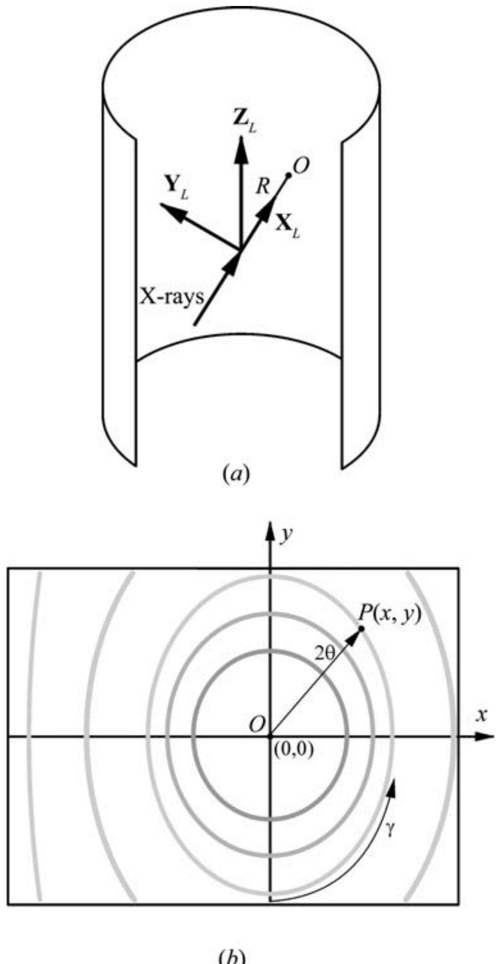

Figure 2.5.6
Cylinder-shaped detector in vertical direction: (*a*) detector position in the laboratory coordinates; (*b*) pixel position in the flattened image.

$$2\theta = \arccos \frac{x \sin\alpha + D\cos\alpha}{(D^2 + x^2 + y^2)^{1/2}} \quad (0 < 2\theta < \pi), \qquad (2.5.6)$$

$$\gamma = \frac{x\cos\alpha - D\sin\alpha}{|x\cos\alpha - D\sin\alpha|} \arccos \frac{-y}{[y^2 + (x\cos\alpha - D\sin\alpha)^2)]^{1/2}}$$
$$(-\pi < \gamma \le \pi). \qquad (2.5.7)$$

2.5.2.2.3. *Pixel position in diffraction space for a curved detector*

The conic sections of the diffraction cones with a curved detector depend on the shape of the detector. The most common curved detectors are cylinder-shaped detectors. The diffraction frame measured by a cylindrical detector can be displayed as a flat frame, typically a rectangle. Fig. 2.5.6(*a*) shows a cylindrical detector in the vertical direction and the corresponding laboratory coordinates X_L, Y_L, Z_L. The sample is located at the origin of the laboratory coordinates inside the cylinder. The incident X-rays strike the detector at a point O if there is no sample or beam stop to block the direct beam. The radius of the cylinder is R. Fig. 2.5.6(*b*) illustrates the 2D diffraction image collected with the cylindrical detector. We take the point O as the origin of the pixel position (0, 0). The diffraction-space coordinates ($2\theta, \gamma$) for a pixel at $P(x, y)$ are given by

$$2\theta = \arccos\left[R\cos\left(\frac{x}{R}\right) \Big/ (R^2 + y^2)^{1/2}\right], \qquad (2.5.8)$$

$$\gamma = \frac{x}{|x|} \arccos\left\{-y \Big/ \left[y^2 + R^2 \sin^2\left(\frac{x}{R}\right)\right]^{1/2}\right\} \quad (-\pi < \gamma \le \pi). \qquad (2.5.9)$$

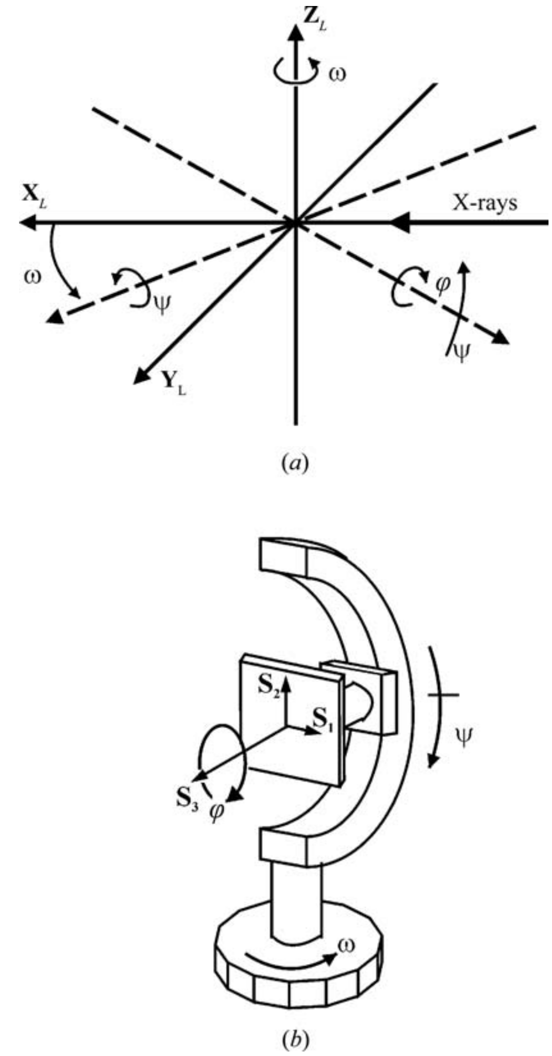

Figure 2.5.7
Sample rotation and translation. (*a*) Three rotation axes in laboratory coordinates; (*b*) rotation axes (ω, ψ, φ) and sample coordinates.

The pixel-position-to-(2θ, γ) conversion for detectors of other shapes can also be derived. Once the diffraction-space coordinates (2θ, γ) of each pixel in the curved 2D detector are determined, most data-analysis algorithms developed for flat detectors are applicable to a curved detector as well.

2.5.2.3. *Sample space and goniometer geometry*

2.5.2.3.1. *Sample rotations and translations in Eulerian geometry*

In a 2D-XRD system, three rotation angles are necessary to define the orientation of a sample in the diffractometer. These three rotation angles can be achieved either by a Eulerian geometry, a kappa (κ) geometry or another kind of geometry. The three angles in Eulerian geometry are ω (omega), ψ (psi) and φ (phi). Fig. 2.5.7(*a*) shows the relationship between rotation axes (ω, ψ, φ) in the laboratory system $\mathbf{X}_L$, $\mathbf{Y}_L$, $\mathbf{Z}_L$. The ω angle is defined as a right-handed rotation about the Z_L axis. The ω axis is fixed in the laboratory coordinates. The ψ angle is a right-handed rotation about a horizontal axis. The angle between the ψ axis and the X_L axis is given by ω. The ψ axis lies on X_L when ω is set at zero. The φ angle defines a left-handed rotation about an axis on the sample, typically the normal of a flat sample. The φ axis lies on the Y_L axis when $\omega = \psi = 0$. In an aligned diffraction system, all three rotation axes and the primary X-ray beam cross at the