The Use of Strain Moments in Determining Strain Distributions in Deformed Crystals

By J.W. Harrison

Metallurgy Division, Atomic Energy Research Establishment, Harwell, England

A method is presented of determining strain distributions in distorted crystals from measurements of distortion coefficients derived from a Fourier analysis of broadened diffraction lines. The moments of the strain distribution are determined approximately from the distortion coefficients and used to determine the expansion coefficients in a series of Hermite polynomials which, together with a weight function, represents the strain distribution. The advantage of the method lies in the fact that when measurements are made on only three reflexions from a distorted crystal a reasonably accurate strain distribution may be derived and intermediate steps in the computation enable an assessment to be made of the importance of the measured distortion coefficients and where emphasis should be placed in improving experimental accuracy. The method is illustrated with the use of the Gaussian as an appropriate weight function, but a suitable choice of the set of polynomials permits a wide range of weight functions to be used.

It has been shown (Wilson 1942, 1943, 1949; Stokes & Wilson 1942, 1944) that the function describing the shape of the lines of the diffraction pattern of a distorted crystal may be represented by a Fourier series.

Averbach & Warren (1949, 1950) used essentially the same formulation in their treatment of experiments on cold-worked metals and their work was extended by Eastbrook & Wilson (1952). It was pointed out by Stokes & Wilson (1944) how the distribution of strains in a distorted crystal could be obtained from a line once the instrumental broadening had been removed, and Warren & Averbach (1950) and Easterbrook & Wilson (1952) showed that the Fourier transform of the Fourier coefficients expressing the distortion of the crystal gave the strain distribution directly. The topic of the X-ray measurement of distorted crystals was reviewed by Warren (1959) and the notation of Warren's article will be used in this paper.

Using Warren's notation the distribution of diffracted power in the $00l$ line from the diffraction pattern of the distorted crystal is given by

$$P(\theta) = K(\theta) N \sum A_n \cos 2\pi n (h_3 - l)$$
$$+ B_n \sin 2\pi n (h_3 - l) \quad (1)$$

where $K(\theta)$ is a slowly varying function of θ, the diffraction angle, N is the number of cells in the coherently diffracting domain, $h_3 - l = 2a_3/\lambda$ $(\sin \theta - \sin \theta_0)$, θ_0 corresponding to the origin used for the diffraction line, a_3 is the quantity ld(d being the interplanar spacing in the $00l$ direction) and λ is the wavelength of the X-rays. The Fourier coefficients A_n and B_n are given by

$$A_n = N_n/N \langle \cos (2\pi Lh_0 e_L/a) \rangle_{\text{average}} \quad (2)$$
$$B_n = -N_n/N \langle \sin (2\pi Lh_0 e_L/a) \rangle_{\text{average}} \quad (3)$$

for cubic crystals. The term e_L is the strain and the suffix L denotes that it is averaged over a distance L in the crystal. When the reflexion is of the type $00l$ then $h_0 = l$. If the crystal is cubic h_0 is given by $h_0^2 = h^2 + k^2 + l^2$.

so that when the length of the unit cell edge is a then $a_3/l = a/h_0$. When the cubic crystal is elastically isotropic the above relations for A_n and B_n hold for all hkl reflexions. In the case of anisotropic crystals the strain distribution may differ in different crystallographic directions and this is reflected in a different set of A_n and B_n for each hkl direction.

The coefficients A_n and B_n may be represented by a product of a 'particle size' term and a distortion term as follows:

$$A_n = A_n^S A_n^D, \qquad B_n = B_n^S B_n^D,$$

where the superscripts denote size(S) and distortion(D). and

$$A_n^S = N_n/N, \qquad B_n^S = N_n/N,$$

$$A_n^D = \langle \cos (2\pi Lh_0 e_L/a) \rangle, \quad B_n^D = -\langle \sin (2\pi Lh_0 e_L/a) \rangle.$$

The term N_n/N, which is related to the distribution of sizes of coherently diffracting domains in the crystal, will not be discussed in this paper. The negative sign in the expression for B_n^D simply indicates a net shift of the diffraction line to lower angles for a positive mean strain in the crystal.

