2.5.4.2.2. *Fundamental equations*

The α and β angles are functions of $\gamma, \omega, \psi, \varphi$ and 2θ. As shown in Fig. 2.5.19(*a*), a pole has three components h_1, h_2 and h_3, parallel to the three sample coordinates S_1, S_2 and S_3, respectively. The pole-figure angles (α, β) can be calculated from the unit-vector components by the following pole-mapping equations:

$$\alpha = \sin^{-1}\left|h_3\right| = \cos^{-1}(h_1^2 + h_2^2)^{1/2}, \qquad (2.5.53)$$

$$\beta = \pm\cos^{-1}\frac{h_1}{(h_1^2 + h_2^2)^{1/2}} \qquad \begin{cases} \beta \geq 0^\circ & \text{if } h_2 \geq 0 \\ \beta < 0^\circ & \text{if } h_2 < 0 \end{cases}, \qquad (2.5.54)$$

where α takes a value between 0 and 90° ($0^\circ \leq \alpha \leq 90^\circ$) and β takes values in two ranges ($0^\circ \leq \beta \leq 180^\circ$ when $h_2 > 0$ and $-180^\circ \leq \beta < 0^\circ$ when $h_2 < 0$). The condition for reflection-mode diffraction is $h_3 > 0$. For transmission diffraction it is possible that $h_3 < 0$. In this case, the pole with mirror symmetry about the S_1S_2 plane to the diffraction vector is used for the pole-figure mapping. The absolute value of h_3 is then used in the equation for the α angle. When $h_2 = 0$ in the above equation, β takes one of two values depending on the value of h_1 ($\beta = 0^\circ$ when $h_1 \geq 0$ and $\beta = 180^\circ$ when $h_1 < 0$). For Eulerian geometry, the unit-vector components $\{h_1, h_2, h_3\}$ are given by equation (2.5.11).

The 2θ integrated intensity along the diffraction ring is then converted to the pole-density distribution along a curve on the pole figure. The α and β angles at each point of this curve are calculated from ω, ψ, φ, γ and 2θ. The sample orientation (ω, ψ, φ) and 2θ for a particular diffraction ring are constants; only γ takes a range of values depending on the detector size and distance.

For a textured sample, the 2θ-integrated intensity of a diffraction ring from a family of (hkl) planes is a function of γ and the sample orientation (ω, ψ, φ), *i.e.* $I_{hkl} = I_{hkl}(\omega, \psi, \varphi, \gamma, \theta)$. From the pole-figure angle-mapping equations, we can obtain the integrated intensity in terms of pole-figure angles as

$$I_{hkl}(\alpha, \beta) = I_{hkl}(\omega, \psi, \varphi, \gamma, \theta). \qquad (2.5.55)$$

The pole density at the pole-figure angles (α, β) is proportional to the integrated intensity at the same angles:

$$P_{hkl}(\alpha, \beta) = K_{hkl}(\alpha, \beta)I_{hkl}(\alpha, \beta), \qquad (2.5.56)$$

where $I_{hkl}(\alpha, \beta)$ is the 2θ-integrated intensity of the (hkl) peak corresponding to the pole direction (α, β), $K_{hkl}(\alpha, \beta)$ is the scaling factor covering the absorption, polarization, background corrections and various instrument factors if these factors are included in the integrated intensities, and $P_{hkl}(\alpha, \beta)$ is the pole-density distribution function. Background correction can be done during the 2θ integration and will be discussed in Section 2.5.4.2.4. The pole figure is obtained by plotting the pole-density function based on the stereographic projection.

