*International Tables for Crystallography* (2018). Vol. H, Section 2.5.4.3.2, pp. 141–142.



Triaxial: all components are not necessarily zero.

Equitriaxial: a special case of triaxial stress where $\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma$.

Strain is a measure of the resulting deformation of a solid body caused by stress. Strain is calculated from the change in the size and shape of the deformed solid due to stress. Analogous to normal stresses and shear stresses are normal strains and shear strains. The normal strain is calculated from the change in length of the solid body along the corresponding normal stress direction. Like the stress tensor, the strain tensor contains nine components:

$$\varepsilon_{ij} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}. \qquad (2.5.65)$$

The directions of all strain components are defined in the same way as for the stress tensor. Similarly, there are six independent components in the strain tensor. Strictly speaking, X-ray diffraction does not measure stresses directly, but strains. The stresses are calculated from the measured strains based on the elasticity of the materials. The stress–strain relations are given by the generalized form of Hooke's law:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \qquad (2.5.66)$$

where $C_{ijkl}$ are elastic stiffness coefficients. The stress–strain relations can also be expressed as

$$\varepsilon_{ij} = S_{ijkl}\sigma_{kl}, \qquad (2.5.67)$$

where $S_{ijkl}$ are the elastic compliances. For most polycrystalline materials without texture or with weak texture, it is practical and reasonable to consider the elastic behaviour to be isotropic and the structure to be homogeneous on a macroscopic scale. In these cases, the stress–strain relationship takes a much simpler form. Therefore, the Young's modulus $E$ and Poisson's ratio $\nu$ are sufficient to describe the stress and strain relations for homogeneous isotropic materials:

$$\begin{aligned}
\varepsilon_{11} &= \frac{1}{E}[\sigma_{11} - \nu(\sigma_{22} + \sigma_{33})], \\
\varepsilon_{22} &= \frac{1}{E}[\sigma_{22} - \nu(\sigma_{33} + \sigma_{11})], \\
\varepsilon_{33} &= \frac{1}{E}[\sigma_{33} - \nu(\sigma_{11} + \sigma_{22})], \\
\varepsilon_{12} &= \frac{1+\nu}{E}\sigma_{12}, \quad \varepsilon_{23} = \frac{1+\nu}{E}\sigma_{23}, \quad \varepsilon_{31} = \frac{1+\nu}{E}\sigma_{31}. \qquad (2.5.68)
\end{aligned}$$

It is customary in the field of stress measurement by X-ray diffraction to use another set of macroscopic elastic constants, $S_1$ and $\frac{1}{2}S_2$, which are given by

$$\tfrac{1}{2}S_2 = (1+\nu)/E \text{ and } S_1 = -\nu/E. \qquad (2.5.69)$$

Although polycrystalline materials on a macroscopic level can be considered isotropic, residual stress measurement by X-ray diffraction is done by measuring the strain in a specific crystal orientation of the crystallites that satisfies the Bragg condition. The stresses measured from diffracting crystallographic planes may have different values because of their elastic anisotropy. In such cases, the macroscopic elasticity constants should be replaced by a set of crystallographic plane-specific elasticity constants, $S_1^{\{hkl\}}$ and $\frac{1}{2}S_2^{\{hkl\}}$, called X-ray elastic constants (XECs). XECs for many materials can be found in the literature, measured or calculated from microscopic elasticity constants (Lu, 1996). In the case of materials with cubic crystal symmetry, the equations for calculating the XECs from the macroscopic elasticity constants $\frac{1}{2}S_2$ and $S_1$ are

$$\begin{aligned}
\tfrac{1}{2}S_2^{\{hkl\}} &= \tfrac{1}{2}S_2[1 + 3(0.2 - \Gamma(hkl))\Delta] \\
S_1^{\{hkl\}} &= S_1 - \tfrac{1}{2}S_2[0.2 - \Gamma(hkl)]\Delta, \qquad (2.5.70)
\end{aligned}$$

where

$$\Gamma(hkl) = \frac{h^2k^2 + k^2l^2 + l^2h^2}{(h^2+k^2+l^2)^2} \text{ and } \Delta = \frac{5(A_{\rm RX} - 1)}{3 + 2A_{\rm RX}}.$$

