Diffraction Line Profiles and Scherrer Constants for Materials with Hexagonal Crystallites

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(Received 23 February 1983; accepted 21 April 1983)

Abstract

Diffraction line profiles and Scherrer constants for use with various measures of diffraction broadening are derived for right hexagonal prisms. A method is described for obtaining the size of crystallites with this form and a comparison is made with a cylindrical model. The technique is applied to annealed ZnO powder obtained from the thermal decomposition of Zn₃(OH)₄(NO₃)₂. The Fourier method is used to show that the crystallites are hexagonal prisms with an average height and edge length of 213 and 87 Å and with the z axis parallel to the axis of the prism and x or y parallel to an edge.

1. Introduction

Size parameters and Scherrer constants for crystallites having a cylindrical or prismatic external form have been discussed by Lele & Anantharaman (1966)* by Wilson (1969b) and more recently by Langford & Louër (1982). In this study we reconsider the important case of the hexagonal prism, that is to say, a right prism with a base defined by a regular hexagon. (See also Louër, Vargas & Langford, 1981.) Earlier work involving the derivation of analytical expressions for diffraction line profiles and size parameters is completed and a comparison is made with the case of cylindrical crystallites.

The model can be applied to materials for which the crystal system has a threefold or sixfold axis, or which are derived from substances having this symmetry. For example, studies of shape based on cylindrical crystallites have been made for Ni(OH)₂ (Louër, Weigel & Langford, 1972), ZnO (Louër, Auffrédic, Langford, Ciosmak & Niepce, 1983) and CdO (Niepce, Mesnier & Louër, 1977; Niepce & Watelle, 1978); the following analysis demonstrates that a more precise determination of the size, shape and orientation of the crystallites is sometimes possible. The procedure can be used to advantage in the study of solid-state decomposition reactions and other chemical processes which yield polycrystalline products.

2. Volume function

The line profile due to small crystallites and the corresponding shape parameters (Scherrer constants, etc.) are derived from the volume function \( V(t) \), the volume common to a crystallite and its 'double' displaced a distance \( t \) in a direction perpendicular to the diffracting planes (Wilson, 1962). In the case of hexagonal prisms of height \( H \) and edge length \( A \) the function \( V(t) \) has two forms: for \( 0 \leq t \leq T \)

\[
V(t) = V_0 \left( 1 - \frac{t}{\tau_1} \right) \left( 1 - \frac{4}{3} \frac{t}{\tau_2} - \frac{C t^2}{T} \right) = V_1(t), \quad (1a)
\]

and for \( T < t < r \)

\[
V(t) = \frac{4}{3} V_0 \left( 1 - \frac{t}{\tau_1} \right) \left( 1 - \frac{t}{\tau_2} \right) \left( 1 - \frac{t}{2T} \right) = V_2(t), \quad (1b)
\]

where \( \tau_1 \) and \( \tau_2 \) are the limiting values of \( t \) for which \( V(t) = 0 \), and \( T \) is an intermediate limit. The equations for \( \tau_1 \), \( \tau_2 \) and \( C \), given below, depend on the relative orientation of the diffraction vector with respect to the prism axes \( X, Y, Z \). If \( \varphi \) is the angle between the normal to the diffracting planes and the \( Z \) axis of the prism, \( \theta \) is the angle between the projection of the diffraction vector on the plane of the prism base (the \( XY \) plane) and the \( X \) axis, and \( \Phi \) is the value of \( \varphi \) for which \( \tau_1 \) and \( \tau_2 \) are equal (Figs. 1a, b and 2), then for \( 0 \leq \varphi \leq \Phi \),

\[
\tau = \frac{H}{\cos \varphi} = \tau_1, \quad (2)
\]

and for \( \Phi \leq \varphi \leq 90^\circ \),

\[
\tau = \sqrt{3A}/\cos \theta \sin \varphi = \tau_2. \quad (3)
\]

*Errors in this paper have been corrected by Langford (1982, footnote on p. 320).
Also,
\[
T = \sqrt{3} A / (\cos \theta + \sqrt{3} \sin \theta) \sin \varphi \\
= \tau_2/(1 + \sqrt{3} \tan \theta),
\]
\[
V_0 = V(t)_{t=0} = \frac{3\sqrt{3}}{2} A^2 H, \quad C = \tan^2 \theta - \frac{1}{3},
\]
\[
\Phi = \arctan \left( \frac{\sqrt{3} A}{H \cos \theta} \right) \quad \text{and} \quad \frac{\tau_2}{\tau_1} = \frac{\tan \Phi}{\tan \varphi}.
\]

