New X-ray Diffraction Line Profile Function Based on Crystallite Size and Strain Distributions Determined from Mean Field Theory and Statistical Mechanics

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Abstract

Analytical profile functions have been derived here for the first time with parameters that directly determine the crystallite size distribution, average crystallite size, or strain distribution. These functions were derived by integrating the Laue interference function $\sin^2(Nx_e)/\sin^2(x_e)$, where $x_e$ is the strain dependent order of the reflection, with the crystallite size or strain distributions determined from mean-field theory and statistical mechanics. These functions are quite general and depend only on four physically measurable parameters of the microstructure: the Bragg or peak d-spacing $d_o$, the average number of lattice planes $<N>$, the rms strain $<\varepsilon^2>^{1/2}$, which is proportional to the average dislocation density $\rho^*$, and the parameter $\beta$ which characterizes the width of the size distribution and is functionally related to the kinetic growth parameter introduced by Rhines and Craig [1] and modified by Doherty [2], of a grain boundary sweep rate constant $\theta^*$. Theoretical values of $\theta^*$ for normal grain growth are shown to be in good agreement with those extracted from experimentally determined grain size distributions of zone-refined Iron [3]. These new profile functions can be fit using a Voight function for most of parameter space except for large values of $\beta$ and small values of $<\varepsilon^2>^{1/2}$ or $\rho^*$, as these analytic functions revert back to the Laue function with $N$ replaced by $<N>$ as they should. However, for small $\beta$ (< 5) the size-profile function is similar in form to a modified Pearson VII function where the exponent $(m - 1)$ is proportional to $\beta$. A general profile function obtained by the integration of the Laue function over both the size and strain distributions, presently exists as a single integral over the strain that is easily integrated numerically, and therefore can be implemented into a least squares fitting routine which will be published in detail elsewhere [4].

Introduction

X-ray line broadening analysis, using integral breadth techniques, typically relies on the assignment of the Lorentzian character of a reflection as due to the grain size distribution and that of its Gaussian character to the strain distribution. This assignment, while not arbitrary, has no solid foundation in theory and will be shown to be valid only under certain conditions. In addition, most profile functions depend on parameters which have no direct microstructural interpretation, rather this information is extracted from the type of analysis technique used. These analysis methods require non-overlapping multiple orders or at the very least reflections of similar size and strain energy dependencies, which is not always possible when analysing thin films. The more robust Fourier techniques (e.g. Warren & Averbach, and Vogel, Haase & Hosemann methods) also require non-overlapping multiple orders, and are generally more difficult to implement. In addition, the average grain size, extrapolated from the initial linear portion of the size dependent Fourier coefficient is plagued from the classical background-hook...
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effect, and the subjective nature of when to truncate the points used in the linear extrapolation, contribute to the uncertainty in the actual extrapolated value. Thus extracting the average grain size is often technique dependent, and a more straightforward approach is needed in determining not only the average grain size but the grain size and strain distributions as well.

The focus of this paper is to produce analytical expressions for x-ray line broadening that contain parameters dependent only on the physical microstructure of a given material. These profile functions should be general enough to apply to a wide class of materials which can then be easily implemented into standard profile fitting routines that utilize the whole peak-profile to extract the relevant physical parameters and not just the integral breadth. This approach is easier to implement than available Fourier techniques, and eliminates the requirement of multiple orders so in principle the microstructural information can be extracted from a single reflection. The approach which was adopted here is somewhat similar to that taken by Lutterotti and Scardi [5], which is to integrate the Laue interference function, as it represents the intensity from a single crystallite of size Nd, over all crystallites utilizing the distributions of crystallite size and strain. However the similarity in the two approaches is outweighed by their differences. Lutterotti and Scardi’s approach was based on fitting preselected points of the profile with a size distribution determined by two or three unphysical Lagrangian multipliers. Our approach is to determine meaningful expressions for both the size and strain distributions based upon a mean field theory and statistical mechanics approach, from which one can calculate a general profile function.

Size Distribution Theory and Function

X-ray scattering from a polycrystalline material with typical x-ray volumes is in essence an averaging process by which the total intensity is the ensemble average of the intensities from hundreds of millions if not billions of crystallites, a truly many bodied problem which lends itself quite well to the mathematical descriptions of statistical mechanics and mean field theory. As the theory of grain growth is a difficult subject, this paper will ignore effects of texture and strain on grain size, as these are subjects better handled elsewhere, and instead focus on randomly oriented growth of a single phase material, which has orientation and strain independent grain boundary surface and interface energies. While the above assumptions seem restrictive, the results are far reaching and applicable to materials which exhibit abnormal growth [6,7].

