PART I
THEORETICAL CONSIDERATIONS ON THE ANALYSIS OF X-RAY DIFFRACTION PROFILES FROM IMPERFECT SOLIDS: APPLICATION OF CONVOLUTION RELATIONS
CHAPTER 1

INTRODUCTORY REMARKS ON X-RAY LINE PROFILE ANALYSIS
1.1 X-ray Line Broadening

1.1.1 Introduction

Following the discovery of the principle of x-ray diffraction by Laue, Friedrich and Knipping (1912), considerable and widespread effort was put into determining the structure of a variety of crystalline substances. These structure determinations led to an enormous increase in knowledge of the crystalline state, and provided the foundation for a thorough theoretical interpretation of a number of the physical properties of the ideal perfect crystal. However, it soon became evident that the diffraction intensities from most real crystals were very different from those one would calculate on the assumption of ideal crystal structures, and it was Darwin (1914, 1922) who, first, found it necessary to assume that crystals did not actually have a perfect structure and postulated the 'mosaic crystal' model. Since then, the interest in the nature and properties of physical imperfections in crystals has risen rapidly.

It has now become apparent that an equally important branch of solid state physics exists: this is the study of defects in the crystal lattice. Crystal imperfections appear to influence the properties of the solids to such an extent that solid state physics has proved in several instances to be equivalent to the study of the properties of the defect crystal as contrasted to those of the perfect crystal.

In the course of defect studies in crystalline materials, x-ray line broadening investigations took a prominent stature for a quite long
It has been known from the early days that the x-ray diffraction lines from cold-worked polycrystals are broadened and that this broadening increases with deformation applied to such crystals (Van Arkel, 1925). This broadening has been interpreted generally in terms of presence of small particle size or elastic distortion in the substance. Dehlinger and Kochendorfer (1939), Kochendorfer (1944), Stokes, Pascoe and Lipson (1943) and Smith and Stickley (1943) showed that the broadening is partly due to strain in the crystalline lattice and partly due to smallness of the crystallites. Theoretical work of Bragg (1942, 1949) supported this view and the results obtained up to 1952 have been very well discussed by Greenough in his review article (Greenough, 1952). Most workers found that the strain broadening predominates and the particle size broadening is relatively small. However, Wood and Rachinger (1949) concluded, from measurements of the variation of broadening with wavelength, that the major part of the broadening was due to particle size. Using more refined x-ray techniques, Auld and Garrod (1952) obtained the opposite result. Again, Williamson and Hall (1953) estimated larger particle size value than that quoted by Wood and Rachinger (1949). It has been suggested that the low values obtained by these workers are due to certain short-comings in experimental technique (Auld and Garrod, 1952; Garrod et al, 1954).

The present day concept, however, attributes the observed broadening for the x-ray diffraction profiles from crystalline materials to be mainly due to the occurrence of faulting in the stacking sequences of close packed layers, a diminution in the size of the coherently diffracting domains and the existence of non-uniform microstrains in the lattice within these
coherently diffracting domains etc. The analysis of the diffraction profiles from polycrystalline materials thus gives an insight of the microstructural changes in the materials quantitatively as well as qualitatively. The earlier X-ray studies were usually content to use peak breadths in terms of Scherrer's half-peak breadth (Scherrer, 1918 ; Jones, 1938) or Laue's integral breadth (Laue, 1926). The line breadth studies has further been enhanced by the recent works by Schoening (1965) and Ruland (1968). Warren and Averbach's more general Fourier method of line shape analysis (Warren and Averbach, 1950, 1952 ; Warren 1959, 1969 ; Wagner, 1966) offers a very elegant and powerful method of analysing line broadening due to particle size, strain and stacking faults in deformed or imperfect materials. The recently developed methods of single line techniques, namely, the 'linlog' method due to Rothmann and Cohen (1969), the parameter fitting method of Gangulee (1974) and the method of Mignot and Rondot (1975) have added further dimension in this particular field of study. Another powerful method, the method of variance developed by Wilson (1962), however, fails to find its wide application due to oversensitiveness in the background level estimation and proper truncation ranges (Wagner 1966 ; Halder and Wagner 1966b).

