ERRORS DUE TO COUNTING STATISTICS IN THE TRIAXIAL STRAIN (STRESS) TENSOR. (U) NORTHWESTERN UNIV EVANSTON IL DEPT OF MATERIALS SCIENCE P RUDNIK ET AL. 01 JUL 85 UNCLASSIFIED TR-18 N00014-80-C-0116
ERRORS DUE TO COUNTING STATISTICS IN THE TRIAXIAL STRAIN
(STRESS) TENSOR DETERMINED BY DIFFRACTION

BY

P. Rudnik and J. B. Cohen
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P. Rudnik and J. B. Cohen

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INTRODUCTION

Knowledge of the errors in a diffraction measurement of residual strains and stresses is useful information, not only in its own right, but also because it permits automation of a measurement to an operator specified precision. There are three sources of these errors:

(1) Instrumental effects, primarily due to sample displacement, separation of the 0 and 2θ axes of the diffractometer, and beam divergence. All three can be estimated, or minimized by employing parallel beam geometry.

(2) Uncertainties in x-ray elastic constants, which can now be evaluated.

(3) Errors in the diffraction peak position related to counting statistics. Equations to evaluate this source have been developed in Ref. 1 for the case of a stress state for which all \( \sigma_{ij} \) \( (i = 1,2,3) = 0 \), with the direction "3" normal to the sample surface, see Fig. 1. This means that the stresses lie only in the surface, e.g., a biaxial stress state \( \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix} \). There are, however, numerous situations when the normal components are appreciable in an x-ray measurement and this is generally the case for neutron diffraction because with neutrons the beam can sample a sizeable volume, at a significant depth below the surface.
FIG. 1: The axial system. Strains are measured with diffraction by measuring the change in spacing of planes normal to the $L_2$ direction. (The axes $P_i$ define the specimen surface.)

TABLE I: STRESS TENSORS (AND STANDARD DEVIATIONS) FOR SPECIMEN C3, REF. 5

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* values given in MPa; $V(d_o)^2 = 0.00016$ A

REFERENCE 5
is the purpose of this paper to derive equations to evaluate the counting statistical error for the entire three dimensional strain (or stress) tensor, 

\[
\begin{bmatrix}
    a_{11} & a_{12} & a_{13} \\
    a_{21} & a_{22} & a_{23} \\
    a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

**BASIC EQUATIONS**

We begin with the general equation for the strains \( \epsilon_{ij} \) and how these affect the interplanar spacing "d". (Refer to Fig. 1 for the axial system.) The measurement is made in the \( \phi \) direction, with a sample tilted \( \phi \) from the normal position (which is with the surface normal bisecting incident and scattered beams). Primed quantities refer to strains in the \( L \) co-ordinate system, unprimed terms are in the \( P \) system.

\[
\langle \epsilon_{11} \rangle_{\phi} = \left( \frac{d_{\phi+} - d_{\phi-}}{2d_{\phi}} \right) = \left[ \langle \epsilon_{11} \rangle \cos^2 \phi + \langle \epsilon_{22} \rangle \sin^2 \phi + \langle \epsilon_{23} \rangle \sin \phi \cos \phi \right]
\]

\[
-\langle \epsilon_{22} \rangle \sin^2 \phi + \langle \epsilon_{23} \rangle + \left[ \langle \epsilon_{11} \rangle \cos \phi + \langle \epsilon_{23} \rangle \sin \phi \right] \sin 2\phi
\]

(1)

Note that the stress-free spacing, \( d_{\phi} \), is involved. While this term can be eliminated for a biaxial stress state, this is not possible for a general strain or stress tensor, and the reader may consult Ref. 8 for a discussion of problems associated with the measurement of this quantity. When \( \epsilon_{23} \) or \( \epsilon_{13} \neq 0 \), \( e_{11} \) is not linear with \( \sin^2 \phi \) and has different curvature for \( \phi \) and \( -\phi \). The carats imply that the strain values are averaged over the depth of penetration of the incident x-ray (neutron) beam and this is to be understood in what follows, as this additional notation is eliminated below.

