

## 2. DIFFRACTION GEOMETRY AND ITS PRACTICAL REALIZATION

in Laue diffraction is considered in detail by Cruickshank, Helliwell & Moffat (1987).

Any relp  $nh$ ,  $nk$ ,  $nl$  ( $n$  integer) will be stimulated by a wavelength  $\lambda/n$  since  $d_{nhnkl} = d_{hkl}/n$ , i.e.

$$\frac{\lambda}{n} = 2 \frac{d_{hkl}}{n} \sin \theta. \quad (2.2.1.5)$$

However,  $d_{nhnkl}$  must be  $> d_{\min}$  as otherwise the reflection is beyond the sample resolution limit.

If  $h$ ,  $k$ ,  $l$  have no common integer divisor and if  $2h$ ,  $2k$ ,  $2l$  is beyond the resolution limit, then the spot on the Laue diffraction photograph is a single-wavelength spot. The probability that  $h$ ,  $k$ ,  $l$  have no common integer divisor is

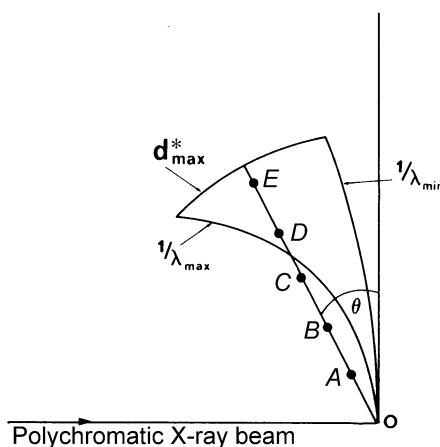


Fig. 2.2.1.3. A multiple component spot in Laue geometry. A ray of multiplicity 5 is shown as an example. The inner point  $A$  corresponds to  $d$  and a wavelength  $\lambda$ , the next point,  $B$ , is  $d/2$  and wavelength  $\lambda/2$ . The outer point  $E$  corresponds to  $d/5$  and  $\lambda/5$ . Rotation of the sample will either exclude inner points (at the  $\lambda_{\max}$  surface) or outer points (at the  $\lambda_{\min}$  surface) and so determine the recorded multiplicity.

$$Q = \left[1 - \frac{1}{2^3}\right] \left[1 - \frac{1}{3^3}\right] \left[1 - \frac{1}{5^3}\right] \dots = 0.832 \dots \quad (2.2.1.6)$$

Hence, for a relp where  $d_{\min} < d_{hkl} < 2d_{\min}$  there is a very high probability (83.2%) that the Laue spot will be recorded as a single-wavelength spot. Since this region of reciprocal space corresponds to 87.5% (i.e.  $7/8$ ) of the volume of reciprocal space within the resolution sphere then  $0.875 \times 0.832 = 72.8\%$  is the probability for a relp to be recorded in a single-wavelength spot. According to W. L. Bragg, all Laue spots should be multiple. He reasoned that for each  $h$ ,  $k$ ,  $l$  there will always be a  $2h$ ,  $2k$ ,  $2l$  etc. lying within the same Laue spot. However, as the resolution limit is increased to accommodate this many more relp's are added, for which their  $hkl$ 's have no common divisor.

The above discussion holds for infinite bandwidth. The effect of a more experimentally realistic bandwidth is to increase the proportion of single-wavelength spots.

The number of relp's within the resolution sphere is

$$\frac{4}{3} \frac{\pi d_{\max}^3}{V^*}, \quad (2.2.1.7)$$

where  $d_{\max}^* = 1/d_{\min}$  and  $V^*$  is the reciprocal unit-cell volume.

The number of relp's within the wavelength band  $\lambda_{\max}$  to  $\lambda_{\min}$ , for  $\lambda_{\max} < 2/d_{\max}^*$ , is (Moffat, Schildkamp, Bilderback & Volz, 1986)

$$\frac{\pi}{4} \frac{(\lambda_{\max} - \lambda_{\min}) d_{\max}^{*4}}{V^*}. \quad (2.2.1.8)$$

Note that the number of relp's stimulated in a  $0.1 \text{ \AA}$  wavelength interval, for example between  $0.1$  and  $0.2 \text{ \AA}$ , is the same as that between  $1.1$  and  $1.2 \text{ \AA}$ , for example. A large number of relp's are stimulated at one orientation of the crystal sample.

The proportion of relp's within a sphere of small  $d^*$  (i.e. at low resolution) actually stimulated is small. In addition, the probability of them being single is zero in the infinite-band-width case and small in the finite-bandwidth case. However, Laue

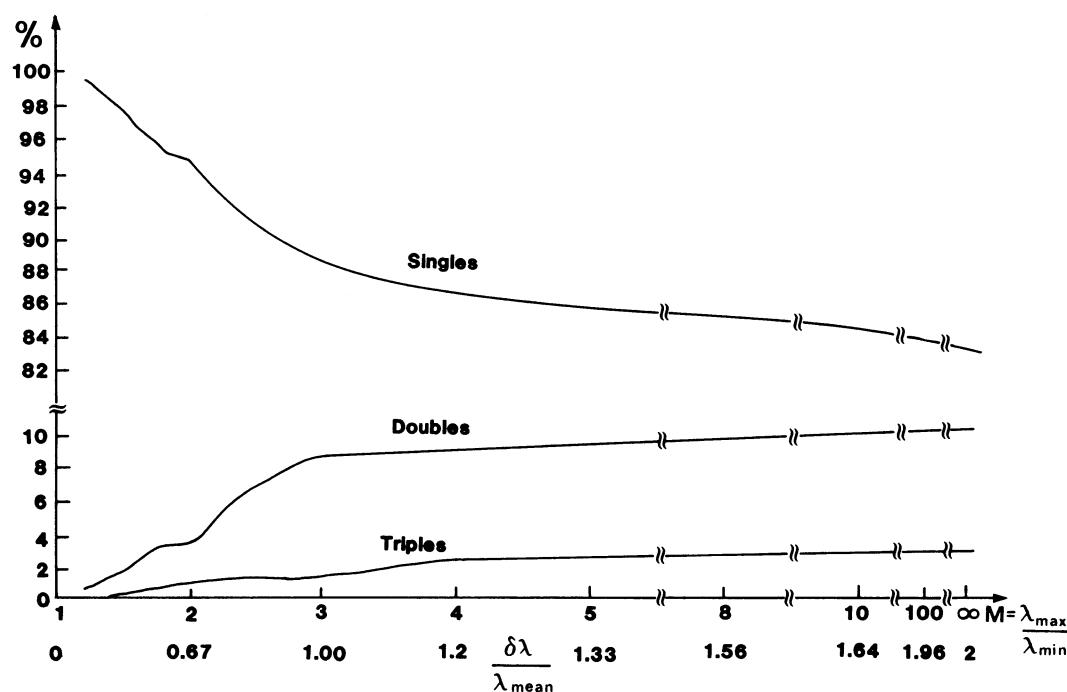


Fig. 2.2.1.4. The variation with  $M = \lambda_{\max}/\lambda_{\min}$  of the proportions of relp's lying on single, double, and triple rays for the case  $\lambda_{\max} < 2/d_{\max}^*$ . From Cruickshank, Helliwell & Moffat (1987).