1.1.2 Concept and development of integral breadth analysis

The Debye - Scherrer pattern from a solid or densely packed aggregate of randomly oriented crystallites begins to exhibit smooth continuous circles only when the number of crystallites irradiated to sufficient for coalescence of the individual reflections spots to take place. By calibrating with known standards and using a conventional beam diameter of approximately
0.5 to 1.0 mm., it is found that perfectly sharp continuous rings require a mean crystallite diameter of the order of $10^{-4}$ cm.

When the individual stress-free crystallites in a polycrystalline sample fall below $10^{-4}$ cm. in diameter, we enter a size range in which the lines in the Debye-Scherrer pattern become appreciably broadened. In the case of conventional powder photographs and in diffractometer readings, the Debye-Scherrer lines progressively broaden as the sizes of the crystallites forming the individual particles in the powder sample continue to be reduced until finally they degenerate into broad diffuse bands which merge slowly into the general background (Taylor, 1961).

The breadth of a diffraction line, which is effectively the angle it subtends at the specimen, treated as point, may be defined in a number of ways. A convenient definition, given originally by Scherrer (1918), expresses the breadth of a line as its angular width in radians at a point where the intensity has fallen to half its maximum value. A somewhat more satisfactory definition of line breadth is given by Von Laue (1926), who defines the breadth of the line in terms of the integrated intensity between the line contour and the background divided by the maximum height of the line as

$$\beta_L = \frac{\int_{2\theta_1}^{2\theta_2} P'(2\theta) \, d(2\theta)}{[P'(2\theta)]_{\text{max}}} \quad \ldots \ldots (1.1)$$

where $2\theta_1$ and $2\theta_2$ are the truncation limits and $P'(2\theta)$ is the measured diffracted power per unit arc length of the diffracting circle.

Its chief advantage is that due weight is given to the contributions made to the line area by the broad base which tails away into the background and which
is ignored in the Scherrer definition.

In his original determination of the intrinsic line broadening, \( \beta \), for crystals of cubical shape, Scherrer (1918) obtained the expression

\[
\beta_s = 2 \sqrt{\frac{\log_2 2}{\pi}} \frac{\lambda}{D \cos \theta} = \frac{0.94 \lambda}{D \cos \theta}
\]

(1.2)

whereas Bragg (1935) obtained a value of 0.89 for the numerical constant. In general, we may write the Scherrer expression in the form:

\[
\beta = \frac{K \lambda}{t \cos \theta}
\]

(1.3)

where \( K \) is referred to as Scherrer constant and \( t \) is the crystallite size defined as the cube root of the volume. Different methods of arriving at the intrinsic broadening, \( \beta \), always lead to an expression of the type given in equation (1.3), but the value of \( K \) depends on the way in which the line broadening and the crystallite size are defined. This problem has been discussed by Warren (1938), Patterson (1939), Von Laue (1926), Jones (1938) and Wilson (1945, 1949, 1950) and in each case a value of \( K \) not very different from unity has been obtained. Since all the crystallites will not have identical shapes, and there may be a size distribution which materially influences the distribution of x-ray intensity in the lines, it is sufficient to define the "mean apparent crystal size" \( D \), in the direction normal to the reflecting planes, equal to \( t/K \), so that

\[
\beta = \frac{1.0 \lambda}{D \cos \theta} \text{ radians}
\]

(1.4)

and \( \beta \), the pure diffraction broadening, is taken as the Laue integral breadth. We can see from this equation that, if \( D \gg 10^{-4} \text{ cm.} \), the diffraction
broadening is negligible and we shall use the expression "crystallites of infinite size" for crystals larger than this.