The pole-density function can be normalized such that it represents a fraction of the total diffracted intensity integrated over the pole sphere. The normalized pole-density distribution function is given by

$$g_{hkl}(\alpha, \beta) = \frac{2\pi P_{hkl}(\alpha, \beta)}{\int_0^{2\pi}\int_0^{\pi/2} P_{hkl}(\alpha, \beta)\cos\alpha \, \mathrm{d}\alpha \, \mathrm{d}\beta}. \qquad (2.5.57)$$

The pole-density distribution function is a constant for a sample with a random orientation distribution. Assuming that the sample and instrument conditions are the same except for the pole-density distribution, we can obtain the normalized pole-density function by

$$g_{hkl}(\alpha, \beta) = \frac{I_{hkl}(\alpha, \beta)}{I_{hkl}^{\text{random}}(\alpha, \beta)}. \qquad (2.5.58)$$

The integrated intensity from the textured sample without any correction can be plotted according to the stereographic projection as an 'uncorrected' pole figure. The same can be done for the sample with a random orientation distribution to form a 'correction' pole figure that contains only the factors to be corrected. The normalized pole figure is then obtained by dividing the 'uncorrected' pole figure by the 'correction' pole figure. This experimental approach is feasible only if a similar sample with a random orientation distribution is available.

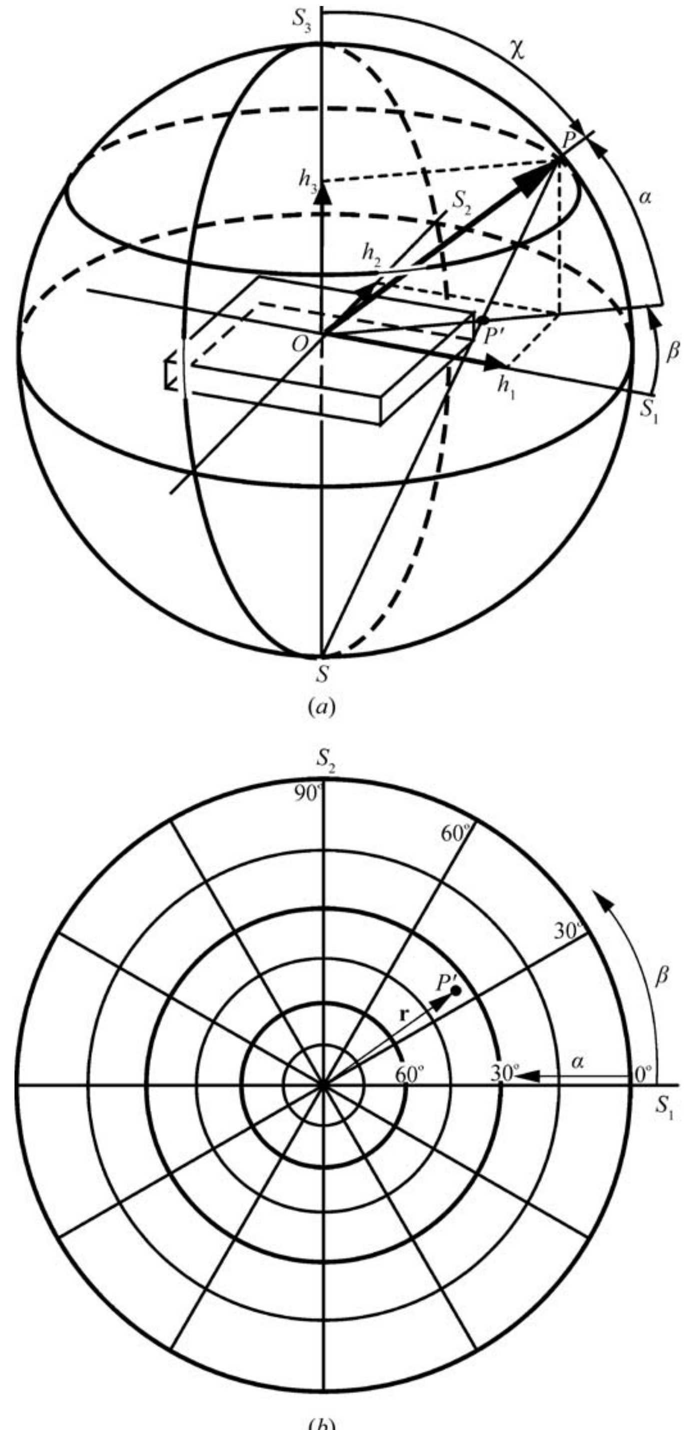

Figure 2.5.19
(*a*) Definition of pole direction angles α and β; (*b*) stereographic projection in a pole figure.

  references