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NON-RANDOM ORIENTATION DISTRIBUTION FUNCTIONS WITH RANDOM POLE FIGURES

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Abstract: It is shown, theoretically and with numerical examples, that the orientation distribution function may vary between zero and two or even more times random while a corresponding pole figure is completely random.

INTRODUCTION

In the literature on textures the opinion has been expressed that from a completely random pole figure one must conclude that the orientation distribution is also completely random.

It is the aim of the present paper to show that the orientation distribution function may vary between zero and two times random (or even more) while a corresponding pole figure is completely random.

1. Non-random ODF with one random pole figure

In the case of cubic crystal symmetry and orthorhombic sample symmetry the orientation distribution function (ODF) can be expressed by the series expansion,

$$f(g) = 1 + \sum_{\lambda=4}^{\infty} \sum_{\mu=1}^{M(\lambda)} \sum_{\nu=0}^{\lambda} C_{\lambda}^{\mu\nu} \, \overset{:.}{T}{}_{\lambda}^{\mu\nu}(g) \qquad (1)$$

where $\overset{:.}{T}{}_{\lambda}^{\mu\nu}(g)$ are generalized spherical functions of the orientation g which may be expressed for example by the Euler angles.

The functions are invariant with respect to the orthorhombic sample symmetry and the cubic crystal symmetry. We consider the special choice of the coefficients:

$$C_\ell^{1n} \neq 0 \quad , \quad C_\ell^{2n} \neq 0 \tag{2}$$

for a given value of ℓ chosen in the set (12,16,18,20,22) and

$$C_\lambda^{\mu\nu} = 0 \quad \text{for} \quad \begin{cases} \lambda \neq \ell \\ \lambda = \ell, \ \nu \neq n \end{cases} \tag{3}$$

In this case the function Eq. (1) takes on the following form

$$f'(g) = 1 + C_\ell^{1n} \, \dot{\dot{T}}_\ell^{1n}(g) + C_\ell^{2n} \, \dot{\dot{T}}_\ell^{2n}(g) \tag{4}$$

The (hkl)-pole figure corresponding to the general case Eq. (1) can be written in the form

$$P_{hkl}(\phi\gamma) = 1 + \sum_{\lambda=4}^{\infty} \sum_{\nu=0}^{\lambda} F_\lambda^\nu(hkl) \, \dot{K}_\lambda^\nu(\phi\gamma) \tag{5}$$

with

$$F_\lambda^\nu(hkl) = \frac{4\pi}{2\lambda + 1} \sum_{\mu=1}^{M(\lambda)} C_\lambda^{\mu\nu} \, \dot{\dot{K}}_\lambda^{*\mu}(hkl) \tag{6}$$

where the $\dot{K}_\lambda^\nu$ and $\dot{\dot{K}}_\lambda^\mu$ are spherical harmonics of orthorhombic and cubic symmetry respectively. In the particular case of Eq. (4) this leads to

$$P'_{hkl}(\phi\gamma) = 1 + F_\ell^n(hkl) \, \dot{K}_\ell^n(\phi\gamma) \tag{7}$$

with

$$F_\ell^n(hkl) = \frac{4\pi}{2\ell + 1} \left[C_\ell^{1n} \, \dot{\dot{K}}_\ell^{*1}(hkl) + C_\ell^{2n} \, \dot{\dot{K}}_\ell^{*2}(hkl) \right] \tag{8}$$

We postulate that the (hkl) pole figure be random

$$P'_{hkl}(\phi\gamma) \equiv 1 \tag{9}$$

According to Eq. (7) this leads to the condition

$$F_\ell^n(hkl) = 0 \tag{10}$$

and from Eq. (8) thus follows

$$C_\ell^{1n} \, \dot{\dot{K}}_\ell^{*1}(hkl) = - C_\ell^{2n} \, \dot{\dot{K}}_\ell^{*2}(hkl) \tag{11}$$

or (provided that $\dot{\dot{K}}_\ell^{*2}$ is not zero)

$$C_\ell^{2n} = - \frac{\dot{\dot{K}}_\ell^{*1}(hkl)}{\dot{\dot{K}}_\ell^{*2}(hkl)} \cdot C_\ell^{1n} \tag{12}$$

With Eq. (12) the ODF Eq. (4) takes on the following form:

$$f'(g) = 1 + C_\ell^{1n}\left[\ddot{T}_\ell^{1n}(g) - \frac{\dot{K}_\ell^{*1}(hkl)}{\dot{K}_\ell^{*2}(hkl)} \cdot \ddot{T}_\ell^{2n}(g)\right] \tag{13}$$

If the coefficient C_ℓ^{1n} is not zero this is a non-random orientation distribution function with a random (hkl) pole figure according to the assumption Eq. (9). If the function $f'(g)$ in Eq. (13) is to represent an orientation density then it must not be negative.