Assuming that the crystallites are large enough to make \( \beta \) negligible, we shall now consider the effects of lattice strains upon the line breadth. According to Stokes and Wilson (1944), the origin of strain broadening may be due to the following two causes:

(i) The metal is broken down to subgrains having dimensions of the order of \( \gtrsim 10^{-5} \) cm., each of which has a uniform expansion or contraction so that its lattice parameter differs from the mean.

(ii) The broadening may be due to distortion of fairly large crystals (\( \gtrsim 10^{-4} \) cm. in linear dimensions), the distortion taking the forms of non-uniform expansions and contractions.

It can be shown that both these causes lead to essentially the same results. The effect of the spacing variations is to distribute the x-ray reflections over a small range of angles round the position of the line for the undistorted crystal.

Following the simplified treatment of Megaw and Stokes (1945), the average strain becomes:

\[
\epsilon = \frac{\beta}{4} \cot \phi \tag{1.5}
\]

and mean stress \( \bar{\sigma} \) will be given by

\[
\bar{\sigma} = \mu \epsilon = \frac{\mu \beta}{4} \cot \phi \tag{1.6}
\]

where \( \beta \) is the pure diffraction breadth in radian measure.
Equations (1.4) and (1.5) enable us to test whether the broadening is due primarily to crystallite size or lattice strain.

Following the early ideas, we may, to a first approximation, assume that, when the fine grain effect and lattice distortion are both operative, their combined effects give the total line broadening, which is the simple sum:

\[ \beta = \beta_{\text{grain size}} + \beta_{\text{lattice distortion}} \quad \cdots \quad (1.7) \]

i.e.

\[ \beta = \frac{\lambda}{D \cos \theta} + 4 \epsilon \tan \theta \quad \cdots \quad (1.8) \]

This may be written in the form:

\[ \frac{\beta \cos \theta}{\lambda} = \frac{1}{D} + 4 \epsilon \frac{\sin \theta}{\lambda} \quad \cdots \quad (1.9) \]

Thus from the corrected breadths, \( \beta \), of the Debye-Scherrer reflections, a plot of \( \frac{\beta \cos \theta}{\lambda} \) versus \( \frac{\sin \theta}{\lambda} \) should be a straight line. The intercept on the \( \frac{\beta \cos \theta}{\lambda} \) axis will yield \( \frac{1}{D} \), the reciprocal of the crystallite size, while the slope will give \( \epsilon \), the average strain. Using the above Cauchy relation, plots of this type have been made by Hall (1949) for filings from aluminium, rhodium, copper and found to be reasonably linear. Kurdyumov and Lysak (1947) assuming Gaussian function used the square relation:

\[ \beta^2 = \beta_{\text{grain size}}^2 + \beta_{\text{lattice distortion}}^2 \quad \cdots \quad (1.10) \]

Actually, there is no valid reason for assuming that the total broadening due to the crystallite size effect and lattice distortion can be
obtained by addition of individual breadths or by any other simple additive process. Simple addition (equation 1.7) is equivalent to assuming that the shape functions for both the size effect and distortion are of the Cauchy forms namely, \( \frac{1}{1 + K_p x^2} \) and \( \frac{1}{1 + K_s x^2} \), whereas the addition of squares (equation 1.10) is equivalent to assuming both broadenings to be of the Gaussian form namely, \( \exp(-K_p x^2) \) and \( \exp(-K_s x^2) \) respectively. According to Guseva and Barbareko (1958) and Lysak (1954), who studied the line broadening effects produced by cold-worked copper and copper-base solid solutions, the crystallite size contribution to the line breadths follows a Cauchy form \( \frac{1}{1 + K_p x^2} \) but the distortion broadening is best represented by a curve of the form \( \frac{1}{(1 + K_s x^2)^2} \), known as double-square type. Warren (1959) has shown that size broadening is of the Cauchy form, while distortion broadening should be represented by a Gaussian expression because of its much steeper rate of fall to the background. This finding is consistent with the work of Guseva and Barbareko (1958).

