

Computer Programs for the Analysis of the Broadening of X-Ray Powder Patterns

E. A. METZBOWER

*Transformations and Kinetics Branch
Metallurgy Division*

April 5, 1971



NAVAL RESEARCH LABORATORY
Washington, D.C.

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) Naval Research Laboratory Washington, D. C. 20390	2a. REPORT SECURITY CLASSIFICATION Unclassified
	2b. GROUP

3. REPORT TITLE COMPUTER PROGRAMS FOR THE ANALYSIS OF THE BROADENING OF X-RAY POWDER PATTERNS

4. DESCRIPTIVE NOTES (Type of report and inclusive dates) A final report on one phase of a continuing problem.
--

5. AUTHOR(S) (First name, middle initial, last name)
--

E. A. Metzbower

6. REPORT DATE April 5, 1971	7a. TOTAL NO. OF PAGES 46	7b. NO. OF REFS 41
8a. CONTRACT OR GRANT NO. NRL Problem M01-23	9a. ORIGINATOR'S REPORT NUMBER(S)	
b. PROJECT NO. Project RR 007-10-46-5430	NRL Report 7253	
c.	9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	
d.		

10. DISTRIBUTION STATEMENT Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY Department of the Navy (Office of Naval Research), Arlington, Va. 22217
-------------------------	--

13. ABSTRACT <p>The report discusses in detail computer programs that have been written to analyze the broadening of x-ray diffraction peaks of hexagonal close-packed metals. The programs allow for the correction of the overlap of the long tails of the diffraction peak, and then correct for polarization and geometric factors, atomic scattering factors, and the $K\alpha$ doublet. Fourier coefficients are calculated using Filon's method of evaluating trigonometric integrals. The Stokes' corrected Fourier coefficients are separated into particle size and distortion coefficients using the Warren-Averbach technique modified for hexagonal close-packed metals. Domain sizes are obtained from fault-unaffected peaks, whereas stacking fault probabilities are obtained from fault-affected peaks.</p>

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
X-Ray Powder Patterns Computer Programs X-Ray Analysis Fourier Analysis of X-Ray Patterns						

DD FORM 1 NOV 65 1473 (BACK)
(PAGE 2)

CONTENTS

Abstract	ii
Problem Status	ii
Authorization	ii
INTRODUCTION	1
THEORY	1
Peak Broadening	1
Fourier Analysis	3
Warren-Averbach Method	3
Warren-Averbach Method Modified for hcp Metals	4
Experimental Considerations	5
PROGRAM ORTAILS	5
PROGRAM XRAY40	6
PROGRAM SEPARATE	10
REFERENCES	10
APPENDIX A - Program ORTAILS	13
APPENDIX B - Program XRAY40	21
APPENDIX C - Program SEPARATE	34

ABSTRACT

The report discusses in detail computer programs that have been written to analyze the broadening of x-ray diffraction peaks of hexagonal close-packed metals. The programs allow for the correction of the overlap of the long tails of the diffraction peak, and then correct for polarization and geometric factors, atomic scattering factors, and the $K\alpha$ doublet. Fourier coefficients are calculated using Filon's method of evaluating trigonometric integrals. The Stokes' corrected Fourier coefficients are separated into particle size and distortion coefficients using the Warren-Averbach technique modified for hexagonal close-packed metals. Domain sizes are obtained from fault-unaffected peaks, whereas stacking fault probabilities are obtained from fault-affected peaks.

PROBLEM STATUS

A final report on one phase of the problem; work in other phases is continuing.

AUTHORIZATION

NRL Problem M01-23
Project RR 007-01-46-5430

Manuscript submitted January 20, 1971.

COMPUTER PROGRAMS FOR THE ANALYSIS OF THE BROADENING OF X-RAY POWDER PATTERNS

INTRODUCTION

The effects of various crystal imperfections such as domain size, elastic strains, and faulting on the diffraction profile of x-ray powder patterns have been studied extensively (1-5). These studies have analyzed the changes in the positions and the profiles of the diffraction lines from powders prepared from metals and alloys by deformation (6, 7,), electrodeposition (8, 9,), vapor deposition (10, 11,), and by chemical processes such as catalytic reactions (12, 13,).

The broadening of the peak profile is assumed to be caused by the reduction in size of the coherently diffracting domains, by elastic strains within these domains, or by faulting on certain planes. Although many studies have been carried out on face-centered (fcc) and body-centered cubic (bcc) lattices, only a few investigations have been made on the broadening of x-ray powder patterns of metals and alloys that have the hexagonal close-packed (hcp) structure (14-25). In hcp metals and alloys the separation of the effects due to either domain size, faulting, or strains can be accomplished because certain $(hk\bar{l})$ peaks are unaffected by faulting, whereas other $(hk\bar{l})$ peaks are affected by faulting.

This report discusses in detail computer programs that have been written to analyze the broadening of x-ray diffraction profiles to hcp metals and alloys. The programs allow for the correction of the overlap of the long tails of the diffraction peak, and then correct for polarization and geometric factors, atomic scattering factors, and the K_{α} doublet by Keating's method (26). Fourier coefficients for both cold-worked and annealed powders are calculated using Filon's method (27) of evaluating trigonometric integrals. Stokes' correction (28) is applied to these Fourier coefficients. The domain size and distortion coefficients are separated by the Warren-Averbach technique modified for hcp metals. Domain sizes and slopes of the curves of the distortion coefficient as a function of the product of the harmonic number and the interplanar spacing are then computed. Finally, the stacking fault probability can be found from these results.

This report was greatly influenced by a similar report by Wagner (29). Several incorporations have been made, such as the corrections for peak overlap, atomic scattering factor, and K_{α} doublet, and especially the method of evaluating the Fourier coefficients. Although primarily written for the analysis of peak profiles from hcp metals, a few minor modifications would make the programs applicable to fcc and bcc metals.

THEORY

Peak Broadening

An x-ray diffractometer must consist of a source, specimen, and detector, all of finite size; otherwise, the diffracted x-ray intensity would be infinitesimal. As a consequence of these finite sizes, the diffraction profile is spread over a range of angles in the neighborhood of those given by Bragg's law. Therefore, one of the problems of x-ray powder diffractometry is the appropriate measurement of line positions and line profiles.

The most obvious measure of the line position is the position of the peak height. Another possible measure of the line position is the centroid or center of gravity, which can be expressed as

$$s_{CG} = \frac{\int_{s_1}^{s_2} s I(s) ds}{\int_{s_1}^{s_2} I(s) ds}, \quad (1)$$

where $I(s)$ is the distribution of scattered x-ray intensity across the diffraction peak as a function of $s = 2 \sin \theta_0 / \lambda$, θ is the Bragg angle, and s_2 and s_1 are the upper and lower limits of integration, i. e., the positions at which the peak profile merges with the background.

Several measures of the dispersion of the line profile have been considered, and no one measure of this peak broadening is universally accepted. The half-width (30) is the angular distance between two points at which the intensity is one-half the peak value. The half-width is an easy quantity to measure experimentally as long as only moderate accuracy is required.

The integral breadth (31) is defined as the integrated intensity of the diffraction peak divided by the peak height;

$$\beta(s) = \frac{1}{I(s_0)} \int_{s_1}^{s_2} I(s) ds. \quad (2)$$

The peak heights occur at $s_0 = 2 \sin \theta_0 / \lambda$, where θ_0 is the Bragg angle of the peak maximum.

The most mathematically satisfying measure of dispersion is the variance (32). The variance is the second moment about the center of gravity and is defined as

$$W(s) = \frac{\int_{s_1}^{s_2} (s - s_{CG})^2 I(s) ds}{\int_{s_1}^{s_2} I(s) ds}. \quad (3)$$

The peak profile $I(s)$ has been expressed as a Fourier series by Bertaut (33) and Warren and Averback (34):

$$I(s) = K \sum_{n=-\infty}^{\infty} C_n \exp [-2\pi n a_3 (s - s_0)], \quad (4)$$

where $a_3 = L$ is the distance normal to the reflecting planes of interplanar spacing $a_3 = d_{hkl}$, and n is the harmonic number. K , a slowly varying function of s , is equal to

$$K = f^2 (1 + \cos^2 2\alpha \cos^2 2\theta) / [\sin^2 \theta (1 + \cos^2 2\alpha)], \quad (5)$$

where f is the average scattering factor of the material, corrected for temperature, and α is the Bragg angle of the monochromator. The complex Fourier coefficients, a measure of peak broadening, are given by

$$C_n = \frac{1}{s_2 - s_1} \int_{s_1}^{s_2} \frac{I(s)}{K} \exp [+2\pi n a_3 (s - s_0)] ds. \quad (6)$$

The Fourier series can be expressed in terms of real quantities as

$$I(s) = K \sum_{n=-\infty}^{\infty} \{ A_n^S \cos [2\pi n a_3 (s - s_0)] + B_n \sin [2\pi n a_3 (s - s_0)] \}. \quad (7)$$

Fourier Analysis

Fourier coefficients have been shown by Warren (2) to be the product of two terms: one, A_n^S , the size coefficient, is a function of particle size; and the other, A_n^D , the distortion coefficient, is a function of strain, i.e.,

$$A_n = A_n^S A_n^D. \quad (8)$$

The size coefficients A_n^S are independent of the order of reflection and can be approximated for small values of $n a_3 = L$ as

$$A_n^S = \exp (-L/D_e), \quad (9)$$

where D_e contains the average size of the coherently diffracting domains $D(hk\bar{l})$ normal to the reflecting planes $(hk\bar{l})$ and the fictitious size $D^F(hk\bar{l})$ due to faulting:

$$\frac{1}{D_e} = \frac{1}{D(hk\bar{l})} + \frac{1}{D^F(hk\bar{l})}. \quad (10)$$

The distortion coefficient A_n^D is dependent on the order of the reflection and may be approximated for small values as

$$A_n^D = \exp \left\{ -2\pi^2 L^2 \left(\langle \epsilon_L^2 \rangle - \langle \epsilon_L \rangle^2 \right) s_0^2 \right\}, \quad (11)$$

where $\epsilon_L = \Delta L/L$, $\langle \epsilon_L^2 \rangle$ is the mean-square strain, and $\langle \epsilon_L \rangle$ is the mean strain.

Warren-Averbach Method

The Warren-Averbach (35) method is applied to separate the size coefficient A_n^S from the distortion coefficient A_n^D . The method requires measuring the peak profiles for several orders (at least two) of the diffraction peak. The distortion coefficient A_n^D approximated by Eq. 11 can be substituted into the expression for the Fourier coefficient, and consequently

$$A_n^S = A_n^S \exp \left[-2\pi^2 L^2 \left(\langle \epsilon_L^2 \rangle - \langle \epsilon_L \rangle^2 \right) s_0^2 \right], \quad (12)$$

which can also be expressed as

$$\ln A_n = \ln A_n^S - 2\pi^2 L^2 \left(\langle \epsilon_L^2 \rangle - \langle \epsilon_L \rangle^2 \right) s_0^2. \quad (13)$$

By plotting $\ln A_n$ as a function of s_0^2 for different diffracting orders for different values of $L = na_3$ and extrapolating to $s_0^2 = 0$, the value of A_n^S for each L is found. The slopes of the $\ln A_n$ vs s_0^2 curves for different values of $L = na_3$ are a measure of the difference between the mean-square strain $\langle \epsilon_L^2 \rangle$ and the square of the mean strain $\langle \epsilon_L \rangle^2$.

The initial slope of curves of A_n^S vs L is a measure of the domain size D_e , since

$$-\left(\frac{dA_n^S}{dL}\right) = \frac{1}{D_e}. \quad (14)$$

Warren-Averbach Method Modified for HCP Metals

In metals with hcp crystal structures, however, it is often very difficult to measure the second order of diffraction from a set of $(hk\bar{l})$ planes. Nevertheless, since certain $(hk\bar{l})$ planes are affected by stacking faults and other $(hk\bar{l})$ planes are unaffected by stacking faults it is possible to use this information to separate the size and distortion coefficients. Assuming that the distortion coefficients can be expressed by Eq. 11, then by plotting for different values of L the $\ln A_n$ vs $s_0^2 (1/d_{h\bar{k}l})$ for *fault-unaffected* peaks, the slope of such a curve is the difference between the mean square strain $\langle \epsilon_L^2 \rangle$ and the square of the mean strain $\langle \epsilon_L \rangle^2$. The intercepts of these plots are the size coefficients for these peaks. The distortion coefficients A_n^D are now utilized to correct the coefficient A_n^S of the *fault-affected* peaks for strain broadening in order to give the size coefficients A_n^S of these profiles.

The initial slopes of curves of the size coefficients as a function of L are a measure of the effective domain size. The slopes are given by

$$\left(-\frac{dA_L^S}{dL}\right) = \frac{1}{D} + \frac{|\ell| d}{c^2} (3\alpha + 3\beta), \quad (15)$$

for $h - k = 3t \pm 1$ and ℓ even, and by

$$\left(-\frac{dA_L^S}{dL}\right) = \frac{1}{D} + \frac{|\ell| d}{c^2} (3\alpha + \beta), \quad (16)$$

for $h - k = 3t \pm 1$ and ℓ odd, and by

$$\left(-\frac{dA_L^S}{dL}\right) = \frac{1}{D}, \quad (17)$$

for $h - k = 3t$ and/or $\ell = 0$, where $c = 2 d_{0002}$, D is the domain size, and α and β are the stacking fault probability and the growth fault probability, respectively.

