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 ω 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 θ 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 ω 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 ω 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 ω. 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 λ_{min} to λ_{max}, defined by the range of incidence angles, θ_{min} to θ_{max}, on the Bragg planes of crystal U. (The width of band U will generally be negligible compared with the range of θ allowed by source width and slit collimation system.) One component of $\Delta\varphi$ is found in the procedure just described. The second component
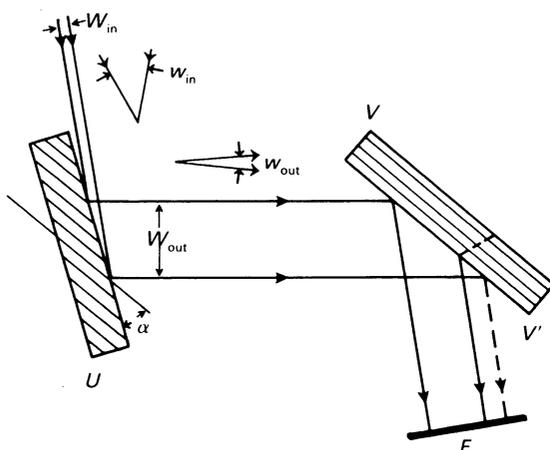
needed to specify the difference between **h**-vector directions of the Bragg planes of V and V' is obtained by repeating the experiment after rotating V by 90° about **h**.

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, ψ) being changed by a 180° rotation about its **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 $\psi = 0°$. Assume that, when ψ is changed by 180°, the rotation of the specimen in its own plane can be made about the **h** vector of V precisely. (This assumption simplifies the diagram.) Then this 180° rotation will not cause any translation of the V band along the θ axis, but does transfer the V' band from V'_0 to the position V'_{180}. With the sense of increasing ω 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 $\psi = 0°$, $\Delta\omega_0 = \theta(V') - \theta(V) + \Delta\varphi$, and, with $\psi = 180°$,
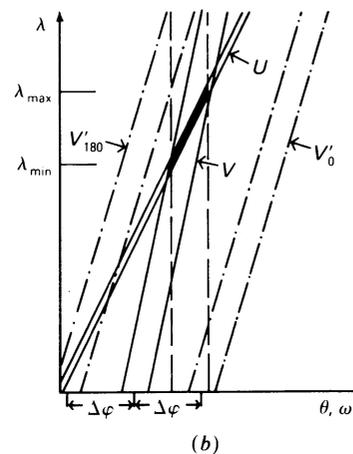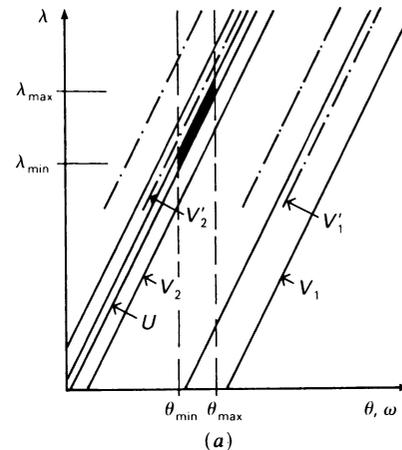

(*a*)

(*b*)

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.

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