Next, we define terms which involve measurements of \( d_{\phi,\phi} \) at plus and minus \( \phi \) tilts of the surface normal.\(^5\)

\[
\epsilon_1 \equiv 1/2[\epsilon_{\phi+} + \epsilon_{\phi-}] = \left( \frac{d_{\phi+} - d_{\phi-}}{2d_{\phi}} \right) \sin \phi
\]

\[
= \epsilon_{11} \cos \phi + \epsilon_{22} \sin \phi \cos \phi + \epsilon_{23} \sin \phi \sin \phi
\]

(2a)

Clearly, \( \epsilon_1 \) should be linear with \( \sin \phi \) and \( \epsilon_{11} \) is the intercept, regardless of \( \phi \).

\[
\epsilon_2 \equiv 1/2[\epsilon_{\phi+} - \epsilon_{\phi-}] = (d_{\phi+} - d_{\phi-})/2d_{\phi}
\]

\[
= [\epsilon_{11} \cos \phi + \epsilon_{22} \sin \phi] \sin |2\phi|. \quad (2b)
\]
Therefore, $a_e$ is linear vs. $\sin|2\phi|$.

Let:

\[
\begin{align*}
    a &= da_e/d\sin^2 \phi, \\
    a_e &= da_e/d\sin|2\phi|
\end{align*}
\]  

(3a)  

(3b)

Then, at: $\phi = 0^\circ$, $a_e = e_{11} - e_{22}$,  

$\phi = 90^\circ$, $a_e = e_{22} - e_{33}$,  

$\phi = 45^\circ$, $a_e = 1/2(e_{11} + e_{22}) + e_{12} - e_{33}$,  

$= e_{12} + 1/2(e_{11} + e_{22})$.

(3c)

and similarly:

at $\phi = 0^\circ$: $a_e = e_{11}$, 

at $\phi = 90^\circ$: $a_e = e_{22}$.

(3d)

Knowledge of the strain tensor permits the calculation of the stress components ($\sigma_{ij}$) from:

\[
\sigma_{ij} = [1/2S_{\nu}(hkl)]^{-1} \{\delta_{ij} - \delta_{ij}[S_{\nu}(hkl)/[3S_{\nu}(hkl)]} + 1/2S_{\nu}(hkl))] \cdot [e_{11} + e_{22} + e_{33}].
\]

(4)

Here, $\delta_{ij}$ is the Kronecker delta function and $S_{\nu}$ and $1/2S_{\nu}$ are the x-ray elastic constants which depend on the indices of the diffraction peak, hkl. (For an isotropic solid these values are $-\nu/E$ and $(1 + \nu)/E$ respectively.)

**VARIANCES DUE TO COUNTING STATISTICS**

For a function $X = f(x_1, x_2, x_3, \ldots)$, assuming the $x_n$ are independent, the variance ($\nu$) is:

\[
\nu(X) = (\frac{dx}{dx_1})^2 \nu(x_1) + (\frac{dx}{dx_2})^2 \nu(x_2) + (\frac{dx}{dx_3})^2 \nu(x_3) + \ldots
\]

(5)

For the straight line, $y = mx + b$, the slope and intercept is given by:

\[
\begin{align*}
    m &= \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} \\
    b &= (\bar{y} - m\bar{x})/N
\end{align*}
\]

(6a)  

(6b)

where $N$ is the number of data points.
Employing Eq. (5):

\[
V(m) = \left[ \frac{\sum \left( y_i - \bar{y} \right)^2}{\sum (x_i - \bar{x})^2} \right] V(x) + \left[ \frac{\sum \left( x_i - \bar{x} \right)^2}{\sum (x_i - \bar{x})^2} \right] V(y)
\]

Therefore:

\[
V(b) = \frac{\sum (x_i - \bar{x})^2}{N} \cdot V(m) = \frac{\sum (x_i - \bar{x})^2}{N} \cdot \frac{\sum (y_i - \bar{y})^2}{\sum (x_i - \bar{x})^2} \cdot V(x)
\]

\[
+ \left[ \frac{\sum (x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right] V(y)
\]

Therefore; in terms of \( a \) vs. \( \sin^2 \phi \):

\[
V(a_i) = \left[ \frac{\sum \left( a_i - \bar{a} \right)^2}{\sum (\sin^2 \phi_i - \sin^2 \phi)^2} \right] V(\sin^2 \phi) + \left[ \frac{\sum \left( \sin^2 \phi_i - \sin^2 \phi \right)^2}{\sum (\sin^2 \phi_i - \sin^2 \phi)^2} \right] V(a_i)
\]

The variance in \( \phi \) is negligible, so the first term can be ignored.