Integral Breadth - The integral breadth $\beta(s)$ can be expressed in terms of the Fourier coefficients C_n . Since

$$\beta(s) = \frac{1}{I(s_0)} \int_{s_1}^{s_2} I(s) ds, \quad (2)$$

and

$$I(s) = K \sum_{n=-\infty}^{\infty} C_n \exp [-2\pi i n a_3 (s - s_0)], \quad (4)$$

then substituting and integrating, one obtains

$$\beta(s) = 1/a_3 \sum C_n. \quad (18)$$

Variance-Wilson (32) has shown that the variance $W(s)$ is the sum of the domain size variance $W^S(s)$ and the strain variance $W^D(s)$;

$$W(s) = W^S(s) + W^D(s), \quad (19)$$

where

$$W^S(s) = \frac{\Delta s_{21}}{2\pi^2 D_e} \quad (20)$$

and

$$W^D(s) = (\langle \epsilon^2 \rangle - \langle \epsilon \rangle^2) s_0^2. \quad (21)$$

Experimental Considerations

Extremely accurate measurements of peak profiles are necessary to apply the analysis of line broadening to cold-worked metals. These measurements require that the diffractometer be aligned, that the sample be prepared carefully, and that the proper choice of χ radiation be used.

In an investigation of titanium-aluminum binary alloys the samples were filed, filtered through a 325-mesh screen, and then placed in a holder, using as a binder a 2-wt% solution of parlodion in amylacetate. Copper $K\alpha$ x rays were used. The diffracted radiation was incident on a LiF curved crystal monochromator which, in turn, diffracted the radiation into a proportional counter. The signal was then fed through a pulse-height analyzer, and the diffracted intensity was recorded as a function of angle on paper tape. The automatic step scanner was set in the preset time mode. The angle was then automatically stepped by a fixed amount (usually 0.02° in 2θ).

PROGRAM ORTAILS

In studying the line profiles of hcp metals, the first problem that must be considered is how to correct for the peak overlap that occurs. Figure 1 shows the diffracted intensity of a titanium 5 wt % aluminum alloy as a function of 2θ , for the $(10\bar{1}0)$, (0002) , and $(10\bar{1}1)$ peaks, and exemplifies the problem of peak overlap. Sato (36) has considered the problem and attempted to solve it by replacing adjacent peaks by either Cauchy or Gaussian distributions and subtracting the "tails" of these distributions from the peak being considered.

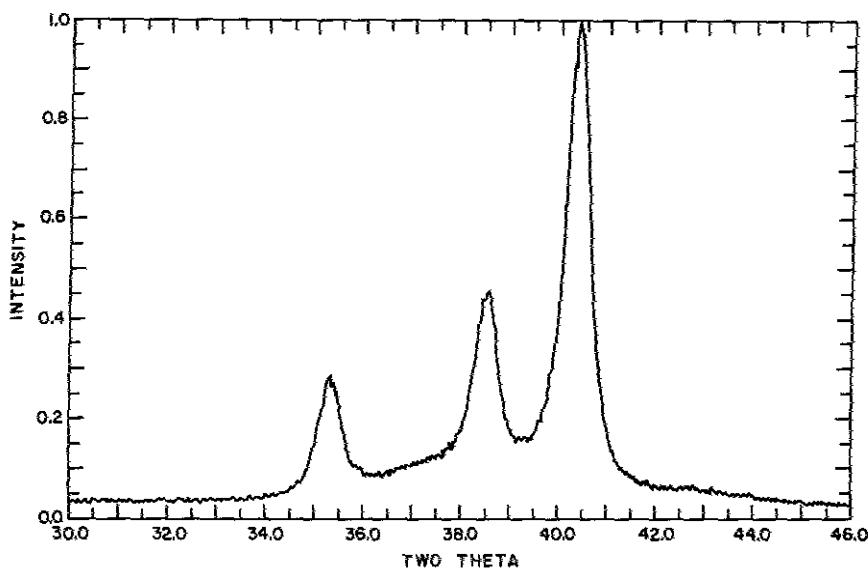


Fig. 1 - Diffracted intensity as a function of 2θ for the $(10\bar{1}0)$, (0002) , and $(10\bar{1}1)$ peaks of a titanium 5wt% aluminum alloy

Every peak in this analysis was approximated by a Cauchy distribution of the form

$$u(x) = \frac{U}{1 + a^2 (x - x_0)^2}, \quad (22)$$

where $u(x_0) = U$, x_0 is the position of the peak maximum, and a is a constant determined from the real peak. This two-constant Cauchy distribution gave an accurate approximation when fitted to the peak of the intensity distribution. If the peak maxima of adjacent peaks were within a certain range of each other ($\Delta 2\theta \leq 5^\circ$, overlap was assumed to occur and was corrected by subtracting the tails of the adjacent Cauchy distribution from the corresponding value of the peak.

The true background of the peaks was taken to be the x-ray intensity of the annealed filings far from any peak. No quantitative method was developed to bring the background of the peak down to the true background.

PROGRAM XRAY 40

The intensity of the line profile corrected for overlap now serves as the input to the main program. These intensities (H_1 in the program) are corrected for the atomic scattering factor (adjusted for temperature) of each type of atom present in the alloy. The atomic scattering factor is

$$f = f_R \exp(-B \sin^2 \theta / \lambda^2), \quad (23)$$

where f_R is the scattering factor of the atom at rest, and B is the Debye-Waller temperature factor of the atom (for values of B , see Ref. 37).

The atomic scattering factor at rest has been represented analytically by Vand and others. (38) and by Forsythe and Wells (39) as

$$f_R = A \exp(-as^2) + B \exp(-bs^2) + C, \quad (24)$$

where $s = \sin \theta / \lambda$, and A , a , B , b , and C are five constants given in Refs. 38 and 39.

The intensities are further corrected for the Lorentz polarization factor for radiation monochromatized by reflection from a curved crystal monochromator at Bragg angle α . This correction is

$$LP = \frac{1 + \cos^2 2\alpha \cos^2 2\theta}{\sin^2 \theta (1 + \cos^2 2\alpha)}. \quad (25)$$

The values of the ordinate 2θ TWOH are converted to equally spaced values of $\sin \theta$ [ET1]

The $K_{\alpha_1} - K_{\alpha_2}$ doublet is separated, using the method of Keating (26). In order to utilize this technique the ordinates must be such that

$$\kappa_j = (4\pi/\lambda) \sin \theta_j, \quad (26)$$

$$(\kappa_{j-1}/\kappa_j)^m = r, \quad (27)$$

where m is an integer convenient for describing the pattern and $r = \lambda_1/\lambda_2$ the ratio of the wavelengths of the K_{α} doublet. Let x be the fraction of the K_{α} radiation in the α_2 component, $1-x$ the fraction of K_{α} radiation in the α_1 component, let $F(\kappa)$ be the pattern that would be produced if all the energy of the characteristic radiation were in the α_1 component, and let $G(\kappa)$ be the observed pattern; then

$$F(\kappa_j) = \frac{1}{1-x} \sum_{n=0}^N \left(\frac{-x}{1-x} \right)^n G(\kappa_{j-nm}), \quad (28)$$

where N is a constant value (≥ 10).

The position of the peak maximum ($\eta_0 = ETMAX$) is determined using a three-point parabola. The value of s_0 [SMAX] is given by $s_0 = 2\eta_0/\lambda$, and the value of $2\theta_0$ is given by $2\theta_0 = 2 \arcsin (\eta_0 180/\pi)$. The center of gravity [ETCG] is given by

$$\eta_{CG} = \sum_{i=1}^N h(\eta_i) (\eta_i - \eta_0) / AREA, \quad (29)$$

where

$$AREA = \sum_{i=1}^N h(\eta_i), \quad (30)$$

and N is the number of data points. Then the center of gravity (s_{CG}) can also be expressed as

$$s_{CG} = 2\eta_{CG}/\lambda. \quad (31)$$

The integral breadth [BSINT] can be evaluated by

$$\beta(s) = 2 AREA \Delta\eta/\lambda h(\eta_0). \quad (32)$$

The variance (W) can be written as

$$W(s) = 4 \left[\sum_{i=1}^N h(\eta_i) (\eta_i - \eta_{CG}) \right] / \lambda^2 \text{ AREA}. \quad (33)$$

The Fourier coefficients have been determined using Filon's method (27) of evaluating trigonometric integrals. This technique was used since the ordinary methods of quadrature often fail at high harmonic numbers because of the rapid oscillations of the trigonometric integrand. The formulas for applying Filon's method can be obtained from the work of Abramowitz (40). The normalized Fourier coefficients can be expressed as

$$HR(L) = \frac{1}{\eta_N - \eta_1} \int_{\eta_1}^{\eta_N} H(\eta_i) \cos \left[\frac{2\pi L (2\eta_i - 2\eta_0)}{\lambda} \right] d\eta / \text{AREA}, \quad (34)$$

$$HI(L) = \frac{1}{\eta_N - \eta_1} \int_{\eta_1}^{\eta_N} h(\eta_i) \sin \left[\frac{2\pi L (2\eta_i - 2\eta_0)}{\lambda} \right] d\eta / \text{AREA}, \quad (35)$$

$$\text{AREA}I = HR(1). \quad (36)$$

Using the interplanar spacing of the reflection plane $a_3 = d_{hkl}$, the interval $2\theta_2 - 2\theta_1$ would have to extend over several tens of degrees. A much smaller interval $2\theta'_2 - 2\theta'_1$, which still encloses the diffraction peak, can be chosen. Therefore, the true harmonic number n is related to an experimental harmonic number n' by

$$n = n' (2\theta_2 - 2\theta_1) / (2\theta'_2 - 2\theta'_1), \quad (37)$$

$$L = n a_3 = n' a'_3, \quad (38)$$

where L is the distance normal to the reflecting planes (hkl) of interplanar spacing $a_3 = d_{hkl}$.

Extraneous broadening due to such things as slit widths, sample size, penetration in the sample, or wavelength spread is usually grouped under the name "instrumental broadening." Instrumental broadening of the peak profile is usually corrected by determining the peak profile of a standard or annealed sample under conditions identical to those of the cold-worked sample. Let $g(z)$ be the intensity function from the annealed sample, and let $h(x)$ be the intensity function from the cold-worked sample; then $f(x-z)$, representing the broadening due to particle size only, can be found from the convolution integral

$$h(x) = \int f(x-z) g(z) dz. \quad (39)$$

Stokes (27) has shown that if the three functions $F(x-z)$, $H(x)$, and $G(z)$ can be expressed as Fourier series over the same interval, then

$$F(x-z) = H(x) | G(z). \quad (40)$$

thus

$$FR(L) = A_L = [HR(L) GR(L) + HI(L) GI(L)] / ([GR(L)]^2 + [GI(L)]^2), \quad (41)$$

$$FI(L) = B_L = [HI(L) GR(L) + HR(L) GI(L)] / ([GR(L)]^2 + [GI(L)]^2), \quad (42)$$

$$|F(L)| = |C_L| = |H(L)| / |G(L)| = ABAR(L), \quad (43)$$

The Stokes-corrected integral breadth $\beta_{st}(s)$ [BSINT] can be written as

$$\beta_{st} = 1/(1 + 2\Delta L \sum A_L),$$

where ΔL is the increment in L values. The corrected integral breadth $\beta_p(s)$ [BINTC] can also be calculated. Let $\beta_h(s)$ [BINT] be the integral breadth of the profile $h(s)$ and $\beta_g(s)$ [BINTS] that of $g(s)$. Wagner and Aqua (4) have shown

$$\beta_p(s) = \beta_h(s) - [\beta_g(s)]^2 / \beta_h(s). \quad (45)$$

The corrected variance $W(s)$ [WC] is the difference between the variance $W_h(s)$ [W] of the broadened profile $h(s)$ and most of the standard profile $W_g(s)$ [WS]:

$$W(s) = W_h(s) - W_g(s). \quad (46)$$

When the Fourier coefficients $A_1(L)$ [ASAVE] and $A_2(L)$ [ABAR] of two orders of reflections are known, it is possible to separate the size coefficient A_L^S from the distortion coefficient A_L^D using the Warren-Averbach method. Their method indicates that

$$\ln A_1(L) = \ln A_1^S(L) - 2\pi^2 L^2 \left(\langle \epsilon_L^2 \rangle - \langle \epsilon_L \rangle^2 \right) s_{01}^2, \quad (47)$$

and

$$\ln A_2(L) = \ln A_2^S(L) - 2\pi^2 L^2 \left(\langle \epsilon_L^2 \rangle - \langle \epsilon_L \rangle^2 \right) s_{02}^2. \quad (48)$$

Note that the size coefficients are independent of order. The two equations can be combined to yield the strains [EPS]

$$\left(\langle \epsilon_L^2 \rangle - \langle \epsilon_L \rangle^2 \right)^{1/2} = \left[\frac{\ln A_2(L) / \ln A_1(L)}{2\pi^2 L^2 (s_{01}^2 - s_{02}^2)} \right]^{1/2} \quad (49)$$

The particle size value can be found by plotting the size coefficient A_L^S [ALP] L extrapolating the linear part of A_L^S for small values of L to the value $L = 0$.