It was Schoening (1965) who first considered mathematically in his more realistic line profile study (described in detail in section 1.3) the Cauchy shape for the particle size broadening and Gaussian as well as double-square shape for the strain broadening, as was pointed out earlier by Lysak (1954) and Guseva et al (1958).

Halder and Wagner (1966a) later on, however, put forward a much simplified empirical form, intermediate between Gaussian and Cauchy forms, in place of Schoening's rigorous method (Schoening, 1965). The following empirical relation has been suggested:

\[
\frac{b_s}{b} = 1 - \left(\frac{b_p}{b}\right)^2
\]

\[\text{(1.11)}\]
where \( b^s \) and \( b^o \) are respectively the integral breadths from particle size and strain broadening and \( b \) is the integral breadth for the true profile. The application of this parabolic relation has been found to yield satisfactory results in many cases.

In addition to the above mentioned works, Ruland (1968) reviewed the principles of the use of line-width relations for the separation of line broadening effects and gave a collection of line-width relations for a number of analytical profile types of practical interest. Ruland (1968) considered the following functional forms:

\[
\begin{align*}
    f_G & = \exp \left(- \pi x^2\right) \\
    f_C & = 1/\left(1 + \pi^2 x^2\right) \\
    f_E & = \exp \left(-2|x|\right) \\
    f_Y & = 1 \quad |x| \leq 0.5 \\
    & = 0 \quad |x| > 0.5 \\
    f_{\phi} & = \sin \pi x/\pi x \\
    f_{\Delta} & = 1 - |x| \quad |x| \leq 1 \\
    & = 0 \quad |x| > 1 \\
    f_{\Psi} & = (\sin \pi x/\pi x)^2
\end{align*}
\]

Some of the line-width relations have been applied recently in cases of f.o.c. alloys (Sen Gupta and De, 1971; Chatterjee and Sen Gupta, 1972 b).

We have so far considered the integral breadths of the line profiles corrected for \( K \alpha_1 - \alpha_2 \) doublet, according to the most widely used Rachinger method (1948), the details of which have been described by
There are also other methods proposed by Papoulis (1955) and Gangulee (1970).

1.2 Instrumental Broadening Correction: Different Methods

1.2.1 Introduction

Instrumental effects comprise of the finite slit widths, imperfect alignment, sample size, unresolved $\alpha_1$ and $\alpha_2$ doublet and its wavelength spread. So, the observed intensity distribution from the sample under investigation which is a convolution of 'true' diffraction profile as well as the 'instrumental' profile is to be corrected for to get the 'true' diffraction profile for the estimation of micro-structural parameters. The existing methods to deal with deconvolution are briefly summarised in the following sections.

1.2.2 Convolution principle

Mathematically, the effect of line broadening is represented by convolution. If $f(x)$ is the line profile resulting from $n$ mutually independent line broadening effects, each of which is given by a characteristic distribution $f_i(x)$, one can write

$$f = f_1 * f_2 * \ldots * f_n \ldots \ldots \ldots (1.13)$$

where * stands for convolution i.e.

$$f_1 * f_2 = \int_{-\infty}^{\infty} f_1(y)f_2(x-y)\,dy \ldots \ldots \ldots (1.14)$$
The Fourier transform $T$ of equation (1.13) gives

$$T(f) = F = F_1 \cdot F_2 \cdots \cdot F_n = \prod_{i} F_i \cdots \cdots \ (1.15)$$

where $\prod$ denotes the product. An unknown broadening distribution $f_k$ can be obtained by inverse Fourier transformation as

$$f_k = T^{-1}(F/ \prod_{i \neq k} F_i ) \cdots \cdots (1.16)$$

1.2.3 Methods based on the breadth of the profiles

The earlier work on instrumental broadening correction based on the measurement of line breadths originated from Scherrer (1918) and Jones (1938). Scherrer (1918) proposed that $\beta$, the breadth for pure or true diffraction profile is related to $B$, the experimentally observed breadth and $b$, the breadth of the geometrical line profile by simple relation:

$$\beta = B - b \cdots \cdots (1.17)$$

This relation holds good only if the respective profiles are of Cauchy type.