Crystallites or domains having the form of a hexagonal prism are most likely to occur in materials whose structure has a threefold or sixfold axis of symmetry. In the particular case of the hexagonal system, or systems which can be referred to hexagonal axes, it is reasonable to assume that the \( z \) direction of the crystallographic axes is parallel to the \( Z \) axis of a crystallite. In the plane of the base two orientations are likely: the \( x \) axis can be parallel to a prism edge (along \( OX \) in Fig. 1b) or perpendicular to an edge (along \( OW \)). In the first case
\[
\varphi = \arccos \left\{ \frac{\sqrt{4}}{3} \left( \frac{\dot{c}}{a} \right)^2 \frac{N + l^2}{2} \right\}^{1/2}
\]
and
\[
\theta = \arccos \left( \frac{(2h + k)/2}{\sqrt{N}} \right),
\]
where \( h, k, l \) are the Miller indices, \( a \) and \( c \) are the dimensions of the unit cell and \( N = h^2 + hk + k^2 \). The second case is equivalent to rotating the crystallographic axes \( \pm 30^\circ \) about the \( Z \) axis. Then, from the symmetry of the hexagonal model, \( \varphi \) is as before and
\[
\theta = \arccos \left( \sqrt{3h/2} / \sqrt{N} \right).
\]
\( V(t) \) is plotted for each case and \( \varphi = 0 \) and \( 90^\circ \) in Fig. 3, together with the equivalent function for cylinders. It should be noted that \( V(t) = V(-t) \) and only the range 0 to \( \tau \) is included in the figure.

The derivatives of \( V(t) \) are required in order to obtain the size parameters (§ 4). In general the volume function for hexagonal prisms can be expressed as

Fig. 2. Limiting values of \( t \) for different values of \( \varphi \), the angle between the diffraction vector and the prism axis.

Fig. 3. Normalized volume functions for crystallites having the form of hexagonal prisms or cylinders. Hexagonal prisms: \( \ldots \ldots \), \( \theta = 0^\circ \), \( \theta = 30^\circ \). Cylinders: \( \ldots \ldots \ldots \) (For \( \varphi = 0^\circ \) the curves for the two models superimpose.)
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\[ V(t) = V_0 \left( 1 - \frac{t}{\tau_1} \right) \sigma(t), \quad (8) \]

where \( \sigma(t) \) is area of overlap in the \( XY \) plane due to a displacement \( (t, \varphi, \theta) \). \( \sigma(t) \) corresponds to the shaded region in Fig. 1(b). The derivative of order \( n \) of \( V(t) \) is thus

\[ \frac{d^n V(t)}{dt^n} = \left[ - \frac{n}{\tau_1} \frac{d^{n-1} \sigma(t)}{dt^{n-1}} + \left( 1 - \frac{t}{\tau_1} \right) \frac{d^n \sigma(t)}{dt^n} \right] V_0. \quad (9) \]

Since \( V(t) \) is a cubic in \( t \), for \( n = 3 \) the derivative of \( V(t) \) is constant and \( V^3(t) = 0 \).

### 3. Line profiles

The diffraction line profile arising from small crystallites is proportional to the Fourier transform of the volume function (Wilson, 1963). Thus, if only size effects are considered,

\[ I(s) = \frac{1}{U} \int_0^T V(t) \cos(2\pi st) \, dt, \quad (10) \]

where \( s \) is the radial distance from the point \( S_0(=2 \sin \theta_0/\lambda) \) in reciprocal space and \( U \) is the volume of the unit cell. For hexagonal prisms, from (1a) and (1b), (10) becomes

\[ I(s) = \frac{2}{U} \left\{ \int_0^T V_1(t) \cos(2\pi st) \, dt + \int_0^T V_2(t) \cos(2\pi st) \, dt \right\}. \quad (11) \]

