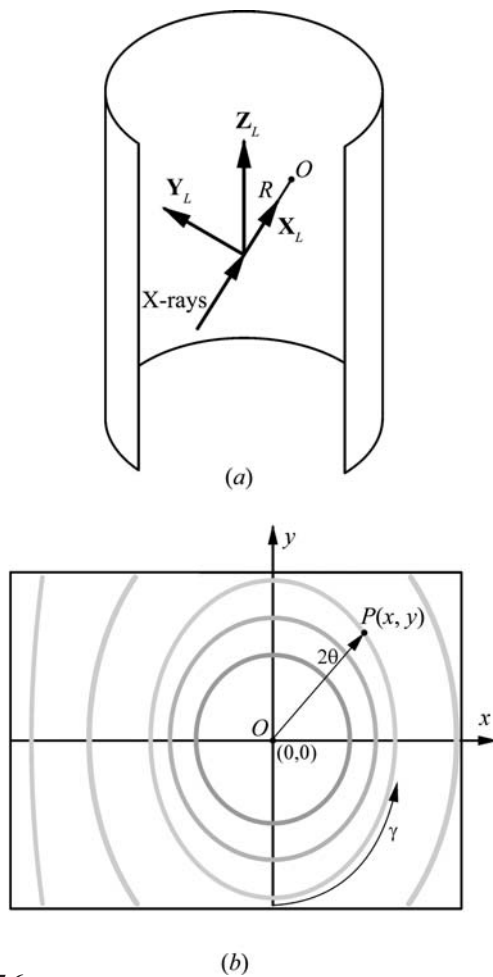


2. INSTRUMENTATION AND SAMPLE PREPARATION


Figure 2.5.6

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

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

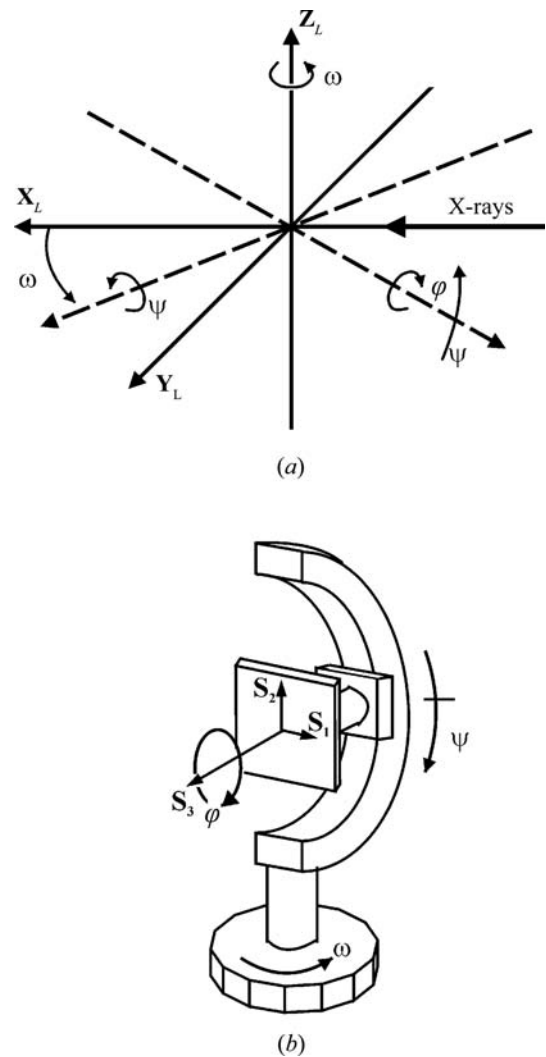
$$\gamma = \frac{x \cos \alpha - D \sin \alpha}{|x \cos \alpha - D \sin \alpha|} \arccos \frac{-y}{[y^2 + (x \cos \alpha - D \sin \alpha)^2]^{1/2}} \quad (-\pi < \gamma \leq \pi). \quad (2.5.7)$$

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

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

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


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- $(2\theta, \gamma)$ conversion for detectors of other shapes can also be derived. Once the diffraction-space coordinates $(2\theta, \gamma)$ 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 X_L, Y_L, 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