Jones (1938) proposed a very useful graphical method for instrumental broadening correction. He obtained direct relations between the ratios of the breadths and their profile shapes for different profiles using the convolution relation (equation 1.14). From the plot of $\beta/B$ vs $b/B$ and considering both Gaussian and Cauchy types of curves, he evaluated the true breadths of the line profile. Later on, many workers namely Warren and Biscoe (1938), Taylor (1941), Wood and Rachinger (1949), Schoening, Niekerk
and Hall (1952), Lysek (1955), Anantharaman and Christian (1956) and Wagner and Aqua (1965) assumed different forms or natures of the respective diffraction profiles to obtain a relation between $B$, $b$ and $\beta$. Some of the important relations which now exist are:

I $\beta = B - b$ (Scherrer 1918) : assuming Cauchy form of profiles.

II $\beta = (B^2 - b^2)^{1/2}$ (Warren and Biscoe, 1938) : assuming Gaussian form of the profiles.

III $\beta = \left[\frac{(B - b)}{b^2} \right]^{1/2}$ (Taylor, 1941).

IV $\beta = \frac{B - b^2}{B}$ (Anantharaman and Christian, 1956 and Wagner and Aqua, 1963) : assuming the diffraction profiles to have natures intermediate between Cauchy and Gaussian — an intermediate parabolic form.

Of these four relations, relation II and relation IV representing pure Gaussian and intermediate parabolic form respectively are usually considered for the instrumental broadening correction and as such are widely used.

Halder (1964) has derived an expression for the integral breadth of the pure diffraction profile (when a Cauchy instrumental profile is convoluted with a pure diffraction profile of unspecified shape to get a Gaussian profile) as

$$\beta = B \exp \left( -\frac{b^2}{\pi B^2} \right) \quad \text{...... (1.18)}$$

He also derived an expression for the line profile as

$$\beta(x) = \frac{2c_2}{bc_1} \exp \left( \frac{b^2}{\pi B^2} \right) \exp \left( -\frac{x^2}{B^2} \right) \cos \left( \frac{2bx}{B^2} \right) \quad \text{...... (1.19)}$$

where $c_1$ and $c_2$ are the constants considered in the Cauchy and
Gaussian functions respectively.

Ruland (1965), considering Gaussian instrumental and Cauchy true diffraction profile, has proposed a relation giving the integral breadth of the true profile as:

\[ \beta = \frac{b \exp \left[-\left(\frac{2}{\sqrt{\pi}} b\right)^2\right]}{1 - \text{erf} \left(\frac{2}{\sqrt{\pi^{1/2}} b}\right)} \]  \hspace{1cm} (1.20)

where \( \text{erf}(x) = \int_0^x \exp(-t^2) \, dt \)

However, Ruland (1968) in his later work, considered different forms of analytical expressions (equation 1.12) for the instrumental profile, in addition to Gaussian and Cauchy forms, and derived the convolution relations with the true profile which has been considered either Gaussian or Cauchy.

1.2.4 Stokes' method

Stokes (1948) gave a general and more rigorous method for the instrumental broadening correction of the observed diffraction profiles. If \( f(y) \), \( h(x) \) and \( g(z) \) are the functions describing respectively the true, observed and the instrumental diffraction profiles, then they can be written in terms of Fourier series in the interval of \(-a/2\) to \(+a/2\) using the complex form (Warren, 1969):

\[ f(y) = \sum_n F(n) \exp(-2\pi i n y/a) \]  \hspace{1cm} (1.21)

\[ g(z) = \sum_{n'} G(n') \exp(-2\pi i n' z/a) \]  \hspace{1cm} (1.22)

and

\[ h(x) = \sum_{n''} H(n'') \exp(-2\pi i n'' x/a) \]  \hspace{1cm} (1.23)
From the important property of the Fourier transforms applied to convolution principles, it turns out that

\[ F(n) = H(n) / G(n) \]  \hspace{1cm} \ldots \ldots (1.24)