The exact evaluation of (11) in any particular case is possible, since \( V^n(t) \) is zero for \( n \geq 4 \). Thus, by successive integration by parts,

\[ I(s) = \frac{1}{U} \left\{ \psi^2 \left[ e_1 + e_2 \cos(2\psi) + e_3 \cos \left( 2\frac{\psi \tau}{T} \right) \right] + \psi^3 \left[ e_4 \sin(2\psi) + e_5 \sin \left( 2\frac{\psi \tau}{T} \right) \right] \right\}, \quad (12) \]

where \( \psi = \pi t \) and
\[ e_1 = -\tau^2 V_1(0)/2, \quad e_2 = \tau^2 V_2^2(T)/2, \quad e_3 = \tau^3 [V_1'(T) - V_2'(T)]/2, \quad e_4 = \tau^3 V_2^2(T)/4, \]
\[ e_5 = \tau^3 [V_1''(T) - V_2''(T)]/4, \quad e_6 = -\tau^4 V_1''/8, \quad e_7 = \tau^4 V_2''/8, \quad e_8 = \tau^4 [V_1'' - V_2'']/8 = -(e_6 + e_7). \]

Figs. 4(a), (b) and (c) show \( I(s) \) for various limiting cases and it can be seen that the oscillations in the tails of the line profiles become less pronounced as \( \varphi \) approaches \( \Phi \) (Fig. 2).

### 4. Size parameters (Scherrer constants, etc.)

The Scherrer constant is a dimensionless number which is used to determine the size of crystallites. In the case of hexagonal prisms it is often of the order of unity, except when the crystallites are thin or long needles. In general it is defined as the ratio between the 'true' size and the apparent size of the crystallites in the direction of the normal to the diffracting planes, or

\[ K = \frac{\text{'true' size}}{\text{apparent size}} = \frac{p}{\varepsilon}, \quad (13) \]

where \( p \) is normally taken as the cube root of the

![Fig. 4](image-url)
Table 1. Comparison of size parameters for crystallites having the form of hexagonal prisms and cylinders: \( \tau \) = limiting value of \( t \), \( \varepsilon_{k,F} \) = variance-slope/Fourier apparent size, \( \varepsilon_{w} \) = FWHM size, \( \varepsilon_{p} \) = integral-breadth size, \( \varepsilon_{r} \) = variance-intercept size and \( M_{R} \) = rotundity parameter

<table>
<thead>
<tr>
<th>Hexagonal prisms</th>
<th>( \varphi (\degree) )</th>
<th>( \theta (\degree) )</th>
<th>( \tau )</th>
<th>( \varepsilon_{k,F}/\tau )</th>
<th>( \varepsilon_{w}/\tau )</th>
<th>( \varepsilon_{p}/\tau )</th>
<th>( \varepsilon_{r}/\tau )</th>
<th>( M_{R} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(-H)</td>
<td>(0)</td>
<td>1.000</td>
<td>1.000</td>
<td>(\infty)</td>
<td>0</td>
<td>(\infty)</td>
<td>0</td>
</tr>
<tr>
<td>(\Phi)</td>
<td>0</td>
<td>(30)</td>
<td>0.429</td>
<td>0.726</td>
<td>0.569</td>
<td>0.548</td>
<td>(\frac{1}{2}) (\cos \Phi \sin \Phi)</td>
<td>0</td>
</tr>
<tr>
<td>(90)</td>
<td>(\sqrt{3}/A)</td>
<td>0.750</td>
<td>0.906</td>
<td>0.778</td>
<td>1.225</td>
<td>0</td>
<td>(H/\tau)</td>
<td>0</td>
</tr>
<tr>
<td>90</td>
<td>(2A)</td>
<td>0.750</td>
<td>1.061</td>
<td>0.889</td>
<td>(\infty)</td>
<td>0</td>
<td>(-HD^{2}/\tau^{3})</td>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cylinders</th>
<th>(\varphi (\degree) )</th>
<th>( \tau )</th>
<th>( \varepsilon_{k,F}/\tau )</th>
<th>( \varepsilon_{w}/\tau )</th>
<th>( \varepsilon_{p}/\tau )</th>
<th>( \varepsilon_{r}/\tau )</th>
<th>( M_{R} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(-H)</td>
<td>(0)</td>
<td>1.000</td>
<td>1.000</td>
<td>(\infty)</td>
<td>0</td>
<td>(\infty)</td>
</tr>
<tr>
<td>(\Phi)</td>
<td>0</td>
<td>(D)</td>
<td>0.440</td>
<td>0.780</td>
<td>0.599</td>
<td>0.627</td>
<td>(-H/\tau)</td>
</tr>
<tr>
<td>90</td>
<td>(\sqrt{D^{2}+H^{2}})</td>
<td>0.785</td>
<td>0.998</td>
<td>0.849</td>
<td>(\infty)</td>
<td>(-H/\tau)</td>
<td>0</td>
</tr>
</tbody>
</table>

Various apparent sizes are compared in Table 1.

