Least-squares analysis of x-ray diffraction line shapes with analytic functions

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Least-squares analysis of x-ray diffraction line shapes with analytic functions

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This is a second paper of a sequence that provides a useful analytic function which is based upon the Warren-Averbach line shape analysis. Once the Fourier coefficients are interrelated in terms of a minimum number of parameters, the rather lengthy Fourier series can be evaluated by reducing it to a convolution of two known functions. One of these functions includes the particle size distribution, strain, and the Cauchy-like contribution to the instrumental broadening. The second includes another strain parameter and the Gaussian contribution to the instrumental broadening. The resultant convolution integral is readily carried out using a nine-point Gaussian-Legendre quadrature. Instrumental parameters are obtained from a separate convolution of Cauchy and Gaussian functions. This procedure reduces the computer time to one-tenth the time required to synthesize the Fourier series and makes it feasible to carry out a least-squares fitting of the profile data. Examples are given for Mo films and for an InSb film.

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INTRODUCTION

In a previous paper,1 it was demonstrated that the Fourier coefficients in the Warren-Averbach line shape analysis2 can be interrelated with five parameters for two orders. They include two strain parameters that describe the falloff of nonuniform microstrain with increasing distance, the average particle size, an instrumental parameter for each order, and an intensity scaling factor for each order. The instrumental parameters are obtained separately by fitting a Cauchy profile to data obtained from ideal samples giving only instrumental broadening. Consequently, the total number of parameters used to fit "n" specimen broadened multiple order profiles is 3 + n. The present paper extends the previous one by giving an analytical expression that reduces computer time to about one-tenth of our previous approach. Also, the requirement that the instrumental broadening must be of a pure Cauchy form has been eliminated.

The new analysis provides useful data even though entire profiles are not available. The classical Warren-Averbach analysis gives a hook effect when for one reason or another the full profile is not measurable. This may introduce considerable error in the results. Examples are given that demonstrate the effect of truncating the number of data points in the peak tails and also the effect of using only one-half of each profile. A 50% truncation still gives acceptable values for all parameters while 75% truncation gives strain parameters that are still quite good but a particle size that is too low.

The new analytical function can be generated quickly enough to make use of nonlinear least-squares fitting routines. By intentionally selecting particle and strain parameters away from the optimum point, error plots can be obtained that show the sharpness of the least-squares fit. A broad error surface would provide a range of strain or particle size parameters and a low confidence level for any single set. Whereas, one that is sharp along a specific parameter axis would represent a high level of confidence in that parameter. Similar surfaces can be generated from the instrumental profiles. This kind of interpretation is not feasible with the classical analysis and becomes especially important when only one peak is used to obtain strain and particle size information.

THEORY

The shape of a diffraction line can be described by2

$$P(h_i) = Y_e \left[ 1 + 2 \sum_{n=1}^{\infty} A_n \cos \left( 2\pi n (h_i - l) \right) \right], \quad (1)$$

where $h_i$ is the usual reciprocal space variable given by

$$h_i = 2d \sin \theta / \lambda, \quad d > \lambda$$

is the average interplanar spacing for (00l) planes, $\theta$ is the angle of incidence, and $\lambda$ is the wavelength. $Y_e$ is considered to be a constant for a reflection. The Fourier coefficient $A_n$ is defined as a product of coefficients. Individual coefficients contain information about the degree of perfection of the specimen, as well as broadening from the instrument. The latter includes the broadening effect from the spectral distribution of wavelengths that are counted from the detector. In order to have the option of working with incomplete profiles, the strain and particle size coefficients were interrelated for different $n$ values by three parameters.1 In this paper, one additional parameter is included to better describe the shape of the instrumental broadening.