In terms of a normalized strain distribution function $P(e_L)$ the distortion terms are given by

$$A_n^D = \int P(e_L) \cos (2\pi Lh_0 e_L/a) \, de_L \quad (4)$$
$$B_n^D = \int P(e_L) \sin (2\pi Lh_0 e_L/a) \, de_L. \quad (5)$$

The strain distribution function itself is given directly as the Fourier transform of the measured A_n^D and B_n^D values, so

$$P(e_L) = L/a \int \{A_n^D \cos (2\pi Lh_0 e_L/a)$$
$$+ B_n^D \sin (2\pi Lh_0 e_L/a)\} \, dh_0. \quad (6)$$

In order to perform the Fourier transformation the coefficients must be determined for enough values of h_0 so that they may be considered a known function of h_0. For elastically isotropic crystals all hkl reflexions

may be used and because of this McKeehan & Warren (1953), with measurements of about seven reflexions from cold-worked tungsten, were able to collect enough data to perform the transformation. Chipman & Warren (1952) also used a Fourier transformation in the treatment of their measurements on neutron irradiated graphite but because of experimental difficulties only three reflexions of the 00l type could be obtained, and this led the authors to doubt the final strain distribution computed from so little data.

The use of a moment method

An attractive approach to the problem of solving the integral equations relating the distortion coefficients to the strain distribution is to use the moments of the strain determinable, approximately, from the coefficients themselves. This may be done as follows. Expanding the strain distribution $P(e_L)$ in terms of a weight function $W(e_L)$ and an orthonormal set of polynomials $P_n(e_L)$ we have

$$P(e_L) = W(e_L) \sum_n a_n P_n(e_L), \qquad (7)$$

in which the a_n are expansion coefficients and the weight function $W(e_L)$ and the set of polynomials $P_n(e_L)$ are so chosen so that

$$\int W(e_L) P_n(e_L) P_m(e_L) de_L = f(n) \delta_{mn} \qquad (8)$$

where δ_{mn} is the Kronecker delta

$$\delta_{mn} = 0 \quad \text{for} \quad m \neq n$$
$$\delta_{mn} = 1 \quad \text{for} \quad m = n,$$

and $f(n)$ is a function of n, the order of the polynomial. Then we find

$$\int P(e_L) P_m(e_L) de_L = a_m f(m). \qquad (9)$$

Now since

$$P_m(e_L) = \sum_n C_n e_L^n \qquad (10)$$

then the integral on the left hand side of equation (9) is equal to $\sum_n C_n \langle e_L^n \rangle$, $\langle e_L^n \rangle$ being the nth moment of the strain distribution. The a_m may then be determined from the expression

$$a_m = 1/f(m) \sum_n C_n \langle e_L^n \rangle \qquad (11)$$

and the distribution function is now determined by using equation (7).

Hermite polynomial expansions have been used by other workers in discussing X-ray problems, in particular by Berry (1947) and Kobe (1959). Berry, while investigating the shape of diffraction lines from colloidal magnesium oxide, used Hermite polynomial expansions to represent observed line shapes in order to unfold the pure diffraction line shape from the observed line contaminated by the response of the X-ray camera. Kobe (1960) has also suggested a method of determining the strain distribution function using strain moments by the use of the Gram–Charlier series (Cramer, 1946) which uses a polynomial expansion of the distribution

function but gives no examples of its use. Kagan & Snovidov (1964), in concluding a paper devoted to the analysis of unresolved components of diffraction lines, mention the possibility of using a moment analysis in determining physical broadening functions and suggest the use of polynomial expansions. The method used in this paper is similar to that suggested by Kobe but avoids the inconvenience of carrying through the analysis in terms of the central moments $\langle (e_L - \langle e_L \rangle)^n \rangle$ and permits the use of several weight functions by a suitable choice of the orthonormal set of polynomials $P_n(e_L)$.