Classical mean field theories [8-11] describe the grain growth process in terms of the growth of a single grain embedded in an ‘environment’ which represents the collective average of all the other grains. This ‘environment’ is described by the collective or mean density of grains of a particular size R, that is, the grain size distribution p(R,t), which can be time dependent. The mean density of grains ρ(R,t) must satisfy the continuity equation for ‘mass’ (density) transport

\[
\frac{\partial \rho(R,t)}{\partial t} = - \frac{\partial}{\partial R} \left( D \frac{\partial \rho(R,t)}{\partial R} \right) - \rho(R,t)v(R) \tag{1}
\]

where D is, as yet, an undefined diffusion constant and v(R) is the grain boundary drift velocity.
given by Hillert [9], which is grain boundary surface curvature driven.

\[ \nu(R) = \mu \gamma \left[ \alpha \left( \frac{1}{R_0} - \frac{1}{R} \right) \right] \]  \hspace{1cm} (2)

Here \( \mu \) is the grain boundary self diffusion or grain mobility constant, \( \gamma \) is the grain boundary surface energy, \( \alpha \) is a geometric constant, and \( R_0 \) is the critical grain radius below which surface curvature forces cause the grain to contract or reduce in size (\( \nu(R) < 0 \)) until consumed by other grains, and above which, expand the grain size (\( \nu(R) > 0 \)) for grain growth. The grain radius \( R \) and critical radius \( R_0 \) are of course time dependent. The expression in the brackets [ ] of equation (2) is Hillert’s mean grain boundary curvature.

The mean field theories to date suffer from at least three inadequate assumptions about the grain growth process which restrict their utility in determining \( \rho(R,t) \). The first assumption is that the principle driving force for grain growth is the reduction of grain boundary surface area, which is incorrect, and instead should be the reduction of the grain boundary surface area per unit volume \( S_b(R) \) [12]. The second assumption is that the diffusion term is negligible as a driving force for grain growth compared with the surface curvature term and is normally dropped from the equation. Strictly speaking, this is true of course only for small grain sizes and actually for large grains the diffusion term becomes quite significant. The physical basis for the introduction of the diffusion term has also been unclear, but it will be shown below that it is related to the kinetics of the growth process. The third inadequacy is related to the property of scaling. It is known [3,12] that for normal grain growth the grain size distribution when scaled to the maximum or average grain size is time invariant. This means that if one searches for a solution to \( \rho(R,t) \) in the form of \( \rho(u(t),t) \) where \( u(t) = R(t)/R_0(t) \) then \( \rho(u(t)) \) is not explicitly dependent on time and \( \partial \rho(u(t))/\partial t = 0 \).

By utilizing the above corrected assumptions and adopting the mean grain boundary curvature given by Hillert [9] we have shown [13] that minimizing \( S_b(R) \) with respect to \( R \) and using a mean field approach given in equation (1) are equivalent, in a mathematical sense, and produce the following simple differential equation for normal grain growth.

\[ \frac{\partial \rho(u)}{\partial u} + \beta (1 - \frac{1}{u}) \rho(u) = 0 \]  \hspace{1cm} (3)

The solution is trivially obtained as

\[ \rho(u) = u^\beta e^{-\beta u} \]  \hspace{1cm} (4)
The physical interpretation of the parameter \( \beta \) comes from the concept of a grain boundary sweep rate constant \( \theta^* \) introduced by Rhines and Craig [1], altered in definition by Doherty [2] and written into a simple empirical equation [11], that can be reduced to equation (3) by utilizing the above assumptions, with \( \beta \) defined in terms of \( \theta^* \) (\( \beta = 1 + 1.5/\theta^* \)). Details of this calculation will be given elsewhere [13]. The parameter \( \theta^* \) is defined (after modification by Doherty) to be the number of grains which vanish when grain boundaries sweep through a volume equivalent to the mean grain volume. Thus, \( \theta^* \) and hence \( \beta \) are parameters which describe the kinetics of the grain growth process. The parameter \( \theta^* \) not only explains the physical basis for the diffusion constant \( D \) in equation (1) but it also explains why the diffusion constant \( D \) has the wrong sign as it represents a loss of grain flux. It is difficult to measure \( \theta^* \) as this would require one to look at the grain microstructure as a function of growth (time). However, Hunderi has estimated \( \theta^* \) for normal grain growth and found \( \theta^* = 1.76 \) based on Hillert's size distribution model [14] and \( \theta^* = 1.67 \) from a computer model of grain growth [15], yielding on average, \( \beta = 1.87 \) using the above expression derived for cross-sectional data.

