about the form of the cross section. Once a shape has been chosen, $\beta_0(s)$ can be calculated, either analytically or numerically, and the maximum in $hLi_c(hL)$ can be found numerically.

The location of the maximum can also be estimated from the approximation (Porod, 1948)

$$i_c(hL) = \exp(-h^2R_c^2/2) \qquad (2)$$

where R_c is the radius of gyration of the cross section about an axis perpendicular to the cross section and passing through the center of mass of the cross section. This approximation is valid for an arbitrary cross section shape. According to (2), $hLi_c(hL)$ has a maximum for $hR_c=1$.

The accuracy of the position of the maximum calculated from (2) was tested for circular and square cross sections and for a rectangular cross section for which one side of the rectangle was 10 times as long as the other. According to the approximate equation, the maxima for the three cross section shapes occur respectively for $hL=2{\cdot}83$, 3·46, and 3·46, while the corresponding values from the exact expression are $hL=2{\cdot}713$, 3·336, and 3·798. For square and circular cross sections, the agreement of the approximate and exact equations is good enough for analysis of many experimental curves, since high accuracy is often not necessary because of other approximations necessary for applying the theory to analysis of experimental data. For the elongated rectangular cross section a considerably greater error results from using the approximate expression. The tests of (2) thus suggest that while it may be sufficiently accurate for cross sections which are not elongated, for highly elongated cross sections, the exact equation probably should be used.

Since a maximum in $\theta^2I(\theta)$ can be expected for the small angle X-ray scattering from all elongated rods, plots of $\theta^2I(\theta)$ can be used to interpret the scattering data from samples consisting of long, rod-shaped particles. Fedorov & Ptitsyn obtained excellent results with the scattering data from a number of samples. Their experience suggests that the use of the $\theta^2I(\theta)$ plot may develop into a useful technique for the analysis of small angle X-ray scattering data.

As Mittelbach & Porod (1961) pointed out when discussing their numerical computations of the intensity of the small angle X-ray scattering from parallelpipeds, equation (1) may often be convenient for numerical calculations of the scattered intensity from highly elongated particles.

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Strain and particle size values from X-ray line breadths. By F. R. L. SCHOENING, *Department of Physics, University of the Witwatersrand, Johannesburg, South Africa*

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The use of the breadth of the diffraction line for obtaining estimates of strain and particle size has the advantage of speed and convenience over the more elaborate analysis of line shapes (Warren, 1959). Therefore breadth analysis is frequently employed although its limitations are generally realized. However, in evaluating breadth data one of two assumptions is sometimes made, either of which is in most cases wrong. It is assumed either that the breadth due to strain and the breadth due to particle size are additive or that the squares of the breadths are additive. This is equivalent to assuming either a Cauchy line shape for particle and strain broadening or a Gauss shape for both broadenings. However, it is known that particle size broadening tends to give a Cauchy line and strain broadening a Gauss or $1/(1+K^2x^2)^2$ line (*cf.* Taylor, 1961). A method for using these more realistic profiles in a breadth analysis is given here.

The observed intensity profile $I_{\text{obs}}(x)$ is the convolution of the strain profile $I_s(x)$ and the particle size profile $I_p(x)$,

$$I_{\text{obs}}(x) = \int_{-\infty}^{+\infty} I_s(x-u)\, I_p(u)\, du\,.$$

The integral can be solved by using the Fourier transforms T of the functions, $T[I_{\text{obs}}(x)] = T[I_s(x)]T[I_p(x)]$. I_{obs} can be obtained by applying the inverse transformation. In the present case considerable simplification is possible because only the integral breadth

$$B_{\text{obs}} = \int_{-\infty}^{+\infty} I_{\text{obs}}(x)dx/I_{\text{obs}}(0)$$

is required. It is

$$\left.\begin{aligned} \int_{-\infty}^{+\infty} I_{\text{obs}}(x)dx &= \int_{-\infty}^{+\infty} T^{-1}\langle T[I_s(x)]T[I_p(x)]\rangle\, dx \\ &= \{T[I_s(x)]\times T[I_p(x)]\}_{u=0} \\ \text{and } I_{\text{obs}}(0) &= \{T^{-1}\langle T[I_s(x)]T[I_p(x)]\rangle\}_{x=0} \end{aligned}\right\} \qquad (1)$$

where x and u are the variables in real and Fourier space respectively. Two cases were considered,

(*a*) $I_p = C_p/(1+K_p^2x^2)$ and $I_s = C_s/(1+K_s^2x^2)^2$

(*b*) $I_p = C_p/(1+K_p^2x^2)$ and $I_s = C_s \exp\{-K_s^2x^2\}$.