In the equations for stress measurement hereafter, either the macroscopic elasticity constants $\frac{1}{2}S_2$ and $S_1$ or the XECs $S_1^{\{hkl\}}$ and $\frac{1}{2}S_2^{\{hkl\}}$ are used in the expression, but either set of elastic constants can be used depending on the requirements of the application. The factor of anisotropy ($A_{\rm RX}$) is a measure of the elastic anisotropy of a material (He, 2009).

2.5.4.3.2. *Fundamental equations*

Fig. 2.5.24 illustrates two diffraction cones for backward diffraction. The regular diffraction cone (dashed lines) is from the powder sample with no stress, so the $2\theta$ angles are constant at all $\gamma$ angles. The diffraction ring shown as a solid line is the cross section of a diffraction cone that is distorted as a result of stresses. For a stressed sample, $2\theta$ becomes a function of $\gamma$ and the sample orientation ($\omega$, $\psi$, $\varphi$), *i.e.* $2\theta = 2\theta(\gamma, \omega, \psi, \varphi)$. This function is uniquely determined by the stress tensor. The strain measured by the $2\theta$ shift at a point on the diffraction ring is $\varepsilon_{(\gamma,\omega,\psi,\varphi)}^{\{hkl\}}$, based on the true strain definition

$$\varepsilon_{(\gamma,\omega,\psi,\varphi)}^{\{hkl\}} = \ln\frac{d}{d_o} = \ln\frac{\sin\theta_o}{\sin\theta} = \ln\frac{\lambda}{2d_o\sin\theta}, \qquad (2.5.71)$$

where $d_o$ and $\theta_o$ are the stress-free values and $d$ and $\theta$ are measured values from a point on the diffraction ring corresponding to ($\gamma$, $\omega$, $\psi$, $\varphi$). The direction of $\varepsilon_{(\gamma,\omega,\psi,\varphi)}^{\{hkl\}}$ in the sample coordinates $S_1$, $S_2$, $S_3$ can be given by the unit-vector components $h_1$, $h_2$ and $h_3$. As a second-order tensor, the relationship between the measured strain and the strain-tensor components is then given by

$$\varepsilon_{(\gamma,\omega,\psi,\varphi)}^{\{hkl\}} = \varepsilon_{ij} \cdot h_i \cdot h_j. \qquad (2.5.72)$$

The scalar product of the strain tensor with the unit vector in the above equation is the sum of all components in the tensor multiplied by the components in the unit vector corresponding to the first and the second indices. The expansion of this equation for $i$ and $j$ values of 1, 2 and 3 results in

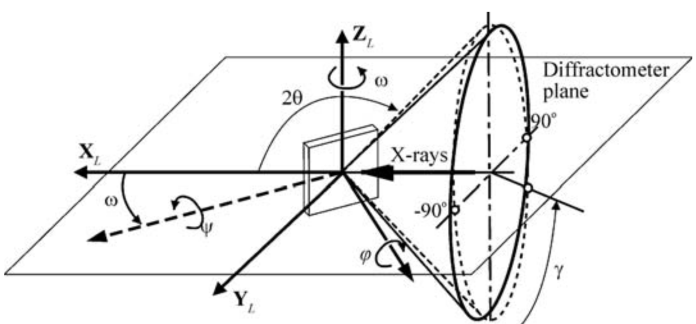


**Figure 2.5.24**
Diffraction-cone distortion due to stresses.

 

$$\varepsilon^{\{hkl\}}_{(\gamma,\omega,\psi,\varphi)} = h_1^2\varepsilon_{11} + 2h_1h_2\varepsilon_{12} + h_2^2\varepsilon_{22} + 2h_1h_3\varepsilon_{13} + 2h_2h_3\varepsilon_{23} + h_3^2\varepsilon_{33}. \tag{2.5.73}$$