Experimental verification of the above model can be accomplished by fitting equation (4) to the measured grain size distribution acquired from two dimensional metallographic cross sections of a material which is known to exhibit normal grain growth. Such a material is zoned-refined Iron. Optically measured grain size distributions of zoned-refined Iron, annealed at 650 C as a function of time, are available from the Handbook of Metals [3].
Figure 1: Simultaneous fitting the alpha-Fe zone-refined size distributions of 25-625 minutes to eq. (4). The first set of numbers in the figure indicate the value of $D_{\text{max}}$ and $\beta$ and the second set the estimated uncertainty.

The combination of the size distributions of Iron, zone-refined from 25 minutes to 625 minutes, are simultaneously fit to equation (4) using a single value of $\beta = 1.86$. This fit emphasizes that the size distribution shape is time invariant, and in good agreement with our theoretical estimate based on Hunderi’s $\theta^*$, and the result is shown in figure 1.

While equation (4) is shown to be a valid size distribution for single phase materials which exhibit normal grain growth, there are other materials such as thin-films which exhibit abnormal grain growth. Abnormal grain growth is basically any grain growth process which is not normal, and is generally associated with additional driving forces which favour specific sets of grains. A specific case of abnormal grain growth is secondary recrystallization, which can be characterized by a bimodal size distribution [6] and hence could be described by two normal grain growth distributions of eq. (4). In addition, Lazecki et. al. [7] suggested that abnormal grain growth could generally be described by a time dependent log-normal size distribution width, which translates here into a time dependent $\beta(t)$ parameter in equation (4). Hence, equation (4) could be used to describe the size distribution in a host of materials at various growth times, and is not necessarily restricted to normal grain growth ($\beta(t) = \text{constant}$).

If we assume, as is commonly done, a columnar-like grain structure perpendicular to the diffracting planes with a uniform strain, then the grain size $R$ can be replaced with $Nd_R$ (R with N,d), and $u$ with $N/N_o$. The Laue function centered about the first order can now be integrated over the size distribution of eq. (4), which is normalized by setting the size distribution integral to unity, resulting in the following analytical size profile function

$$f(d, N_o, \beta, \theta) = \frac{1}{2 \sin^2 \Lambda} (1 - \cos[(\beta + 1) \tan^{-1}(\frac{2N_o A}{\beta})])$$

$$\frac{(1 + \left(\frac{2N_o A}{\beta}\right)^2)^{\frac{\beta + 1}{2}}}{(1 + \left(\frac{2N_o A}{\beta}\right)^2)^{\frac{\beta + 1}{2}}}$$

where $A$ is given by

$$A = \pi \left(\frac{2d}{\lambda} \sin \theta \cdot 1\right).$$

If $\theta$ is expanded about the peak position $\theta_b$ then $2N_o A/\beta$ can be approximated by

$$\frac{2N_o A}{\beta} = 2\pi \frac{N_o d_b \cos \theta_b}{\lambda} 2 \sin (\theta - \theta_b) = a(\beta) \frac{(2\theta - 2\theta_b)}{FWHM}$$

(7)
Where the FWHM is given by the Debeye-Scherrer equation (the reciprocal of which is in the brackets \([\ ]\) of eq. (7)) and \(a(\beta)\) is a constant dependent on \(\beta\). After substituting eq. (7) into eq. (5) the denominator of eq. (5) looks similar to a Pearson VII function where the exponent \(m\) is functionally related to \(\beta\). However, it can be shown that a better approximation to eq. (5) would be the following ‘modified’ Pearson VII function

\[
\frac{I_0}{(1 + k^2(\frac{2\theta - 2\theta_p}{FWHM})^2)^m}
\]

(8)

where \(k\), and \(m\) are functions of \(\beta\), and for \(\beta < 5\) given in the following approximate expressions

\[
k \sim \frac{.056}{\sqrt{\beta + 1} - 1}, \quad m \sim .231\beta + 1 .
\]

(9)

These approximations, in equations (8) and (9) give a physical justification for using a Pearson VII function, albeit in modified form, over other physically ambiguous but well fitting functions like the pseudo-Voight.
Figure 2: θ–2θ x-ray diffraction pattern of a fiber axis textured bilayer thin-film of a (111) NiFe layer deposited onto a highly oriented (002) hexagonal beta-Ta layer, where the NiFe (111) reflection shows finite size oscillations produced by a uniform NiFe grain or crystallite size.