Also, from Eq. (2a):

\[
V(a_i) = \left[ \frac{\sum \left( d_i - \bar{d} \right)^2}{d(d_{\phi^+})} \right]^2 V(d_{\phi^+}) + \left[ \frac{\sum \left( d_i - \bar{d} \right)^2}{d(d_{\phi^-})} \right]^2 V(d_{\phi^-}) + \left[ \frac{\sum \left( d_i - \bar{d} \right)^2}{d(d_{\phi^-})} \right]^2 V(d_{\phi^-})
\]

Writing Bragg's law in the form \( d = \frac{\lambda}{2 \sin \theta} \), adopting the convention that \( \theta^+, \theta^- \) are the \( \theta \) values (in degrees) for the peaks at \( +\phi \), \( -\phi \) respectively, and employing Eq. (5):

\[
V(d_{\phi^+}) = \frac{\lambda}{180} \left( \frac{\cos \theta^+/2 \sin \theta^+}{\sin \theta^+} \right)^2 V(2\theta^+)/2
\]

and similarly for \( V(d_{\phi^-}) \). Recalling Eq. (2a):

\[
\left[ \frac{d\theta}{d(d_{\phi^+})} \right]^2 = \left[ \frac{d\theta}{d(d_{\phi^-})} \right]^2 = \frac{1}{4\omega^2}
\]
Thus, we may rewrite Eq. (7):

\[
V(A,\theta) = \left[ \frac{\Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)}{\Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)^2} \right]^{2} \cdot \frac{1}{4d_{0}^{4}} \left\{ \left( \frac{x}{180} \right)^{2} \frac{\lambda^{2}}{8} \left[ \frac{(\cos^{2}\theta)}{\sin^{2}\theta} \right] \right\} V_{1}(2\theta) + \left( \cos^{2}\theta \right) V_{1}(2\theta) \]

(11)

In a similar manner for \( a_{2} \) vs. \( \sin|2\phi| \), where \( a_{2} \equiv (d_{\phi_2} - d_{\phi_1})/2d_{0} = d'_{-}/2d_{0} \):

\[
V(A_{2}) = \left[ \frac{\Sigma(\sin|2\phi_1| - \sin|2\phi_2|)}{\Sigma(\sin|2\phi_1| - \sin|2\phi_2|)^2} \right]^{2} \cdot \frac{1}{4d_{0}^{4}} \left\{ \left( \frac{x}{180} \right)^{2} \frac{\lambda^{2}}{8} \left[ \frac{(\cos^{2}\theta)}{\sin^{2}\theta} \right] \right\} V_{1}(2\theta) + \left( \cos^{2}\theta \right) V_{1}(2\theta) \]

(12)

We now propagate these values into the strain and stress tensors.

**THE STRAIN TENSOR**

Abbreviating the intercept of \( a_{1} \) vs. \( \sin^{2}\phi \) as \( I \), then at any \( \theta \):

\[
\epsilon_{33} = I \quad \text{(of } a_{1} \text{ vs. } \sin^{2}\phi \text{)}, \quad \text{(13a)}
\]

\[
V(\epsilon_{33}) = V(A_{1}) + V(I) \quad \text{(13b)}
\]

\[
V(I) = \frac{\Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)^2}{\Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)^2} \cdot \frac{\Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)^2}{\Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)^2} V(a_{1}) \]

\[
= \frac{1}{\Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)^2} \Sigma(\sin^{2}\phi_1 - \sin^{2}\phi_2)^2 V(a_{1}) \quad \text{(13c)}
\]

Now, from Eqs. (3c), at \( \theta = 0^\circ \):

\[
\epsilon_A = \epsilon_{11} - \epsilon_{33} = \epsilon_{11} - I, \quad \text{(14)}
\]

\[
V(\epsilon_{11}) = 2V(\epsilon_{12}) + V(I).
\]

