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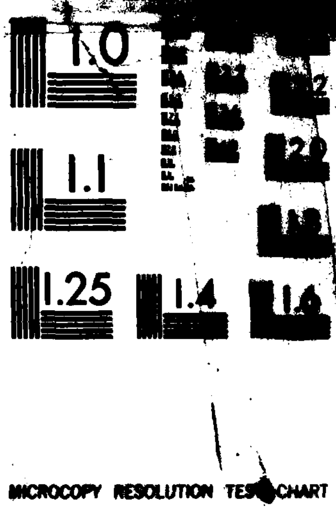
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ERRORS DUE TO COUNTING STATISTICS IN THE TRIAXIAL STRAIN (STRESS) TENSOR DETERMINED BY DIFFRACTION

BY

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

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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.[1] There are three sources of these errors:

(1) Instrumental effects, primarily due to sample displacement, separation of the θ and 2θ axes of the diffractometer, and beam divergence. All three can be estimated[2], or minimized by employing parallel beam geometry.[3]

(2) Uncertainties in x-ray elastic constants, which can now be evaluated.[4]

and (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 σ_{i3} ($i = 1,2,3$) = 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 $\begin{vmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{vmatrix}$. There are, however, numerous situations when the normal components are appreciable in an x-ray measurement[5,6] 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[7]. It

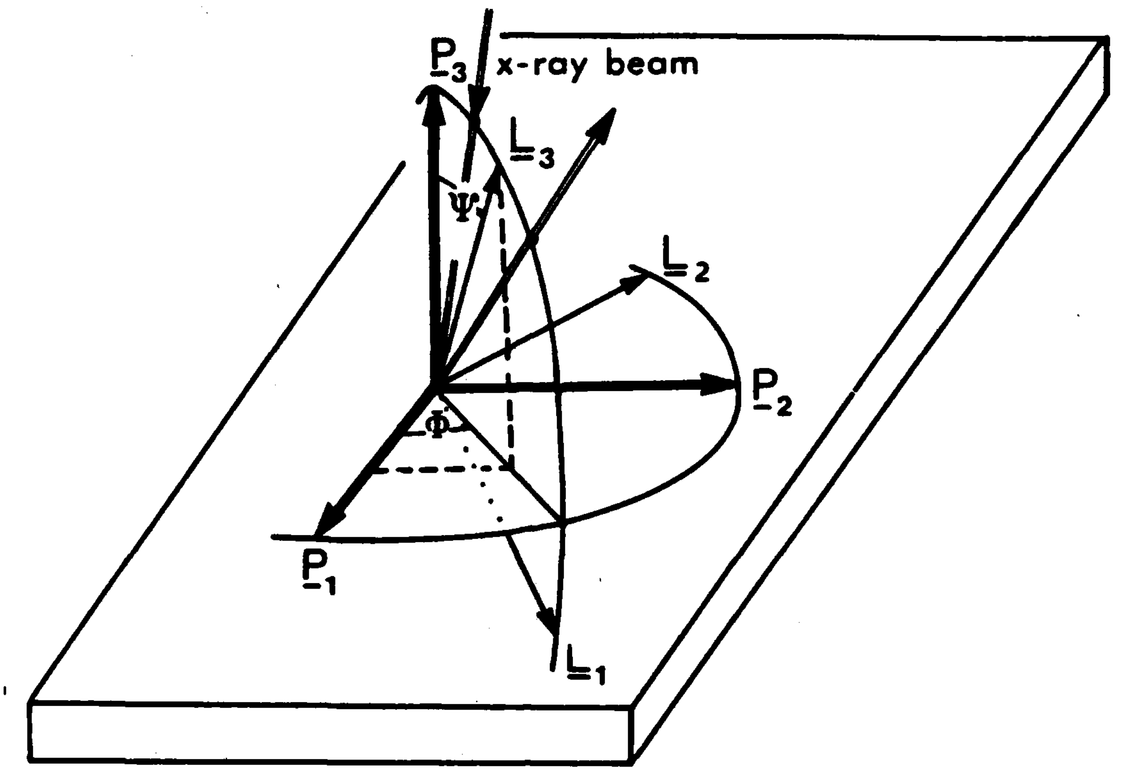

FIG. 1: The axial system. Strains are measured with diffraction by measuring the change in spacing of planes normal to the L_3 direction. (The axes P_i define the specimen surface.)