The Fourier coefficient in Eq. (1) can be written in two ways that are experimentally indistinguishable. These are given by

$$A_n = (A \gamma)^n (A \beta)^n A \delta (A \rho)^n \quad (2a)$$

$$A_n = (A \gamma)^n (A \beta)^n A \delta (A \rho)^n (A \psi)^n. \quad (2b)$$

In the following discussion, a brief description is given of the individual Fourier coefficients. The strain coefficient can be written as

$$\text{(Continued...)}$$
\[ (A^p)^* = [\exp(-2\pi^2 <\epsilon^2 > >)]^*, \quad (3) \]

where \( q = 2(r + 1) \) and \( r \) allows the total \( n \)th neighbor strain to be related to the first according to

\[ <\epsilon^2 > ^{1/2} = |n| <\epsilon^2 > ^{1/2}. \quad (4) \]

The restriction \(-1/2 < r < 0 \) is imposed \(^1\) with \( r = -1/2 \) taken to represent the strains associated with a dislocation network. \(^2\) The second definition of the strain coefficient is given as a product of the individual terms corresponding to the two extreme strain distributions found in certain sputtered films,

\[ (A^p)^* = [\exp(-2\pi^2 <\epsilon^2_{ID} >)]^* \quad r = -1/2, \quad (5a) \]

\[ (A^p)^* = [\exp(-2\pi^2 <\epsilon^2_{UD} >)]^* \quad r = 0, \quad (5b) \]

where the mean-square strain \( <\epsilon^2_{ID} > \) is related to pure dislocation sources and \( <\epsilon^2_{UD} > \) has been associated with atoms becoming embedded in films during the sputtering process. \(^3\) The alternate expressions [Eqs. (5a) and (5b)] can be obtained by convoluting the strain distributions associated with these defects. The strain field giving \( <\epsilon^2_{ID} > \) and the related broadening requires the special constraints found in film specimens with only one surface free to move. It could be set equal to zero for more conventional studies of cold-worked metals having point defects in solids with unconstrained free surfaces.

The particle size coefficient is given by

\[ A^p_s = 1 - \frac{n}{N_3} + \frac{4}{27} \left( \frac{n}{N_3} \right)^3, \quad n < \frac{3}{2} N_3, \quad (6a) \]

\[ A^p_s = 0, \quad n \geq \frac{3}{2} N_3, \quad (6b) \]

where \( N_3 \) is the average number of unit cells per column. The first two terms in Eq. (6a) represent the fraction of \( n \)th neighbors for columns of the same height. The cubic term allows for the distribution of heights within an entire sample. In the present case, it has been approximated by the column length distribution of a sphere.

The first of the instrumental coefficients is relatable to the Cauchy-like character of the instrumental broadening and is defined by

\[ A^p_c = \exp(-2\pi\rho), \quad (7) \]

where \( \rho \) representing a shape fitting parameter. This coefficient is obtained by taking the Fourier transform of the normalized Cauchy function, i.e.,

\[ g_1(h_3) = (1/\rho\alpha)(1 + h_3/\alpha h_3)^{-1}, \quad (8) \]

while

\[ A^p_c = \exp(-\pi\rho h_3^2), \quad (9) \]

is obtained from the Fourier transform of a normalized Gaussian function given by

\[ g_2(h_3) = (1/\rho\alpha)\exp(-\pi h_3^2/\alpha h_3^2). \quad (10) \]

It is well known that when Fourier coefficients are multiplied, this is equivalent to convoluting the original functions from which the coefficients were derived. \(^5\) Equation (1) can be interpreted in this sense. One can begin with an ideal sample giving very sharp reflection points described by delta functions. If one introduces internal boundaries, the reflections become broadened and this can be introduced by convoluting the delta function with the appropriate particle size function. Likewise, the effect of dislocation strain fields or other strain distributions that produce broadening can be introduced by successive convolutions. This is imagined as a systematic and independent process of introducing various defects that give successive broadening effects. In the case of strain broadening, one can introduce a single strain distribution as given by Eq. (4) or convolute with two extreme distributions having \( r = -1/2 \) and \( <\epsilon^2 > \) can be determined from a best fit of

\[ (1/n)\langle \epsilon^2_{ID} \rangle + <\epsilon^2_{UD} > = n^2 <\epsilon^2 > = \langle \epsilon^2 >. \quad (11) \]

