Charts for Analysing Crystallite Distribution Function Plots for Cubic Materials

By G. J. Davies, D. J. Goodwill and J. S. Kallend

Department of Metallurgy, University of Cambridge, Pembroke Street, Cambridge, England

Charts are given which provide a rapid and unambiguous way of attributing ideal orientations to regions of crystallite orientation distribution plots for materials having cubic symmetry.

The use of the crystallite orientation distribution function in textural studies is becoming well established (Roe, 1966; Bunge & Haessner, 1968; Morris & Heckler, 1968; Bunge & Roberts, 1969; Kallend & Davies, 1969). The crystallite distribution function expresses the probability of a crystallite having the orientation described by the Euler angles ψ, θ and φ. These angles relate the crystallographic axes of the crystallite to chosen axes in the sample sheet material, e.g. normal direction, rolling direction, transverse direction (Fig. 1). Fig. 1 gives the normal mathematical convention for Euler angles (Mathews & Walker, 1965) as adopted by Roe (1966) and subsequently by Morris & Heckler (1968) and Kallend & Davies (1969). Bunge & Haessner (1968) and Bunge & Roberts (1969) on the other hand have taken the θ-rotation about the crystallographic a axis. The two conventions are related by

$$\psi_{\text{Roe}} = \psi_{1,\,\text{Bunge}} - \pi/2$$
$$\theta_{\text{Roe}} = \Phi_{\text{Bunge}}$$
$$\varphi_{\text{Roe}} = \psi_{2,\,\text{Bunge}} + \pi/2$$

and the necessary conversions must be made in comparing the results from the different sources.

The results of analyses of crystallite orientation distributions are normally represented graphically by plotting the probabilities in Eulerian space and taking constant sections of one of the Euler angles, most usually constant-φ sections.

Using these sections the textural elements can be considered in terms of ideal orientations (hkl) $[uvw]$, which correspond to Euler angles given by

$$\cos \psi = \frac{w}{(u^2 + v^2 + w^2)^{1/2}} \cdot \frac{(h^2 + k^2 + l^2)^{1/2}}{(h^2 + k^2)^{1/2}} \ (h, k \neq 0)$$

$$\cos \theta = \frac{l}{(h^2 + k^2 + l^2)^{1/2}}$$

$$\cos \varphi = \frac{-h}{(h^2 + k^2)^{1/2}} \ (h, k \neq 0)$$

For the special case in which $h = k = 0$ then

$$\cos (\psi + \varphi) = \frac{u}{(u^2 + v^2 + w^2)^{1/2}} \cdot$$

These ideal orientations are those commonly used in rolling studies in which (hkl) refers to a crystallographic plane lying in the plane of the sheet specimen and $[uvw]$

is a crystallographic direction in this plane and parallel to the rolling direction.

Alternatively, an ideal orientation can be found from known Euler angles using

$$h = -\sin \theta \cos \varphi \quad k = \sin \theta \sin \varphi \quad l = \cos \theta$$
$$u = \cos \psi \cos \theta \cos \varphi - \sin \psi \sin \varphi$$
$$v = -\cos \psi \cos \theta \sin \varphi - \sin \psi \cos \varphi$$
$$w = \cos \psi \sin \theta$$

and rationalizing the resulting indices.

In most cases this analysis is unnecessarily time-consuming and to facilitate the analysis of crystallite distribution plots a set of charts has been prepared for cubic materials. These charts show all the textural components (hkl) $[uvw]$ for cubic materials formed by permuting h, k, l, u, v, w through 3 to -3. The resulting Euler angles are taken within the ranges

$$0 \leq \psi \leq \pi/2 \quad 0 \leq \theta \leq \pi/2 \quad 0 \leq \varphi \leq \pi/2$$

which are adequate for a complete description of textures with cubic symmetry.
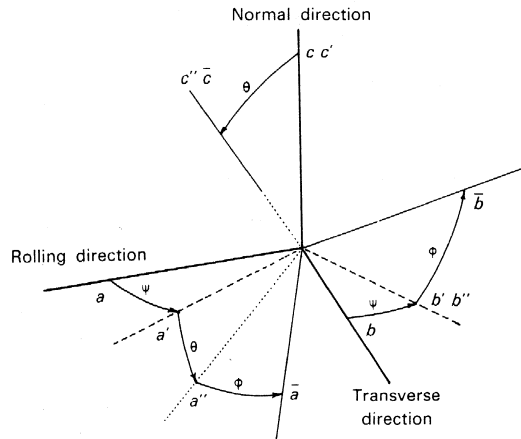