The parameter $\beta$ in eq. (5) controls the shape of the reflection, and for small values of $\beta$ ($\beta \sim 1$) the profile is almost completely Lorentzian and for moderate values of $\beta$ ($\beta \sim 5$) the profile has a predominant Gaussian character. Profile shape changes from Lorentzian to Gaussian with increasing $\beta$ indicates that integral breadth techniques are valid only for small values of $\beta$. It is not surprising then to find that eq. (5) can also be fit quite well to a Voight function for most of parameter space, except for large values of $\beta$. It is not difficult to show that for large $\beta$ eq. (5) reduces to the Laue function with $N$ replaced by $N_0$ as the size distribution becomes a very sharply peaked (gaussian like) function around $N=N_0$. That is to say, the size distribution is uniform for large values of $\beta$.

The physical implications of a uniform size distribution are borne out in the following example. During the initial stages of growth, after grain nucleation, the grain boundaries of highly textured polycrystalline materials are known to be relatively immobile [3]. This immobility of grain boundaries for highly textured very thin-films results in little or no grain occlusion [16], that is during growth, grain loss and hence $\theta^*$ is small, or alternately $\beta$ is large, resulting in a uniform grain size distribution. Such is the case in figure 2 (above) which shows a θ–2θ XRD pattern for a bilayer of a highly textured (111) fcc-NiFe film 100 angstroms thick grown on a seed layer of hexagonal beta Tantalum 35 angstroms thick. The damping of the finite size oscillations on the high 2θ side of the (111) NiFe reflection is due to a bi-modal strain distribution. The damping of finite size oscillations due to rms-strains, is discussed in the next section, and the profile fitting results of the data in figure 2 will be published elsewhere [4]. Figure 2 clearly demonstrates that it is extremely important to use a profile function like equation (5) in the analysis of highly textured thin-films which exhibit finite size oscillations, in order to extract relevant microstructural information.

While eq. (5) is expressed in terms of $N_0$ which is the peak of the size distribution, it is trivial to show that the average $N$, <$N>$, is related to $N_0$, through the relation <$N>$ = $N_0$(β+1)/β. So, eq. (5) can easily be expressed in terms of <$N>$ (i.e. the average grain size <$N>$) by this simple scaling. Scaling by <$N>$ is necessary if one is to calculate the Fourier coefficient by integrating the size distribution in equation (4). One can also show that the initial linear extrapolation of the normalized Fourier coefficient $A_n$ does indeed intersect at $n = <$<$N>$> for any value of $\beta$ as it should.

**Strain Distribution Theory and Function**

The approach taken here in determining the strain distribution is through the mathematical description of the mean strain density or strain probability offered by statistical mechanics. In statistical mechanics, the mean density or probability $P(q)$ of a parameter $q$, assumed here to be a continuous variable, can be shown to obey the continuity equation for $q$-space (i.e. has no explicit time dependence or is time invariant) if $P(q)$ is proportional to $e^{H(q)}$ where $H(q)$ is the
Hamiltonian or total energy of the system, and \( k \) is a Lagrangian multiplier which satisfies the equation for the average energy \( U_\varepsilon \) of the system given below [17].

\[
U_\varepsilon = \langle H(q) \rangle = \frac{\int H(q)e^{-kH(q)}dq}{\int e^{-kH(q)}dq} 
\]  

(10)

Most of the effort in determining \( P(q) \) is writing out an expression for \( H(q) \), which allows the problem to be tractable but yet retains some physical significance, and usually involves several simplistic approximations. We have assumed that the mechanical coupling or interaction between grains can be described by a single grain mean field energy approximation. By utilizing this approximation, the grains are mathematically decoupled, and the hamiltonian can straightforwardly be replaced with the single grain mean field energy \( E_\varepsilon \).