The integral breadth particle size D_I [DINTP] and strain E_I [EPSP] can be calculated as

$$D_I = \frac{\beta_1 s_{02}^2 - \beta_2 s_{01}^2}{\beta_1^2 s_{01}^2 + \beta_2^2 s_{02}^2} \quad (50)$$

and

$$\epsilon_I = \beta_1 \beta_2 (\beta_2 - \beta_1) / 4 \left(\beta_1 s_{02}^2 - \beta_2 s_{01}^2 \right), \quad (51)$$

where β_1 and β_2 are the corrected integral breadth, and s_{01} and s_{02} are the peak maximums of the first and second order reflection, respectively. The value of D_I [DINT] can also be calculated from the size coefficients A_L^S as

$$D_I = 1 / \left(1 + 2\Delta L \sum A_L^S \right). \quad (52)$$

PROGRAM SEPARATE

If, however, two orders of reflections can not be measured, the separation of the size and distortion coefficients is still possible. This technique utilizes the fact that if $h-k=3t$ ($t = 0, \pm 1, \pm 2$, etc), or $t=0$, then the Fourier coefficient which is independent of faulting can be expressed as

$$A_n = A_n^S \exp \left[-2\pi^2 L^2 \langle \epsilon_L^2 \rangle - \langle \epsilon_L^2 \rangle^2 / d^2 \right]$$

When the $\ln(A_n)$ vs $1/d^2$ for different hkl reflections not affected by faulting and for different values of $L = na_3$ are plotted, the slopes of these curves become a measure of the difference between the mean square and the mean strain squared. The distortion coefficients calculated in this manner can be utilized to correct for strain broadening those Fourier coefficients of those reflections affected by faulting, thus separating the size and distortion coefficients of fault-affected peaks.

This program has as an input for each reflection the hkl value, $1/d^2 hkl$, the Fourier coefficients, and $L = na_3$, for all values of L . The program computes for fault-unaffected peaks the natural logarithm of their Fourier coefficients and the slope of these natural logarithms as a function of the inverse of the square of the d spacings. From this information, the distortion coefficients of each peak and then the size coefficients of fault-affected peaks are calculated.

REFERENCES

1. Greenough, G.B., Prog. Met. Phys. 3: 176 (1952)
2. Warren, B.E., Prog. Met. Phys. 8: 147 (1958)
3. Wagner, C.N.J., "Local Atomic Arrangements Studied by X-Ray Diffraction," ed. (J.B. Cohen and J.E. Hilliard,) New York: Gorder and Breach, 1966
4. Otte, H.M., J. Appl. Phys. 38: 217 (1967)
5. Warren, B.E., "X-Ray Diffraction," Reading, Mass.: Addison-Wesley, 1969
6. Welch, D.O., and Otte, H.M., "Adv. X-Ray Anal." 6:96 (1963)
7. Wagner, C.N.J., Boisseau, J.P., and Aqua, E.N., Trans. TMS-AIME 233:1280 (1965)
8. Hinton, R.W., Schwartz, L.H., and Cohen, J.B., J. Electrochem. Soc. 110:103 (1963)
9. Eichkorn, G., and Fischer, H., Z. Metallk, 55:582 (1964)
10. Vook, R.W., and Witt, F., J. Vac Sci. Techn. 2:49 (1965)
11. Light, T.B., and Wagner, C.N.J., J. Vac. Sci. Techn. 3:1 (1966)
12. Herbstein, F.H., and Smuts, J., J. Catalysis 2:69 (1963)
13. Royen, P., Tolksdorf, W., Granzer, F. and Schuster, H., Acta Cryst. 17:1246 (1964)

14. Mitra, G.B., and Halder, N.C., *Acta Cryst.* 17:817 (1964)
15. Mogard, J.H., and Averbach, B.L., *Acta Met.* 6:552 (1958)
16. Lele, S., and Anantharaman, T.R., *Phys. Stat. Sol.* 5:K121 (1964)
17. Mitra, G.B., and Misra, N.K., *Acta Cryst.* 22:454 (1967)
18. Stratton, R.P. and Kitchingman, W.J., *Brit. J. Appl. Phys.* 16:1311 (1965)
19. Stratton, R.P., and Kitchingman, W.J., *Brit. J. Appl. Phys.* 17:1039 (1966)
20. Sen Gupta, S.P., and Goswami, K.N., *Brit. J. Appl. Phys.* 18:193 (1967)
21. Krishnan, R., *Z. Metalik* 58:811 (1967)
22. Sharan, B., Agnihotri, O.P., *J. Appl. Phys.* 39:1489 (1968)
23. Pittinato, G.F., and Neumann, J.P., *Mat. Sci. Engr.* 3:151 (1968)
24. De, M., and Sen, S., *Brit. J. Appl. Phys.* 1:1141 (1968)
25. Lele, S., and Anantharaman, T.R., *Z. Metallk.* 58:461 (1967)
26. Keating, D.T., *Rev. Sci. Instrum.* 30:725 (1959)
27. Filon, L.N.G., *Proc. Roy. Soc. Edinburgh*, 49:38 (1928-1929)
28. Stokes, A.R., *Proc. Phys. Soc. London* 61:382 (1948)
29. Wagner, C.N.J., Yale Univ., Dept of Engineering and Applied Sci., Tech. Rept. No. 15, Apr. 1966
30. Scherreu, P., *Nachr. Ges. Wiss. Gottingen*, Sept. 26, 1918, pp. 98-100
31. Laue, M., *Z. Krist.* 64:115 (1929)
32. Wilson, A.J.C., *Proc. Phys. Soc. (London)* 80:286 (1962)
33. Bertaut, F., *C.R. Acad. Sci. Paris* 228:492 (1949)
34. Warren, B.E., and Averbach, B.L., *J. Appl. Phys.* 21:595 (1950)
35. Warren, B.E., and Averbach, B.L., *J. Appl. Phys.* 23:497 (1952)
36. Sato, S., *Jap. J. Appl. Phys.* 1:210 (1962)
37. "International Tables for X-Ray Crystallography," Vol. II, p. 233, Birmingham, England:Kynoch Press, 1959.
38. Vand, V., Eiland, P.F., and Pepinsky, R., *Acta Cryst.* 10:303 (1957)
39. Forsyth, J.P., and Wells, M., *Acta Cryst.* 12:412 (1959)

40. "Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables." Applied Mathematics Series 55, National Bureau of Standards, M. Abramowitz and I.A. Stegun, Ed. Washington, D.C.: Superintendent of Documents, 1964 p. 890.
41. Wagner, C.N.J., and Aqua, E.N., Adv X-Ray Anal. 7:46 (1964)

Appendix A
Program ORTAILS

Control or Data Cards	Format	
WLGTH DWLGTH	2F10.6	WLGTH=wavelength and DWLGHT=wavelength $(\lambda K\alpha_2 - \lambda K\alpha_1)$
IJK	I2	parameter=0 do program $\neq 0$ go to end of program
TWOH(1)	F10.6	TWOH(1)= $2\theta_1$ value for first data point
DTWOH	F10.6	DTWOH= $\Delta 2\theta$ interval be- tween data points
NPK	I1	NPK=number of peaks ≤ 3
(TWH(I)=1, NPK)	F8.4	TWH(I), =approx, position of peaks
NDP	I3	NDP=number of data points ≤ 900
(H(I), I=1, NDP)	10F7.1	H(I)=intensity data

```

PROGRAM ORTALS
DIMENSION H(1000),H1(1000),H2(1000),E1(1000)
DIMENSION TWH(1000),X(1000),THW(9),HC1(1000),HC2(1000),HC3(1000)
DIMENSION ABUFFER(254)
TYPE INTEGER MAR
100 FORMAT(2F10.6)
101 FORMAT(I2)
102 FORMAT(F10.6)
103 FORMAT(I1)
104 FORMAT(3F6.4)
105 FORMAT(1H0,I5X,* THE NUMBER OF PEAKS IS *,I2,* AND THEY ARE LOCATE
1D AT *//,2X,F7.2)
106 FORMAT(1H1,*THE INITIAL TWO THETA VALUE IS *,F10.6,* AND THE TWO
1THETA INCREMENT IS *,F10.6//)
107 FORMAT(I3)
108 FORMAT(2X,*THE NUMBER OF DATA POINTS IS *,I3//)
109 FORMAT(10F7.1)
110 FORMAT((10F6.0))
111 FORMAT(5X,*THE PEAK IS AT *,I4,* WHICH HAS THE TWO THETA VALUE *,
1F10.4,* AND HAS THE INTENSITY OF *,F10.4//)
112 FORMAT(5X,*THE FIRST PEAK IS AT *,I4,* WHICH HAS A TWO THETA VALUE
1 OF *,F10.4,* AND AN INTENSITY OF *,F10.4//)
113 FORMAT(5X,*THE SECOND PEAK IS AT *,I4,* WHICH HAS A TWO THETA VAL
1UE OF *,F10.4,* AND AN INTENSITY OF *,F10.4//)
114 FORMAT(5X,*THE THIRD PEAK IS AT *,I4,* WHICH HAS A TWO THETA VALUE
1 OF *,F10.4*, AND AN INTENSITY OF *,F10.4//)
115 FORMAT(//* SELECT NOT SATISIFIED, NXN = 0. */
READ 100,WLNGTH,DWLNGTH
CALL PLOTS(ABUFFER,254,10)
RADIAN = 3.14159/180.
1 READ 101,IJK
IF(IJK,EQ,0) 2,68
2 CONTINUE
READ 102,TWH(1)
READ 102,DTW0H
READ 103,NPK
READ 104,(TWH(I),I=1,NPK)
PRINT 105,NPK,(TWH(I),I=1,NPK)
PRINT 106,TWH(1),DTW0H
READ 107,NDP
PRINT 108,NDP
X(1) = 0.
DO 3 I=2,NDP
TWH(I) = TWH(I-1) + DTW0H
3 X(I) = X(I-1) + DTW0H
READ 109,(H(I),I=1,NDP)
PRINT 110,(H(I),I=1,NDP)
CALL MAX(H,NDP,L1MAX)
LMAX1 = L1MAX
DO 4 I=1,NDP
4 E1(I) = (10./H(L1MAX))*H(I)
X5 = DTW0H*NDP + 1.
X7 = X5 + 2.
CALL PLOT(10.,0.,-3)
CALL AXIS(0.,0.,9HINTENSITY,9,10.,90.,1.,0.,1.,4HF4,1)
CALL AXIS(0.,0.,9HTWO THETA,=9,X5,0.,1.,TWH(1),1.,4HF6,2)

```

```

CALL LINE(X,E1,NDP,1,-1,0,.1)
CALL PLOT(X7,0,,-3)
CALL PLOTS(0,0)
CALL PLOT1=10.,0,,-3)
IF(NPK,EQ,4) 5,6
5 CALL MAX(H,NDP,LMAX1)
PK1POS = TWOH(LMAX1)
PK1INT = H(LMAX1)
PRINT 111,LMAX1,PK1POS,PK1INT
PRINT 110,(H(I),I=1,NDP)
GO TO 13
6 IF(NPK,EQ,2)7,9
7 N1 = (0.5*(TWH(1) + TWH(2)))/DTWH = TWOH(1)/DTWH
CALL MAX(H,N1,LMAX1)
PK1POS = TWOH(LMAX1)
PK1INT = H(LMAX1)
PRINT 112,LMAX1,PK1POS,PK1INT
PRINT 110,(H(I),I=1,N1)
J=0
IN1 = N1+1
DO 8 I=IN1,NDP
J=J+1
8 H1(J)=H(I)
JN1 = J
CALL MAX(H1,JN1,LMAX2)
PK2POS = TWOH(LMAX2+N1)
PK2INT = H1(LMAX2)
PRINT 113,LMAX2,PK2POS,PK2INT
PRINT 110,(H1(I),I=1,JN1)
GO TO 13
9 IF(NPK,EQ,3) 10,68
10 N1 = (0.5*(TWH(1) + TWH(2)))/DTWH = TWOH(1)/DTWH
CALL MAX(H,N1,LMAX1)
PK1POS = TWOH(LMAX1)
PK1INT = H(LMAX1)
PRINT 112,LMAX1,PK1POS,PK1INT
PRINT 110,(H(I),I=1,N1)
N2 = (0.5*(TWH(2)+TWH(3)))/DTWH = TWOH(1)/DTWH
J=0
IN1 = N1+1
DO 11 I=IN1,N2
J=J+1
11 H1(J) = H(I)
JN1 = J
CALL MAX(H1,JN1,LMAX2)
PK2POS = TWOH(LMAX2+N1)
PK2INT = H1(LMAX2)
PRINT 113,LMAX2,PK2POS,PK2INT
PRINT 110,(H1(I),I=1,JN1)
IN2 = N2+1
JJ=0
N3=NDP
DO 12 I=IN2,NDP
JJ=JJ+1
12 H2(JJ)=H(I)
JN2=JJ
CALL MAX(H2,JN2,LMAX3)
PK3POS = TWOH(LMAX3+N2)
PK3INT = H2(LMAX3)
PRINT 114,LMAX3,PK3POS,PK3INT
PRINT 110,(H2(I),I=1,JN2)
13 IF(NPK,EQ,1) 14,15
14 THAL=TWOH(1)
PRINT 110,(H(I),I=1,NDP)

