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Determination of the odd part of the texture function

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Résumé. — Lors du calcul du développement en série de la fonction de distribution des orientations (F.D.O.) à partir de figures de pôles expérimentales, seule la partie paire (rangs l pair) a pu être considérée à ce jour, puisque les figures de pôles sont nécessairement centro-symétriques.

Si l'on tient compte de la condition de non-négativité de la F.D.O., et ce plus particulièrement dans les *domaines nuls* dans lesquels la F.D.O. prend la valeur zéro, il est également possible de déterminer la partie impaire du développement par une méthode d'approximation.

A partir de mesures d'orientations individuelles, il est également possible de déterminer les parties paires et impaires de la F.D.O.

Abstract. — By calculating the series expansion of the orientation distribution function (O.D.F.) from experimental pole-figures, previously only the even part (l even) could be considered, since the pole-figures are necessarily centro-symmetric.

When the condition of non-negativity of the O.D.F. is taken into account, particularly in the *null-domains* in which the O.D.F. is zero, it is also possible to determine the odd part of the development by means of an approximation method.

From individual orientation measurements, it is also possible to determine the even and odd parts of the O.D.F.

The orientation distribution function (O.D.F.) of crystallites in a polycrystalline material can be represented by a series of generalized spherical harmonics :

$$f(g) = \sum_{l=0(1)}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} T_l^{mn}(g). \quad (1)$$

The coefficients C_l^{mn} can be calculated from pole-figures :

$$\tilde{P}_h(\mathbf{y}) = \frac{1}{2\pi} \int_{[\pm h \parallel \mathbf{y}]} f(g) d\gamma. \quad (2)$$

The integral extends over all orientations g for which the crystallographic directions $\pm \mathbf{h}$ lie in the sample direction $\mathbf{y}$. From this we obtain :

$$P_h(\mathbf{y}) = 4\pi \sum_{l=0(1)}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} \times \frac{C_l^{mn}}{2l+1} [k_l^{*m}(\mathbf{h}) + k_l^{*m}(-\mathbf{h})] k_l^n(\mathbf{y}). \quad (3)$$

Because of the relation :

$$k_l^m(-\mathbf{h}) = (-1)^l k_l^m(\mathbf{h}) \quad (4)$$

it is not possible to calculate the coefficients with odd l from polycrystalline diffraction experiments. This has recently been pointed out by S. Matties [1]. Therefore, all previous texture analyses have neglected the odd part. As shown by Pospiech [2] *ghosts* may therefore arise. If we denote by $f^s(g)$ the part with even l in relation (1) and by $f^a(g)$ that with odd l we have :

$$f(g) = f^s(g) + f^a(g). \quad (5)$$

However, all previous methods based on series expansion give only the $f^s(g)$ part.

Now, it should be noted that the pole-figures (relation 3) frequently possess *null-domains* Z_h^0 in which $\tilde{P}$ is zero. For each rotation g , for which any pole $+\mathbf{h}$ or $-\mathbf{h}$ falls into a domain Z_h^0 of the corresponding pole-figure, the orientation density $f(g)$ must be zero.

These orientations constitute the *null-domain* Z^0 in the space of orientations g . This domain can be constructed, for instance, by the method of Imhof [4].

From relation (5), $f^a(g)$ is known in the *null-domain* :

$$f^a(g) = -f^s(g). \quad (6)$$

The coefficients C_l^{mn} of the odd part $f^a(g)$ can be approximated by the condition :

$$\int_{Z_0} \left[-f^s(g) - \sum_{l=1(2)}^L \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} T_l^{mn}(g) \right]^2 \times dg = \text{Min}. \quad (7)$$

If we set :

$$\int_{Z_0} f^s(g) T_\lambda^{mn}(g) dg = -a_\lambda^{mn} \quad (8)$$

$$\int_{Z_0} T_\lambda^{mn}(g) T_{\lambda'}^{m'n'}(g) dg = \alpha_{\lambda\lambda'}^{mn'm'n'} \quad (9)$$

the coefficients C_l^{mn} for odd l , are obtained by solving the linear equation system :

$$\sum_{l=1(2)}^L \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} \alpha_{ll'}^{mm'nn'} = a_{ll'}^{m'n'}. \quad (10)$$

The crystal directions $+\mathbf{h}$ and $-\mathbf{h}$ are indistinguishable in polycrystalline experiments, but not in individual crystal experiments. (Measurement of all the orientations g_i of individual crystallites in a polycrystal.) From the orientations g_i of a sufficient amount of crystallites, the coefficients C_l^{mn} can be determined from the relation (3, 5) :

$$C_l^{mn} = (2l+1) \frac{\sum_i V_i T_l^{mn}(g_i)}{\sum_i V_i} \quad (l = 0(1) \dots \infty). \quad (11)$$

This relation holds also for odd l . However, it also has only been used for the determination of the even part [5, 6].

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