Determination of the strain moments

Following Kobe (1960) we expand the right hand sides of equations (2) and (3) and find

$$A_n^D = 1 - (1/2!)(2\pi Lh_0/a)^2 \langle e_L^2 \rangle + (1/4!) \times (2\pi Lh_0/a)^4 \langle e_L^4 \rangle - \ldots \quad (12)$$

$$B_n^D = -(2\pi Lh_0/a)\langle e_L \rangle + (1/3!)(2\pi Lh_0/a)^3 \langle e_L^3 \rangle - \ldots \quad (13)$$

where $\langle e_L^n \rangle$ is the nth moment of the strain distribution averaged over the length L in the crystal. For a set of m diffraction lines we have then two sets of m equations for determining m even and odd moments respectively. Because the expansions used for the sine and cosine terms are not rapidly convergent some error will be introduced by using only the first few terms of each expansion. However some improvement may be made to this first approximation to the moments by a method to be discussed below which involves computing a first approximation to the strain distribution and then comparing distortion coefficients computed from this first approximation with those actually observed. From the differences in the coefficients corrections may be made to the approximate moments to derive an improved strain distribution and the process repeated iteratively. The moments having been determined, equations (7) to (11) define the scheme of determining the strain function.

The choice of a suitable polynomial expansion for the strain function is determined by a suitably approximate weight function. The advantage of the representation (7) is that if a reasonable guess can be made as to the form of the weight function then the terms $a_n P_n(e_L)$ serve merely as nth order correction terms and are not required to represent the function itself. Physically it seems reasonable to choose $W(e_L)$ to be the Gaussian function since experimental observations (McKeehan & Warren 1953) indicate that this is a good approximation. The use of this function then determines the use of Hermite polynomials $H_n(e_L)$ for the orthonormal set $P_n(e_L)$, since the identity

$$\int \exp(-be_L^2) H_n(b^{\frac{1}{2}} e_L) H_m(b^{\frac{1}{2}} e_L) b^{\frac{1}{2}} de_L = 2^n \pi^{\frac{1}{2}} n! \delta_{mn} \quad (14)$$

leads simply to the following equation for determining the expansion coefficients:

$$a_n = 1/(2^n n!) \int P(e_L) \, H_n(b^{\frac{1}{2}} e_L) \, de_L \qquad (15)$$

where

$$P(e_L) = b^{\frac{1}{2}} \pi^{-\frac{1}{2}} \exp\left(-b e_L^2\right) \Sigma \, a_n \, H_n(b^{\frac{1}{2}} e_L) . \qquad (16)$$

The multiplier $b^{\frac{1}{2}} \pi^{-\frac{1}{2}}$ is chosen to normalize the integral of $P(e_L)$ over all positive and negative strains to unity, b being a parameter of the weight function.

Using the identity

$$H_n(b^{\frac{1}{2}} e_L) = \sum_{k=0}^{k \le n/2} \frac{(-1)^k \, e_L^{n-2k} \, b^{(n-2k)/2} \, 2^n \, n!}{k! \, (n-2k)! \, 2^{2k}} \qquad (17)$$

for the nth Hermite polynomial, and substituting in equation (15) we find

$$a_n = \sum_{k=0}^{k \le n/2} \frac{(-1)^k \, \alpha_{n-2k} \, b^{(n-2k)/2}}{k! \, (n-2k)! \, 2^{2k}} \qquad (18)$$

where

$$\alpha_{n-2k} = \int P(e_L) \, e_L^{n-2k} \, de_L; \qquad (19)$$

that is, α_{n-2k} is the $(n-2k)$th moment of $P(e_L)$.

To determine the coefficients a_n the value of b must be known. Since the second moment of the weight function is identically equal to $(2b)^{-1}$ and because, in a first approximation, this is the most important moment in determining the shape of the distribution function $P(e_L)$, b is put equal to $(2\alpha_2)^{-1}$ where α_2 is the second moment of the distribution determined from the set of equations (12). It will be noticed that when $P(e_L)$ is exactly Gaussian then all a_n for $n \neq 0$ are identically zero and b is given exactly by the relation