Similarly, for \( \theta = 90^\circ \):
\[ e_{11} = s \varepsilon_1 + I, \]
\[ V(e_{11}) = V(s \varepsilon_1) + V(\varepsilon_1) + V(I), \] (15)

and for \( \phi = 45^\circ \):

\[ e_{12} = s \varepsilon_2 + e_{33} - 0.5 (e_{11} + e_{22}) \]
\[ + e_{33} - 0.5 (s \varepsilon_3 + s \varepsilon_3), \]
\[ V(e_{12}) = V(s \varepsilon_3) + 0.25 [V(\varepsilon_1) + V(\varepsilon_1)]. \] (16)

From Eqs. (3d):

\[ V(e_{12}) = V(s \varepsilon_3), \] (17)

\[ V(e_{23}) = V(s \varepsilon_3). \] (18)

**THE STRESS TENSOR**

We define \( Q = s/(3s + 1/2s_1) \) (which is \([-s/2-s] \) for an isotropic solid). Then Eq. (4) may be written, for the diagonal stress components, as:

\[ \sigma_{ij} = (1/2s_1)^{-1} [(1-Q)e_{ii} - Qe_{kk} - Qe_{jj}]. \] (19)

Here \( i = 1,2,3; \ j = 2,3,1; k = 3,1,2. \)

From Eq. (19):

\[ V(\sigma_{11})^{1/2} = (1/2s_1)^{-1} \{ (1-Q)2V(\varepsilon_{11}) + Q^2[V(\varepsilon_{kk}) + V(\varepsilon_{jj})]\}^{1/2}. \] (20)

Therefore, with Eqs. (13-15):

\[ V(\sigma_{11})^{1/2} = (1/2s_1)^{-1} \{ (1-Q)^2V(\varepsilon_{11}) + Q^4[V(\varepsilon_{kk}) + V(\varepsilon_{jj})]\}^{1/2}, \] (21)

\[ V(\sigma_{22})^{1/2} = (1/2s_1)^{-1} \{ (1-Q)^2V(\varepsilon_{22}) + (1-2Q + Q^2)V(\varepsilon_{11})\}^{1/2}, \] (22)

\[ V(\sigma_{33})^{1/2} = (1/2s_1)^{-1} \{ (1-Q)^2V(\varepsilon_{33}) + Q^4[V(\varepsilon_{kk}) + V(\varepsilon_{jj})]\}^{1/2}, \] (23)
Similarly:

\[ V(\sigma_{z_2})^{\frac{1}{2}} = (1/2S_2)^{-1} \left[ V(\sigma_{x_2}) + 0.25 \left[ V(\sigma_{\phi_1}) + V(\sigma_{x_1}) \right] \right]^{\frac{1}{2}}, \]  
\[ (24) \]

\[ V(\sigma_{y_2})^{\frac{1}{2}} = (1/2S_2)^{-1} V(\sigma_{x_2})^{\frac{1}{2}}, \]  
\[ (25) \]

\[ V(\sigma_{z_2}) = (1-2S_2)^{-1} V(\sigma_{x_2})^{\frac{1}{2}}. \]  
\[ (26) \]

EXAMPLES

To illustrate the typical magnitudes of the errors due to counting statistics, we employed data from Ref. 5, for a ground steel specimen, that is we used the peak positions and the variances in these positions with Eq. (9). [Formulae to calculate the variance for the parabolic fit employed in Ref. 5 are given in Ref. 1; for other types of fits the appropriate equation may be substituted.] The resultant errors are given in Tables I-III. For the first two tables it was assumed that the error in \( d_\phi \) was the actual measured value. If there is no preferred orientation, the intensity of the peak changes little with the \( \phi \)-tilt. In this case, Tables I and II show the effect of the uncertainty in \( d_\phi \); reducing this error all the stress components by the same proportion, except \( \sigma_{z_2}, \sigma_{x_2}, \) which remain relatively unaffected, because the role of the error in \( d_\phi \) is damped by \((d_\phi)^2\) in Eq. (12).