Fig. 1. Diagram illustrating the three successive rotations through the Euler angles ψ, θ and φ which relate the crystal axes to the sheet reference axes. Axes a, b, c, coincident with the sheet reference axes are rotated successively by ψ about c to a', b', c'; by θ about b' to a'', b'', c''; by φ about c'' to $\bar{a}, \bar{b}, \bar{c}$. $\bar{a}, \bar{b}, \bar{c}$ represent the final position of the crystal axes.
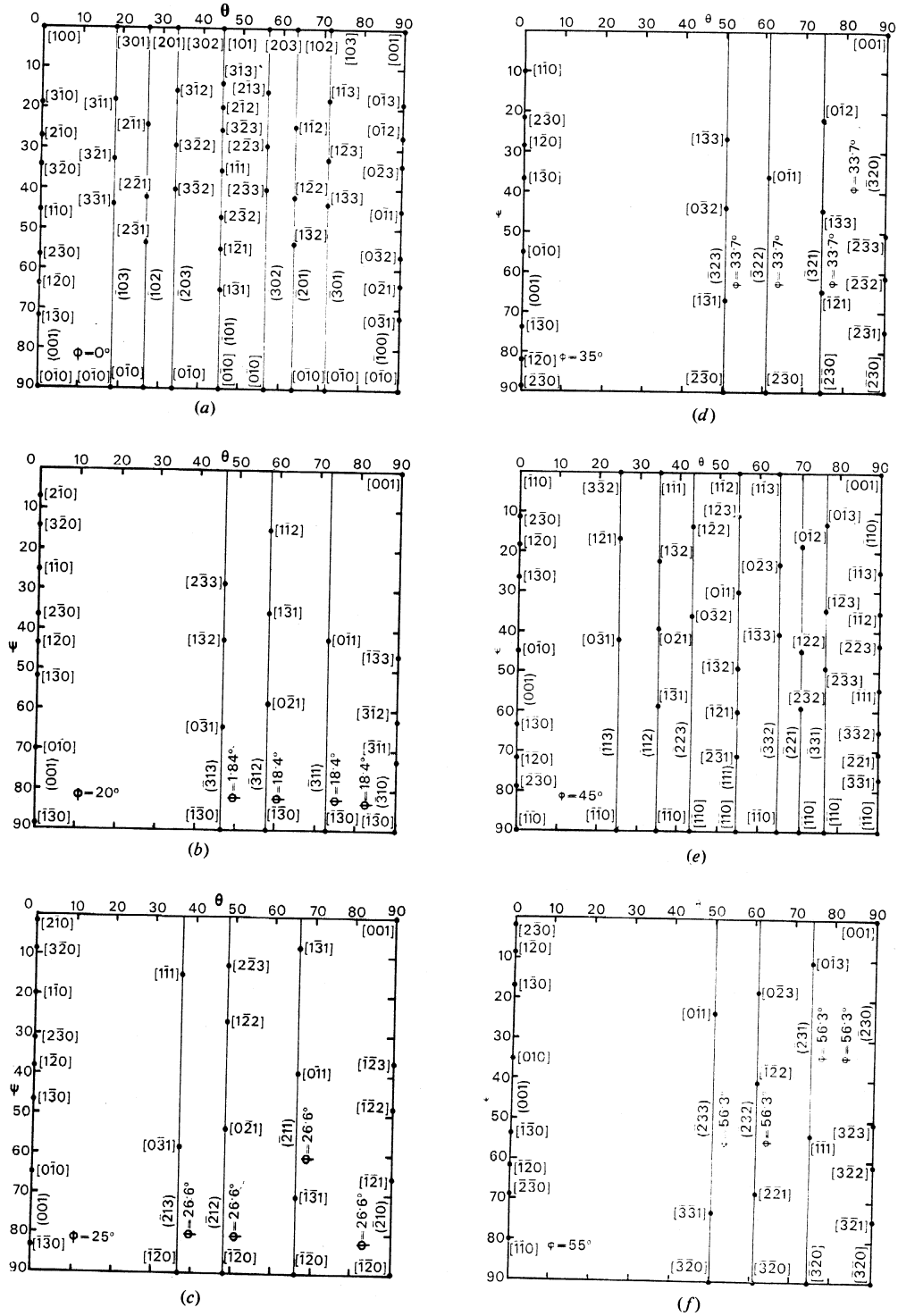
Fig. 2. Constant-φ sections through the Eulerian space (a) $\varphi = 0°$, (b) $\varphi = 20°$, (c) $\varphi = 25°$, (d) $\varphi = 35°$, (e) $\varphi = 45°$, (f) $\varphi = 55°$.

(g)

(h)