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

		DATA SET 1			
537.62	(161.94)	-24.03	(78.81)	-39.15	(4.58)
		550.04	(161.66)	2.31	(3.56)
				78.29	(130.57)
		DATA SET 2			
520.60	(137.25)	-4.03	(66.60)	-34.17	(3.21)
		555.19	(137.03)	0.11	(2.69)
				82.20	(110.67)
		DATA SET 3			
535.03	(158.28)	-20.13	(77.06)	-40.19	(5.72)
		555.98	(157.99)	-0.98	(4.56)
				86.66	(127.69)
		DATA SET 4			
538.53	(146.23)	-30.63	(70.95)	-38.03	(3.83)
		565.37	(146.14)	0.76	(3.89)
				88.18	(117.92)

AVERAGE			REFERENCE 5		
532.95	-19.69	-37.89	541	-20	-38
	556.65	0.55		565	1
		83.83			86

* values given in MPa; $V(d_0)^{\frac{1}{2}} = 0.00016$ Å

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

$$\begin{vmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{vmatrix}.$$

BASIC EQUATIONS

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

$$\langle\varepsilon'_{33}\rangle_{\phi\psi} = (d_{\phi\psi} - d_0)/d_0 = [\langle\varepsilon_{11}\rangle \cos^2\phi + \langle\varepsilon_{22}\rangle \sin^2\phi + \langle\varepsilon_{12}\rangle \sin 2\phi$$

$$-\langle\varepsilon_{33}\rangle] \sin^2\psi + \langle\varepsilon_{33}\rangle + [\langle\varepsilon_{13}\rangle \cos\phi + \langle\varepsilon_{23}\rangle \sin\phi]\sin 2\psi \qquad (1)$$

Note that the stress-free spacing, d_0, 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 ε_{23} or $\varepsilon_{13} \neq 0$, ε'_{33} is not linear with $\sin^2\psi$ and has different curvature for $+\psi$ and $-\psi$. 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 $d_{\phi,\psi}$ at plus and minus ψ tilts of the surface normal.[5]

$$a_1 \equiv 1/2[\varepsilon'_{\phi\psi+} + \varepsilon'_{\phi\psi-}] = \{d_{\phi\psi+} + d_{\phi\psi-})/2d_0\}-1$$

$$= \varepsilon_{33} + [\varepsilon_{11} \cos^2\phi + \varepsilon_{22} \sin^2\phi + \varepsilon_{12} \sin 2\phi - \varepsilon_{33}])\sin^2\psi \qquad (2a)$$

Clearly, a_1, should be linear with $\sin^2\psi$ and ε_{33} is the intercept, regardless of ϕ.

$$a_2 \equiv 1/2[\varepsilon_{\phi\psi+} - \varepsilon_{\phi\psi-}] = (d_{\phi\psi+} - d_{\phi,\psi-})/2d_0$$

$$= [\varepsilon_{13} \cos\phi + \varepsilon_{23} \sin\phi]\sin|2\psi|. \qquad (2b)$$

Therefore, a_2 is linear vs. $\sin|2\psi|$.

Let:

$$\ell_1 = da_1/d\sin^2\psi, \tag{3a}$$

$$\ell_2 = da_2/d\sin|2\psi| \tag{3b}$$

Then, at: $\phi = 0°,\ {}_0\ell_1 = \varepsilon_{11} - \varepsilon_{33}$,

$\phi = 90°,\ {}_{90}\ell_1 = \varepsilon_{22} - \varepsilon_{33}$,

$$\phi = 45°,\ {}_{45}\ell_1 = 1/2(\varepsilon_{11} + \varepsilon_{22}) + \varepsilon_{12} - \varepsilon_{33}, \quad = \varepsilon_{12} + 1/2({}_0\ell_1 + {}_{90}\ell_1). \tag{3c}$$

and similarly:

at $\phi = 0°$: ${}_0\ell_2 = \varepsilon_{13}$,

$$\text{at } \phi = 90°: {}_{90}\ell_2 = \varepsilon_{23}. \tag{3d}$$

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

$$\sigma_{ij} = [1/2S_2(hk\ell)]^{-1}\{\varepsilon_{ij} - \delta_{ij}\{S_1(hk\ell)/[3S_1(hk\ell) + 1/2S_2(hk\ell)]\}\cdot[\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}]\}. \tag{4}$$