But all these three coefficients involve real and imaginary parts and so,

\[ F(n) = \left[ H_r(n) + i \cdot H_i(n) \right] / \left[ G_r(n) + i \cdot G_i(n) \right] \]  \hspace{1cm} \ldots \ldots (1.25)

This on simplification yields

\[ F_r(n) = \left[ H_r(n) \cdot G_r(n) - H_i(n) \cdot G_i(n) \right] / \left[ G_r^2(n) + G_i^2(n) \right] \]  \hspace{1cm} \ldots \ldots (1.26)

\[ F_i(n) = \left[ H_i(n) \cdot G_r(n) + H_r(n) \cdot G_i(n) \right] / \left[ G_r^2(n) + G_i^2(n) \right] \]  \hspace{1cm} \ldots \ldots (1.27)

From the two experimental profiles, one observed from the imperfect sample giving \( h(x) \) and other from the well-annealed sample with large domain or grain size and free of strain giving \( g(z) \), the cosine and sine coefficients can be determined and they can be combined to give coefficients \( F_r(n) \) and \( F_i(n) \). The inverse Fourier transforms finally give the true broadening function as follows:

\[ f(y) = \sum_n \left\{ F_r(n) \cos \left( \frac{\pi \cdot n \cdot y}{a} \right) + F_i(n) \sin \left( \frac{\pi \cdot n \cdot y}{a} \right) \right\} \]  \hspace{1cm} \ldots \ldots (1.28)

1.2.5 Variance method for instrumental correction

Wilson (1962) introduced the concept of variance i.e., the second moment of the diffraction profile and defined it as

\[ W(2\theta) = \int (2\theta - 2\theta_c)^2 I(2\theta) \, d(2\theta) / \int I(2\theta) \, d(2\theta) \]  \hspace{1cm} \ldots \ldots (1.29)

where \( 2\theta_c \), the first moment, gives the position of the centroid or centre.
of gravity of the peak profile and defined as:

\[
\bar{\Theta} = \int \Theta I(\Theta) \, d(\Theta) / \int I(\Theta) \, d(\Theta)
\]

Now, if \( W'(\Theta) \) is the variance of the observed profile, which includes the effects of the instrumental aberrations and \( W''(\Theta) \) is the variance of the aberration functions, generally obtained from the profiles of the well-annealed samples, then according to Wilson (1962) and Papoulis (1955) the variances are additive and the true variance \( W(\Theta) \) is given by:

\[
W(\Theta) = W'(\Theta) - W''(\Theta)
\]

From the plot of \( W'(\Theta) \) and \( W''(\Theta) \) vs the angular range or the integration interval \( \Delta 2\Theta \), respective variances are to be determined from the linear portion of the plots, i.e., from the region of constant slope on using the property that the variances of diffraction profiles are linear functions of the range over which the variances are considered (Langford and Wilson, 1963; Aqua, 1966; Misra and Mitra, 1967; De and Sen Gupta, 1970, 1973). Recently, the non-additivity relations, curvature and satellite-group corrections, in the variance analysis have been discussed by Edwards and Toman (1970, 1971a,b), which need further consideration.

### 1.3 Schoening's Method of Convolution:

In evaluating breadth data it is assumed 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 double-square line. Schoening's (1965) method is concerned with these more realistic profiles, and needs detailed mention in view of our present work on simultaneous convolutions.