$$b = (2\alpha_2)^{-1} . \qquad (20)$$

Method of computation

To determine the moments of the strain distribution the two sets of simultaneous equations defined by equations (12) and (13) were solved by a process of matrix inversion and the moments finally computed from the inverse matrix and the distortion coefficients.
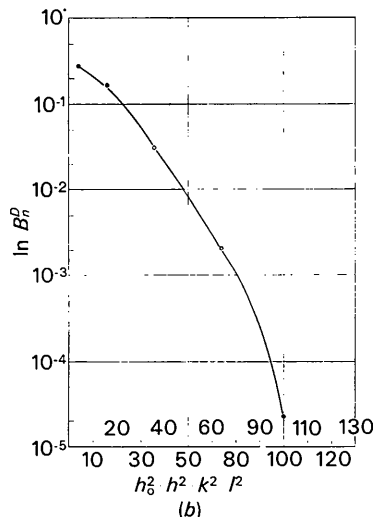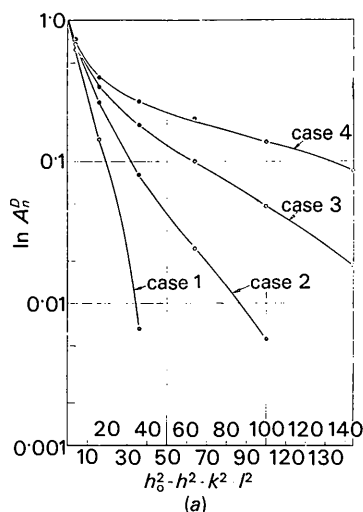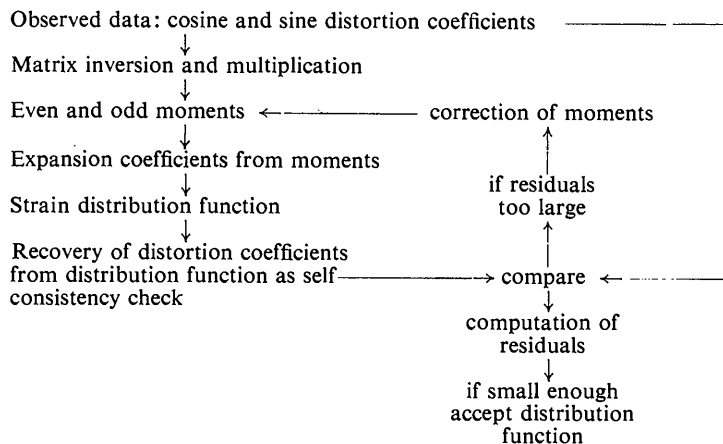

Fig. 1. (a) Average cosine terms. (b) Average sine terms for all cases.

Table 1. *Scheme of computation*

Observed data: cosine and sine distortion coefficients
↓
Matrix inversion and multiplication
↓
Even and odd moments ←—————— correction of moments
↓   ↑
Expansion coefficients from moments
↓   if residuals
Strain distribution function   too large
↓   ↑
Recovery of distortion coefficients
from distribution function as self—————→ compare ←————
consistency check   ↓
                              computation of
                                 residuals
                                    ↓
                              if small enough
                              accept distribution
                                  function

It proved of value to effect the computation in this way since, as discussed below, inspection of the inverse matrix made it clear how error in the measured distortion coefficients would finally affect the computed moments. Furthermore, the inverse matrix may be used to improve the approximation to the moments computed from the series expansions of (12) and (13). If we consider the equation relating the magnitude of the moments with the distortion terms we have

$$\alpha_{2m} = \sum_{j=1}^{n} a_{mj}^{-1} C_i$$

where α_{2m} is the $2m$th moment, C_i is the ith cosine coefficient and the a_{mj}^{-1} are the elements of the inverse cosine matrix. The error in the moments $\Delta\alpha_{2m}$ due to error ΔC_i in the coefficients is therefore given by

$$\Delta\alpha_{2m} = \sum_{j=1}^{n} a_{mj}^{-1} \Delta C_i .$$

Now computing a distribution function from the observed coefficients allows a recomputation of distortion coefficients corresponding to this distribution. Let these coefficients be written as C_i^1, the superscript indicating the first approximation to the distribution function. Comparing the C_i^1 with the C_i and writing

$$\Delta^1 C_i = C_i - C_i^1 \text{ we may compute}$$

$$\Delta^1\alpha_{2m} = \sum_{j=1}^{n} a_{mj}^{-1} (C_i - C_i^1) ,$$

where $\Delta^1\alpha_{2m}$ is the first order correction to the moments. The process may be repeated with the corrected moments to compute a better approximation to the distribution function, until the differences between the observed and computed distortion coefficients become stationary. Obviously with a small number of observed coefficients it will not always be possible to reduce the differences indefinitely since the higher approximations to the distribution function are being computed with a number of moments limited by the number of observed diffraction lines.