Or, taking the true strain definition,

$$h_1^2\varepsilon_{11} + 2h_1h_2\varepsilon_{12} + h_2^2\varepsilon_{22} + 2h_1h_3\varepsilon_{13} + 2h_2h_3\varepsilon_{23} + h_3^2\varepsilon_{33} = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right), \tag{2.5.74}$$

where $\theta_o$ corresponds to the stress-free $d$-spacing and $\theta$ are measured values from a point on the diffraction ring. Both $\theta$ and $\{h_1, h_2, h_3\}$ are functions of $(\gamma, \omega, \psi, \varphi)$. By taking $\gamma$ values from 0 to 360°, equation (2.5.74) establishes the relationship between the diffraction-cone distortion and the strain tensor. Therefore, equation (2.5.74) is the fundamental equation for strain measurement with two-dimensional X-ray diffraction.

Introducing the elasticity of materials, one obtains

$$-\frac{\nu}{E}(\sigma_{11} + \sigma_{22} + \sigma_{33}) + \frac{1+\nu}{E}(\sigma_{11}h_1^2 + \sigma_{22}h_2^2 + \sigma_{33}h_3^2 + 2\sigma_{12}h_1h_2 + 2\sigma_{13}h_1h_3 + 2\sigma_{23}h_2h_3) = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right) \tag{2.5.75}$$

or

$$S_1(\sigma_{11} + \sigma_{22} + \sigma_{33}) + \tfrac{1}{2}S_2(\sigma_{11}h_1^2 + \sigma_{22}h_2^2 + \sigma_{33}h_3^2 + 2\sigma_{12}h_1h_2 + 2\sigma_{13}h_1h_3 + 2\sigma_{23}h_2h_3) = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right). \tag{2.5.76}$$

It is convenient to express the fundamental equation in a clear linear form:

$$p_{11}\sigma_{11} + p_{12}\sigma_{12} + p_{22}\sigma_{22} + p_{13}\sigma_{13} + p_{23}\sigma_{23} + p_{33}\sigma_{33} = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right), \tag{2.5.77}$$

where $p_{ij}$ are stress coefficients given by

$$p_{ij} = \begin{cases} (1/E)[(1+\nu)h_i^2 - \nu] = \tfrac{1}{2}S_2h_i^2 + S_1 & \text{if } i = j, \\ 2(1/E)(1+\nu)h_ih_j = 2\tfrac{1}{2}S_2h_ih_j & \text{if } i \neq j. \end{cases} \tag{2.5.78}$$

In the equations for the stress measurement above and hereafter, the macroscopic elastic constants $\frac{1}{2}S_2$ and $S_1$ are used for simplicity, but they can always be replaced by the XECs for the specific lattice plane $\{hkl\}$, $S_1^{\{hkl\}}$ and $\frac{1}{2}S_2^{\{hkl\}}$, if the anisotropic nature of the crystallites should be considered. For instance, equation (2.5.76) can be expressed with the XECs as

$$S_1^{\{hkl\}}(\sigma_{11} + \sigma_{22} + \sigma_{33}) + \tfrac{1}{2}S_2^{\{hkl\}}(\sigma_{11}h_1^2 + \sigma_{22}h_2^2 + \sigma_{33}h_3^2 + 2\sigma_{12}h_1h_2 + 2\sigma_{13}h_1h_3 + 2\sigma_{23}h_2h_3) = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right). \tag{2.5.79}$$

