International Tables for Crystallography (2018). Vol. H, Figure 2.5.24, p. 141.

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:

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

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:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \tag{2.5.66}$$

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

$$\varepsilon_{ij} = S_{ijkl}\sigma_{kl}, \tag{2.5.67}$$

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 ν are sufficient to describe the stress and strain relations for homogeneous isotropic materials:

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

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

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

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

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

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 2θ angles are constant at all γ 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, 2θ becomes a function of γ and the sample orientation (ω, ψ, φ), *i.e.* $2\theta = 2\theta(\gamma, \omega, \psi, \varphi)$. This function is uniquely determined by the stress tensor. The strain measured by the 2θ shift at a point on the diffraction ring is $\varepsilon_{(\gamma,\omega,\psi,\varphi)}^{\{hkl\}}$, based on the true strain definition

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

where d_o and θ_o are the stress-free values and d and θ are measured values from a point on the diffraction ring corresponding to (γ, ω, ψ, φ). 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

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

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

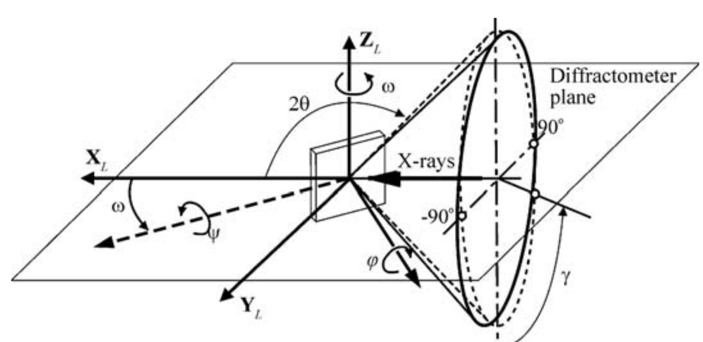

Figure 2.5.24
Diffraction-cone distortion due to stresses.