International Tables for Crystallography (2018). Vol. H, Section 2.5.2.2.2, pp. 121–122.

satisfied, the diffraction vector is normal to the diffracting lattice planes and its magnitude is reciprocal to the d-spacing of the lattice planes. In this case, the diffraction vector is equivalent to the reciprocal-lattice vector. Each pixel in a 2D detector measures scattered X-rays in a given direction with respect to the incident beam. We can calculate a diffraction vector for any pixel, even if the pixel is not measuring Bragg scattering. Use of the term 'diffracted beam' hereafter in this chapter does not necessarily imply that it arises from Bragg scattering.

For two-dimensional diffraction, the incident beam can be expressed by the vector $\mathbf{s}_0/\lambda$, but the diffracted beam is no longer in a single direction, but follows the diffraction cone. Since the direction of a diffraction vector is a bisector of the angle between the incident and diffracted beams corresponding to each diffraction cone, the trace of the diffraction vectors forms a cone. This cone is referred to as the diffraction-vector cone. The angle between the diffraction vector and the incident X-ray beam is $90^\circ + \theta$ and the apex angle of a vector cone is $90^\circ - \theta$. It is apparent that diffraction-vector cones can only exists on the $-X_L$ side of the diffraction space.

For two-dimensional diffraction, the diffraction vector is a function of both the γ and 2θ angles, and is given in laboratory coordinates as

$$\mathbf{H} = \frac{\mathbf{s} - \mathbf{s}_0}{\lambda} = \frac{1}{\lambda}\begin{bmatrix} \cos 2\theta - 1 \\ -\sin 2\theta \sin\gamma \\ -\sin 2\theta \cos\gamma \end{bmatrix}. \qquad (2.5.4)$$

The direction of the diffraction vector can be represented by its unit vector, given by

$$\mathbf{h}_L = \frac{\mathbf{H}}{|\mathbf{H}|} = \begin{bmatrix} h_x \\ h_y \\ h_z \end{bmatrix} = \begin{bmatrix} -\sin\theta \\ -\cos\theta \sin\gamma \\ -\cos\theta\cos\gamma \end{bmatrix}, \qquad (2.5.5)$$

where $\mathbf{h}_L$ is a unit vector expressed in laboratory coordinates and the three components in the square brackets are the projections of the unit vector on the three axes of the laboratory coordinates, respectively. If γ takes all values from 0 to 360° at a given Bragg angle 2θ, the trace of the diffraction vector forms a diffraction-vector cone. Since the possible values of θ lie within the range 0 to 90°, h_x takes only negative values.

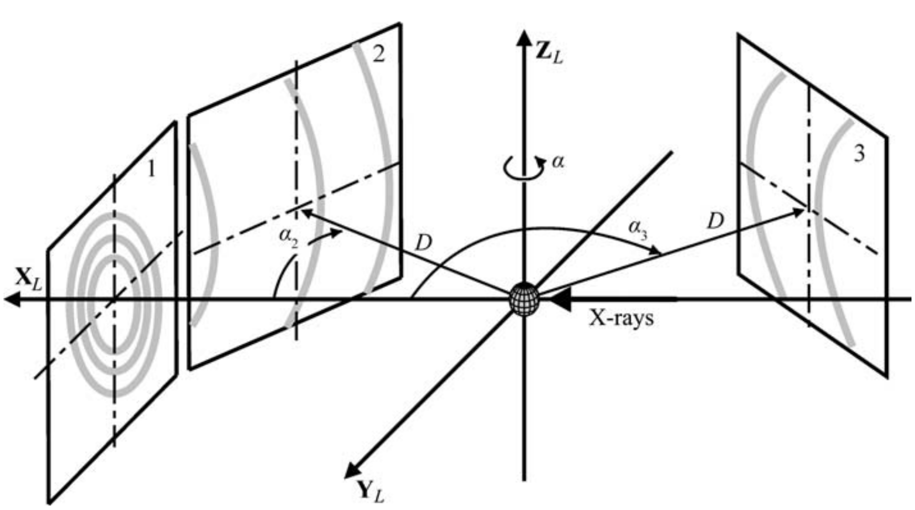

Figure 2.5.4
Detector positions in the laboratory-system coordinates.

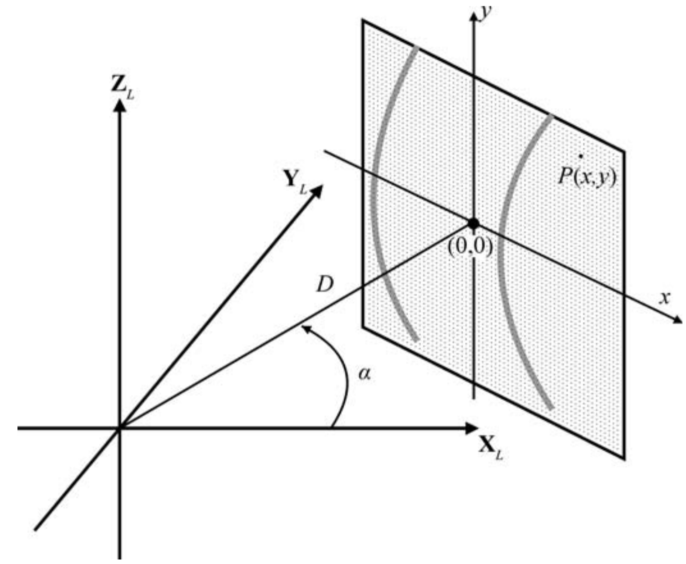

Figure 2.5.5
Relationship between a pixel P and detector position in the laboratory coordinates.