```

```

      CALL PRFLDT2(H,NDF,THAL)
      CALL PLDTSTD,0)
      CALL PLGT(-10.,0.,-3)
      GO TO 68
15 IF(NPK.EQ.2)16,19
16 X01 = PK1POS
      A01PI = PK1INT
      CALL SELECT(H,N1,LMAX1,NXN)
      IF(NXN.EQ.0) GO TO 70
      PK1INT1 = H(LMAX1+NXN)
      PK1POS1 = TW0H(LMAX1+NXN)
      DIF1 = (PK1POS1-PK1POS)**2
      BB1 = (1./DIF1)*(PK1INT/PK1INT1 - 1.)
      A01 = A01PI * 3.14159
      AX1 = TW0H(LMAX1) - 5.00
      DO 17 I=1,501
      XNEW1 = AX1 + (I-1)*DTW0H
17 HC1(I) = A01PI/(1.+BB1*(XNEW1-X01)**2)
      X02 = PK2POS
      CALL SELECT(H1,JN1,LMAX2,NXN)
      IF(NXN.EQ.0) GO TO 70
      PK2INT1 = H(LMAX2+NXN)
      PK2POS1 = TW0H(N1+LMAX2+NXN)
      DIF2 = (PK2POS1-PK2POS)**2
      BB2 = (1./DIF2)*(PK2INT/PK2INT1 - 1.)
      A02PI = PK2INT
      A02 = A02PI * 3.14159
      AX2 = TW0H(N1+LMAX2) - 5.00
      DO 18 I=1,501
      XNEW2 = AX2 + (I-1)*DTW0H
18 HC2(I) = A02PI/(1.+BB2*(XNEW2-X02)**2)
      GO TO 24
19 IF(NPK.EQ.3) 20,68
20 X01 = PK1POS
      A01PI = PK1INT
      A01 = A01PI * 3.14159
      CALL SELECT(H,N1,LMAX1,NXN)
      IF(NXN.EQ.0) GO TO 70
      PK1INT1 = H(LMAX1+NXN)
      PK1POS1 = TW0H(LMAX1+NXN)
      DIF1 = (PK1POS1-PK1POS)**2
      BB1 = (1./DIF1)*(PK1INT/PK1INT1 - 1.)
      AX1 = TW0H(LMAX1) - 5.00
      DO 21 I=1,501
      XNEW1 = AX1 + (I-1)*DTW0H
21 HC1(I) = A01PI/(1.+BB1*(XNEW1-X01)**2)
      X02 = PK2POS
      A02PI = PK2INT
      A02 = A02PI * 3.14159
      CALL SELECT(H1,JN1,LMAX2,NXN)
      IF(NXN.EQ.0) GO TO 70
      PK2INT1 = H(LMAX2+NXN)
      PK2POS1 = TW0H(N1+LMAX2+NXN)
      DIF2 = (PK2POS1-PK2POS)**2
      BB2 = (1./DIF2)*(PK2INT/PK2INT1 - 1.)
      AX2 = TW0H(N1+LMAX2) - 5.00
      DO 22 I=1,501
      XNEW2 = AX2 + (I-1)*DTW0H
22 HC2(I) = A02PI/(1.+BB2*(XNEW2-X02)**2)
      X03 = PK3POS
      A03PI = PK3INT
      A03 = A03PI * 3.14159
      CALL SELECT(H2,JN2,LMAX3,NXN)
      IF(NXN.EQ.0) GO TO 70

```

```

PK3INT1 = H2(LMAX3+NXN)
PK3POS1 = TW0H(N2+LMAX3+NXN)

```

```

DIF3 = (PK3POS1-PK3POS)**2
BB3 = (1./DIF3)*(PK3INT/PK3INT1 - 1.)
AX3 = TW0H(N2+LMAX3) = 5.00

```

```

DO 23 I=1,501
XNEW3 = AX3 * (I=1)*DTW0H
23 HC3(I) = A03P1/(1.+BB3*(XNEW3-XG3)**2)

```

```
GO TO 39
```

```
24 COMP1 = PK2POS + PK1POS
```

```
IF((TW0H(N1+LMAX2)-TW0H(LMAX1)),GT,5.) GO TO 34
IF(AX2,GE,TW0H(1)) 25,28
```

```
25 I=N1+LMAX2-290
```

```
C AX2=TW0H(1)
```

```
IF(I,LT,N1) 26,33
```

```
26 IJ=0
```

```
DO 27 KJ=1,N1
```

```
IJ=IJ+1
H(KJ) = H(KJ) - HC2(IJ)
IF(IJ,GE,501) 28,27
```

```
27 CONTINUE
```

```
28 CONTINUE
```

```
GO TO 33
```

```
29 IZ250=(N1+LMAX2)
```

```
C HC2(I)=TW0H(1)
```

```
IF(I,LT,N1) 30,33
```

```
30 IJ=1
```

```
DO 31 KJ=1,N1
```

```
H(KJ) = H(KJ)-HC2(IJ)
```

```
IJ=IJ+1
```

```
IF(IJ,GE,501) 32,31
```

```
31 CONTINUE
```

```
32 CONTINUE
```

```
33 CONTINUE
```

```
34 CONTINUE
```

```
THAL=TW0H(1)
```

```
PRINT 110,(H(I),I=1,N1)
```

```
CALL PRPL9T2(H,N1,THAL)
```

```
IF((TW0H(N1+LMAX2)-TW0H(LMAX1)),GT,5.) GO TO 38
```

```
35 IJ=251+N1+1-LMAX1
```

```
DO 36 KJ=1,JN1
```

```
H1(KJ) = H1(KJ)-HC1(IJ)
```

```
IJ=IJ+1
```

```
IF(IJ,GE,501) 37,36
```

```
36 CONTINUE
```

```
37 CONTINUE
```

```
38 CONTINUE
```

```
THAL = TW0H(N1+1)
```

```
PRINT 110,(H1(I),I=1,JN1)
```

```
CALL PRPL9T2(H1,JN1,THAL)
```

```
CALL PL9TS(0,0)
```

```
CALL PL9T1(-10.,0.,-3)
```

```
GO TO 68
```

```
39 COMP1 = PK2POS + PK1POS
```

```
COMP2 = PK3POS - PK2POS
```

```
IF((TW0H(N1+LMAX2)-TW0H(LMAX1)),GT,5.) GO TO 49
```

```
IF(AX2,GE,TW0H(1)) 40,44
```

```
40 I=N1+LMAX2-250
```

```
C AX2=TW0H(1)
```

```
IF(I,LT,N1) 41,48
```

```
41 IJ=0
```

```
DO 42 KJ=1,N1
```

```
IJ=IJ+1
```

```
H(KJ) = H(KJ)-HC2(IJ)
```

```
IF(IJ,GE,501) 43,42
```

```

42 CONTINUE
43 CONTINUE
  GO TO 45
44 I=250*(N1*LMAX2)
C H02(I)=TWOH(1)
  IF(I,LT,N1) 45,48
45 IJ=I
  DO 46 KJ=1,N1
    H(KJ)=H(KJ)-HC2(I,J)
    IJ=IJ+1
  IF(IJ,GE,501) 47,46
46 CONTINUE
47 CONTINUE
48 CONTINUE
49 CONTINUE
  THAL=TWOH(1)
  PRINT 110,(H(I),I=1,N1)
  CALL PRPLQT2(H,N1,THAL)
  IF((TWOH(N1+LMAX2)-TWOH(LMAX1)),GT,5,) GO TO 62
  IF((TWOH(N2+LMAX3)-TWOH(N1+LMAX2)),GT,5,) GO TO 62
  IF(LX3,GE,TWOH(N1+1)) 50,54
50 I=N2+LMAX3-251
C LX3=TWOH(1)
  IF(I,GE,(N1+1),AND,I,LE,N2) 51,58
51 IJ=I-(N1+1)
  DO 52 KJ=1,501
    H(IJ)=H(IJ)-HC3(KJ)
    IJ=IJ+1
  IF(KJ,GE,JN1,OR,IJ,GE,JN1) 53,52
52 CONTINUE
53 CONTINUE
  GO TO 57
54 I=N2+LMAX3-251
  HC3(I)=TWOH(1)
  IF(I,GE,N1) 55,58
55 IJ=N1+1-I
  DO 56 KJ=1,JN1
    H1(KJ)=H1(KJ)-HC3(IJ)
    IJ=IJ+1
  IF(IJ,GE,501) 57,56
56 CONTINUE
57 CONTINUE
58 CONTINUE
59 IJ=251+N1+1-LMAX1
  DO 60 KJ=1,JN1
    H1(KJ)=H1(KJ)-HC1(IJ)
    IJ=IJ+1
  IF(IJ,GE,501) 61,60
60 CONTINUE
61 CONTINUE
62 CONTINUE
  THAL=TWOH(N1+1)
  PRINT 110,(H1(I),I=1,JN1)
  CALL PRPLQT2(H1,JN1,THAL)
63 CONTINUE
  IF((TWOH(N2+LMAX3)-TWOH(N1+LMAX2)),GT,5,) GO TO 67
64 IJ=251+N2+1-(N1+LMAX2)
  DO 65 KJ=1,JN2
    H2(KJ)=H2(KJ)-HC2(IJ)
    IJ=IJ+1
  IF(IJ,GE,501) 66,65
65 CONTINUE
66 CONTINUE
67 CONTINUE

```

```

THAL=TWOH(N2+1)
PRINT 110,(H2()),I#1,JN2)
CALL PRPL0T2(H2,JN2,THAL)
CALL PLOTS(0,0)
CALL PLOT(-10.,0.,-3)
68 CONTINUE
CALL PL0TS(0,0)
IF(IJK,NE,0) 71,69
69 GO TO 1
70 PRINT 115
71 CALL STOPPLOT
END

```

```

SUBROUTINE SELECT(A,N,L,NX)
DIMENSION A(N)
NX = 17

```

```

1 Q1 = A(L+NX)
Q2 = A(L+NX)
QAV = 0.5*(Q1+Q2)
AQ1 = 1,1*Q1
AQ2 = 1,1*Q2
RQ1 = 0.9*Q1
BQ2 = 0.9*Q2
IF(QAV,GT,AQ1) 5,2
2 IF(QAV,GT,AQ2) 5,3
3 IF(QAV,LT,BQ1) 5,4
4 IF(QAV,LT,BQ2) 5,8
5 NX = NX + 1
IF(L+NX,GT,N) 7,6
6 IF(L+NX,LE,1) 7,1
7 NX = 0
8 RETURN
END

```

```

SUBROUTINE PRPL0T2(XX,NDP,THAL)
DIMENSION XX(NDP),E1(1000),F1(1000)
DIMENSION TWOH(1000)

```

```

100 FORMAT(F4.0,3I3,F8.5)
101 FORMAT(3F6.2,F8.5)
102 FORMAT(10F6.0)
WAVE = 1,54050
WAVE2 = 1,54434
TWOH(1)=THAL
D9 1 I#2,NDP
1 TWOH(1)=TWOH(1-1)*0.02
CALL MAX(XX,NDP,LMAX)
THAM=TWOH(LMAX)
THAH=TWOH(NDP)
YM=NDP-1,
JN=LMAX-1
JO=LMAX
JP=LMAX+1
PRINT 100 ,YM,JN,JO,JP,WAVE2
PRINT 101 ,THAL,THAM,THAH,WAVE
PRINT 102 ,(XX()),I#1,NDP)
PUNCH 100 ,YM,JN,JO,JP,WAVE2

```

```

PUNCH 101 ,THAL,THAM,THAH,WAVE
PUNCH 102 ,(XX(1),1,1,NDP)
X5=0.02*NDP+1,
X7=X5+2,
DO 2 I=1,NDP
E1(I)=X(10)/XX(LMAX)*XX(I)
2 F1(I)=I-1+0.02
CALL AXIS(0.,0.,9HINTENSITY,9,10.,90.,1,0.,1.,4WF4,1)
CALL AXIS(0.,0.,9HTW0 THETA,=9,X5,0.,1.,TW0H(1),1.,4WF6,2)
CALL LINE(F1,E1,NDP,1,-1,0.,1)
CALL PLOT(X7,0.,-3)
CALL PLOTS(0,0)
CALL PLOT(-10.,0.,-3)
RETURN
END

```

```

SUBROUTINE MAX(A,N,L)
DIMENSION A(N)
BIGA=A(1)
1
DO 2 I=2,N
IF(BIGA.GT.A(I)) GO TO 1
BIGA=A(I)
L=I
1 CONTINUE
2 CONTINUE
RETURN
END

```

```

SUBROUTINE MIN(A,N,L)
DIMENSION A(N)
SMALLA=A(1)
1
DO 2 I=2,N
IF(SMALLA.LT.A(I)) GO TO 1
SMALLA=A(I)
L=I
1 CONTINUE
2 CONTINUE
RETURN
END

```

Appendix B
Program XRAY40

Control or Data Cards	Format	
WLGTH, DWLGTH	2F10.6	WLGTH=wavelength and DWLGTH=wavelength difference ($\lambda K\alpha_2 - \lambda K\alpha_1$)
NA	12	NA=number of atomic species in alloy
(SK(J) J=1, NA)	F5.2	SK(J)=atomic percent of each atomic species in alloy
(SA(J), SB(J), SD(J), SE(J), SH(J), J=1, NA)	F7.3, F6.3 F7.3, F6.2 F7.3, F4.2	SA, SB, SC, SD, SE, are con- stants in equation for atomic atomic scattering factor, SH-Const for temperated dependence of atomic scat- tering factor
IJK	12	IJK-parameter -1 do program =1- go to end of the program
IH, IK, II, IL, Spec, Comp,	4I2, 3A6	(IHIIIL)=HKIL Spec, Comp, State characterize the sample
NFC, VIK	I2, F10.5	NFC=number of Fourier coefficients wanted ≤ 100 VIK=interval in Δl between Fourier coefficients
NRAC	I1	NRAC=0 no $K\alpha_2$ correction =1 do $K\alpha_2$ correction
NACW	I1	NACW=1 annealed peak only, =2 this peak annealed, cold work peak to follow =3 this peak cold work follows annealed peak, use previously calculated $GR(L)$ and $GI(L)$ =4 this peak cold worked, read $GR(L)$ and $GR(L)$ values

