

## 2. DIFFRACTION GEOMETRY AND ITS PRACTICAL REALIZATION

crystal-surface normal, is also the ratio of spatial widths of the incoming to the outgoing beams,  $W_{in}/W_{out}$ . In the case of symmetric Bragg reflection, the perfect crystal  $U$  would totally reflect (in the zero-absorption case) over a small angular range,  $w_S$ . In the asymmetric case, the ranges of total reflection are  $w_{in}$  for the incoming rays and  $w_{out}$  for the outgoing. Dynamical-diffraction theory [IT B (1996, Part 5)] shows that  $w_{out} = bw_{in} = b^{1/2} w_S$ , so that  $w_{in} W_{in} = w_{out} W_{out}$  (as would be expected from energy conservation). Thus, highly asymmetric reflection from the reference crystal  $U$  not only provides a spatially wide beam, able to cover a large area of  $V$  without recourse to any mechanical traversing motion of the components  $S$ ,  $U$  or  $V$ , but also produces a desirably narrow angular probe for studying the angular breadth of reflection of  $V$ . In practice, values of  $b$  lower than 0.1 can be used.

Du Mond diagrams for the  $+ -$  arrangement are shown in Fig. 2.7.3.4(a) and (b). For simplicity, the curves (slope  $d\lambda/d\theta = 2d \cos \theta$ ) are represented by straight lines. In the  $+ -$  setting,  $\theta_V - \theta_U = \omega$  and  $\Delta\theta_V = \Delta\theta_U$ . In Fig. 2.7.3.4(a), the narrow band labelled  $U$  passing through the origin represents the beam of angular width  $w_{out}$  leaving  $U$ . It is assumed that all of the specimen crystal  $V$  has the same interplanar spacing as  $U$  but that it contains a slightly misoriented minor region  $V'$  (which may be located as shown in Fig. 2.7.3.3). When  $\omega$  differs substantially from zero, the bands corresponding to crystal  $V$  and its minor part  $V'$  lie in positions  $V_1$  and  $V'_1$ , respectively, in Fig. 2.7.3.4(a). (Only the relevant part of the latter band is drawn, for simplicity.) The offset along the  $\theta$  axis between  $V_1$  and  $V'_1$  is the component  $\Delta\varphi$  of the misorientation between  $V$  and  $V'$  that lies in the plane of incidence. If  $\omega$  is reduced step-wise, a double-crystal topograph image being obtained at  $F$  at each angular setting,  $\Delta\varphi$  can be found from film densitometry, which will show at what settings band  $U$  is most effectively overlapped by band  $V$  or by band  $V'$ . When  $\omega$  is reduced to zero, the specimen crystal bands are at  $V_2$  and  $V'_2$ . The drawing shows that  $V'$  has then passed right through the setting for its Bragg reflection, which occurred at a small positive value of  $\omega$ . Since the  $U$  and  $V$  bands have identical slopes, their overlap occurs at all wavelengths when  $\omega = 0$ . In practice, only the shaded area is involved, corresponding to the wavelength range  $\lambda_{min}$  to  $\lambda_{max}$ , defined by the range of incidence angles,  $\theta_{min}$  to  $\theta_{max}$ , on the Bragg planes of crystal  $U$ . (The width of band  $U$  will generally be negligible compared with the range of  $\theta$  allowed by source width and slit collimation system.) One component of  $\Delta\varphi$  is found in the procedure just described. The second component

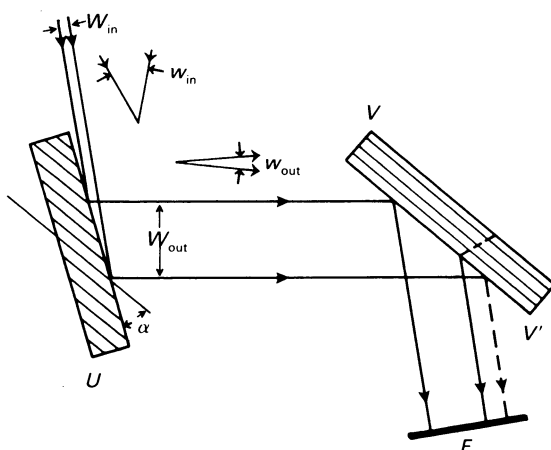


Fig. 2.7.3.3. Double-crystal topographic arrangement,  $+ -$  setting. Asymmetric reflection from reference crystal  $U$ . Specimen crystal divided into regions  $V$  and  $V'$ .