Here, δ_{ij} is the Kronecker delta function and S_1 and $1/2S_2$ are the x-ray elastic constants which depend on the indices of the diffraction peak, $hk\ell$. (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 (V) is[9]:

$$V(X) = \left(\frac{dX}{dx_1}\right)^2 V(x_1) + \left(\frac{dX}{dx_2}\right)^2 V(x_2) + \left(\frac{dX}{dx_3}\right)^2 V(x_3) + \ldots \tag{5}$$

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

$$m = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} \tag{6a}$$

$$b = (\Sigma y_i - m\Sigma x_i)/N \tag{6b}$$

where N is the number of data points.

Employing Eq. (5):

$$V(m) = \left[\frac{\sum_i (y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2}\right]^2 V(x) + \left[\frac{\sum_i (x_i - \bar{x})}{\sum_i (x_i - \bar{x})^2}\right]^2 V(y) \tag{6c}$$

Therefore:

$$V(b) = \frac{\Sigma(x_i - \bar{x})^2}{N} \cdot V(m) = \frac{\Sigma(x_i - \bar{x})^2}{N} \cdot \left\{ \left[\frac{\Sigma(y_i - \bar{y})}{\Sigma(x_i - \bar{x})^2}\right]^2 V(x) + \left[\frac{\sum_i (x_i - \bar{x})}{\Sigma(x_i - \bar{x})^2}\right]^2 V(y)\right\} \tag{6d}$$

Therefore; in terms of a_1 vs. $\sin^2\phi$:

$$V(\ell_1) = \left[\frac{\sum_i (a_{1\,i} - \bar{a}_1)}{\sum_i (\sin^2\phi_i - \overline{\sin^2\phi})^2}\right]^2 V(\sin^2\phi) + \left[\frac{\sum_i(\sin^2\phi_i - \overline{\sin^2\phi})}{\sum_i(\sin^2\phi_i - \overline{\sin^2\phi})^2}\right]^2 V(a_1) \tag{7}$$

The variance in ϕ is negligible, so the first term can be ignored.

Also, from Eq. (2a):

$$V(a_1) = \left[\frac{da_1}{d(d_{\theta\phi+})}\right]^2 V(d_{\theta\phi+}) + \left[\frac{da_1}{d(d_{\theta\phi-})}\right]^2 V(d_{\theta\phi-}) + \left[\frac{da_1}{d(d_0)}\right]^2 V(d_0) \tag{8}$$

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

$$V(d_{\theta,\phi+}) = (\pi/180)^2 (\lambda\cos\theta^+/2\sin^2\theta^+)^2 \; V(2\theta^+)/2 \tag{9}$$

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

$$\left[\frac{da_1}{d(d_{\theta\phi+})}\right]^2 = \left[\frac{da_1}{d(d_{\theta\phi-})}\right]^2 = \frac{1}{4d_0^{\,2}}, \tag{10a}$$

$$-\frac{da_1}{d(d_0)} = \frac{[d_{\phi\psi+} + d_{\phi\psi-}]^2}{4d_0^4} = d_+^2/4d_0^4. \quad (10b)$$

Thus, we may rewrite Eq. (7):

$$V(\ell_1) = \left[\frac{\sum_i(\sin^2\psi_i - \overline{\sin^2\psi})}{\sum_i(\sin^2\psi_i - \overline{\sin^2\psi})^2}\right]^2 \frac{1}{4d_0^2}\{(\pi/180)^2 \frac{\lambda^2}{8}[(\frac{\cos\theta^2}{\sin^2\theta^+})^2 V_i(2\theta^+)$$

$$+ (\frac{\cos\theta^-}{\sin^2\theta^-})^2 V_i(2\theta^-)] + (d_+^2/d_0^2)V(d_0)\} \quad (11)$$

