The plane given by X_L and Y_L is the diffractometer plane. The axis Z_L is perpendicular to the diffractometer plane. The axes X_L, Y_L and Z_L form a right-handed rectangular coordinate system with the origin at the instrument centre. The incident X-ray beam propagates along the X_L axis, which is also the rotation axis of all diffraction cones. The apex angles of the cones are determined by the 2θ values given by the Bragg equation. The apex angles are twice the 2θ values for forward reflection ($2\theta \leq 90^\circ$) and twice the value of $180^\circ - 2\theta$ for backward reflection ($2\theta > 90^\circ$). For clarity, only one diffraction cone of forward reflection is displayed. The γ angle is the azimuthal angle from the origin at the six o'clock direction with a right-handed rotation axis along the opposite direction of incident beam ($-X_L$ direction). A given γ value defines a half plane with the X_L axis as the edge; this will be referred to as the γ plane hereafter. The diffractometer plane consists of two γ planes at $\gamma = 90^\circ$ and $\gamma = 270^\circ$. Therefore many equations developed for 2D-XRD should also apply to conventional XRD if the γ angle is given as a constant of 90° or 270°. A pair of γ and 2θ values represents the direction of a diffracted beam. The γ angle takes a value of 0 to 360° for a complete diffraction ring with a constant 2θ value. The γ and 2θ angles form a spherical coordinate system which covers all the directions from the origin of sample (instrument centre). The γ–2θ system is fixed in the laboratory system $\mathbf{X}_L$, $\mathbf{Y}_L$, $\mathbf{Z}_L$, which is independent of the sample orientation and detector position in the goniometer. 2θ and γ are referred to as the diffraction-space parameters. In the laboratory coordinate system $\mathbf{X}_L$, $\mathbf{Y}_L$, $\mathbf{Z}_L$, the surface of a diffraction cone can be mathematically expressed as

$$y_L^2 + z_L^2 = x_L^2 \tan^2 2\theta, \qquad (2.5.1)$$

with $x_L \geq 0$ or $2\theta \leq 90^\circ$ for forward-diffraction cones and $x_L < 0$ or $2\theta > 90^\circ$ for backward-diffraction cones.