2.5.2.2. *Detector space and pixel position*

A typical 2D detector has a limited detection surface, and the detection surface can be spherical, cylindrical or flat. Spherical or cylindrical detectors are normally designed for a fixed sample-to-detector distance, while a flat detector has the flexibility to be used at different sample-to-detector distances so as to choose either high resolution at a large distance or large angular coverage at a short distance.

2.5.2.2.1. *Detector position in the laboratory system*

The position of a flat detector is defined by the sample-to-detector distance D and the detector swing angle α. D and α are referred to as the detector-space parameters. D is the perpendicular distance from the goniometer centre to the detection plane and α is a right-handed rotation angle about the Z_L axis. Detectors at different positions in the laboratory coordinates X_L, Y_L, Z_L are shown in Fig. 2.5.4. The centre of detector 1 is right on the positive side of the X_L axis (on-axis), $\alpha = 0$. Both detectors 2 and 3 are rotated away from the X_L axis with negative swing angles ($\alpha_2 < 0$ and $\alpha_3 < 0$). The detection surface of a flat 2D detector can be considered as a plane, which intersects the diffraction cone to form a conic section. Depending on the swing angle α and the 2θ angle, the conic section can appear as a circle, an ellipse, a parabola or a hyperbola.

2.5.2.2.2. *Pixel position in diffraction space for a flat detector*

The values of 2θ and γ can be calculated for each pixel in the frame. The calculation is based on the detector-space parameters and the pixel position in the detector. Fig. 2.5.5 shows the relationship of a pixel $P(x, y)$ to the laboratory coordinates X_L, Y_L, Z_L. The position of a pixel in the detector is defined by the (x, y) coordinates, where the detector centre is defined as $x = y = 0$. The diffraction-space coordinates $(2\theta, \gamma)$ for a pixel at $P(x, y)$ are given by

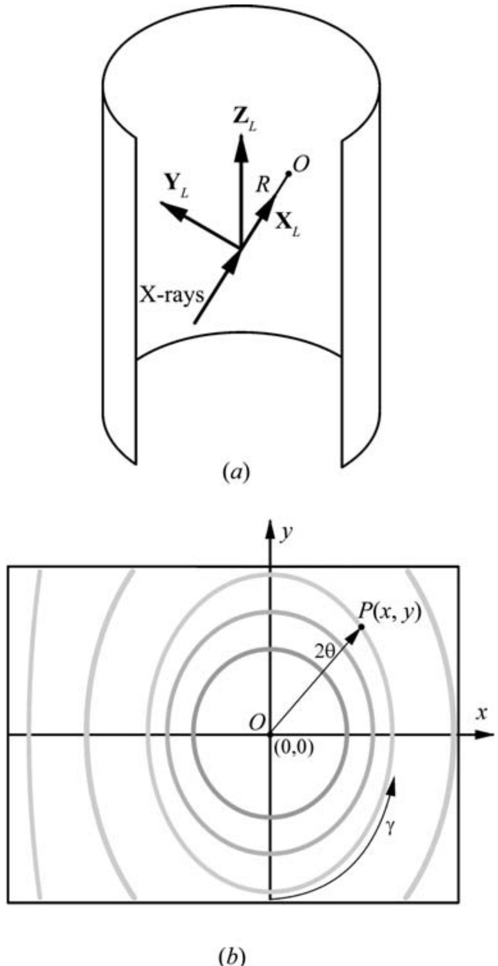

Figure 2.5.6
Cylinder-shaped detector in vertical direction: (a) detector position in the laboratory coordinates; (b) pixel position in the flattened image.

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

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

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 (2θ, γ) for a pixel at $P(x, y)$ are given by

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

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

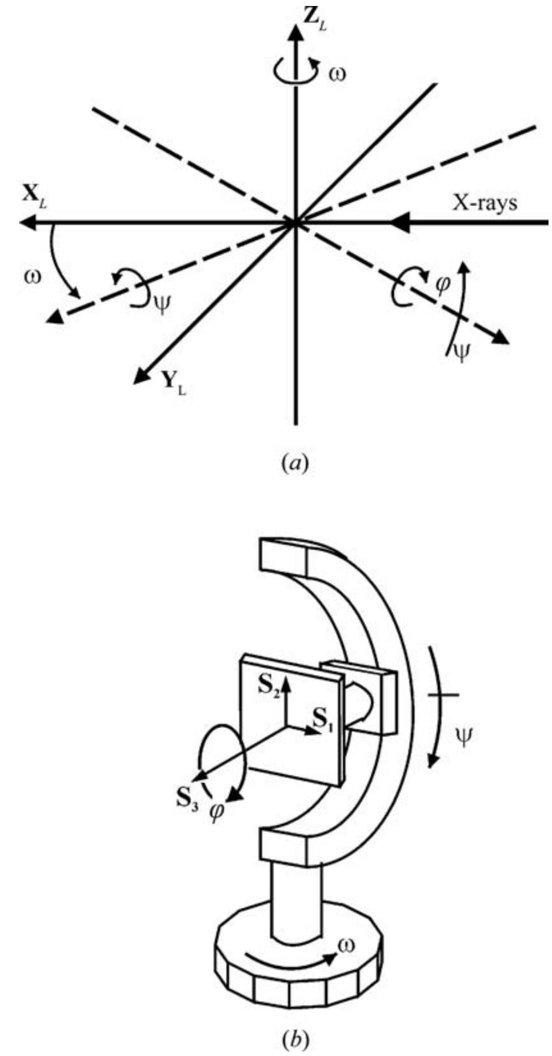

Figure 2.5.7
Sample rotation and translation. (a) Three rotation axes in laboratory coordinates; (b) rotation axes (ω, ψ, φ) and sample coordinates.

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