needed to specify the difference between  $\mathbf{h}$ -vector directions of the Bragg planes of  $V$  and  $V'$  is obtained by repeating the experiment after rotating  $V$  by  $90^\circ$  about  $\mathbf{h}$ .

Next consider the more general case when  $V'$  differs from  $V$  in both orientation and interplanar spacing, and both  $V'$  and  $V$  have slightly different interplanar spacings from  $U$ . The difference in orientation between  $V'$  and  $V$ ,  $\Delta\varphi$ , and their difference in interplanar spacing,  $d(V') - d(V)$ , can be distinguished by taking two series of double-crystal topographs, the orientation of the specimen in its own plane (its azimuthal angle,  $\psi$ ) being changed by a  $180^\circ$  rotation about its  $\mathbf{h}$  vector between taking the first and second series. As shown schematically in the Du Mond diagram, Fig. 2.7.3.4(b), the  $U$ ,  $V$ , and  $V'$  bands now all have slightly different slopes. [Reference crystal  $U$  is reflecting the same small wavelength band as in Fig. 2.7.3.4(a).] The setting represented in the diagram is that putting  $V$  at the maximum of its Bragg reflection. Let the  $V'$  band be then at position  $V'_0$ , for the case when  $\psi = 0^\circ$ . Assume that, when  $\psi$  is changed by  $180^\circ$ , the rotation of the specimen in its own plane can be made about the  $\mathbf{h}$  vector of  $V$  precisely. (This assumption simplifies the diagram.) Then this  $180^\circ$  rotation will not cause any translation of the  $V$  band along the  $\theta$  axis, but does transfer the  $V'$  band from  $V'_0$  to the position  $V'_{180}$ . With the sense of increasing  $\omega$  taken as that translating the specimen bands to the right and  $\Delta\omega$  taken as the difference in readings between peak reflection from  $V$  and that from  $V'$ , the diagram shows that, with  $\psi = 0^\circ$ ,  $\Delta\omega_0 = \theta(V') - \theta(V) + \Delta\varphi$ , and, with  $\psi = 180^\circ$ ,

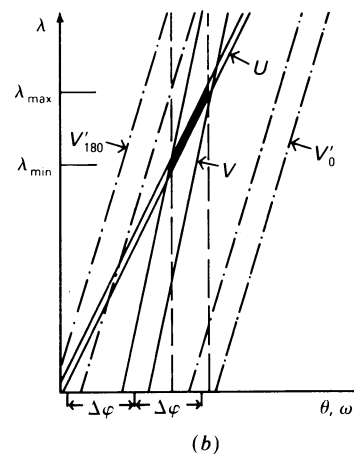
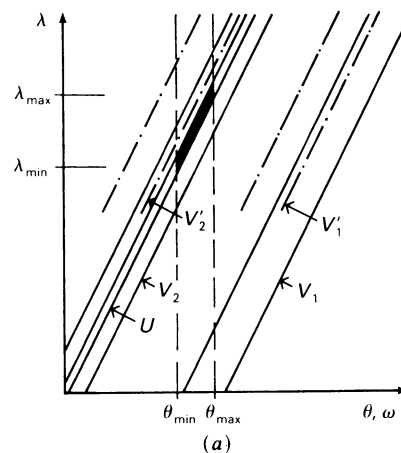


Fig. 2.7.3.4. Du Mond diagrams for  $+ -$  setting in Fig. 2.7.3.3. (a) Case when specimen region  $V'$  is misoriented with respect to  $V$ , but  $U$ ,  $V$ , and  $V'$  all have the same interplanar spacing. (b) Case when  $V'$  differs from  $V$  in both orientation and interplanar spacing, and both differ from  $U$  in interplanar spacing.