(i)
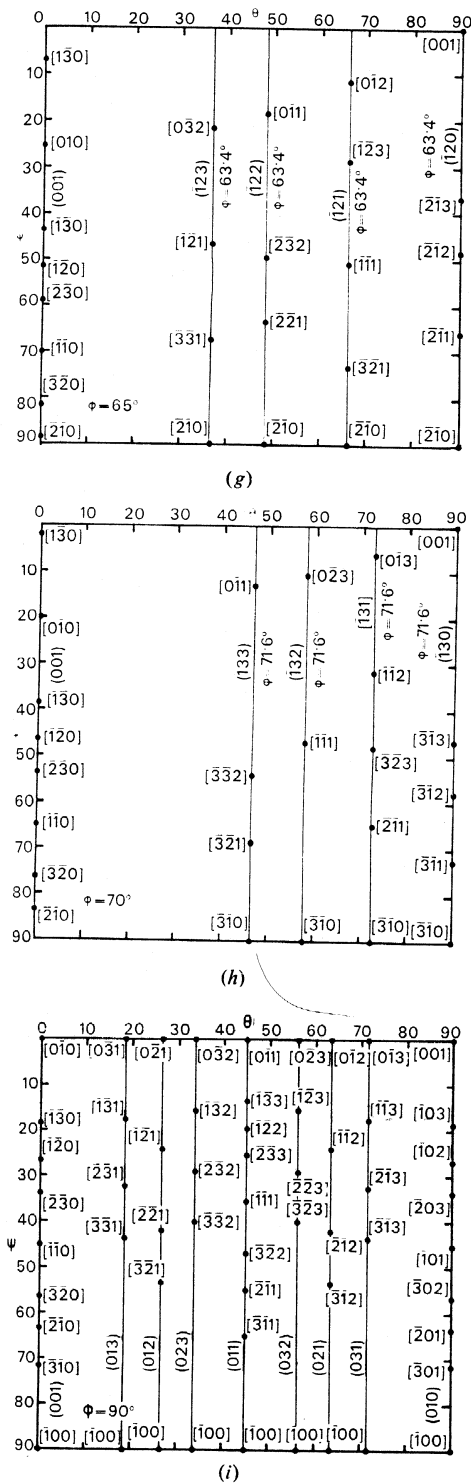
Fig 2. (cont.)

(g) $\varphi = 65°$, (h) $\varphi = 70°$, (i) $\varphi = 90°$.
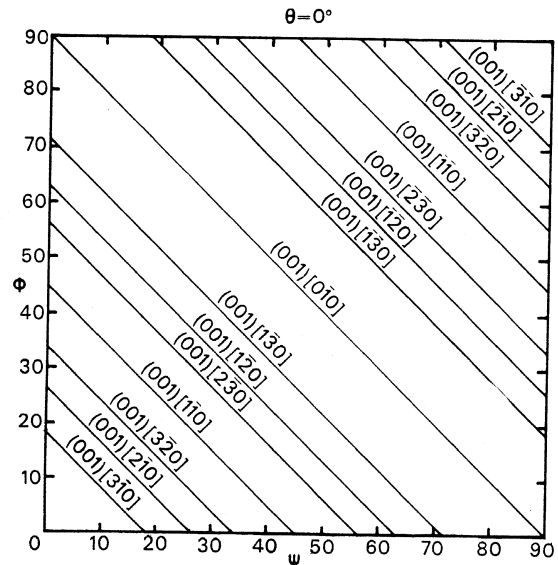
$\theta = 0°$
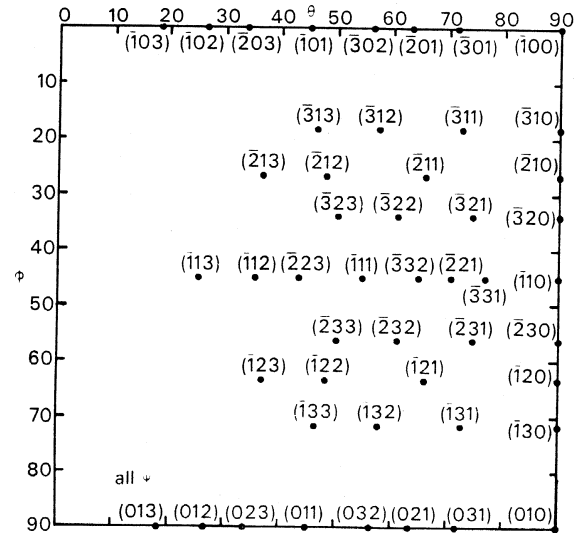
Fig. 3. The section $\theta = 0°$.

Fig. 4. The positions of the lines representing (hkl) for all ψ values.

Each ideal orientation, (hkl) $[uvw]$, is represented by a unique point in the region of Eulerian space considered.

Fig. 2(a) to (i) gives constant-φ sections through the Eulerian space. As can be seen from the expressions given above, specifying (hkl) determines θ and φ, while $[uvw]$ is needed to determine ψ. Hence the (hkl) are represented by lines of constant θ in the constant-φ sections and the corresponding $[uvw]$ as points along these lines. Each point in the charts thus represents a component (hkl) $[uvw]$. It is not practical to produce constant-φ sections for every φ value and hence where the

actual φ value differs by a small amount from the value on the section this is given on the chart. In practice this means that the point representing the appropriate (hkl) $[uvw]$ lies either just above or just below the given section.

As referred to earlier, some ambiguity exists for the ideal orientations (001) $[uv0]$ and these appear as points on all sections. Fig. 3 shows the $\theta = 0$ section which gives the lines representing these orientations.

Fig. 4 shows the positions of (hkl) lines for all ψ values. These are the lines which appear as constant-θ on the constant-φ sections.

Using these sets of charts, ideal orientations can be attributed to the high density regions of crystallite orientation distribution function plots both rapidly and unambiguously. This will enhance the understanding of the data contained in the plots as well as permitting comparison with textural data obtained by more conventional methods (Dillamore & Roberts, 1965).

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