NSTR	I1	NSTR=0 no strain calculation =1 do strain calculation using this peak and following =2 do strain calculation using this peak and preceding
ALPHA1	F10.6	ALPHA1=monochromator angle
TWOH(1)	F10.6	TWOH(1)= $2\theta_1$, value of first data point
DTWOH	F10.6	DTWOH= $\Delta 2\theta$, interval between data points
NDP	I3	NDP=number of data points ≤ 900
(HI(I), I=1, NDP)	10F6.0	H1(I)=intensity data
(GR(L), GI(L), L=2, NFC1)	8F10.6	IF NACW =4, NFC values of GR(L) and GI(L) follow the intensity data. The interval between data points ΔL must be equal to VIK.

```

C PROGRAM XRAY40
C ANALYSIS OF THE BROADENING OF POWDER PATTERN PEAKS
DIMENSION SA(99),SB(99),SC(99),SD(99),SH(99),SHY(99)
DIMENSION THSH(900),ET1(900),ET2(900),ET3(900),ET(900),H1(900),
1H2(900),H3(900),HR(101),HI(101),HBAR(101),GR(101),OI(101),H(900),
2GBAR(101),FR(101),FI(101),ABAR(101),ASAVE(101),BAL(101),ETA(900)
DIMENSION BALG(101),OBA(101)
DIMENSION ALPH(101),BETA(101),GAMMA(101)
DIMENSION ET5(900),ET6(900),YX(900),YZ(900)
DIMENSION X(900),A(900),XX(101),YY(101),ZZ(101),ALP(101),EPS(101)
DIMENSION ET4(900)
DIMENSION ABUFFER(254)
DIMENSION TITLEN(3),TITLEN(3),TITLER(7)
DIMENSION TITLET(3),TITLE1(2),TITLE2(3)
DATA(TITLET(1)=24H INITIAL INTENSITIES )
DATA(TITLE1(1)=16H ALP VERSUS BAL )
DATA(TITLE2(1)=24H EPSILON VERSUS BAL )
DATA(TITLEN(1)=24H GBAR (+) VERSUS BAL )
DATA(TITLEN(1)=24H ABAR (+) VERSUS BAL )
DATA(TITLER(1)=56H FINAL KALPHA INTENSITIES AT EQUAL INTERVAL OF
1 ETA )
```

C

```

100 FORMAT (2E10.6)
101 FORMAT (12)
102 FORMAT (F5.2)
103 FORMAT (F7.3,F6.3,F7.3,F6.2,F7.3,F4.2)
104 FORMAT (12)
105 FORMAT (4J2,3A6)
106 FORMAT (1H1-25HANALYSIS OF REFLECTION      :4I2+3A6//)
107 FORMAT (12,E10.5)
108 FORMAT (18)
109 FORMAT (F10.6)
110 FORMAT (13)
111 FORMAT (//31H THE ORIGINAL DATA POINTS ARE    // )
112 FORMAT (12H THOH(1) = F8.3,2X,13H AND DTHOH = F6.3,2X,11H AND NDP
18,14,//)
113 FORMAT (10F6.0)
114 FORMAT (10F9.1)
115 FORMAT (12H ET2(1) IS ,F8.5,2X,13H AND BETA IS ,F10.5,2X,13H)
116 FORMAT (//34H THE FINAL INTENSITY VALUES ARE   //)
117 FORMAT (//10H NET IS ,15//)
118 FORMAT (4I2)
119 FORMAT (F10.5)
120 FORMAT (1H1,37H POSITION OF PEAK MAXIMUM, ETA(MAX) = F10.5//)
121 FORMAT (3H POSITION OF PEAK MAXIMUM, THOHMAX = F8.3//)
122 FORMAT (3H POSITION OF PEAK MAXIMUM, SMAX = F10.5//)
123 FORMAT (20H S SQUARE, SSMAX = F10.5//)
124 FORMAT (3D9 POSITION OF MAXIMUM HEIGHT = 13//)
125 FORMAT (3DH CENTER OF GRAVITY, ETCG) = F10.5//)
126 FORMAT (2DH CENTER OF GRAVITY, SCG = F10.5//)
127 FORMAT (18H AREA UNDER PEAK = E15.8//)
128 FORMAT (20H INTEGRAL BREADTH = F12.8//)
129 FORMAT (18H VARIANCE = E15.8//)
130 FORMAT (18H DELTA S = F15.5//)
131 FORMAT ( 39H PEAK MAXIMUM D SPACING = ,F12.5//)
132 FORMAT ( 35H CENTER OF GRAVITY D SPACING = ,F12.5//)
133 FORMAT (7W.OH) ,4I2,21H = OBSORT IS EQUAL TO ,FD.9//)
134 FORMAT (18X,3HBAL,15X,5HGR(L),15X,5HHI(L),15X,7HGBAR(L),15X,
135 FORMAT (6X,E8.2,F20.4)
136 FORMAT (8F10.6)
137 FORMAT (F80.8)
138 FORMAT (1H1,48H USE READ-IN VALUES OF G(L) FOR STOKES CORRECTION//)
139 FORMAT (//10X,3HBAL,15X,5HGR(L),15X,5HHI(L),15X,7HGBAR(L),15X,
1 7HGBAR(L),15X,7HABAR(L)  //)
```

```

140 FORMAT (5DH USE COMPUTED VALUES OF G(L) FOR STOKES CORRECTION//)
141 FORMAT (1F/6X,3HBAL,12X,3HHR(L),10X,3HN)(L),10X,3HGR(L),10X,
   1 3HQ1(L),10X,3HFR(L),10X,3HFI(L),10X,7HABAR(L)      //)
142 FORMAT (F82.2,F15.4)
143 FORMAT (F12.2,F15.4)
144 FORMAT (2DH CORRECTED VARIANCE, HC = E15.8//)
145 FORMAT (1F/44H STOKES CORRECTED INTEGRAL BREADTH, BINT = F20.8//)
146 FORMAT (37H CORRECTED INTEGRAL BREADTH, BINTC = F12.8//)
147 FORMAT (1W1,34H STRAIN DETERMINATION FOR PEAKS ,412.6H AND ,
   1 412.6H//)
148 FORMAT (1BX,3HBAL,1BX,13HABAR(L) PEAK ,412.10X,13HABAR(L) PEAK ,
   142.10X,13HABAR(L) PARTICLE ,15X,7HBRSTGN//)
CALL PLDTSCABUFFER,254,10)
READ 100,NLGTM,DWLGTH
READ 101,NA
READ 102,ISK(J),JN1,NA)
READ 103,ISA(J)*SB(J),SC(J),SD(J),SE(J),SH(J),JN1,NA)
SA1 = 0;
SB1 = 0;
SC1 = 0;
SD1 = 0;
SE1 = 0;
SH1 = 0;
DO 1 I=1,NA
  SA1 = SA1 + SK(I)*SA(I)
  SB1 = SB1 + SK(I)*SB(I)
  SC1 = SC1 + SH(I)*SC(I)
  SD1 = SD1 + SK(I)*SD(I)
  SE1 = SE1 + SK(I)*SE(I)
  1 SH1 = SH1 + SK(I)*SH(I)
999 CONTINUE
READ 104,JJK
IF (IJK,EQ,-1) GO TO 997
READ 105,JH,IK,II,IL,SPEC,COMP,STATE
PRINT 106,IN,IK,II,IL,SPEC,COMP,STATE
READ 107,NFC,VIK
READ 108,MRAC
READ 108,NACW
READ 108,NSTR
READ 109,ALPHA1
READ 109,TWHSH(1)
READ 109,BTHSH
READ 110,NDP
PRINT 111
PRINT 112,TWHSH(1),DTWHSH,NDP
READ 113,M1(I),I=1,NDP)
PRINT 114,(M1(I),I=1,NDP)
IF (NACW,BQ,3) 3,2
  2 CALL MAX(M1,NDP,LMAX)
  GMAX = M1(LMAX)
  PEAK1 = GMAX
  3 RATIO = 10./PEAK1
  X(1) = 0.
  A(1)=RAT1BNH1(1)
  DO 4 I=2,NDP
    X(I) = X(I-1) + DTWHSH
    4 A(I) = M1(I) * RATIO
    YMIND = TWHSH(1)
    X5 = DTWHSH * NDP + 1.
    X7 = X5 + 2.
    CALL AX15(10.,0.,1,TITLET(1),24,10.,90,1,0,1,4HPC4,X)
    CALL AX15(10.,0.,10,-1,X5,0,1,1,YMIND/1.,4HPC6,Z)
    CALL LINBIX,A,NDP,1,1,0,1)
    CALL PLDT(X7,0,,-3)

```

```

C   CORRECTION FOR POLARIZATION AND GEOMETRIC FACTOR, AND CONVERSION
C   OF TWOH SCALE TO ETA = SIN(TWOH/2) SCALE
C   RADIANT = 3,14159/180,
C   XKFACT=(COS(ALPHA1*RADIANT/2.,1))**2
C   DO 5 I=2,NDP
C   5 TWOH(I)=TWOH(I-1)+DTWOH
C   CORRECTION FOR ATOMIC SCATTERING FACTORS
C
C   S=(SIN((TWOH(1)*3,14159)/(2,*180,))/WLGTH)**2
C   AL=1*(SA1*EXP(-SB1*S)+SC1*EXP(-SD1*S)+SE1)*EXP(-SH1*S)
C   S=(SIN((TWOH(NDP)*3,14159)/(2,*180,))/WLGTH)**2
C   AH=1*(SA1*EXP(-SB1*S)+SC1*EXP(-SD1*S)+SE1)*EXP(-SH1*S)
C   AL=(AH/AL)**2
C   DO 6 J=1,NDP
C   7 Z=J-1
C   6 H1(J)=H1(J)*(AL+Z*(1.+AL))/(NDP-1)
C   DO 7 I=1,NDP
C   H1(I)=H1(I)*(1.+XKFACT)*(SIN(TWOH(I)*RADIANT/2.,1))**2
C   1 (1.+XKFACT*(COS(TWOH(I)*RADIANT))**2)
C   7 ET1(I)=SIN(TWOH(I)*RADIANT/2.,)
C   IF(NRAC,60,0) GO TO 12
C
C   RACHINGER CORRECTION OF KALPHA INTENSITIES, BACKGROUND CORRECTION
C   AND CONVERSION TO EQUALLY SPACED ETA INTERVALS
C   ET2(1)=ET2(1)
C   ET2(NDP)=ET1(NDP)
C   NETA=NDP
C   NDPM1=NDP-1
C   DPM1=NDRM1
C   DETA=(ET1(NDP)-ET1(1))/DPM1
C   ET5(1)=(4,*3,14159/WLGTH)*ET1(1)
C   ET5(NDP)=(4,*3,14159/WLGTH)*ET1(NDP)
C   DO 8 I=2,NDRM1
C   ET2(I)=ET2(I-1)+DETA
C   8 ET5(I)=(4,*3,14159/WLGTH)*ET1(I)
C   ARL=WLGTH/(WLGTH+DWLGTH)
C   MAR=10
C   AMAR=MAR
C   QMAR=1./AMAR
C   RLQMAR=1./ARL**QMAR
C   ET6(1)=ET5(1)
C   DO 9 I=2,800
C   ET6(I)=ET6(I-1)*RLQMAR
C   IF(ET6(I),GT,ET5(NDP)) GO TO 10
C   9 CONTINUE
C   INSTA=900
C   GO TO 11
C   10 INETA=I-1
C   GO TO 11
C   11 CALL INTERP(ET5,ET6,H1,YX,NDP,INETA)
C   CALL ARANORG(YX,YZ,INETA,MAR)
C   CALL AINTERP(ET6,ET2,YZ,H3,INETA,NETA)
C   CALL BORDER(H3,NETA)
C   GO TO 13
C
C   BACKGROUND CORRECTION AND CONVERSION TO EQUALLY SPACED ETA INTERVAL
C   (NO RACHINGER CORRECTION )
C   12 ET2(1)=ET1(1)
C   ET2(NDP)=ET1(NDP)
C   NETA=NDP
C   NDPM1=NDRM1
C   DPM1=NDRM1

```

```

DETA = (ED1(NDP)-ET1(1))/OPM1
DO 13 182/NBDM1
13 ET2(1) = ET1(1)+DETA
    CALL INTERP (ET1,ET2,H1,H3,NDP,NETA)
    SLOPE = (H3(NETA)-H3(1))/(ET2(NETA)-ET2(1))
    H3SAVE = H3(1)
    DO 14 181/NETA
14 H3(1) = H3(1)+H3SAVE+SLOPE*(ET2(1)-ET2(1))
15 CONTINUE
    PRINT 125/ET2(1),DETA
C
C   CALCULATION OF PEAK MAXIMUM (3 POINT PARABOLA)
    CALL MAXIM(H3,NETA,NMAX)
    PNUM = 3,*H3(NMAX-3)+H3(NMAX-2)+H3(NMAX+2)
    PDEN = 2,*H3(NMAX-1)+H3(NMAX+1)+H3(NMAX+2)
    ETAMAX = ET2(NMAX+4)+DETA*PNUM/PDEN+1,5
    PNU = 4,*H3(NMAX-3)+H3(NMAX-2)+H3(NMAX+3)
    PDL = 2,*H3(NMAX)+H3(NMAX-3)+H3(NMAX-3)
    ETAMA = ED2(NMAX+3)+DETA*PNU/PDL+1,5
    RN = 1,*H3(NMAX+1)+H3(NMAX+2)+H3(NMAX+4)
    RD = 1,*H3(NMAX+1)+H3(NMAX+2)+H3(NMAX+4)
    ETAM = ET2(NMAX+2)+DETA*PN/PD+1,5
    ETHAX = (ETAMAX + ETAMA + ETAM)/3,
    NET = NETA
    DO 16 181/NET
16 ET3(1) = ET2(1)
    H(1) = H(1)
    NET4=NET=0
    PRINT 126
    PRINT 127/NET
    DO 17 181/NET
17 ET2(1) = ET3(1)*100,
    IF(NACH,88,3) 17,18
    CALL MAXIM(NET,NET,NMAX)
18 RATIO = 9,/PEAK2
    PEAK2 = H(1)
    ET4(1) = ET3(1)
    ET4(NET) = ET3(NET)
    DET4 = 1604(NET)+ET4(1)/(INET+1)
    A(1) = H(1)*RATIO
    DO 20 182/NET
    A(1) = H(1)*RATIO
20 ET4(1) = ET4(1-1)+100,+DET4
    YMIN1 = ET4(1)
    X5 = ET4(NET)+1,
    X7 = X5+2,
    CALL AXIS1(0,,1,,0,-1,X5,0,,1,,YMIN1,,01,4HF6,3)
    CALL AXIS1(0,,0,,TITLER(1),56,10,,90,,1,,1,,1,,4HF6,2)
    CALL PLOT1-ET4(1),1,,3)
    CALL LINE (ET4,A,NET,1,rcl,0,,1)
    CALL PLOT1X7,0,,3)
C   POSITION OF PEAK MAXIMUM AND CENTER OF GRAVITY, INTRODUCED BY
C   AND VARIANCE IN S = ZSIN(TWGH/2)/WLGH
    THGMM = 2,*ASIN(ETMAX)/RADIAN
    SMAX = ETMAX*2./WLGH
    SSMAX = SMAX*SMAX
    HMAX = H(SMAX)
    AREA = 0,
    AM = 0,
    VAR = 0,
    DO 22 181/NET
22 ET(1) = ET3(1)+ETMAX
    AREA = AREA +(H(1)