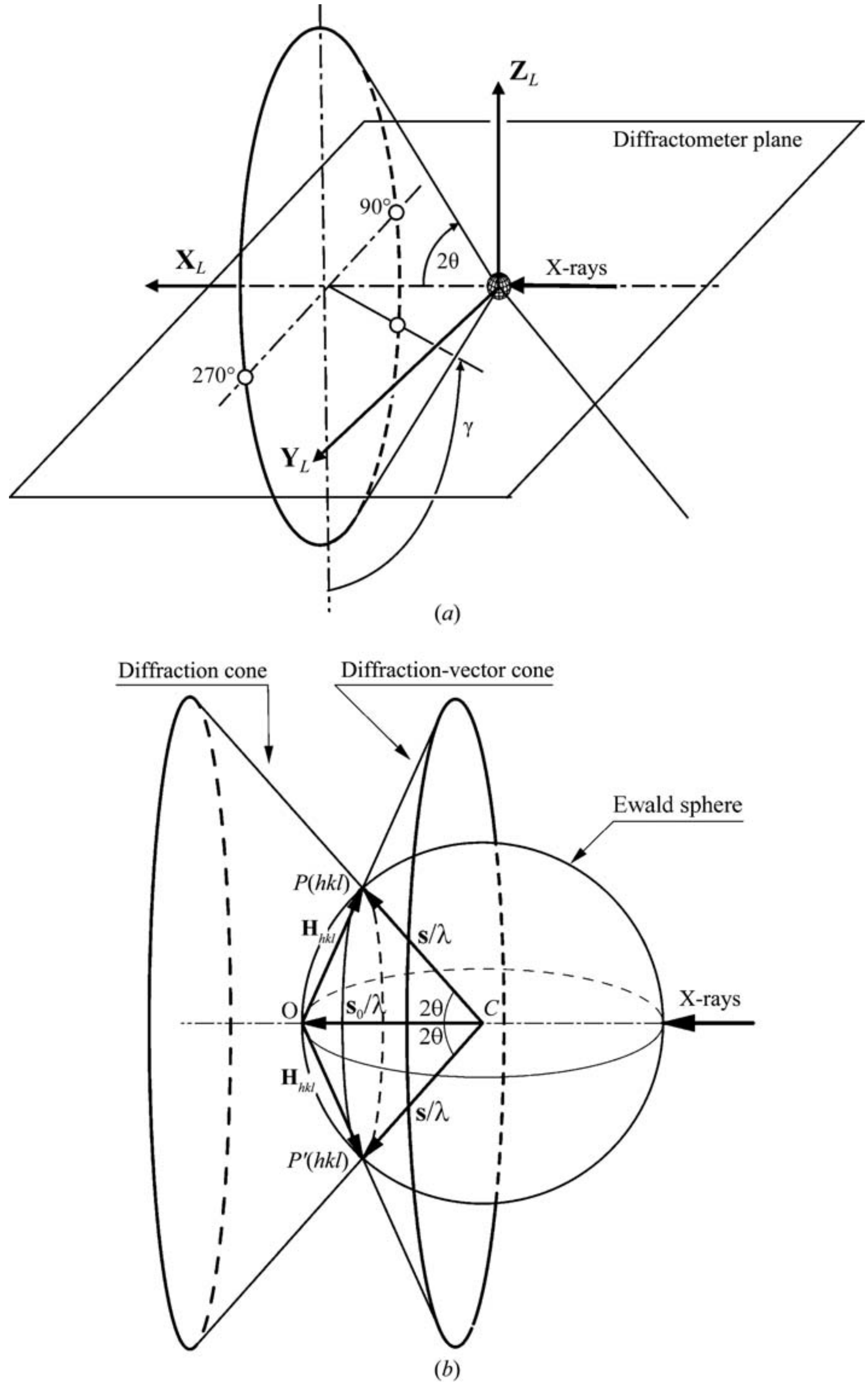

Figure 2.5.3
The diffraction cone and the corresponding diffraction-vector cone.

2.5.2.1.2. *Diffraction-vector cones in laboratory coordinates*

Fig. 2.5.3(*b*) shows the diffraction-vector cone corresponding to the diffraction cone in the laboratory coordinate system. C is the centre of the Ewald sphere. The diffraction condition can be given by the Laue equation as

$$\frac{\mathbf{s} - \mathbf{s}_0}{\lambda} = \mathbf{H}_{hkl}, \qquad (2.5.2)$$

where $\mathbf{s}_0$ is the unit vector representing the incident beam, $\mathbf{s}$ is the unit vector representing the diffracted beam and $\mathbf{H}_{hkl}$ is the reciprocal-lattice vector. Its magnitude is given as

$$\left|\frac{\mathbf{s} - \mathbf{s}_0}{\lambda}\right| = \frac{2\sin\theta}{\lambda} = \left|\mathbf{H}_{hkl}\right| = \frac{1}{d_{hkl}}, \qquad (2.5.3)$$

in which d_{hkl} is the d-spacing of the crystal planes (hkl). It can be easily seen that it is the Bragg law in a different form. Therefore, equation (2.5.2) is the Bragg law in vector form. In the Bragg condition, the vectors $\mathbf{s}_0/\lambda$ and $\mathbf{s}/\lambda$ make angles θ with the diffracting planes (hkl) and $\mathbf{H}_{hkl}$ is normal to the (hkl) crystal plane. In order to analyse all the X-rays measured by a 2D detector, we extend the concept to all scattered X-rays from a sample regardless of the Bragg condition. Therefore, the index (hkl) can be removed from the above expression. $\mathbf{H}$ is then a vector which takes the direction bisecting the incident beam and the scattered beam, and has dimensions of inverse length given by $2\sin\theta/\lambda$. Here 2θ is the scattering angle from the incident beam. The vector $\mathbf{H}$ is referred to as the scattering vector or, alternatively, the diffraction vector. When the Bragg condition is

  references