Table 1 shows the scheme of the computation.

Application of the method

Preliminary computations were made with distortion coefficients computed from artificial strain distributions. These strain distributions were constructed by using two Gaussian functions so displaced along the strain axis as to produce asymmetrical distributions. Table 2 lists the parameters used in generating these functions. The average cosine and sine terms were computed by numerical integration with $L = 100$ Å and $a = 4.123$ Å and terms were computed for six orders of

diffraction with h_0 equal to 2, 4, 6, 8 and 10. Fig. 1 shows the computed average cosine and sine terms while the solid lines in Fig. 2 shows the shape of the synthetic distribution functions. By progressively increasing the ratio of the parameters in the exponents of the Gaussian terms the synthetic strain functions themselves were made more asymmetrical. The open circles in Fig. 2 show for comparison the strain functions computed from the synthetic distortion coefficients. The agreement between the theoretical and 'experimental' curves is seen to be quite good. A remarkable feature is that for cases 2, 3 and 4, each of which contains two Gaussian terms, the ratio of whose exponents is 2, 4 and 8 respectively, a single parameter in the weight function is enough to approximate the theoretical curves quite well. One might expect to improve the agreement by increasing the number of measured orders. By using more orders to determine the strain moments some gain is made in determining the lower orders more accurately. Inspection of Table 3 gives an example of how the ratio of the exact moments to the moments computed from the distortion coefficients varies with the number of orders measured for case 4, the most skew distribution considered. For the case of six orders the lower moments are certainly determined more accurately but the error of the higher moments becomes intolerable. Fig. 3(a) is a comparison of the theoretical and computed distributions for case 4 and shows the effect of error in the higher moments. Fig. 3(b) shows the distribution computed for the same case, that is using six orders, but in which only the first six moments have been used, the expansion having been stopped at the sixth Hermite polynomial. There is a little improvement in the fit in comparison with the three order computation, but not enough to justify the extra experimental effort, in a particular case, of measuring three more orders. The increasing error in the determination of the moments from the set of equations derived by expanding the average cosine and sine terms is of course due to the use of these poorly convergent expansions. For reasonably large arguments of the cosine and sine, that is for large values of h_0 and the ratio L/a, many more terms would be required to represent these functions accurately.

Table 2.

$$P(\varepsilon_L) = \frac{aA^{\frac{1}{2}}}{\pi^{\frac{1}{2}}} \exp\left(-Ae_L^2\right) + \frac{bB^{\frac{1}{2}}}{\pi^{\frac{1}{2}}} \exp\left\{-B\left(e_L - e_L'\right)^2\right\}$$

Case No.	a	A	b	B	e_L'
1	0.3	$6.56 . 10^4$	0.7	$6.56 . 10^4$	0.002
2	0.4	$1.312 . 10^5$	0.6	$6.56 . 10^4$	0.002
3	0.4	$2.624 . 10^5$	0.6	$6.56 . 10^4$	0.002
4	0.4	$5.248 . 10^5$	0.6	$6.56 . 10^4$	0.002

Table 3. *Ratio of exact to computed moments for case* 4

Number of moment	1	2	3	4	5	6	7	8	9	10	11	12
Ratio:												
3 Orders	1.12	1.07	1.68	1.51	5.04	4.14						
6 Orders	1.05	0.98	1.23	1.08	1.83	1.47	3.82	2.84	12.83	8.84	92.9	59.8