```

```

22 AM = AM + H(I)*ET(I)
ETCG = AM*AREA + ETMAX
SCG = ETCG*2./WLGTH
DO 23 I=1,NET
ETA(I) = ET3(I) - ETCG
23 VAR = VAR + H(I)*ETA(I)*BTA(I)
BINT = AREA*DETA/HMAX*2./WLGTH
W = VAR/AREA*2./WLGTH*2./WLGTH
DELTA$ = IETA(NET)-ETA(1)*2./WLGTH
DPM = 1./SMAX
DCG = 1./SCG
CHI = 1./ETMAX - ETMAX
PUNCH 128,IW,IK,II,IL
PUNCH 129,SSMAX
PRINT 120,ETMAX
PRINT 121,TWOMM
PRINT 122,SMAX
PRINT 123,SSMAX
PRINT 124,NMAX
PRINT 125,ETCG
PRINT 126,SCG
PRINT 127,AREA
PRINT 128,BINT
PRINT 129,W
PRINT 130,DELTA$
PRINT 131,DPM
PRINT 132,DCG
PRINT 133,IW,IK,II,IL,CHI

```

C
C CALCULATION OF FOURIER COEFFICIENTSC
C CALCULATION OF FOURIER COEFFICIENTS BY THE TRIGONOMETRIC INTEGRAL
C
TECHNIQUE OF FILON

```

VIK=2,
NET1=NET-1)/2
NET2=NET8
NFC1=NFC*8
MNEC1=MNEC1
1F(NRAC,NE,0) GO TO 25
DO 24 I=1,NET
24 ETA(I)=ET1(I)
25 ETANET=ETA(NET)
ETA=ETA($)
PI=3.141592653
TP1=2.*PI
DO 26 L=1,NFC1
EL=L
BAL(L)=EL+VIK
HRL=0,
26 HLL=0,
ALPHA(1)=0,
BETA(1)=0,66666666666666
GAMMA(1)=2,333333333333
DO 27 L=2,NFC1
THETA=BAL(L)*TP1*2.*DETA/WLGTH
ALPHA(L)=ISQ*/THETA)*(1.+0,B*SINF(2.*THETA)/THETA-2.*B*COSF(2.*THETA)/THETA)
12./THETA**2)
BETA(L)=(2./THETA**2)*(1.+COSF(THETA)**2-SINF(2.*THETA)/THETA)
27 GAMMA(L)=14./THETA**2)*(SINF(THETA)/THETA-COSF(THETA))
DO 29 L=1,NFC1
ARGX0=BAL(L)*TP1*R,*ETA1/WLGTH
ARGX2=HBM(L)*TP1*2.*ETANET/WLGTH

```

```

SUM2NC=0,5*(H(NET)*COSF(ARGX2N)+H(1)*COSF(ARGX0))
SUM2N2C=0,
SUM2N6=-0,5*(H(NET)*SINF(ARGX2N)+H(1)*SINF(ARGX0))
SUM2N18=0,
DO 128 1=1,NET,2
  ARGEVEN=SUM2N18+TP1*2,NETALTY/HLGTH
  ARGODD=BAR(L)*TP1*2,ETA(1)*1/HLGTH
  SUM2NC+SUM2NO+H(1)*COSF(ARGEVEN)
  SUM2N2C+SUM2N1C+H(1)*1*COSF(ARGOODD)
  SUM2N8+SUM2N9+H(1)*SINF(ARGEVEN)
128 SUM2N18+SUM2N18+H(1)*1*SINF(ARGOODD)
  ARBAR=DETA*(ALPHA(L)*(H(1)*COSF(ARGX0)-H(NET)*COSF(ARGX2N))+1*BETA(L)*SUM2NC+GAMMA(L)*SUM2N1C)
  HR(L)=BARH*ETANET
  AREA1=BETA*(ALPHA(L)*(H(1)*COSF(ARGX0)-H(NET)*COSF(ARGX2N))+1*BETA(L)*SUM2N8+GAMMA(L)*SUM2N18)
  HI(L)=BARH*ETANET
  GO TO CONTINUE
  AREAHR=L17
  DO 130 L=1,NR01
    HR(L)=HR(L)/AREA
    HI(L)=HI(L)/AREA
130 HBAR(L)=SQRT(HR(L))+HI(L)*HI(L)
C
C ANNEALED PEAKS ONLY
IF(NACW,NE,31) GO TO 132
PRINT 134
  DO 31 L=1,NFC1
31 PRINT 135,BAL(L),HR(L),HI(L),HBAR(L)
  BUNCH 136(BAL(L),HI(L),L=2,NFC1)
  HBAR(NFC1)=0.
  GO TO 132
C
C ANNEALED PEAK, COLDWORKED PEAK TO FOLLOW
32 IF(NACW,NE,2) GO TO 34
  DO 33 L=1,NFC1
    OR(L)=HR(L)
    OI(L)=HI(L)
33 GBAR(L)=HBAR(L)
  BINTS=BINT
  WS=0
  GO TO 999
C
C STOKES CORRECTION (USE READ IN VALUES OF GBAR)
34 IF(NACW,NE,5) GO TO 40
  READ 107,NFG,VG
  NFG1=NFG+1
  READ 136,108A(L),L=2,NFG1)
  READ 137,BINTS
  GBA(1)=1
  NF=NFG1-NFC1
  FF=NF
  VVG=VG*FF
  IF(VVVG,0,0) GO TO 36
  DO 35 L=1,NR01
    GBAR(L)=1
35 BALG(L)=VG*CL
  CALL INTERP1(BALG,BAL,GBA,GBAR,NFG1,NFC1)
  GO TO 38
36 DO 37 L=1,NFC1
37 GBAR(L)=GBAR(L)
38 PRINT 138
  PRINT 139
  DO 39 L=1,NFC1
    ABAR(L)=HBAR(L)/GBAR(L)

```

39 PRINT 135;BAL(L),HR(L),HI(L),HBAR(L),GBAR(L),ABAR(L)
GO TO 45

C C STOKES CORRECTION (USE READ IN VALUES OF GR AND GI)

40 IF(NACW,NE,4) GO TO 41
READ 136,1GR(L),GI(L),L=2,NFC1
GR(1)=1,
GI(1)=0,
PRINT 138

C C STOKES CORRECTION (USE COMPUTED VALUES OF GR AND GI)

41 IF(NACW,NE,3) PRINT 140
PRINT 141
DO 42 L=1,NFC1
FR(L) = (BR(L)*GR(L) + HI(L)*GI(L))/(GR(L)*GR(L)+GI(L)*GI(L))
FI(L) = (HI(L)*GR(L) - GI(L)*HR(L))/(GR(L)*GR(L)+GI(L)*GI(L))
ABAR(L) = SQRT(FR(L)*FR(L)+FI(L)*FI(L))
42 PRINT 142;BAL(L),HR(L),HI(L),GR(L),GI(L),FR(L),FI(L),ABAR(L)
43 DO 44 I=1,NFC1

L1

PUNCH 143;BAL(L),ABAR(L)

XX(I) = 0,04*BAL(I)

44 YY(I) = 5,0*ABAR(I)

X5 = XX(NFC1) + 1,

X7 = X5 + 2,

YMIN2 = BAL(I)

CALL AXIS1D(Y,0,,TITLEM(I),24,10,,99,,1,,0,1,,4HF4,1)

CALL AXIS1D(Y,0,,0,-1,X5,0,,1,,YMIN2,99,,4HF6,2)

CALL LINE1XX,YY,NFC1,1,0,0,0,1)

CALL PLOTIXX7,0,,3)

WC5W=WS

PRINT 144;WC

45 DIN=0,1,

DO 46 L=2,NFC1

46 DIN=DIN*ABAR(L)/2,

BSINT = 1/DIN/VIK

PRINT 145;BSINT

BINTC = BINT-BINTS*BINTS/BINT

PRINT 156;BINTC

IF(NSTR=1) WT,48,BD

47 ABAR=NFC1/10,

FR(NFC1) = 0,

GO TO 999

48 IHSAVE = IM

IKSAVE = IK

IISAVE = IJ

ILSAVE = IL

SCGS = SCB

BINTCS = BINTC

SSMAXS = SSMAX

DO 49 I=1,NFC1

49 ASAVE (I) = ABAR(I)

GO TO 999

C

C SEPARATION OF PARTICLE SIZE AND STRAIN

50 PRINT 147;IHSAVE,IKSAVE,IISAVE,ILSAVE,IM,IK,II,IL

PRINT 148;IMSAVE,IKSAVE,IISAVE,ILSAVE,IM,IK,II,IL

CALL STRAIN (ASAVE,ABAR,SCGS,SCB,NFC,VIK,DOG,1,1,1,1,1,1)

1 SSMAXS,SSMAX,ALP,BRS)

DO 51 I=1,NFC1

XX(I) = 0,04*BAL(I)

YY(I) = 5,0*ABAR(I)

51 ZZ(I) = 5,0*EPS(I)

X5 = XX(NFC1) + 1,

```

X7 = X5 + 2,
YMIN3 = BNL(1)
CALL AXIS10,,0,XTITUR1(1)/14,10,-90,1,0,0,0,20,4HFS,2
CALL AXIS10,,0,-1,X5,0,1,YMIN3,25,,4HF6,2
CALL LINE1XX,YY,NFC1,1,-1,0,,1
CALL PLOT1X7,0,-3
CALL AXIS10,,0,XTITUR2(1),24,10,-90,1,0,0,0,20,4HFS,2
CALL AXIS10,,0,XTITUR2(1),24,10,-90,1,0,0,0,20,4HFS,2
CALL LINE1XX,YY,NFC1,1,-1,0,,1
CALL PLOTS(0,0)
GO TO 999
297 CONTINUE
CALL STOPBLDT
END

```

```

SUBROUTINE MAX(A,N,L)
C
C      MAXIMUM VALUE OF ARRAY A OF LENGTH N IS AT L
C
DIMENSION A(N)
L=1
SMALLA = A(1)
DO 1 I=2,N
1 IF(SMALLA<=A(I)) GO TO 1
SMALLA = A(I)
L=1
1 CONTINUE
RETURN
END

```

```

SUBROUTINE INTERP(XB,XA,YB,YA,NB,NA)
C
C      QUADRATIC INTERPOLATION PROCEDURE
C
DIMENSION XA(NA),YA(NA),XB(NB),YB(NB)
NBEG = 1
NA1 = NA+2
NB1 = NB+2
YA(NA) = YB(NB)
DO 3 J=1,NA1
DO 1 K=NBEG,NB1
1 IF(XB(K)<=XA(J)) GO TO 2
2 Y12 = (YB(K+1)-(XB(K)-XA(J))*YB(K)*(XB(K+1)-XA(J)))/(XB(K)-XB(K+1))
3 Y23 = (YB(K)+(XB(K+3)-XA(J))*YB(K+1)*(XB(K)-XA(J)))/(XB(K+1)-XB(K+3))
YA(J) = (Y12*(XB(K+1)-XA(J))-Y23*(XB(K+1)-XA(J)))/(XB(K+1)-XB(K+3))
3 NBEG = K
RETURN
END

```

SUBROUTINE ARANCOR(G,F,N,M)

```

C
C   RACHINGER CORRECTION BY KRATINGS METHOD
C

DIMENSION G(N),F(N)
B = .5
XN=N
SLOPE=(G(N)-G(1))/(XN-1.)
GSAVE=G(1)
DO 1 I=1,N
X1=I
1 G(I)=G(I)-GSAVE*SLOPE*(X1-1.)
DO 3 J=1,N
F(J)=G(N)
DO 2 I=1,20
JNM = J+M
IF(JNM.LT.1) GO TO 3
F(J)=F(N) + (B**I)*G(JNM)
2 CONTINUE
3 CONTINUE
RETURN
END