In a similar manner for a_2 vs. $\sin|2\psi|$, where $a_2 \equiv (d_{\phi\psi-} - d_{\phi\psi-})/2d_0 = ^{d-}/2d_0$:

$$V(\ell_2) = \left[\frac{\sum_i \sin|2\psi_i| - \overline{\sin|2\psi|})}{\sum_i(\sin|2\psi_i| - \sin|2\psi|)^2}\right]^2 \frac{1}{4d_0^2}\{(\frac{\pi}{180})^2(\frac{\lambda^2}{8})[(\frac{\cos\theta^+}{\sin^2\theta^+})^2 V_i(2\theta^+)$$

$$+ (\frac{\cos\theta^-}{\sin^2\theta^-})^2 V_i(2\theta^-)] + (d_-^2/d_0^2)\ V(d_0)\} \quad (12)$$

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

THE STRAIN TENSOR

Abbreviating the intercept of a_1 vs. $\sin^2\psi$ as I, then at any ϕ:

$$\varepsilon_{33} = I \text{ (of } a_1 \text{ vs. } \sin^2\psi), \quad (13a)$$

$$V(\varepsilon_{33}) = V(\ell_1) + V(I) \quad (13b)$$

$$V(I) = \frac{\Sigma(\sin^2\psi_i - \overline{\sin^2\psi})^2}{N} \cdot \left[\frac{\Sigma(\sin^2\psi_i - \overline{\sin^2\psi})}{\Sigma(\sin^2\psi_i - \overline{\sin^2\psi})^2}\right]^2 V(a_{1\,i})$$

$$= \frac{1}{N}\ \frac{[\Sigma(\sin^2\psi_i - \overline{\sin^2\psi})]^2}{\Sigma(\sin^2\psi_i - \sin^2\psi)^2}\ V(a_{1\,i}) \quad (13c)$$

Now, from Eqs. (3c), at $\phi = 0°$:

$$_0\ell_1 = \varepsilon_{11} - \varepsilon_{33} = \varepsilon_{11} - I, \quad (14)$$

$$V(\varepsilon_{11}) = 2V(_0\ell_1) + V(I).$$

Similarly, for $\phi = 90°$:

$$\varepsilon_{22} = {}_{90}\ell_1 + I,$$

$$V(\varepsilon_{22}) = V({}_{90}\ell_1) + V({}_{0}\ell_1) + V(I), \tag{15}$$

and for $\phi = 45°$:

$$\varepsilon_{12} = {}_{45}\ell_1 + \varepsilon_{33} - 0.5\,(\varepsilon_{11} + \varepsilon_{22})$$
$$+ {}_{45}\ {}_{1} - 0.5\,({}_{0}\ell_1 + {}_{90}\ell_1),$$
$$V(\varepsilon_{12}) = V({}_{45}\ell_1) + 0.25\,[V({}_{0}\ell_1) + V({}_{90}\ell_1)]. \tag{16}$$

From Eqs. (3d):

$$V(\varepsilon_{12}) = V({}_{0}\ell_2), \tag{17}$$

$$V(\varepsilon_{23}) = V({}_{90}\ell_2). \tag{18}$$

THE STRESS TENSOR

We define $Q = S_1/(3S_1 + 1/2S_2)$ (which is $[^{-\nu}/1\text{-}2\nu]$ for an isotropic solid). Then Eq. (4) may be written, for the diagonal stress components, as:

$$\sigma_{ij} = (1/2S_2)^{-1}[(1-Q)\varepsilon_{ii} - Q\varepsilon_{kk} - Q\varepsilon_{jj}]. \tag{19}$$

Here $i = 1,2,3$; $j = 2,3,1$; $k = 3,1,2$.

