Any relp (*hkl*) lying in the region of reciprocal space between the $1/\lambda_{\max}$ and $1/\lambda_{\min}$ Ewald spheres and the resolution sphere $1/d_{\min}$ will diffract (the shaded area in Fig. 2.2.1.1). This region of reciprocal space is referred to as the accessible or stimulated region. Fig. 2.2.1.2 shows a predicted Laue pattern from a well aligned protein crystal. For a description of the indexing of a Laue photograph, see Bragg (1928, pp. 28, 29).

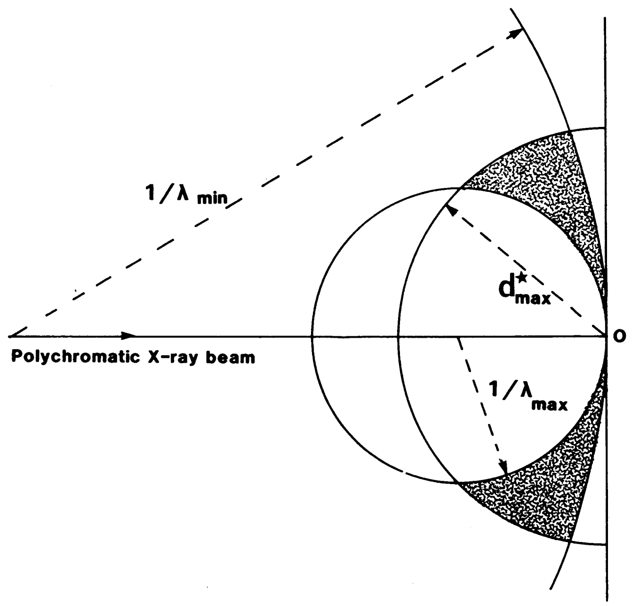

Fig. 2.2.1.1. Laue geometry. A polychromatic beam containing wavelengths $\lambda_{\min}$ to $\lambda_{\max}$ impinges on the crystal sample. The resolution sphere of radius $d^*_{\max} = 1/d_{\min}$ is drawn centred at O, the origin of reciprocal space. Any reciprocal-lattice point falling in the shaded region is stimulated. In this diagram, the radius of each Ewald sphere uses the convention $1/\lambda$.

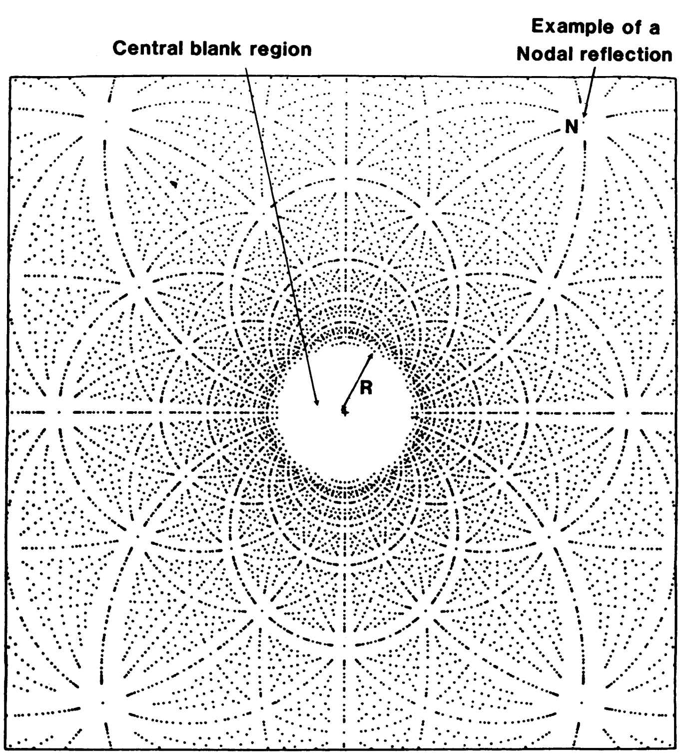

Fig. 2.2.1.2. A predicted Laue pattern of a protein crystal with a zone axis parallel to the incident, polychromatic X-ray beam. There is a pronounced blank region at the centre of the film (see Subsection 2.2.1.2). The spot marked *N* is one example of a nodal spot (see Subsection 2.2.1.4).

For a Laue spot at a given θ, only the ratio λ/d is determined, whether it is a single or a multiple relp component spot. If the unit-cell parameters are known from a monochromatic experiment, then a Laue spot at a given θ yields λ since d is then known. Conversely, precise unit-cell lengths cannot be determined from a Laue pattern alone; methods are, however, being developed to determine these (see Carr, Cruickshank & Harding, 1992).

The maximum Bragg angle $\theta_{\max}$ is given by the equation

$$\theta_{\max} = \sin^{-1}(\lambda_{\max}/2d_{\min}). \qquad (2.2.1.2)$$

2.2.1.2. *Crystal setting*

The main use of Laue photography has in the past been for adjustment of the crystal to a desired orientation. With small-molecule crystals, the number of diffraction spots on a monochromatic photograph from a stationary crystal is very small. With unfiltered, polychromatic radiation, many more spots are observed and so the Laue photograph serves to give a better idea of the crystal orientation and setting prior to precession photography. With protein crystals, the monochromatic still is used for this purpose before data collection *via* an area detector. This is because the number of diffraction spots is large on a monochromatic still and in a protein-crystal Laue photograph the stimulated spots from the *Bremsstrahlung* continuum are generally very weak. Synchrotron-radiation Laue photographs of protein crystals can be recorded with short exposure times. These patterns consist of a large number of diffraction spots.

Crystal setting *via* Laue photography usually involves trying to direct the X-ray beam along a zone axis. Angular mis-setting angles ε in the spindle and arc are easily calculated from the formula

$$\varepsilon = \tan^{-1}(\Delta/D), \qquad (2.2.1.3)$$

where Δ is the distance (resolved into vertical and horizontal) from the beam centre to the centre of a circle of spots defining a zone axis and D is the crystal-to-film distance.

After suitable angular correction to the sample orientation, the Laue photograph will show a pronounced blank region at the centre of the film (see Fig. 2.2.1.2). The radius of the blank region is determined by the minimum wavelength in the beam and the magnitude of the reciprocal-lattice spacing parallel to the X-ray beam (see Jeffery, 1958). For the case, for example, of the X-ray beam perpendicular to the a^*b^* plane, then

$$\lambda_{\min} = c(1 - \cos 2\theta), \qquad (2.2.1.4a)$$

where

$$2\theta = \tan^{-1}(R/D) \qquad (2.2.1.4b)$$

and R is the radius of the blank region (see Fig. 2.2.1.2), and D is the crystal-to-flat-film distance. If $\lambda_{\min}$ is known then an approximate value of c, for example, can be estimated. The principal zone axes will give the largest radii for the central blank region.

2.2.1.3. *Single-order and multiple-order reflections*

In Laue geometry, several relp's can occur in a Laue spot or ray. The number of relp's in a given spot is called the multiplicity of the spot. The number of spots of a given multiplicity can be plotted as a histogram. This is known as the multiplicity distribution. The form of this distribution is dependent on the ratio $\lambda_{\max}/\lambda_{\min}$. The multiplicity distribution

references