```

SUBROUTINE AINTERP(XB,XA,YB,YA,NB,NA)

```

C
C   QUADRATIC INTERPOLATION PROCEDURE DIFFERENT X-AXES
C

DIMENSION XA(NA),YA(NA),XB(NB),YB(NB)
YA(NA)=YB(NB)
RADIAN = 3.14159/180.
NB1 = NB - 1
NBEG = 1
AMULT=XB(1)/XA(1)
DO 3 J=1,NA
ETJ=AMULT*XA(J)
DO 1 K=NBEG,NB1
IF(XB(K).GT.ETJ) GO TO 2
1 CONTINUE
2 Y12 = (YB(K+1)*(XB(K)-ETJ)-YB(K)*(XB(K+1)-ETJ))/(XB(K)-XB(K+1))
Y23 = (YB(K)*(XB(K+1)-ETJ)-YB(K+1)*(XB(K)-ETJ))/(XB(K+1)-XB(K))
YA(J) = (Y12*(XB(K+1)-ETJ)+Y23*(XB(K+1)-ETJ))/(XB(K+1)-XB(K-1))
3 NBEG = K
RETURN
END

```

SUBROUTINE WORDER(LA,N)

ORDERSING OF AN ARRAY A OF LENGTH N ABOUT ITS MAXIMUM ELEMENT

```

C
DIMENSION A(N),E1(500),E2(500)
CALL MAX1(LA,N,L1)
DO 1 I=N,N
1 E1(I)=ABSE(A(I))
J=0
DO 2 I=L1,N
2 E2(I)=ABSE(A(I))
J=N-J
DO 3 I=L1,N
3 E1(LMIN)=87777778
DO 4 I=L1,N
4 E2(LMAX)=800000000
CALL MAX2(E2,JN,LMAX)
A(LMAX)=A(LMIN)
E2(LMAX)=E2(LMIN)
RETURN
END

```

SUBROUTINE MIN1(A,N,M)

MINIMUM VALUE OF ARRAY A OF LENGTH N IS AT L

```

C
DIMENSION A(N)
SMALL=A(1)
L=1
DO 1 I=2,N
1 IF(A(I)<SMALL) GO TO 1
SMALL=A(I)
L=I
1 CONTINUE
RETURN
END

```

SUBROUTINE STRAIN (A,B,SCG1,SCG2,NFC,VIK,DUG,B11,B12,S21,S22,ALP,
1-ERS)

C

C SEPARATION OF PARTICLE SIZE AND DISTORTION COEFFICIENTS

DIMENSION A(101),B(101),EPS(101),ALP(101),TITLE(6),BAL(101)

100 FORMAT(6X,' THE VALUES OF THE PARTICLE COEFFICIENT PRELIMINAR')

101 FORMAT(E18.2,F18.4)

102 FORMAT(F8.3,F8.3)

103 FORMAT(//#4H INTEGRAL BREADTH PARTICLE SIZE, DINT = F10.2//)

104 FORMAT(//#4H INTEGRAL BREADTH PARTICLE SIZE, DINTR = F10.2//)

105 FORMAT(3SH INTEGRAL BREADTH STRAIN, EPSP = F10.2//)

NFC1=0,NFC0=1

DO 1,L=1,NFC0

EL=L-1

BAL(L)=EL*VIK

Y1=A(L)*GIA(L)

Y2=A(L)*GIB(L)

X1=B(SCG1)*2

X2=B(SCG2)*2

BC=(Y2-Y1)/(X2-X1)

IF(BC,G1,0.) EPS(L)=SQRT(BC)/(SQRT(2.)*3.14159*BAL(L))

IF(BC,LE,0.) EPS(L)=0.

IF(BC,GT,0.) ALP(L)=EXP(XZ)

IF(BC,LE,0.) ALP(L)=A(L)

1 EPS(L)=EPS(L)*100.

PUNCH 180

PUNCH 100

PUNCH 100

DO 2,L=NFC0

PUNCH 181,BAL(L),ALP(L)

2 PRINT 102,BAL(L),ALP(L),EPSP(L),EPS(L)

DI=1,

DO 3 L=2,NFC1

3 DI=DI+ALP(L)*2,

DINT=VIK+DI

PRINT 103,DINT

EXPLAINT(DINT)=SS1

DINT=SX/1B|1*B|1*SS2=B|2*B|2*SS1

EPSP=(SQRT(B|1*B|2*(B|2*B|1)/SX/4.,))+100,

PRINT 104,EPSP

A(NFC2)=0,

B(NFC2)=0,

ALP(NFC1)=0,

EPS(NFC1)=0,

RETURN

END

Appendix C
Program SEPARATE

Control or Data Cards	Format	
NFC	I2	NFC=number of Fourier coefficients
IH1, IK1, IH1, IL1	4I2	IH1IK1IH1IL1=(HKIL) Miller-Bravais indices of Peak
AA1	F10.5	AA1 = $1/d_{hkl}^2$
(BAL(I), A1 (I), I=1, NFC)	F12.2, F15.4	BAL=na ₃ AL=Fourier coefficient

11/19/70

```

PROGRAM SEPARATE
DIMENSION A1(101),A2(101),A3(101),A4(101),A5(101),A6(101),A7(101)
DIMENSION A8(101),A9(101),A0(101)
DIMENSION B1(101),B2(101),B3(101),B4(101),B5(101),B6(101),B7(101)
DIMENSION B8(101),B9(101),B0(101)
DIMENSION C1(101),C1(101),C3(101),C4(101),C5(101),C6(101),C7(101)
DIMENSION C8(101),C9(101),C0(101)
DIMENSION D1(101),D1(101),D3(101),D4(101),D5(101),D6(101),D7(101)
DIMENSION D8(101),D9(101),D0(101)
DIMENSION DD1(101),DD1(101),DD3(101),DD4(101),DD5(101),DD6(101)
DIMENSION DD7(101),DD8(101),DD9(101),DD0(101)
DIMENSION W(100),YI(100),DELY(100),B(30),SR(30),T(30),ST(10)
DIMENSION C2(11),SC(11),AI(30,30),XI(100)
DIMENSION SM(10)
DIMENSION STR1(101),STR2(101),DSTR1(101),DSTR2(101)
DIMENSION STR(30),AYK(101),BYK(101)
DIMENSION APAR(101),RMSSTR(101)
DIMENSION STRAIN(101),PARSIZ(101)
DIMENSION XK(101),YK(101)
DIMENSION AVSL0(101),ABAL(101),BAL(101)
DIMENSION ABUFFER(254)
DIMENSION SLOPE(101)

99 FORMAT(I2)
100 FORMAT(4I2)
101 FORMAT(F10.5)
102 FORMAT(F12.2,F15.4)
103 FORMAT(1H0,5X,* THE HKIL VALUES ARE *,4I2//)
104 FORMAT(5X,* THE VALUE OF 1./D(HKIL) SQUARED IS *,F10.5//)
105 FORMAT(5X,* THE VALUES OF ABAR ARE *//,(10F7.4))
106 FORMAT(5X,* THE VALUES OF THE NATURAL LOG OF APAR ARE *//,
1(1X,10F9.5))
107 FORMAT(1H1,2X,* BAL *,4X,* STRAIN *,6X,* SLOPE *,7X,* PARTICLE SIZ
1E *,//)
108 FORMAT(1X,F6.1,3X,F10.6,3X,F12.8,5X,F10.6)
109 FORMAT(//,4X,*L*,4X,*BAL*,3(6X,*SLOPE*,6X,*DOM SIZE*)//)
110 FORMAT(//,3X,I2,2X,F5.1,3(2X,E15.7,2X,F6.1))
111 FORMAT(5X,* THE VALUE OF XC IS *,F10.6//)
112 FORMAT(//,2X,* DD1 = *,F10.6,* DD2 = *,F10.6,* DD3 = *,F10.6,* DD4
1 = *,F10.6,* DD5 = *,F10.6,* DD6 = *,F10.6,* DD7 = *,F10.6//)
113 FORMAT(1H0,2X,* THE DISTORTION COEFFICIENTS ARE *//,(10F7.4))
114 FORMAT(//2X,* THE PARTICLE SIZE COFFICIENTS ARE *//,(10F7.4))
CALL PLOTS(ABUFFER,254,18)
NOUT=1
READ 99,IJK
90 READ 99,NFC
NOUT=NOUT+1
NFC=NFC+1
READ 100,IH1,IK1,II1,IL1
READ 101,AA1
READ 102,(BAL(I),A1(I),I=1,NFC)
PRINT 103,IH1,IK1,II1,IL1
PRINT 104,AA1
PRINT 105,(A1(I),I=1,NFC)
READ 100,IH2,IK2,II2,IL2
READ 101,AA2
READ 102,(BAL(I),A2(I),I=1,NFC)

```

```

PRINT 103,IK2,IK2,II2,IL2
PRINT 104,AA2
PRINT 105,(A2(I),IK1,NFC)
READ 100,IK3,IK3,II3,IL3
READ 101,AA3
READ 102,(BAL(I),A3(I),I=1,NFC)
PRINT 103,IK3,IK3,II3,IL3
PRINT 104,AA3
PRINT 105,(A3(I),I=1,NFC)
READ 100,IK4,IK4,II4,IL4
READ 101,AA4
READ 102,(BAL(I),A4(I),I=1,NFC)
PRINT 103,IK4,IK4,II4,IL4
PRINT 104,AA4
PRINT 105,(A4(I),I=1,NFC)
READ 100,IK5,IK5,II5,IL5
READ 101,AA5
READ 102,(BAL(I),A5(I),I=1,NFC)
PRINT 103,IK5,IK5,II5,IL5
PRINT 104,AA5
PRINT 105,(A5(I),I=1,NFC)
READ 100,IK6,IK6,II6,IL6
READ 101,AA6
READ 102,(BAL(I),A6(I),I=1,NFC)
PRINT 103,IK6,IK6,II6,IL6
PRINT 104,AA6
PRINT 105,(A6(I),I=1,NFC)

DO 1 I=1,NFC
BBAL(I)=0.06666667*BAL(I)
AP1(I)=10.*A1(I)
AP2(I)=10.*A2(I)
AP3(I)=10.*A3(I)
AP4(I)=10.*A4(I)
AP5(I)=10.*A5(I)
AP6(I)=10.*A6(I)
1 ABAL(I)=0.04*BAL(I)

CALL LINE(10.,0.,0.,-1,10.,0.,1.,0.,18.,14HF4.2)
CALL LINE(0.,0.,0.,1,10.,0.,-1,0.,0.,14HF4.2)
CALL LINE(BBAL,AP1,NFC,1,-1,0.,0.)
CALL LINE(BBAL,AP2,NFC,1,-1,0.,0.)
CALL LINE(BBAL,AP3,NFC,1,-1,0.,0.)
CALL LINE(BBAL,AP4,NFC,1,-1,0.,0.)
CALL LINE(BBAL,AP5,NFC,1,-1,0.,0.)
CALL LINE(BBAL,AP6,NFC,1,-1,0.,0.)
CALL PLOT(12.,0.,-3)
DO 2 I=1,NFC
B1(I) = LOGF(A1(I))
B2(I) = LOGF(A2(I))
B3(I) = LOGF(A3(I))
B4(I) = LOGF(A4(I))
B5(I) = LOGF(A5(I))
B6(I) = LOGF(A6(I))
2 CONTINUE

PRINT 106,(B1(I),I=1,NFC)
PRINT 106,(B2(I),I=1,NFC)

```

```

PRINT 106,(B3(I),I=1,NFC)
PRINT 106,(B4(I),I=1,NFC)
PRINT 106,(B5(I),I=1,NFC)
PRINT 106,(B6(I),I=1,NFC)
XI(1) = AA1
XI(2) = AA2
XI(3) = AA3
M=3 S KM#1 S IWR0 S ISH#0 S LP#0
DO 3 L=1,NFC
SM(1) = B1(L)
SM(2) = B2(L)
SM(3) = B3(L)
CALL LSQPOL(M,KM,IW,ISW,LP,SIGMA,XI,SM,W,YI,DELY,B,SB,T,ST,OB,SC)
1AI,STR)
PARSIZ(L) = EXPF(B(1))
SLOPE(L) = B(2)
STRAIN(L) = -SLOPE(L)/(19,7392088+BAL(L)*#2)
PRINT 107,BAL(L),STRAIN(L),SLOPE(L)
PRINT 108,BAL(L),PARSIZ(L)
3 CONTINUE
DO 4 L=1,NFC
APAR(L) = 10,*PARSIZ(L)
4 CONTINUE
DO 6 L=2,NFC
RMSSTR(L) = 1000,*SQRTF(STRAIN(L))
6 CONTINUE
CC = 2.0/SQRTF(AA2)
PRINT 111,CC
AD1 = 1./SQRTF(AA1)
AD2 = 1./SQRTF(AA2)
AD3 = 1./SQRTF(AA3)
AD4 = 1./SQRTF(AA4)
AD5 = 1./SQRTF(AA5)
AD6 = 1./SQRTF(AA6)
PRINT 112,AD1,AD2,AD3,AD4,AD5,AD6
CALL ORDER(PARSIZ,NFC,MM)
DO 13 I=1,NFC
C1(I)=EXPF(AA1*SLOPE(I))
C2(I)=EXPF(AA2*SLOPE(I))
C3(I)=EXPF(AA3*SLOPE(I))
C4(I)=EXPF(AA4*SLOPE(I))
C5(I)=EXPF(AA5*SLOPE(I))
C6(I)=EXPF(AA6*SLOPE(I))
D1(I) = A1(I)/C1(I)
D2(I) = A2(I)/C2(I)
D3(I) = A3(I)/C3(I)
D4(I) = A4(I)/C4(I)
D5(I) = A5(I)/C5(I)
D6(I) = A6(I)/C6(I)
13 CONTINUE
DO 14 I=1,NFC
DD1(I) = 10.0 * D1(I)
DD2(I) = 10.0 * D2(I)
DD3(I) = 10.0 * D3(I)
DD4(I) = 10.0 * D4(I)
DD5(I) = 10.0 * D5(I)