Effect of the accuracy of the distortion coefficients

Table 4 shows the inverse matrices for the cosine and sine terms for the case $L/a = 23\cdot8$. The error $\Delta\alpha_{2m}$ in the $2m$th moment is given by

$$\Delta\alpha_{2m} = \sum_{j=1}^{3} a_{mj}^{-1} c_i$$

where c_i is the error in the ith cosine coefficient and the a_{mj}^{-1} are the elements of the inverse matrix. A similar expression is used for the error in the odd moments using the elements of the inverse sine matrix and errors in the sine terms. The tolerable error in the distortion coefficients then depends on the magnitudes of the elements of the inverse matrix which depend in turn on the L/a ratio and the range of h_0 values used in the experiment. For example, assuming that the absolute error in the cosine coefficients for case 4 is 0·01 and that the signs of the errors are so chosen as to give the largest possible error in the even moments, we find for the case of three measured orders

$$\Delta\alpha_2 = 3\cdot7310^{-7} \quad \Delta\alpha_4 = 2\cdot1910^{-11} \quad \Delta\alpha_6 = 6\cdot2410^{-16}$$

where the computed moments were

$$\alpha_2 = 6\cdot8910^{-6} \quad \alpha_4 = 1\cdot4910^{-10} \quad \alpha_6 = 2\cdot7610^{-15}.$$

The percentage errors in the first three even moments due to these errors in the coefficients are then 5·4, 14·6 and 22·6% respectively, which are quite acceptable. All of the distributions discussed above in fact were computed with distortion coefficients themselves first computed to six significant figures and then with the coefficients rounded off to two significant figures. In every case the loss of accuracy with the rounded off values was negligible.

Measurements on cold-worked metals

McKeehan & Warren (1953) studied cold work in thoriated tungsten by an X-ray method and derived a strain distrubtion from measurements of about seven reflexions. From Fig. 4 of their paper, distortion coefficients were estimated for the 200, 400 and 600 reflexions for averaging distances 125 Å and 200 Å respectively. For both cases the coefficients of the 600 reflexions were put equal to zero since the published curves indicate that they are certainly less than 0·01. A_L^D (400) was also put equal to zero for the case of $L = 200$ Å for the same reason. This last case then becomes a rather extreme instance of a measurement being available for only one reflexion combined with very crude approximations for two other lines. Fig. 4 compares the strain distributions computed by the moment method with those of the original paper. Inspection of the inverse cosine matrix showed that for these cases there was not a sensitive dependence of computed moments on distortion coefficients and hence the good agreement of the two methods. An attempt to compute the distribution for the distance 60 Å failed because in this case

it was obvious from the cosine inverse matrix that the values of the coefficients could not be read from the published curve accurately enough to allow computation of an accurate set of moments. Attempts to compute strain distributions from the results of Warren & Averbach (1950) and Wagner (1957) failed for the same reason.
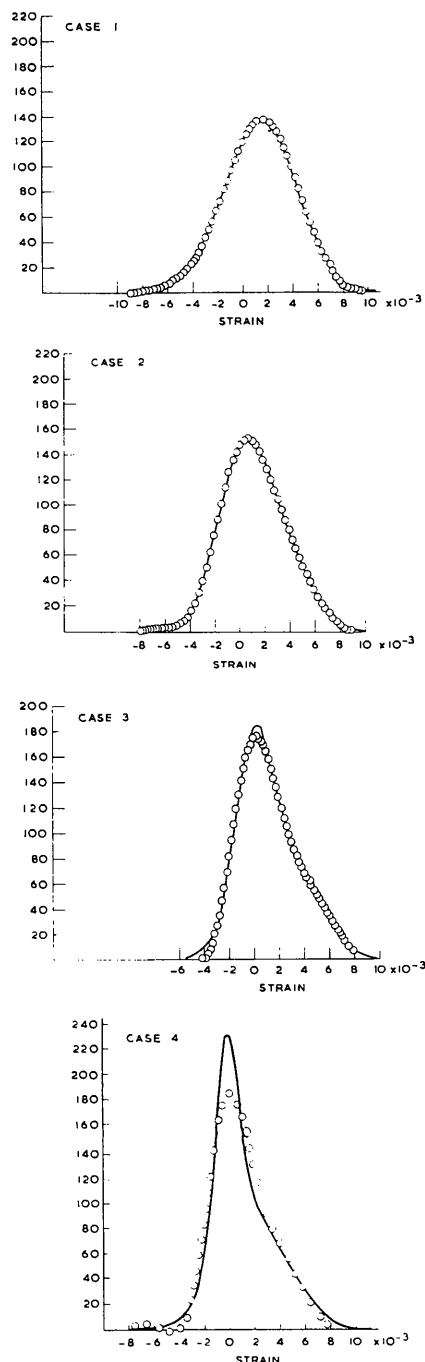