Equation (1) is cumbersome to use as a Fourier series having many terms and can be put into a much more useful form for computer calculations. This sum is best carried out as an equivalent integration. The following definitions are required to change variables and to simplify the equations:

\[ u = n/N_3, \quad h_3 = N_3 h_3 \quad (12) \]

and

\[ \gamma = 2\pi N_3(a + \pi <\epsilon^2_{ID} >), \quad (13a) \]

\[ \beta = \pi N_3^2(a_0 + 2\pi <\epsilon^2_{UD} >). \quad (13b) \]

This enables one to write the integral

\[ P(h_3^2) = \int_0^{1/2} \left( 1 - u + \frac{4}{27} u^3 \right)e^{-\gamma u + \beta u^2} \cos(2\pi h_3^2 u) du. \quad (14) \]

A useful result can be obtained by setting \( \beta = 0 \) and evaluating the sum of three integrals of the type,

\[ \int u^m e^{-\gamma s} \cos(\rho u^3) du = \exp(-s u), \quad (15) \]

\[ \int \frac{m(m - 1)}{\rho^2} u^{m-2} \cos(\rho u^3 - 3\phi) du = \frac{m-1}{\rho^2} u^{m-3} \cos(\rho u^3 - 4\phi) + \cdots, \quad (15) \]

Table I. Nine-and nineteen-point roots and weight factors for the Gauss-Legendre quadrature. \(^7\)

<table>
<thead>
<tr>
<th>Roots (( z_i ))</th>
<th>Weight factors (( W_i ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nine-point</td>
<td></td>
</tr>
<tr>
<td>0.000 000</td>
<td>0.330 239</td>
</tr>
<tr>
<td>± 0.324 253</td>
<td>0.312 347</td>
</tr>
<tr>
<td>± 0.613 371</td>
<td>0.260 611</td>
</tr>
<tr>
<td>± 0.836 031</td>
<td>0.180 648</td>
</tr>
<tr>
<td>± 0.968 160</td>
<td>0.081 274</td>
</tr>
<tr>
<td>Nineteen-point</td>
<td></td>
</tr>
<tr>
<td>0.000 000</td>
<td>0.161 054</td>
</tr>
<tr>
<td>± 0.160 359</td>
<td>0.158 969</td>
</tr>
<tr>
<td>± 0.316 564</td>
<td>0.152 766</td>
</tr>
<tr>
<td>± 0.604 571</td>
<td>0.142 607</td>
</tr>
<tr>
<td>± 0.600 545</td>
<td>0.128 754</td>
</tr>
<tr>
<td>± 0.720 966</td>
<td>0.111 567</td>
</tr>
<tr>
<td>± 0.822 715</td>
<td>0.091 490</td>
</tr>
<tr>
<td>± 0.903 156</td>
<td>0.069 045</td>
</tr>
<tr>
<td>± 0.960 208</td>
<td>0.044 814</td>
</tr>
<tr>
<td>± 0.992 407</td>
<td>0.019 462</td>
</tr>
</tbody>
</table>
TABLE II. Least-squares analysis of two Mo films on (111) Si and one InSb on (111) GaAs.

<table>
<thead>
<tr>
<th>Sample</th>
<th>(&lt;L&gt;) (A)</th>
<th>(&lt;\varepsilon_{1p}&gt;^{1/2}\times 10^2)</th>
<th>(&lt;\varepsilon_{1U}&gt;^{1/2}\times 10^3)</th>
<th>(\phi/M)</th>
<th>(\phi/M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo/Si</td>
<td>186</td>
<td>1.37</td>
<td>0.310</td>
<td>6.91</td>
<td></td>
</tr>
<tr>
<td>Mo/Si</td>
<td>884</td>
<td>1.30</td>
<td>0.143</td>
<td>4.60</td>
<td></td>
</tr>
<tr>
<td>InSb/GaAs</td>
<td>1337</td>
<td>0.42</td>
<td>0.042</td>
<td>12.8</td>
<td></td>
</tr>
</tbody>
</table>

where \(p = (b^2 + \gamma^2)^{1/2}\), \(\cos \phi = -\gamma/p\), \(\phi = \pi - \tan^{-1}(b/\gamma)\).