From Eq. (19):

$$V(\sigma_{ii})^{\frac{1}{2}} = (1/2S_2)^{-1}\,\{(1-Q)^2 V(\varepsilon_{ii}) + Q^2[V(\varepsilon_{kk}) + V(\varepsilon_{jj})]\}^{\frac{1}{2}}. \tag{20}$$

Therefore, with Eqs. (13-15):

$$V(\sigma_{11})^{\frac{1}{2}} = (1/2S_2)^{-1}\,\{(2-4Q + 4Q^2)V({}_{0}\ell_1) + Q^2 V({}_{90}\ell_1)$$
$$+ (1-2Q + 3Q^2\ V(I)\}^{\frac{1}{2}}, \tag{21}$$

$$V(\sigma_{22})^{\frac{1}{2}} = (1/2S_2)^{-1}\,\{(1-2Q + 4Q^2)V({}_{0}\ell_1) + (1-2Q + Q^2)V({}_{90}\ell_1)$$
$$+ (1-2Q + 3Q^2)V(I)\}^{\frac{1}{2}}, \tag{22}$$

$$V(\sigma_{33})^{\frac{1}{2}} = (1/2S_2)^{-1}\{(1-2Q + 4Q^2)V({}_{0}\ell_1) + Q^2 V({}_{90}\ell_1)$$
$$+ (1-2Q + 3Q^2)V(I)\}^{\frac{1}{2}} \tag{23}$$

Similarly:

$$V(\sigma_{12})^{\frac{1}{2}} = (1/2S_2)^{-1}[V(_{45}\ell_1) + 0.25\,[V(_0\ell_1) + V(_{90}\ell_1)]^{\frac{1}{2}}, \tag{24}$$

$$V(\sigma_{13})^{\frac{1}{2}} = (1/2S_2)^{-1}V(_0\ell_2)^{\frac{1}{2}}, \tag{25}$$

$$V(\sigma_{23}) = (1-2S_2)^{-1}V(_{90}\ell_2)^{\frac{1}{2}}. \tag{26}$$

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 this 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 $d_{\phi,\psi}$ was the actual measured value. If there is no preferred orientation, the intensity of the peak changes little with the ψ-tilt. In this case, Tables I and II show the effect of the uncertainty in d_0; reducing this error all the stress components by the same proportion, except σ_{13}, σ_{23}, which remain relatively unaffected, because the role of the error in d_0 is damped by $(d-)^2$ in Eq. (12).

If there is preferred orientation, the peak intensity can vary greatly with ψ and there will be large variances contributing to $V(\ell_1)$ from weak peaks. This was minimized in the following way. The average variance, σ_i, in the 2θ peak position for $+\psi$ and $-\psi$ was obtained and the weighting factor c_i was formed:

$$c_i = (1/\sigma_i^2) \;/\; \sum_i (1/\sigma_i^2) \tag{27}$$

The Eqs. 11 and 12 were then altered to multiply $V_i(2\theta^+)$, $V_i(2\theta^-)$ 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 ψ. 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 $V(d_0)^{1/2} = 0.00004$ Å *

DATA SET 1

539.74	(48.24)	-24.03	(24.50)	-39.15	(4.58)
		552.16	(47.26)	2.30	(3.56)
				80.41	(38.96)

DATA SET 2

520.60	(40.52)	-4.03	(19.95)	-34.17	(3.21)
		555.19	(39.73)	0.11	(2.69)
				82.20	(32.75)

DATA SET 3

535.03	(47.81)	-20.14	(24.35)	-40.19	(5.72)
		555.98	(46.81)	-0.98	(4.56)
				86.66	(38.84)

DATA SET 4

538.53	(42.84)	-30.63	(21.10)	-38.03	(3.83)
		565.37	(42.51)	0.76	(3.89)
				88.18	(34.67)

*values given in MPa

TABLE III: WEIGHTED STRESS TENSOR AND STANDARD DEVIATIONS*

DATA SET 1

536.24	(48.56)	-24.62	(24.56)	-38.33	(4.59)
		554.65	(47.60)	2.90	(3.65)
				80.68	(39.22)

DATA SET 2

520.29	(41.84)	-6.04	(20.11)	-34.82	(3.55)
		560.22	(40.60)	1.56	(2.73)
				85.29	(33.76)

DATA SET 3

532.56	(48.15)	-7.90	(24.93)	-39.66	(5.81)
		549.83	(47.16)	-2.81	(4.57)
				82.21	(39.16)

DATA SET 4

539.23	(42.88)	-31.22	(21.23)	-38.28	(3.85)
		565.17	(42.65)	-0.59	(3.94)
				88.98	(34.68)

* $V(d_0)^{1/2} = 0.00004$ Å; 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. $\sin^2\psi$ 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.

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13. 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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