The transforms and the integral breadths B as function of particle size L and strain e are

(*a*) $T[I_p] = C_p\pi K_p^{-1} \exp\{-2\pi|u|/K_p\}$

$T[I_s] = \frac{1}{2}\pi C_s K_s^{-2}(K_s+2\pi u) \exp\{-2\pi u/K_s\}$

$B_p = \pi/K_p = \lambda/L \cos\theta$, $B_s = \pi/2K_s = e \tan\theta$

$$(b)\quad T[I_p]=C_p\pi K_p^{-1}\exp\{-2\pi|u|/K_p\}$$
$$T[I_s]=\sqrt{\pi}C_sK_s^{-1}\exp\{-\pi^2u^2/K_s^2\}$$
$$B_p=\pi/K_p=\lambda/L\cos\theta,\quad B_s=\sqrt{\pi}/K_s=e\tan\theta\,.$$

Using these relations in (1) gives

$$(a)\quad B_{\rm obs}=(2B_s+B_p)^2(4B_s+B_p)^{-1}$$
$$(b)\quad B_{\rm obs}=\tfrac{1}{2}B_s\exp\{-(B_p/B_s)^2/\pi\}(\tfrac{1}{2}-\mathrm{erf}\{\sqrt{2/\pi}B_p/B_s\})^{-1} \qquad (2)$$

where $\mathrm{erf}\{x\}=\sqrt{1/2\pi}\int_0^x\exp\{-t^2/2\}dt$ as tabulated (*Handbook of Chemistry and Physics*, 1963).

An easy separation of strain broadening from particle size is possible if two orders of reflexions from the same plane are used. The method is demonstrated and numerical data are given for the most frequently occurring case of the *n*th and 2*n*th order (*e.g.* 111 and 222, 200 and 400). In general any two reflexions at θ_1 and θ_2 can be used, but a graph, different from that given in Fig. 1, has to be plotted if $(\sin\theta_1)/\sin\theta_2\neq\frac{1}{2}$.

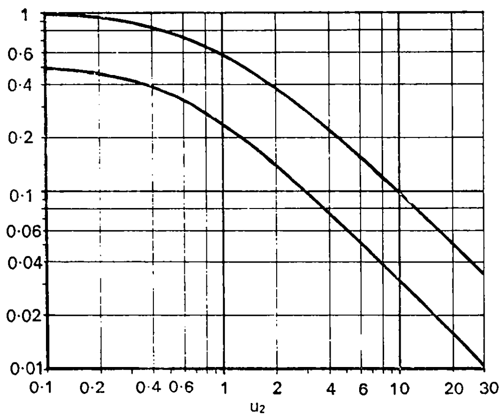

Fig. 1. Top curve: $1/LB_2$. Bottom curve: $B_1B_2-\frac{1}{2}$, plotted *versus* u_2.

The following abbreviations are introduced:

$$\left.\begin{aligned}B_i&=B_{i\rm obs}(\cos\theta_i)/\lambda\\ u_i&=Le(\sin\theta_i)/\lambda\end{aligned}\right\}\ i=1,2$$
$$a=(\sin\theta_1)/\sin\theta_2\,,$$