This result is given by

\[
P(h_0) = \frac{1}{2N_{1}Y_0} \left( \frac{2\pi h_0^2 - \gamma^2 + 8/9 \cos \left[ 3\pi h_0^2 + 3 \tan^{-1}(2\pi h_0^2/\gamma) \right] }{2\pi h_0^2 + \gamma^2} \right)^{1/2} - \text{FLC}
\]

and

\[
\text{FLC} = \frac{e^{-(1/2) \pi}}{[2\pi h_0^2 + \gamma^2]^{3/2}} \left( \frac{4}{3} \cos \left[ 3\pi h_0^2 + 3 \tan^{-1}(2\pi h_0^2/\gamma) \right] \right)
+ \frac{8}{9} \frac{\cos \left[ 3\pi h_0^2 + 4 \tan^{-1}(2\pi h_0^2/\gamma) \right] }{[2\pi h_0^2 + \gamma^2]^{1/2}}.
\]  

The first term in Eq. (16) can be obtained from Eq. (14) by allowing the upper limit to go to infinity. A finite limit introduces an additional term given by FLC. This finite limit correction, of course, results from the 3/2 cutoff point of the particles size coefficient given in Eq. (6a). If the term \(e^{-\tau w}\) were to converge to zero before \(A_{\infty}\), the FLC can be neglected.

Although the complete solution has not yet been obtained, Eq. (16) can be used to analyze cold-worked metals under certain restricted conditions. First, the specimen broadening must be due only to small particle size and dislocation originated strain \((\tau = -\gamma)\). Second, the instrumental broadening must either be relatively small or a pure Cauchy function. The latter is approximately attained with a well-focused monochromater that removes the \(K_{\alpha 2}\) component of the \(K_{\alpha}\) doublet and ideal diffractometer conditions.

In order to complete the calculation of Eq. (14) with \(\beta \neq 0\), it must be recognized that this term originates from a Gaussian function with a half-width determined by \(<\varepsilon_{1U}>\) and \(a_{\beta}^2\), i.e.,

\[
g_3(h_0^0) = Y_0 \exp \left[ -\pi h_0^2/3N_{1}^2 \left( a_{\beta}^2 + 2\pi <\varepsilon_{1U}>/1.2 \right) \right].
\]  

or, that the cosine transform of Eq. (17) gives the original term \(e^{-i\omega x}\) when properly normalized. Equation (17) remains Gaussian after convoluting the Gaussian strain broadening with the Gaussian contribution from instrumental broadening.

Unfortunately, one must resort to a numerical convolution of Eq. (16) with Eq. (17) to obtain the final result. This can be carried out accurately using a nine-point Gauss-Legendre quadrature. 6,7 The required convolution integral is

\[
P_{\beta}^{*}(h_0^0) = Y_0^{*} \int_{-b}^{b} g_3(x)P_{1}^{*}(h_0^0 - x)dx,
\]  

where \(Y_0^{*}\) is a scaling constant and the limits \(\pm b\) are established to encompass most of the area of \(g_3(x)\). A typical value that has been used and one which does not introduce a significant termination error is 99.9%. The numerical integration by Gauss-Legendre quadrature is normally carried out with the new variable \(z\) that causes the limits to be \(\pm 1\).

\[
P_{\beta}^{*}(h_0^0) = Y_0^{*} \int_{-\infty}^{\infty} g_3(bz)P_{1}^{*}(h_0^0 - bz)dz,
\]  

or as a nine-point quadrature,
FIG. 2. Instrumental fit using Eq. (20) for two orders from a Mo powder. The fit for every third data point is illustrated.

SEVERAL EXAMPLES OF LINE SHAPE FITTING

All of the following examples of line shape fitting deal with sputtered films. Two of the data sets were obtained from samples containing Mo films on (111)-oriented Si single-crystal substrates prepared under different conditions. A third sample contained a (111)-oriented single crystal InSb film on a (111) GaAs crystal. The greatest line broadening was obtained from one of the Mo films while the smallest was obtained from the InSb film. All data were collected with a diffracted beam quartz monochromator, a fine focus Siemens diffraction tube, and a 0.05-mm receiver slit. The monochromator was set to reject the $K_a^2$ line.

