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

Or, taking the true strain definition,

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

where θ_o corresponds to the stress-free d-spacing and θ are measured values from a point on the diffraction ring. Both θ and $\{h_1, h_2, h_3\}$ are functions of $(\gamma, \omega, \psi, \varphi)$. By taking γ 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

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

or

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

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

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

where p_{ij} are stress coefficients given by

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

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

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

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 (2θ-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 (ω, ψ, φ) (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:

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

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 (σ_φ) and shear stress (τ_φ) at any arbitrary angle φ can be given by

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

$$\tau_\varphi = \sigma_{13}\cos\varphi + \sigma_{23}\sin\varphi. \quad (2.5.82)$$

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

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

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

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

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

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