1 and 2 referring to the two orders of the reflexion. Therewith, and using (2),

$$(a)\left\{\begin{aligned}&B_1/B_2=(au_2+\tfrac{1}{2})^2(2u_2+\tfrac{1}{2})(2au_2+\tfrac{1}{2})^{-1}(u_2+\tfrac{1}{2})^{-2}\\ &1/LB_2=\tfrac{1}{2}(2u_2+\tfrac{1}{2})(u_2+\tfrac{1}{2})^{-2}\end{aligned}\right.$$

$$(b)\left\{\begin{aligned}&B_1/B_2=a\exp\{(1-1/a^2)/\pi u_2^2\}(\tfrac{1}{2}-\mathrm{erf}\{\sqrt{2/\pi}/u_2\})\\ &\quad\times(\tfrac{1}{2}-\mathrm{erf}\{\sqrt{2/\pi}/u_2a\})^{-1}\\ &1/LB_2=(2/u_2)\exp\{1/\pi u_2^2\}(\tfrac{1}{2}-\mathrm{erf}\{\sqrt{2/\pi}/u_2\})\end{aligned}\right.$$

The results of the calculations of B_1/B_2 and $1/LB_2$ as functions of u_2 and for $a=\frac{1}{2}$ are given in Table 1 and are shown in Fig. 1 for case (*b*).

Table 1. *Values of* B_1/B_2 *and* $1/LB_2$ *calculated as functions of* u_2

	(*a*)		(*b*)	
u_2	B_1/B_2	$1/LB_2$	B_1/B_2	$1/LB_2$
0·1	0·9803	0·9722	0·9888	0·9849
0·2	0·9446	0·9184	0·9620	0·9464
0·3	0·9077	0·8594	0·9270	0·8955
0·4	0·8738	0·8025	0·8898	0·8421
0·6	0·8174	0·7025	0·8257	0·7409
0·8	0·7742	0·6213	0·7775	0·6549
1·0	0·7407	0·5556	0·7397	0·5843
1·5	0·6836	0·4375	0·6769	0·4568
2·0	0·6480	0·3600	0·6394	0·3736
3·0	0·6064	0·2653	0·5974	0·2729
4·0	0·5830	0·2099	0·5747	0·2147
6·0	0·5576	0·1479	0·5510	0·1504
8·0	0·5441	0·1142	0·5387	0·1157
10·0	0·5357	0·0930	0·5311	0·0939
15·0	0·5242	0·0635	0·5210	0·0639
20·0	0·5183	0·0482	0·5157	0·0484
30·0	0·5123	0·0325	0·5105	0·0326
40·0	0·5093	0·0245	0·5080	0·0246
60·0	0·5062	0·0165	0·5053	0·0165
80·0	0·5047	0·0124	0·5040	0·0124
100·0	0·5037	0·0099	0·5021	0·0099

The use of Fig. 1 may be illustrated by taking the broadening of the 200 and 400 reflexions which were observed with Cu radiation from a film of gold deposited in vacuum on sodium chloride. The integral breadths are $B_{1\rm obs}(2\theta_{200}=44{\cdot}4^\circ)=0{\cdot}0037$ rad 2θ and $B_{2\rm obs}(2\theta_{400}=98{\cdot}2^\circ)=0{\cdot}0070$ rad 2θ after correction for $\alpha_1-\alpha_2$ overlap and instrumental broadening. These breadths give $B_1=0{\cdot}00224$ Å^{-1}, $B_2=0{\cdot}00298$ Å^{-1} and $B_1/B_2=0{\cdot}753$. The $(B_1/B_2)-\frac{1}{2}$ and $1/LB_2$ curves in Fig. 1 give, respectively, $u_2=0{\cdot}92$ and $1/LB_2=0{\cdot}61$ from which $L=550$ Å and $e=u_2\lambda/L\sin\theta_2=0{\cdot}0034$ is obtained as final result.

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A further development of the crystal setter.

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Some of the well known graphical, analytical methods which are used to find the arc corrections of a goniometer head with crossed arcs from oscillation photographs require the use of the following convention: the crossed arcs of the goniometer head have a special position relative to the primary beam (one arc parallel or both arcs at 45° to the beam) (Kratky & Krebs, 1936; Hendershot, 1937; Weisz & Cole, 1948; Jeffrey, 1949*a*, *b*; Bunn, 1949; Davies, 1950, 1961). In our method (Kulpe, 1963; Kulpe & Dornberger-Schiff, 1965) a similar convention is given. To