Table II illustrates the results of a least-squares analysis of all three samples as performed on an IBM 370 system. These results include the average x-ray particle size ($\langle L \rangle$), two strain parameters, and the sum of squares deviation per point for fitting two orders ($\phi/M$). The Mo results made use of the (110) and (220) reflections while the InSb data used the (111) and (444). Figure 1 illustrates the fit to the actual data using Eq. (19) while Fig. 2 illustrates the fit for a pair of

TABLE III. Curve fitting with incomplete profiles of equally spaced points—No background truncation (a) and lower one-half of profile (b). Sample 2 Mo/Si.

<table>
<thead>
<tr>
<th>Data set</th>
<th>$M$</th>
<th>$\langle L \rangle$</th>
<th>$\langle \epsilon_{1d} \rangle^{1/2}$</th>
<th>$\langle \epsilon_{1u} \rangle^{1/2}$</th>
<th>$\phi/M$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) 20 FWHM</td>
<td>302</td>
<td>884</td>
<td>1.30</td>
<td>0.143</td>
<td>4.60</td>
</tr>
<tr>
<td>(b) $%$ of points (lower 2$\theta$)</td>
<td>154</td>
<td>1001</td>
<td>1.29</td>
<td>0.154</td>
<td>3.26</td>
</tr>
<tr>
<td>(c) 50% back. t.</td>
<td>154</td>
<td>867</td>
<td>1.31</td>
<td>0.141</td>
<td>7.89</td>
</tr>
<tr>
<td>(d) 75% back. t.</td>
<td>74</td>
<td>730</td>
<td>1.35</td>
<td>0.130</td>
<td>9.25</td>
</tr>
<tr>
<td>(e) 90% back. t.</td>
<td>30</td>
<td>608</td>
<td>1.39</td>
<td>0.115</td>
<td>4.94</td>
</tr>
</tbody>
</table>
instrumental curves using Eq. (20). The small deviation on
the high side of the second order peak is due to incomplete
rejection of the $K_{\alpha 2}$ line. A computer time of 222 sec
was required to obtain a best fit for sample 2 and this took 12
separate calculations for each pair of profiles to arrive at the
minimum sum of the squares with 302 data points. Each pair
of reflections requires about 19 sec of computer time to gen-
erate profiles for a given set of parameters when 302 data
points are used.

In many applications, one cannot obtain reliable data
for an entire profile because of overlapping peaks. Sample 2
was reanalyzed with various subsets of data points deleted
from each peak within a pair. These results are illustrated in
Table III. The first entry contains data over a $2\theta$ range of
twenty times the full width at the half maximum (FWHM)
arranged with the peak approximately at the center of
each interval. The same number of points were selected to
represent each peak and all points were equidistant on the $h_1$
scale. If only the points on the low side of each peak are used,
one still finds good agreement with the full analysis.
The rather large particle size of ~ 900 Å, which was found in this
sample, is expected to be subject to error because of the small
broadening associated with this size. The effect of back-
ground truncations of 50, 75, and 90% is also given. It would
appear that this analysis still gives a very reasonable particle
size with a 50% truncation of background. However, with
75 and 90% truncations, the particle size gives increasingly
obvious deviations. It is surprising to find that the strain
parameters remain nearly constant even with considerable
truncation. These results indicate that reliable particle size
and strain information can be obtained from incomplete pro-
files when two orders are used. This agreement cannot be
to be expected when using the conventional Warren-Averbach
line shape analysis.

In order to relate the sensitivity of $\phi/M$ to variations of
$<L>$, $<\varepsilon_{10}>$, and $<\varepsilon_{10}^2>$, these were varied holding the
other two fixed at the minimum (see Figs. 3, 4, and 5, respec-
tively). Figure 3 illustrates this response curve to variations in
$<L>$. Also illustrated are the truncation points b, c, d.

![Graph](image_url)

**FIG. 3.** Misfit $\phi/M$ vs normalized $<L>$,
$<L>/<L>_m$, for three samples, where $<L> = <d> \times N$. Both strain
parameters are held at the optimum values as given in Table II.