```

```

DD6(1) = 10.0 * D6(1)
14 CONTINUE
NF=NFC-1
CALL AXIS(0.,0.,3H L ,-3,10.,0.,1.,0.,15.,14HF6,2)
CALL AXIS(0.,0.,12H RMS STRAIN , 12,10.,90.,1.,0.,.001,14HF7,3)
CALL LINE(BBAL(2),RMSSTR(2),NF,1,-1,0.,1)
CALL PLOTS(0,0)
CALL PLDT(12,,0,,*3)
CALL AXIS(0.,0.,26H PARTICLE SIZE COEFFICIENT,26,10.,90.,1.,0.,1)
14HF4,2)
CALL AXIS(0.,0.,3H L ,-3,10.,0.,1.,0.,15.,14HF6,2)
CALL LINE(BBAL,DD3,NFC ,1,-1,0.,1)
CALL LINE(BBAL,DD4,NFC ,1,-1,0.,1)
CALL LINE(BBAL,DD6,NFC ,1,-1,0.,1)
CALL LINE(BBAL,ARAR,NFC ,1,-1,0.,1)
CALL STOPPLOT
END

```

```

SUBROUTINE MAX (A,N,L)
DIMENSION A(N)
BIGA = A(1)
L = 1
DO 1 I=2,N
IF(A(I),LE,BIGA) GO TO 1
BIGA = A(I)
L = I
1 CONTINUE
RETURN
END

```

```

SUBROUTINE ORDER(A,N,L)
DIMENSION A(N)
L=1
BIGA=A(1)
DO 1 I=2,N
IF(A(I),GT,BIGA) GO TO 2
BIGA=A(I)
L=I
1 CONTINUE
GO TO 3
2 L=I
3 RETURN
END

```

```

SUBROUTINE LSQPOL(M,KM,IW,ISW,LP,SIGMA,X,F2,W,Y,DELY,B,SB,T,ST,C) LSQPL 1
1SC,A,STR)
C E2 UCSD LSQPOL F 63
C CORRECTED APRIL, 1964
C MODIFIED OCT, 16, 1964
C F60, F62, F63
DIMENSION S(30),X(100),F2(100),ST(30),SB(30), LSQPL 3
1 F(100),PM(100),P(100),B(30),DELY(100),W(100), LSQPL 4
2A(30,30),T(30),Y(100),BM(11,11), LSQPL 5
DIMENSIONND(11,11),C(11),SC(11) LSQPL 6
DIMENSION STR(30)
IJK=0
LL=0
9 FM=0,0
A(1,1)=1.0
A(2,2)=1.0
FBAR=0.0
XBAR=0.0
D010I=1,M
IF(IW)1009,1010,1009
1010 W2=1.0
W(I)=1.0
GOT01011
1009 W2=SQRTE(W(I))
1011 FM=FM+W(I)
F(I)=W2*F2(I)
PM(I)=W2
FBAR=FBAR+F(I)*PM(I)
10 XBAR=XBAR+X(I)*PM(I)**2
XBAR=XBAR/FM
T(1)=FBAR/FM
A(2,1)=XBAR
PXF=0.0
PXP=0.0
D020I=1,M
P(I)=(X(I)-XBAR)*PM(I)
PXF=PXF+P(I)*F(I)
20 PXP=PXP+P(I)*P(I)
T(2)=PXF/PXP
PMXPM=FM
S(1)=PMXPM
KM=KM+1
B(1)=T(1)*A(1,1)+T(2)*A(2,1)
B(2)=T(2)*A(2,2)
60 D0 190 K=2,KM
IF(K,GT,2)65,165
65 XPXP=0.0
XPXPM=0.0
B(K)=0.0
D070J=1,M
XP=X(J)*P(J)
XPXP=XPXP+XP*P(J)
70 XPXPM=XPXPM+XP*PM(J)
ALPHA=XPXP/PXP
BETA=XPXPM/PMXPM
PPXF=0.0
LSQPL 7
LSQPL 8
LSQPL 9
LSQPL 10
LSQPL 11
LSQPL 12
LSQPL 13
LSQPL 14
LSQPL 15
LSQPL 16
LSQPL 17
LSQPL 18
LSQPL 19
LSQPL 20
LSQPL 21
LSQPL 22
LSQPL 23
LSQPL 24
LSQPL 25
LSQPL 26
LSQPL 27
LSQPL 28
LSQPL 29
LSQPL 30
LSQPL 31
LSQPL 32
LSQPL 33
LSQPL 34
LSQPL 35
LSQPL 36
LSQPL 37
LSQPL 38
LSQPL 39
LSQPL 40
LSQPL 41
LSQPL 42
LSQPL 43
LSQPL 44
LSQPL 45
LSQPL 46
LSQPL 47
LSQPL 48
LSQPL 49
LSQPL 50

```

```

PPXPP=0,0
D090I=1,M
80 PT=P(I)
81 P(I)=X(I)*PT+ALPHA*PT+BETA*PM(I)
82 PPXF=PPXF+P(I)*F(I)
83 PPXPP=PPXPP+P(I)*P(I)
90 PM(I)=PT
T(K)=PPXF/PPXPP
PMXP=PPXPP
PPXPP=PPXPP
A(K,1)=ALPHA*A(K-1,1)+BETA*A(K-2,1)
A(K,K-1)=A(K-1,K-2)-A(K-1,K-1)*ALPHA
A(K,K)=1,0
IF(K=3)150,150,110
110 K1=K-2
D0120I=2,K1
120 A(K,I)=A(K-1,I-1)-ALPHA*A(K-1,I)+BETA*A(K-2,I)
150 D0160I=1,K
160 B(I)=B(I)+T(K)*A(K,I)
165 SIG2=0,0
D0180I=1,M
Y(I)=POLYE1(X(I),K,B)
175 DELY(I)=Y(I)-F2(I)
180 SIG2=SIG2+(DELY(I)**2)*W(I)
SIG2=SIG2/FLGATE(M-K)
SIGMA=SQRTF(SIG2)
S(K)=PXP
D0499I=1,K
499 ST(I)=SIGMA/SQRTF(S(I))
D0501I=1,K
SB(I)=0,0
D0500J=1,K
500 SB(I)=SB(I)+(A(J,I))*ST(J)**2
501 SB(I)=SQRTF(SB(I))
IF(LP)658,183,658
658 IF(K=2)652,651,652
651 D(1,1)=1,0
D(2,2)=1,0
D(2,1)=0,0
D(3,3)=3,/2,
D(3,2)=0,
D(3,1)=-1,/2,
D(4,4)=5,/2,
D(4,3)=0,
D(4,2)=-3,/2,
D(4,1)=0,
D(5,5)=35,/8,
D(5,4)=0,
D(5,3)=30,/8,
D(5,2)=0,
D(5,1)=3,/8,
D(6,6)=63,/8,
D(6,5)=0,
D(6,4)=-70,/8,
D(6,3)=0,
D(6,2)=15,/8,
LSQPL 51
LSQPL 52
LSQPL 53
LSQPL 54
LSQPL 55
LSQPL 56
LSQPL 57
LSQPL 58
LSQPL 59
LSQPL 60
LSQPL 61
LSQPL 62
LSQPL 63
LSQPL 64
LSQPL 65
LSQPL 66
LSQPL 67
LSQPL 68
LSQPL 69
LSQPL 70
LSQPL 71
LSQPL 72
LSQPL 73
LSQPL 74
LSQPL 75
LSQPL 76
LSQPL 77
LSQPL 78
LSQPL 79
LSQPL 80
LSQPL 81
LSQPL 82
LSQPL 83
LSQPL 84
LSQPL 85
LSQPL 86
LSQPL 87
LSQPL 88
LSQPL 89
LSQPL 90
LSQPL 91
LSQPL 92
LSQPL 93
LSQPL 94
LSQPL 95
LSQPL 96
LSQPL 97
LSQPL 98
LSQPL 99
LSQPL100
LSQPL101
LSQPL102
LSQPL103
LSQPL104
LSQPL105
LSQPL106

```

D(7,7)=231./16,	LSQPL108
D(6,1)=0,	LSQPL109
D(7,6)=0,	LSQPL110
D(7,5)=315./16,	LSQPL110
D(7,4)=0,	LSQPL111
D(7,3)=105./16,	LSQPL112
D(7,2)=0,	LSQPL113
D(7,1)=5./16,	LSQPL114
D(8,8)=429./16,	LSQPL115
D(8,7)=0,	LSQPL116
D(8,6)=693./16,	LSQPL117
D(8,5)=0,	LSQPL118
D(8,4)=315./16,	LSQPL119
D(8,3)=0,	LSQPL120
D(8,2)=-35./16,	LSQPL121
D(8,1)=0,	LSQPL122
D(9,9)=6435./128,	LSQPL123
D(9,8)=0,	LSQPL124
D(9,7)=-12012./128,	LSQPL125
D(9,6)=0,	LSQPL126
D(9,5)=6930./128,	LSQPL127
D(9,4)=0,	LSQPL128
D(9,3)=-1260./128,	LSQPL129
D(9,2)=0,	LSQPL130
D(9,1)=35./128,	LSQPL131
D(10,10)=12155./128,	LSQPL132
D(10,9)=0,	LSQPL133
D(10,8)=-25740./128,	LSQPL134
D(10,7)=0,	LSQPL135
D(10,6)=18018./128,	LSQPL136
D(10,5)=0,	LSQPL137
D(10,4)=-4620./128,	LSQPL138
D(10,3)=0,	LSQPL139
D(10,2)=315./128,	LSQPL140
D(10,1)=0,	LSQPL141
D(11,11)=46189./256,	LSQPL142
D(11,10)=0,	LSQPL143
D(11,9)=-109395./256,	LSQPL144
D(11,8)=0,	LSQPL145
D(11,7)=90090./256,	LSQPL146
D(11,6)=0,	LSQPL147
D(11,5)=-30030./256,	LSQPL148
D(11,4)=0,	LSQPL149
D(11,3)=3465./256,	LSQPL150
D(11,2)=0,	LSQPL151
D(11,1)=-63./256,	LSQPL152
650 BM(I)=0,	LSQPL153
652 D0700II=1,K	LSQPL154
J=K-1I+1	LSQPL155
VARA=0.0	LSQPL156
III=K-J	LSQPL157
IF(III)702,701,702	LSQPL158
702 D0703JJ=1,III	LSQPL159
JK=K-JJ+1	LSQPL160
703 VARA=VARA+D(JK,J)*BM(K,JK)	LSQPL161
	LSQPL162

701 BM(K,J)*(A(K,J)-VARA)/D(J,J)	LSQPL163
1F(K=2)700,704,700	LSQPL164
704 BM(1,1)*A(1,1)/D(1,1)	LSQPL165
700 CONTINUE	LSQPL166
705 D0708I=1,K	LSQPL167
C(I)=0.0	LSQPL168
SC(I)=0.0	LSQPL169
D0707J=1,K	LSQPL170
C(I)=C(I)+BM(J,I)*T(J)	LSQPL171
707 SC(I)=SC(I)+(BM(J,I)*ST(J))**2	LSQPL172
708 SC(I)=SQRTF(SC(I))	LSQPL173
183 CONTINUE	LSQPL174
IBLANKS=1H	LSQPL175
D0 1100 I=1,K	
IJK=IJK+1	
STR(IJK) = B(I)	
1100 CONTINUE	
192 PRINT 1,(IBLANKS,I,B(I),SB(I),I=1,K)	LSQPL176
1 FORMAT(41H1C0EFFICIENTS OF Y=B1*B2*X*ETC AND ERRORS//(3(A1,2HB(I2,LSQPL177	
12H)*E15,7,6H ERRB=E10,3)))	LSQPL178
185 PRINT 186,SIGMA,(IBLANKS,I,T(I),ST(I),I=1,K)	LSQPL179
186 FORMAT(8H0SIGMA =E16,7//45H COEFFICIENTS OF Y=T1*P1*T2*P2*ETC AND LSQPL180	
1ERRORS//(3(A1,2HT(I2,2H)*E15,7,6H ERRT=E10,3)))	LSQPL181
IF(LP)187,670,187	LSQPL182
187 PRINT 188,(IBLANKS,I,C(I),SC(I),I=1,K)	LSQPL183
188 FORMAT(23H0 LEGENDRE POLYNOMIALS/45H COEFFICIENTS OF Y=C1*L1+C2*LLSQPL184	
12+ETC AND ERRORS//(3(A1,2HO(I2,2H)*E15,7,6H ERRC=E10,3)))	LSQPL185
670 PRINT 2,(I,X(I),P2(I),Y(I),DELY(I),W(I),I=1,M)	LSQPL186
2 FORMAT(47H0 I X(I) P(I)	LSQPL187
137HY(I) DELY(I) W(I)/(16.5E16,7))	LSQPL188
190 CONTINUE	LSQPL189
211 IF(ISW) 210,220,210	LSQPL190
210 D02151=2,KM	LSQPL191
215 PRINT 5,I,(A(I,J),J=1,I)	LSQPL192
5 FORMAT (29H0 ORTHOGONAL POLYNOMIAL COEFF	LSQPL193
16HFOR K=15//(8E15,6))	LSQPL194
220 KM=KM-1	LSQPL195
RETURN	
END	LSQPL196

FUNCTION POLYE1(X,K,B)	LSQPL197
DIMENSION B(30)	LSQPL198
10 S=B(K)	LSQPL199
KK=K-1	LSQPL200
20 D0 40 I=1,KK	LSQPL201
30 IK=K-I	LSQPL202
40 S=X*S+B(IK)	LSQPL203
POLYE1=S	LSQPL204
50 RETURN	LSQPL205
END	LSQPL206