4.1. Half-width size
The Scherrer constant corresponding to the full width of the line profile at half maximum intensity (FWHM), \(2s_{w}\), is obtained from \(I(s)\) (12). Then
\[
K_{w} = \frac{p}{\varepsilon_{w}} = 2ps_{w}, \tag{14}
\]
and \(\varepsilon_{w}\) is the most direct measure of apparent size. Calculation of \(s_{w}\), and hence \(\varepsilon_{w}\) or \(K_{w}\), requires the solution of the equation \(I(s_{w}) = I(0)/2\). This is difficult to achieve directly, but a close approximation can be obtained by the successive application of Newton's method:
\[
\psi_{w} = \pi s_{w} \tau = g - \frac{I(g) - I(0)/2}{I'(g)}, \tag{15}
\]
where \(g\) is an approximate value of \(\psi_{w}\) and \(I'(g)\) is obtained from the derivative of (12).

4.2. Integral-breadth size
The integral-breadth Scherrer constant is
\[
K_{\beta} = \frac{p}{\varepsilon_{\beta}}, \tag{16}
\]
where \(\varepsilon_{\beta}\) is 'the volume average of the thickness of the crystallites measured in a direction perpendicular to the diffracting planes' (Wilson, 1963, pp. 96 ff). Hence
\[
\varepsilon_{\beta} = \frac{1}{V_{0}} \int_{0}^{T} V(t) \, dt = \frac{2}{V_{0}} \left\{ \int_{0}^{T} V_{1}(t) \, dt + \int_{T}^{0} V_{2}(t) \, dt \right\}
\]
and
\[
= 2 \left[ \frac{a_{1}}{2} + \frac{a_{2}}{2} T + \frac{a_{3}}{4} T^{2} \right]
\]
where
\[
a_{1} = \frac{1}{3}, \quad a_{2} = \frac{4}{3} - C, \quad a_{3} = C, \tag{17}
\]
and
\[
b_{1} = -1 - 1 - 1, \quad b_{2} = \frac{1}{3} + 1 + \frac{1}{2T}, \quad b_{3} = \frac{1}{2T}, \tag{18}
\]
and
\[
4.3. Variance slope and Fourier size
The Scherrer constant for use with the slope of the variance-range function or in the Fourier method is given by
\[
K_{k,F} = \frac{p}{\varepsilon_{k,F}}, \tag{19}
\]
where \(\varepsilon_{k,F}\) is the ratio of the volume of the crystallite \(V_{0}\) to its projected area \(V'(t)\) in the direction of the diffraction vector (Wilson, 1962). It is thus equal to the inverse of the initial slope of the Fourier transform of the profile, \(V'(t)\) at \(t = 0\), or
\[
\varepsilon_{k,F} = -\frac{V_{0}}{V'(0)}. \tag{20}
\]
In the neighbourhood of \(t = 0\) the volume function is equal to \(V'(t)\) and
\[
\varepsilon_{k,F} = \left( \frac{4}{3} + \frac{1}{\tau} \right)^{-1}. \tag{21}
\]
4.4. Variance intercept size

The Scherrer constant corresponding to the intercept of the variance function, $K_T$, is obtained from Wilson (1962, p. 53):

$$L = p^2 V''(0)/V_0,$$

(20)

where $L$ is the taper parameter (Wilson, 1963, pp. 101–102) and

$$K_T = L^{1/2} = \frac{p}{\varepsilon_T}.$$  

(21)

The apparent size, from (20) and (1), is then

$$\varepsilon_T = \tau_2 \left( \frac{8\tau_2}{3\tau_1} - 2C \right)^{-1/2}.$$  

(22)

4.5. Variance–range function

The variance of a diffraction peak, suggested by Tournarie (1956) and developed by Wilson (1962), is given by

$$W(\sigma) = \frac{\int_{-\sigma}^{+\sigma} I(s)s^2 ds}{\int_{-\infty}^{+\infty} I(s) ds},$$

(23)

and can be used to estimate the size of crystallites. If one considers only the linear part of the variance–range function (23), then

$$W(\sigma) = W_0 + k\sigma,$$

(24)

where $W_0 = -(2\varepsilon_T)^{-2}$ and $k = (\pi^2 \tau_{k_F})^{-1}$.