If there is preferred orientation, the peak intensity can vary greatly with \( \phi \) and there will be large variances contributing to \( V(x_2) \) from weak peaks. This was minimized in the following way. The average variance, \( \sigma_1 \), in the \( 2\theta \) peak position for \( \pm \phi \) and \( -\phi \) was obtained and the weighting factor \( c_1 \) was formed:

\[ c_1 = (1/\sigma_1) / \frac{1}{1} (1/\sigma_1) \]  
\[ (27) \]

The Eqs. 11 and 12 were then altered to multiply \( V(2\theta^+) \), \( V(2\theta^-) \) terms by this weighting for Table III. There is only a small difference (between Tables II and III) because of the lack of texture in the specimen; the peak intensity changed only by about 8 pct with \( \phi \). With more severe preferred orientation the effect will be larger.

CONCLUDING REMARKS

There are now adequate equations for calculating errors in stress.
### TABLE II: STRESS TENSOR AND STANDARD DEVIATIONS WHEN $V(d_0) = 0.00004$ A *

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<td>565.37 (42.51)</td>
<td>0.76 (3.89) 88.18 (34.67)</td>
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*Values given in MPa

### TABLE III: WEIGHTED STRESS TENSOR AND STANDARD DEVIATIONS *

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<tr>
<td>536.24 (48.56)</td>
<td>-24.62 (24.56) -38.33 (4.59)</td>
</tr>
<tr>
<td>554.65 (47.60)</td>
<td>2.90 (3.65) 80.68 (39.22)</td>
</tr>
</tbody>
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<tr>
<th>Data Set 2</th>
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<tr>
<td>520.29 (41.84)</td>
<td>-6.04 (20.11) -34.82 (3.55)</td>
</tr>
<tr>
<td>560.22 (40.60)</td>
<td>1.56 (2.73) 85.29 (33.76)</td>
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<table>
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<tbody>
<tr>
<td>532.56 (48.15)</td>
<td>-7.90 (24.93) -39.66 (5.81)</td>
</tr>
<tr>
<td>549.83 (47.16)</td>
<td>-2.81 (4.57) 82.21 (39.16)</td>
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<td>539.23 (42.88)</td>
<td>-31.22 (21.23) -38.28 (3.85)</td>
</tr>
<tr>
<td>565.17 (42.65)</td>
<td>-0.59 (3.94) 88.98 (34.68)</td>
</tr>
</tbody>
</table>

* $V(d_0) = 0.00004$ A; values given in MPa
measurements due to instrumental effects, counting statistics and in the x-ray elastic constants. We would like to conclude this paper with a plea to the community making stress measurements via diffraction to regularly report these errors with their data. It is all too common for investigators to repeat a measurement (of stress or an elastic constant) once and to use the difference as an error estimate. Another practice is to dust a stress-free powder on the specimen surface and to use a (single) measurement of the stresses measured with this powder as an error estimate. Finally, some report an error in a slope vs. sin²φ obtained by least-squares, but ignore the uncertainty in each point in this plot in estimating errors. None of these procedures is particularly satisfying in a statistical sense. Of course, if time permits, the average of, say, ten repetitions of a measurement is the best of all error estimates. If this cannot be done, error estimates from the available equations are far more satisfactory than the currently all-too-common procedures.

ACKNOWLEDGEMENTS

This research was supported by ONR under contract No. N00014-80-C116. We thank Dr. I. C. Noyan for his advice.

REFERENCES

3. **Report Title**

ERRORS DUE TO COUNTING STATISTICS IN THE TRIAXIAL STRAIN (STRESS) TENSOR DETERMINED BY DIFFRACTION

4. **Technical Notes**

TECHNICAL REPORT # 18

5. **Authors** (First name, middle initial, last name)

P. Rudnik
Jerome B. Cohen

6. **Report Date**

July 1, 1985

7. **Contract or Grant No.**

N00014-80-C-116

8. **Originator's Report Number(s)**

18

9. **Distribution Statement**

Distribution of document is unlimited

11. **Abstract**

The errors are derived for the diffraction measurement of the three dimensional stress and strain tensor due to counting statistics.
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<td>Residual stresses</td>
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<tr>
<td>Errors in residual stresses</td>
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<td>Counting statistical errors in stresses</td>
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