![Graph](image_url)

**FIG. 4.** Misfit error vs normalized $<\varepsilon_{10}>$, $<\varepsilon_{10}^2>/<\varepsilon_{10}^2>_m$, for three samples. $<L>$ and $<\varepsilon_{10}>$ are held at the optimum values given in Table II.

and $\varepsilon$ corresponding to the $<L>$ values given in Table III
(sample 2). It can be seen that all of these points are within
$\phi/M < 10^{-4}$. Plots within this range would appear to give
good visual fits with the data. An examination of Figs. 3, 4,
and 5 show that sample 2 has a relatively broad response
curve for particle size variations and sharp curves for the
strain parameters. This is because the major contribution to
the line broadening is due to strain and not particle size.
Sample 3 has the smallest broadening contribution from
strain and is primarily broadened by particle size. As one
might expect, the particle size response curve is the sharpest.
These curves are useful for evaluating the various contribu-
tions to the line broadening and therefore the degree of confi-
dence that may be associated with the parameters defining
the minimum points. Data from sample 1 is influenced by all
three types of broadening giving three relatively sharp re-
sponse curves.

Thus far all of the data have been analyzed as multiple
order pairs. It is tempting to examine the misfit generated
when only one peak is used for the analysis. If the broadening
associated with each effect is sufficiently distinctive, one
might expect to extract all three parameters from one peak.
Unfortunately, a one peak analysis has not given a unique set. Table IV gives results from separate analyses of the first and second order peaks as well as for an analysis of a pair from sample 2. When the least-squares program is initiated with \(<\epsilon_{1D}^2> = 0.5 \times 10^{-3}, <\epsilon_{1U}^2> = 0.5 \times 10^{-5}\) and \(N_3 = 50, 100, 150, 200, 250, \) and 300 successively, different compositions of parameters usually have low \(\phi/M\) values when only one peak is used. However, for the first order fit alone, both \(<L>\) and \(<\epsilon_{1D}^2>\) have a large range of values with equally low \(\phi/M\), while only \(<\epsilon_{1U}^2>\) appears to be well defined. For the second order, different initial values of \(<L>\) again converge to different points, all of which give low \(\phi/M\) values. When two orders are used, a unique minimum is obtained. The convergence illustrated in Table IV is typical of all paired profiles that have been studied. It is possible that when the total broadening approaches the instrumental broadening, several minimum points will be observed with nearly the same \(\phi/M\) even when a pair is used. This situation has not been observed thus far. Obviously, when this occurs, unique results cannot be obtained from the data. The present data indicates that a single peak analysis of strain and particle size does not give a unique minimum and is to be avoided.

As a final point, the calculations leading to Eq. (19) are based upon the distribution given by 1/n \(<\epsilon_{1D}^2> + <\epsilon_{1U}^2>\) rather than \(n^2 <\epsilon_{1D}^2>\) as given in Eq. (11). In a previous paper,\(^1\) it was pointed out that the profiles are insensitive to the small differences in strain associated with these distributions. This is true because the slowly varying intensity that gives strain information at low \(n\) is not usually measurable because of overlapping tails. Likewise, at large \(n\), the strain does not introduce an important effect on the profile because of the small number of pairs of cells that contribute to the intensity profile. The profile is largely shaped by pairs of cells having a separation within the range

\[
\frac{N_3}{20 < n < N_3},
\]

(21)

The strain has been plotted using both distributions within this range for sample 2 (see Fig. 6). The \(n^2 <\epsilon_{1D}^2>\) strain distribution has been shown to agree with Warren-Averbach analysis strain data\(^2\) but the data scatter most often exceeds the small oscillation introduced by the two term strain distribution. Consequently, either distribution is acceptable. In either case, the nonuniform strain \(<\epsilon_n^2>\) should not be interpreted out of the range given by Eq. (21). The parameters \(<\epsilon_{1U}^2>, <\epsilon_{1D}^2>,\) and \(<\epsilon_n^2>\) only have meaning when used to calculate \(<\epsilon_n^2>\) over the designated range.

**ACKNOWLEDGMENTS**

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