Let $I_p$ and $I_s$ respectively denote the intensity distribution for particle size and strain factors. Two cases were considered by Schoening (1965), and these are:

**case a**:\n\[ I_p = \frac{C_p}{(1 + K_p x^2)} \quad \text{and} \quad I_s = \frac{C_s}{(1 + K_s x^2)^2} \] (Particle size is Cauchy and strain is double-square)

**case b**:\n\[ I_p = \frac{C_p}{(1 + K_p x^2)} \quad \text{and} \quad I_s = \frac{C_s}{\exp(-K_s x^2)} \] (Particle size is Cauchy and strain is Gaussian)

Considering these two cases, the observed integral breadth $B_{\text{obs}}$ can be expressed in terms of the observed intensity profiles $I_{\text{obs}}(x)$ as,

\[ B_{\text{obs}} = \int_{-\infty}^{\infty} \frac{I_{\text{obs}}(x)}{I_{\text{obs}}(0)} \, dx \]  

The integral can be solved by using the properties of Fourier transforms namely,

\[ \int_{-\infty}^{\infty} I_{\text{obs}}(x) \, dx = \{ \mathcal{T}[I_p(x)] \cdot \mathcal{T}[I_s(x)] \}_{u=0} \]  

and

\[ I_{\text{obs}}(0) = \{ \mathcal{T}^{-1} \cdot \mathcal{T}[I_p(x)] \cdot \mathcal{T}[I_s(x)] \}_{x=0} \]

where $x$ and $u$ are the variables in real and Fourier space respectively.

Using the transforms and the integral breadths as a function of particle size $L$ and strain $e$ in equation (1.34) for the above cases we get:
\( B_{\text{obs}} = (2B' + B) \) \( (4B' + B)^{-1} \) \quad \ldots \quad (1.37) 

where \( B' = \mu/K' = \lambda/L \cos \theta \) and \( B' = \mu/K' = e \tan \theta \) \ldots \quad (1.38) 

\( B_{\text{obs}} = \frac{1}{2} \) \( B \) \exp \left\{ - \left( B'/B \right)^2/\pi \right\} \left( \frac{1}{2} - \text{erf} \left\{ \sqrt{2/\pi} \frac{B'}{B} \right\} \right) \quad \ldots \quad (1.39) 

where \( B' = \mu/K' = \lambda/L \cos \theta \) and \( B' = \mu/K' = e \tan \theta \) \ldots \quad (1.40) 

and \( \text{erf} (x) = \frac{1}{\sqrt{\pi}} \int_0^x \exp (-t^2) \, dt \) \quad \ldots \quad (1.41) 

An easy separation of strain broadening from particle size broadening is possible if two pairs of reflections (i.e. 111, 222 and 200, 400 in case of f.c.c. system) are used. The following abbreviations are introduced:

\[
\begin{align*}
B_i &= B_{\text{obs}} \left( \cos \Theta_i \right) / \lambda \\
U_i &= L \cos \Theta_i / \lambda \\
\alpha &= \left( \sin \Theta_1 \right) / \sin \Theta_2
\end{align*}
\]

With these abbreviations (equation 1.42), equations (1.37) and (1.39) becomes

\[ B'/B_2 = \left( \frac{1}{2} \right) \left( \frac{1}{2} \right)^2 \left( \frac{1}{2} + \frac{1}{2} \right)^{-1} \left( u_2 + \frac{1}{2} \right)^{-1} \quad \ldots \quad (1.43) 

\[ B'/B_2 = \frac{1}{2} \left( \frac{1}{2} \right) \left( u_2 + \frac{1}{2} \right) \frac{1}{2}^{-2} \quad \ldots \quad (1.43) 
\]

\[ B'/B_2 = \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \right)^2 \left( \frac{1}{2} + \frac{1}{2} \right)^{-1} \left( u_2 + \frac{1}{2} \right)^{-1} \quad \ldots \quad (1.44) 

\[ 1/L B_2 = \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \right)^2 \left( \frac{1}{2} + \frac{1}{2} \right)^{-1} \left( u_2 + \frac{1}{2} \right)^{-1} \quad \ldots \quad (1.44) 
\]
The results of the calculations of $B_1/B_2$ and $1/LB_2$ as functions $u_2$ and for $a = 1/2$ are given for the cases $a$ and $b$ and this allows the determinations of $L$ (particle size) and $g$ (strain) from $B_1/B_2$. 