

2. DIFFRACTION GEOMETRY AND ITS PRACTICAL REALIZATION

The terminology used today for different methods is essentially the same as originally used except that the rotation method now tends to mean limited angular ranges (instead of 360°) per diffraction photograph/image. The Weissenberg method in its modern form now employed at a synchrotron is a screenless technique with limited angular range but still with detector translation coupled to crystal rotation.

The diffraction spots lie on curved arcs where each curve corresponds to the intersection with a film of a cone. With a flat film the intersections are conic sections. The curved arcs are obviously recognizable for the protein crystal case where there are a large number of spots.

2.2.2.1. Monochromatic still exposure

In a monochromatic still exposure, the crystal is held stationary and a near-zero wavelength-bandpass (e.g. $\delta\lambda/\lambda = 0.001$) beam impinges on it. For a small-molecule crystal, there are few diffraction spots. For a protein crystal, there are many (several hundred), because of the much denser reciprocal lattice. The actual number of stimulated relp's depends on the reciprocal-cell parameters, the size of the mosaic spread of the crystal, the angular beam divergence as well as the small, but finite, spectral spread, $\delta\lambda/\lambda$. Diffraction spots are only partially stimulated instead of fully integrated over wavelength, as in the Laue method, or over an angular rotation (the rocking width) in rotating-crystal monochromatic methods.

2.2.2.2. Crystal setting

Crystal setting follows the procedure given in Subsection 2.2.1.2 whereby angular mis-setting angles are given by equation (2.2.1.3). When viewed down a zone axis, the pattern on a flat film or electronic area detector has the appearance of a series of concentric circles. For example, with the beam parallel to $[00\bar{1}]$, the first circle corresponds to $l = 1$, the second to $l = 2$, etc. The radius of the first circle R is related to the interplanar spacing between the $(hk0)$ and $(hk1)$ planes, i.e. λ/c (in this example), through θ , by the formulae

$$\tan 2\theta = R/D; \quad \cos 2\theta = 1 - \lambda/c. \quad (2.2.2.1)$$

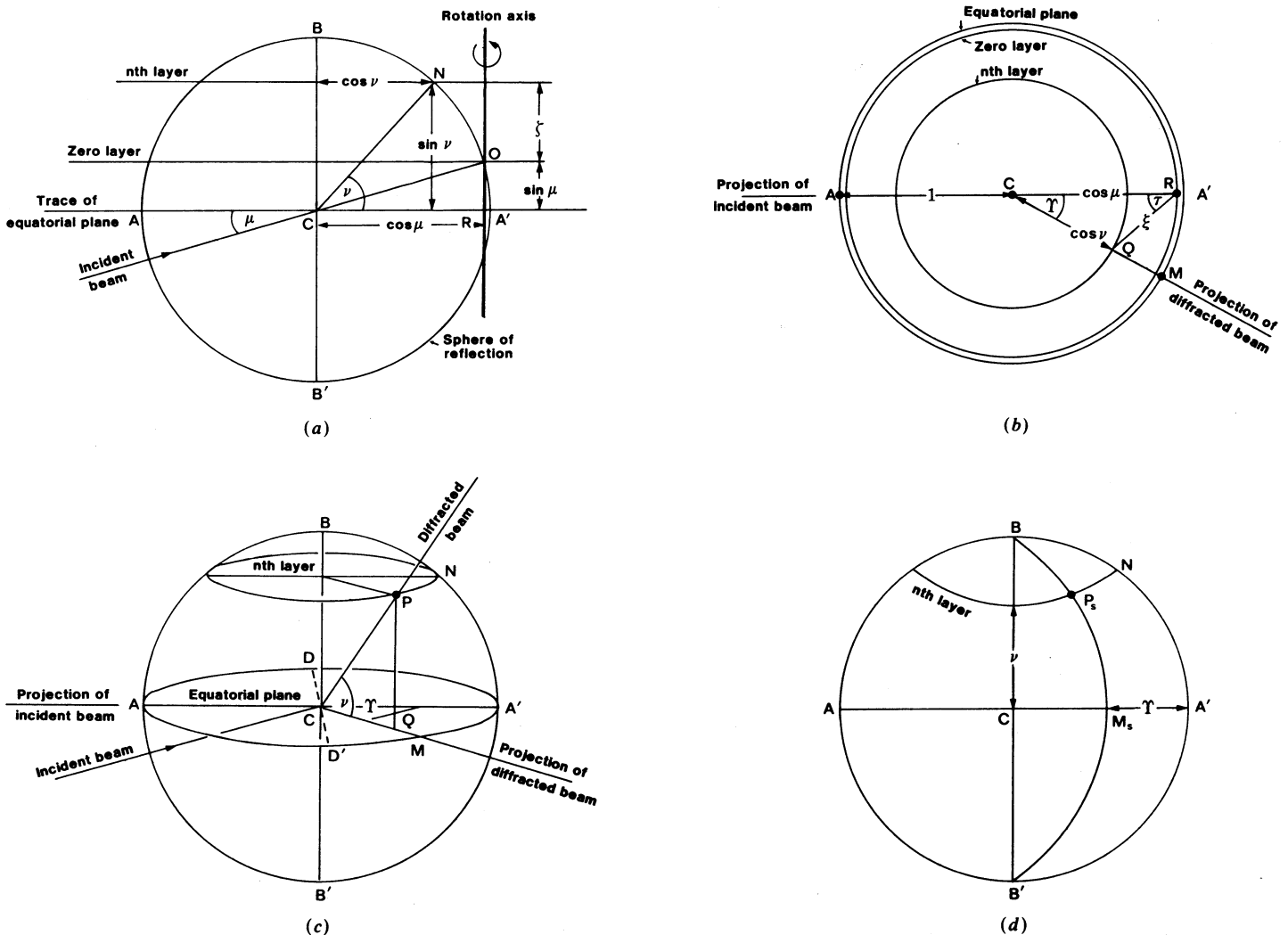


Fig. 2.2.3.1. (a) Elevation of the sphere of reflection. O is the origin of the reciprocal lattice. C is the centre of the Ewald sphere. The incident beam is shown in the plane. (b) Plan of the sphere of reflection. R is the projection of the rotation axis on the equatorial plane. (c) Perspective diagram. P is the relp in the reflection position with the cylindrical coordinates ζ, ξ, φ . The angular coordinates of the diffracted beam are ν, γ . (d) Stereogram to show the direction of the diffracted beam, ν, γ , with DD' , normal to the incident beam and in the equatorial plane, as the projection diameter. From Evans & Lonsdale (1959).