4.6. Rotundity parameter

The rotundity parameter (Mitra, 1964) is defined as

$$M_R = -p^2 V''''(0)/V(0),$$

(25)

and for hexagonal prisms

$$M_R = \sqrt{3} \cos \varphi \sin^2 \varphi (1 - 4 \sin^2 \theta).$$

(26)

The rotundity parameter thus depends only on the orientation of the prisms with respect to the diffraction vector and not on the dimensions of the prisms. $M_R$ passes through a maximum when $\varphi = \arctan \sqrt{2} = 54.736^\circ$ (Fig. 5).

5. Comparison between hexagonal prisms and cylinders

It is of interest to compare hexagonal prisms with the cylindrical case, so that the appropriate model can be selected in any particular application. From Fig. 3 it can be seen that, for $\varphi \neq 0^\circ$, the volume function for a cylinder lies between the curves $\theta = 0^\circ$ and $\theta = 30^\circ$ for the hexagonal case, but both models clearly give the same estimate of size for $\varphi = 0^\circ$ (e.g. 00l reflections in the hexagonal system). Also, the various size parameters given in Table I have similar values for each shape. How then can one choose which is the better model to apply in practice? In order to distinguish between the two models, reflections with $\varphi \neq 0^\circ$ are considered and it is convenient to use lines for which $\varphi = 90^\circ$. At this stage it is necessary to assume a particular orientation of the crystallographic axes unless this is known $a$ priori. Then the curves of the Fourier coefficients of $A_n$ vs $n$ or the variance–range curves will superimpose in the cylindrical case for all such reflections (e.g. hk0 in the hexagonal system), but for hexagonal prisms they will differ (Fig. 3). Other measures of breadth behave in the same way. For each reflection whose diffraction vector lies in the basal plane, $A$ can then be obtained from § 4 in the case of hexagonal prisms, or $D$, the diameter of the cylinders, from Langford & Louër (1982). A check on these estimates of size can then be made by using data for which $0 < \varphi < 90^\circ$ (e.g. hkl reflections), when the observed apparent size should be the same as that calculated from the mean estimate of $D$ or $A$ and $H$ from reflections with $\varphi = 0$ and $\varphi = 90^\circ$ (e.g. hk0 and 00l lines).

It should be noted that a good cylindrical fit does not necessarily mean that the crystallites are in fact cylinders; the implication is that on average they may be regarded as having this form (Louër et al., 1983). This could occur, for example, when the prism section is not a regular hexagon, or when the crystallographic axes do not have the same orientation in all crystallites. Furthermore, it is only possible to distinguish between the two shapes if the data for all lines are of high quality and the analysis is carried out with care. That is to say, good counting statistics are essential (Wilson, 1967, 1968, 1969a), the step length must not be too large (Langford, 1968), each line must be scanned over as wide a range as is practicable, with a meaningful correction for overlapping tails where appropriate, and in general a correction should be made for any intensity lost by truncation (Langford, 1982).
In order to make a direct comparison between the two models it is convenient to assume that the cylinders and prisms have equal volumes. Then, since \( H \) is the same in each case,

\[
D = \left( \frac{6 \sqrt{3}}{\pi} \right)^{1/2} A = 1.8188 A.
\]

### 6. Practical considerations

It has been shown in §§ 4 and 5 that several parameters to describe the morphology of a single crystallite can be obtained from diffraction theory. In practice, however, a powder sample contains a large number of crystallites and, even if they all have the same shape, it is unlikely that their dimensions will be identical. A distribution of size means that the oscillations which appear in the tails of the theoretical profiles (Fig. 4) will not be observed experimentally. In practice it is thus the mean apparent dimensions and the behaviour of the Fourier transform of the diffraction profile for different crystallographic directions which are of interest. This is particularly true for crystallites having the form of a prism with a hexagonal or circular cross section and with the principal axis parallel to a main symmetry axis of the crystal structure.