Fig. 2. Shape of the distribution function for cases 1–4. Full lines: theoretical strain functions. Circles: results computed from synthetic distortion coefficients.

Table 4. *Inverse matrices for the case* $L/a = 23\cdot8$

Cosine terms

i / j	1	2	3
1	$3\cdot37 \cdot 10^{-5}$	$-3\cdot37 \cdot 10^{-6}$	$2\cdot49 \cdot 10^{-7}$
2	$1\cdot64 \cdot 10^{-9}$	$-5\cdot05 \cdot 10^{-10}$	$4\cdot21 \cdot 10^{-11}$
3	$4\cdot26 \cdot 10^{-14}$	$-1\cdot70 \cdot 10^{-14}$	$2\cdot84 \cdot 10^{-15}$

Sine terms

i / j	1	2	3
1	$5\cdot03 \cdot 10^{-3}$	$-1\cdot00 \cdot 10^{-3}$	$1\cdot12 \cdot 10^{-4}$
2	$1\cdot22 \cdot 10^{-7}$	$-7\cdot53 \cdot 10^{-8}$	$9\cdot42 \cdot 10^{-9}$
3	$2\cdot11 \cdot 10^{-12}$	$-1\cdot69 \cdot 10^{-12}$	$4\cdot23 \cdot 10^{-13}$
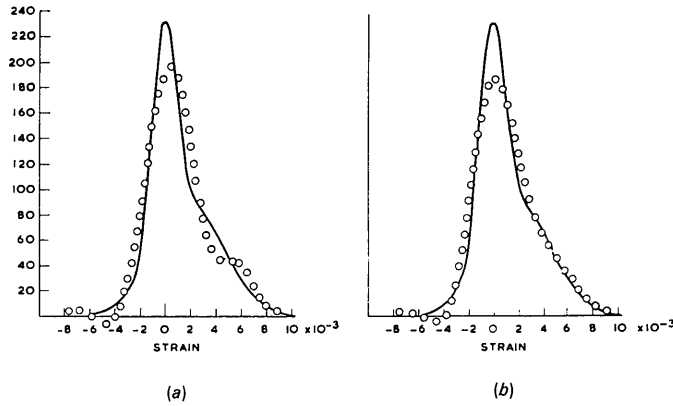
Fig. 3. Comparison of theoretical (full lines) and computed distributions (circles) for case 4. (*a*) 6 orders and 12 polynomials used; (*b*) 6 orders and 6 polynomials used.
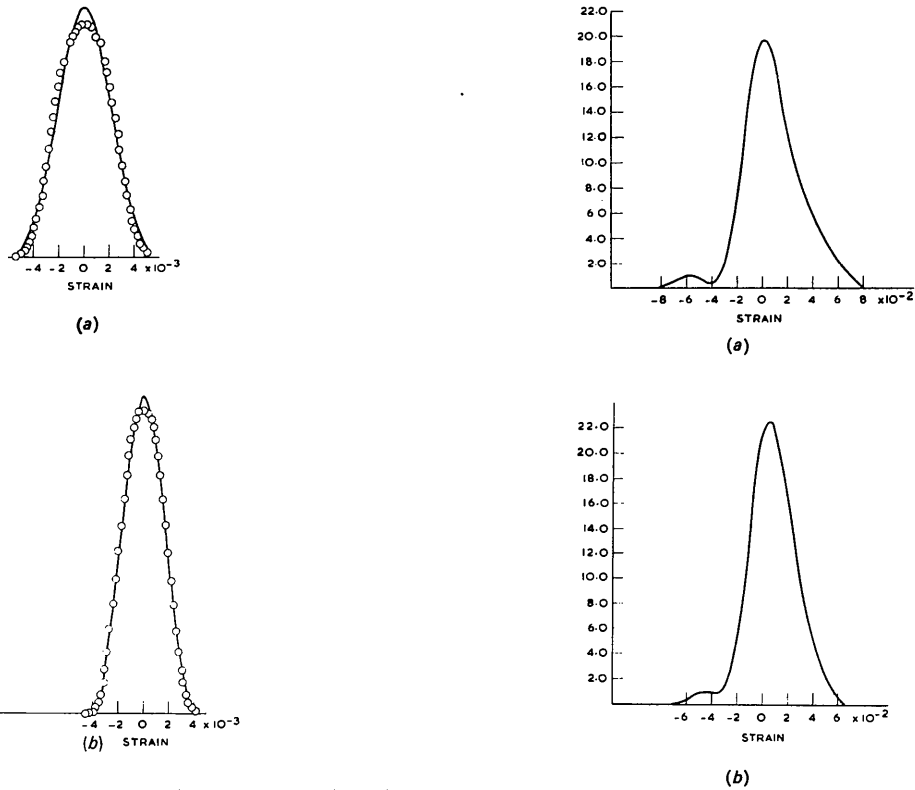
Fig. 4. Full line: strain distribution derived by McKeehan & Warren (1953) for cold-worked thoriated tungsten. Circles: distribution computed by the moment method. (*a*) $L = 125$ Å, (*b*) $L = 200$ Å.