It is known that in materials with high dislocation densities, like strain hardened or cold-worked metals, there are uniformly strained regions of an otherwise perfect lattice in between regions of high dislocation densities. Dislocations generated inside the grain are, for the most part, swept through the grain, by forces which minimize the strain energy, and pile-up at obstacles like grain boundaries. If the grains are coupled mechanically, the dislocation arrays generated in each grain can redistribute themselves in the pile up to minimize the strain energy. These uniformly strained regions of the lattice in between networks of dislocations can then be averaged, in a mean-field sense, so that the grain can be described by an overall uniform strain which is dependent on some volume averaged dislocation density \( \rho^* \) and grain volume \((Nd)A\). The mean-field strain energy \( E_\varepsilon \) can be written as

\[
E_\varepsilon = \frac{N(\varepsilon - \varepsilon_0^*)^2}{G_{(h,k,l)}\rho^*}(Nd)A 
\]  

(11)

where \( G_{(h,k,l)} \) is a constant which is dependent on the burgers vector \( b \), shear modulus \( G \) and various other lattice constants, and \( \varepsilon_0^* \) is related to the back or internal stress generated from a dislocation array pile-up at the grain boundary [18]. Utilizing equations (10) and (11) the strain probability can be given as

\[
P(\varepsilon) = e^{-\frac{-N^2(\varepsilon - \varepsilon_0^*)^2}{f(N)}} 
\]  

(12)

where the function \( f(N) = \langle N^2(\varepsilon - \varepsilon_0^*)^2 \rangle = a_{(h,k,l)}p^*N \), and \( a_{(h,k,l)} \) is a direction specific constant which we will henceforth fold into some effective \( p^* \). Thus \( f(N) \) is proportional to the average dislocation density and the grain size \( N \). The linear dependence of \( f(N) \) on \( N \) was first deduced by Rothman and Cohen [19] by averaging the strain energy of single dislocations. A more general, but complex power law form of \( f(N) =aN^2r \) was deduced by Adler and Houska [20] from the Fourier analysis of several strain hardened or cold worked bulk materials and thin films.
Adler and Houska found that the parameter \( r \), was narrowly bound for a wide variety of materials, between about .4 and .6, and for which the average \( (r - \frac{1}{2}) \) also produces a linear function of \( N \). We have shown that a linear dependence of \( f(N) \) on \( N \) is a natural consequence of a statistical mechanics description of \( P(\varepsilon) \) using the strain fields from dislocation networks.

While there are many types of expressions for \( f(N) \) which could be applicable to a wide variety of materials like \( f(N) = a + bN \), which represents the convolution of a ‘Gaussian’ \( N^2 \) and a ‘Lorentzian’ \( N \) exponent term [20], they require at least an additional parameter which may be unnecessary. The exact \( N \) dependence of \( f(N) \) is only important when determining the simultaneous size and strain profile function in later sections, and for this purpose the linear form of \( f(N) \) given above will be used as this was shown by Adler and Houska to be fairly general, and it is more tractable than the other forms discussed above.

The d-spacing, \( d \), is strain dependent and strictly speaking given as \( d = d_0(1 + \varepsilon) \), where \( d_0 \) is the equilibrium lattice parameter. To facilitate the derivation, \( d_0 \) is replaced with \( d_b \) and the strain is re-scaled so that \( d = d_b(1 + (\varepsilon - \varepsilon_b)) \), and it is assumed that \( \varepsilon_b = \varepsilon_0 \) in equation (12). The strain distribution profile function \( F(d_b,f(N),N,\theta) \) can be obtained by integrating (12) with the Laue interference function and the above d spacing definition. The integration limits are strictly speaking over \(-1 \leq \varepsilon \leq \infty\), however it can be shown that for all practical values of the parameters the lower limit of \( \varepsilon \) can be extended to \(-\infty \leq \varepsilon_b \), with negligible error, and the integral expression is given below

\[
F(d_b,f(N),N,\theta) = \int_{-\infty}^{\infty} e^{-N^2(\varepsilon - \varepsilon_b)^2} \sin^2(\pi NL(1 + (\varepsilon - \varepsilon_b))) \, d\varepsilon
\]

(13)

where \( L \) is the order of the reflection given by \( L = (2d/\lambda)\sin(\theta) \). The integral in (13) is difficult to evaluate with ‘apparent’ singularities in the denominator of the Laue function. However, by assuming that \( N \) is an integer (as was implied in the derivation of the Laue function), and integrating the Laue function by parts \( N-1 \) times, an alternate expression for the Laue function can be developed.