The cylindrical model has been applied to ZnO obtained from the thermal decomposition of the hydroxynitrate \( \text{Zn}_3(\text{OH})_6(\text{NO}_3)_2 \) (Louèr et al., 1983). During a study of the initial sintering of this oxide (Vargas, 1981; Louèr, Vargas & Auffrédic, 1983), modifications to the form of the crystallites were observed which are shown here to provide a practical example of the use of the hexagonal-prism model developed in §§ 2, 3 and 4. The specimen was again obtained from the thermal decomposition of the hydroxynitrate at 553 K, but the sample was then maintained at 703 K for 25 h in a dynamic vacuum of 13.3 mPa (Vargas, 1981). Five reflections (100, 110, 102, 103 and 004) were step-scanned by means of a Compagnie Générale de Radiologie powder diffractometer and with strictly monochromatic Cu K\( \alpha_1 \) radiation. The experimental conditions and the technique used have been described in a previous paper (Louèr et al., 1983). The Fourier method was used to illustrate the application of the hexagonal-prism model in an analysis of size broadening.

### 7. Results and conclusions

The cosine coefficients \( A_L \) for the small-crystallite profiles are plotted in Figs. 6(a), (b). Inspection of these curves indicates that the crystallites are not spheres, for which they would superimpose, and the right cylinder is not an ideal model, since the curves for the 100 and 110 reflections are different. The apparent sizes obtained from the initial slopes of Fig. 6 are listed in Table 2 and again there is clearly an anisotropy of shape. If it is assumed that the crystallites are right prisms, with their axes parallel to the \( z \) direction, the average height from the 004 line is 213 Å. If it is further assumed that the cross section of the prisms is a regular hexagon, then the edge length obtained from both the 100 and 110 reflections is 87 Å. These values for \( H \) and \( A \) can then be inserted in (19) to calculate the apparent size for the remaining reflections (i.e. 102 and 103). It can be seen from Table 2 that there is

<table>
<thead>
<tr>
<th>hkl</th>
<th>( e_{\text{f}} ) (Å)</th>
<th>( e_{\text{cyl}} ) (Å)</th>
<th>( e_{\text{hex}} ) (Å)</th>
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<tr>
<td>100</td>
<td>130</td>
<td>121</td>
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</tr>
<tr>
<td>110</td>
<td>112</td>
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</tr>
<tr>
<td>102</td>
<td>118</td>
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<td>103</td>
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<td>120</td>
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</tr>
<tr>
<td>004</td>
<td>213</td>
<td>213</td>
<td>213</td>
</tr>
</tbody>
</table>

![Fig. 6. Fourier cosine coefficients for annealed ZnO. (a) 102, 103, +004; (b) 110, 100.](image-url)
excellent agreement between the calculated and experimental values for these lines, confirming that a hexagonal model adequately describes the shape of the crystallites.

For completeness the apparent sizes obtained from an assumed cylindrical form are included in Table 2. In this instance the mean height is again 213 Å and the diameter is 154 Å. The experimental and calculated apparent sizes then differ, but only by 6 to 7%, indicating that, to this order of accuracy, the cylinder is still a reasonable model.

There is a high degree of internal consistency in the above result and the crystallites are clearly right hexagonal prisms with the a or b side of the unit cell parallel to an edge. The experimental and calculated apparent sizes agree to better than 2%, but the procedure for determining the size from the Fourier cosine coefficients is particularly susceptible to truncation effects (Young, Gerdes & Wilson, 1967; Langford, 1982) and the absolute error may well be somewhat greater.

In this work we have listed the various parameters from which the dimensions and orientation of crystallites having the form of a right hexagonal prism can be determined. Volume functions, essentially $A_n$ versus $n$ curves, and the corresponding diffraction line profiles are also given, and a comparison is made with the cylindrical case. A study of the size and shape of the crystallites in annealed ZnO, by using the Fourier method to analyse the diffraction broadening, demonstrates that the hexagonal model can be applied in practice to give accurate estimates of the mean dimensions of the crystallites and also their orientation. It is further shown that the cylindrical model is a reasonable approximation to the form of the crystallites.

The authors are indebted to Professors A. J. C. Wilson and D. Grandjean for their continuing interest in this work and to Dr J. P. Auffrédic for preparing the zinc oxide sample.

References