Fig. 5. Strain distribution in reactor-irradiated graphite, obtained by the moment method from Chipman & Warren's (1952) data. (*a*) $L = 20\cdot1$ Å, (*b*) $L = 26\cdot8$ Å.

Measurements on irradiated materials

For the sake of comparing the distributions in cold worked metals with cases in which the strain was introduced by another means two experiments involving neutron damage were treated.

Fig. 5 shows the distributions obtained by the moment method from the experimental data of Chipman & Warren (1952) from the 002, 004 and 006 reflexions from reactor-irradiated graphite. An interesting feature of the distributions is their change in shape for quite a small change in the averaging distance. While the broadening of the base of the curve towards positive strains as the averaging distance is decreased is probably a real effect consistent with a model of islands of interstitial atoms producing an expanded lattice in their vicinity, the small peaks, which could be thought to arise from regions of contracted lattice due to vacancies, are more likely due to errors in the higher moments of the distribution function.

Measurements have been made on the first five $h00$ reflexions from neutron irradiated single-crystal magnesium oxide by T. W. Baker of this laboratory. Fig. 6 shows a comparison of the distributions determined using all reflexions and a Fourier inversion and only three reflexions and the moment method.
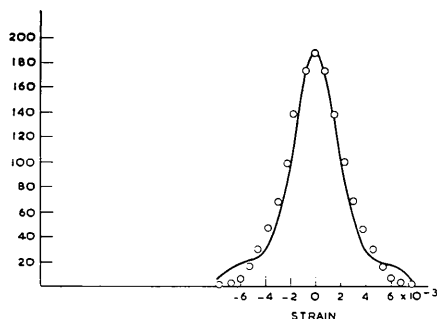

Fig. 6. Strain distribution in neutron-irradiated magnesium oxide, from measurements made by Baker (1964). Full line: distribution computed by the moment method with the use of 3 reflexions. Circles: distribution computed by Fourier inversion of measurements for 5 reflexions.

Conclusions

In conclusion the following remarks may be made concerning the use of this method.

1. When properly chosen measurements are made on three reflexions from a distorted crystal a reasonably accurate strain distribution may be derived.
2. Intermediate steps in the computation enable assessments to be made of the importance of the respective distortion coefficients determined from the measurements and where emphasis should be placed in improving experimental accuracy.
3. Although the method has been illustrated using the Gaussian as an appropriate weight function a suitable choice of the set of orthonormal polynomials permits a wide range of weight functions to be used.

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