\[
\sin^2(\pi NL(1 + (\varepsilon - \varepsilon_b))) = N - 2 \sum_{k=1}^{N-1} (N-k) \cos(2kL(1 + (\varepsilon - \varepsilon_b)))
\]

(14)

Equation (14) expresses the Laue function as a sum of cosines of different frequencies and substituting it into equation (13) makes the integration of (13) straight forward.

\[
F(d_b,f(N),N,\theta) = N - 2 \sum_{k=1}^{N} (N-k)e^{-f(N)/\pi^2L^2} \frac{1}{N^2} \cos(2\pi kL)
\]

(15)
If \( f(N) = \rho^*N \), then for \( \rho^* = 0 \) (i.e., a perfect crystallite lattice of size \( N \)), it can be seen that equation (15) reverts back to the Laue function of (14) with a uniform strain \( \varepsilon = \varepsilon_0 \), again as it should. The exponential in equation (15) acts as a defect damping mechanism to finite size oscillations given in the cosine term. While equation (15) appears simple, the sum over \( k \) is difficult to evaluate as it becomes a double integral or sum, when integrated or summed over the size distribution in equation (4). For this reason we will use the size distribution function to integrate the strain distribution of eq. (12) in the next section.

**Profile Function of Simultaneous Size and Strain Effects**

The general size and strain dependent profile function \( f(d_p,N_0,\beta,\rho^*,\theta) \), is determined by a double integration of the Laue function over size \( (N) \) and strain \( (\varepsilon) \) using the distributions of equations (4) and (12) after they are simultaneously normalized. This double integration can be accomplished by either integrating the strain function of equation (15) over the size \( N \), which leaves a double integration or sum over \( k \) and \( N \), or by integrating the Laue interference function over the size distribution in equation (4) taking into account the \( N \) dependence of the strain distribution in equation (12) and then integrating over the strain. For the reasons given above we have chosen the latter, and have formulated the following single integral expression for the general size and strain profile function \( f(d_p,N_0,\beta,\rho^*,\theta) \)

\[
f(d_p,N_0,\beta,\rho^*,\theta) = A_0 \int_{-\infty}^{\infty} \frac{1}{2\sin^2(B(\varepsilon))(1 + \frac{N_0}{\rho^* \beta})^{\frac{\beta + 1}{2}}} \left( 1 - \frac{\cos((\beta + 1)\tan^{-1}(\alpha))}{(1 + \alpha^2)^{\frac{\beta + 1}{2}}} \right) d\varepsilon
\]

where

\[
A_0 = \sqrt{\frac{N_0}{\pi \rho^* \beta}} \frac{\Gamma(\beta + 1)}{\Gamma(\beta + \frac{1}{2})}, \quad (17)
\]

\[
B(\varepsilon) = \pi(\frac{2d_p}{\lambda} \sin\theta)(1 + \varepsilon) - 1) \quad , \quad (18)
\]

and

\[
\alpha = \frac{2N_0 B(\varepsilon)}{\beta + \frac{N_0}{\rho^* \varepsilon^2}} \quad . \quad (19)
\]
Equations (16-19) have been easily implemented into a standard least squares refinement package with an instrument function convolution and the details of this implementation will be given elsewhere [4]. We have also derived other analytic forms of equations (15) and (16), based on the more general forms of the strain distribution given above, but these depend on the difficult evaluation of the Whittaker function $D_v(z)$ with a complex argument $z$ that is easily evaluated only for integral values of $v$ and will be given elsewhere [21].

Summary

We have produced here for the first time analytic x-ray line profile functions for size or strain which are only dependent on physically relevant parameters of the microstructure of a given material. Although these functions are expected to be fairly general in their application, only experimental verification can prove their usefulness. One of these parameters, $\beta$, is related mathematically to the $\theta^*$ kinetic parameter of growth defined by Rhines and Craig [1] and Doherty [2]. This connection must be proven experimentally and will be the focus of further papers on the x-ray analysis of thin film size distributions and their comparison to optically analysed TEM micrographs [22]. At present the line profile function for size and strain exists as a single integral over the strain and this has been implemented into a non-linear least squares fitting routine and the details are given elsewhere [4]. Numerical integration of more general strain and size distribution profile functions are of course possible, but they involve a more time consuming double integral and their comparisons to equation (16) are the subject of further work [21].

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