The fundamental equation (2.5.74) may be used to derive many other equations based on the stress–strain relationship, stress state and special conditions. The fundamental equation and the derived equations are referred to as 2D equations hereafter to distinguish them from the conventional equations. These equations can be used in two ways. One is to calculate the stress or stress-tensor components from the measured strain ($2\theta$-shift) values in various directions. The fundamental equation for stress measurement with 2D-XRD is a linear function of the stress-tensor components. The stress tensor can be obtained by solving the linear equations if six independent strains are measured or by linear least-squares regression if more than six independent measured strains are available. In order to get a reliable solution from the linear equations or least-squares analysis, the independent strain should be measured at significantly different orientations. Another function of the fundamental equation is to calculate the diffraction-ring distortion for a given stress tensor at a particular sample orientation $(\omega, \psi, \varphi)$ (He & Smith, 1998). The fundamental equation for stress measurement by the conventional X-ray diffraction method can also be derived from the 2D fundamental equation (He, 2009).

2.5.4.3.3. *Equations for various stress states*

The general triaxial stress state is not typically measured by X-ray diffraction because of low penetration. For most applications, the stresses in a very thin layer of material on the surface are measured by X-ray diffraction. It is reasonable to assume that the average normal stress in the surface-normal direction is zero within such a thin layer. Therefore, $\sigma_{33} = 0$, and the stress tensor has five nonzero components. In some of the literature this stress state is denoted as triaxial. In order to distinguish this from the general triaxial stress state, here we name this stress state as the 'biaxial stress state with shear'. In this case, we can obtain the linear equation for the biaxial stress state with shear:

$$p_{11}\sigma_{11} + p_{12}\sigma_{12} + p_{22}\sigma_{22} + p_{13}\sigma_{13} + p_{23}\sigma_{23} + p_{\rm ph}\sigma_{\rm ph} = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right), \tag{2.5.80}$$

where the coefficient $p_{\rm ph} = \frac{1}{2}S_2 + 3S_1$ and $\sigma_{\rm ph}$ is the pseudo-hydrostatic stress component introduced by the error in the stress-free $d$-spacing. In this case, the stresses can be measured without the accurate stress-free $d$-spacing, since this error is included in $\sigma_{\rm ph}$. The value of $\sigma_{\rm ph}$ is considered as one of the unknowns to be determined by the linear system. With the measured stress-tensor components, the general normal stress $(\sigma_\varphi)$ and shear stress $(\tau_\varphi)$ at any arbitrary angle $\varphi$ can be given by

$$\sigma_\varphi = \sigma_{11}\cos^2\varphi + \sigma_{12}\sin 2\varphi + \sigma_{22}\sin^2\varphi, \tag{2.5.81}$$

$$\tau_\varphi = \sigma_{13}\cos\varphi + \sigma_{23}\sin\varphi. \tag{2.5.82}$$

Equation (2.5.81) can also be used for other stress states by removing the terms for stress components that are zero. For instance, in the biaxial stress state $\sigma_{33} = \sigma_{13} = \sigma_{23} = 0$, so we have

$$p_{11}\sigma_{11} + p_{12}\sigma_{12} + p_{22}\sigma_{22} + p_{\rm ph}\sigma_{\rm ph} = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right). \tag{2.5.83}$$

In the 2D stress equations for any stress state with $\sigma_{33} = 0$, we can calculate stress with an approximation of $d_o$ (or $2\theta_o$). Any error in $d_o$ (or $2\theta_o$) will contribute only to a pseudo-hydrostatic term $\sigma_{\rm ph}$. The measured stresses are independent of the input $d_o$ (or $2\theta_o$) values (He, 2003). If we use $d_0'$ to represent the initial input, then the true $d_o$ (or $2\theta_o$) can be calculated from $\sigma_{\rm ph}$ with

$$d_0 = d_0' \exp\left(\frac{1-2\nu}{E}\sigma_{\rm ph}\right), \tag{2.5.84}$$

$$\theta_0 = \arcsin\left[\sin\theta_0' \exp\left(\frac{1-2\nu}{E}\sigma_{\rm ph}\right)\right]. \tag{2.5.85}$$

Care must be taken that the $\sigma_{\rm ph}$ value also includes the measurement error. If the purpose of the experiment is to