$$f'(g) \geqslant 0 \tag{14}$$

This condition leads to a restriction for the permitted values of the coefficient C_ℓ^{1n}. If we replace the functions $\ddot{T}_\ell^{\mu n}$ by their upper limit

$$|\ddot{T}_\ell^{\mu\nu}(g)| \leqslant 1 \tag{15}$$

We thus obtain the condition

$$|C_\ell^{1n}|\left[1 + \frac{|\dot{K}_\ell^{*1}(hkl)|}{|\dot{K}_\ell^{*2}(hkl)|}\right] \leqslant 1 \tag{16}$$

which leads to the condition for the maximum absolute value of the coefficient C_ℓ^{1n}

$$|C_\ell^{1n}|_{max} = \frac{|\dot{K}_\ell^{*2}(hkl)|}{|\dot{K}_\ell^{*1}(hkl)| + |\dot{K}_\ell^{*2}(hkl)|} \tag{17}$$

The values of the cubic spherical harmonics have been tabulated (see Ref. 1). With these values one easily obtains the following maximum values for the coefficients C_ℓ^{1n} in Eq. (13) (compare Table I).

$|C_\ell^{1n}|_{max} =$ (18)

ℓ \ (hkl)	(100)	(110)	(111)
12	0.262376	0.616048	0.824811
16	0.330666	0.182709	0.944293
18	0.289795	0.721933	0.419833
20	0.371170	0.495857	0.975382
22	0.373890	0.312079	0.763246

(hkl)	ℓ	K^1_ℓ	K^2_ℓ	$\lvert K^1_\ell\rvert + \lvert K^2_\ell\rvert$	$\lvert C^{1,n}_\ell\rvert_{max.}$	K^1_ℓ / K^2_ℓ	$\lvert C^{2,n}_\ell\rvert_{max.}$	$\sqrt{\frac{4\pi}{2\ell+1}}$	$\lvert C^1_\ell\rvert_{max.}$	$\lvert C^2_\ell\rvert_{max.}$
	12	0.924258	0.328762	1.253021	0.262376	2.811327	- 0.737624	0.708982	0.186020	- 0.522962
	16	0.989941	0.489053	1.478994	0.330666	2.024202	- 0.669334	0.617089	0.204050	- 0.413039
(100)	18	- 0.727509	- 0.296856	1.024365	0.289795	2.450712	- 0.710205	0.582779	0.168887	- 0.413893
	20	1.044404	0.616464	1.660868	0.371170	1.694184	- 0.628830	0.553622	0.205488	- 0.348134
	22	- 0.764143	- 0.456319	1.220463	0.373890	1.674580	- 0.626110	0.528444	0.197580	- 0.330864
	12	- 0.447688	0.718311	1.165999	0.616048	- 0.623250	0.383952	0.708982	0.436767	0.272215
	16	0.498838	0.111517	0.610355	0.182709	4.473183	- 0.817291	0.617089	0.112748	- 0.504341
(110)	18	- 0.316864	0.822660	1.139524	0.721933	- 0.385170	0.278067	0.582779	0.420727	0.162052
	20	- 0.521182	0.512617	1.033799	0.495857	- 1.016709	0.504143	0.553622	0.274517	0.279104
	22	0.397370	0.180268	0.577638	0.312079	2.204322	- 0.687921	0.528444	0.164916	- 0.363528
	12	- 0.121713	0.573042	0.694755	0.824811	- 0.212398	0.175189	0.708982	0.584776	0.124205
	16	0.057939	- 0.982131	1.040070	0.944293	- 0.058993	0.055707	0.617089	0.582713	0.034376
(111)	18	0.454180	- 0.328664	0.782844	0.419833	- 1.381899	0.580167	0.582779	0.244670	0.338109
	20	- 0.0271167	1.076393	1.103561	0.975382	- 0.025239	- 0.024618	0.553622	0.539993	0.013629
	22	- 0.265028	0.854396	1.119425	0.763246	- 0.310194	0.236754	0.528444	0.403332	0.125111

The term in brackes in Eq. (13) takes on positive and negative values of about the same magnitude. If the coefficient C_ℓ^{1n} is chosen as the maximum value according to Eq. (18) then the second term in Eq. (13) varies between plus and minus 1 and the orientation distribution function f'(g) itself varies between

$$0 \leqslant f'(g) \leqslant 2 \tag{19}$$

while its corresponding (hkl) pole figure is random. [Of course other pole figures of the same texture, for example the (h'k'l') pole figure, will generally not be random.]

2. Non-random fiber texture with one random pole figure

A fiber texture (axially symmetric texture) is completely described by the inverse pole figure (of the fiber axis) (see Ref. 1). In the case of cubic crystal symmetry a fiber texture can thus be represented by the series expansion

$$R(\phi\beta) = 1 + \sum_{\lambda=4}^{\infty} \sum_{\mu=1}^{M(\lambda)} C_\lambda^\mu \, \dot{K}_\lambda^\mu(\phi\beta) \tag{20}$$

The (hkl) pole figure of this texture can be written

$$P_{hkl}(\phi) = 1 + \sum_{\lambda=4}^{\infty} F_\lambda(hkl) \, \bar{P}_\lambda(\phi) \tag{21}$$

where $\bar{P}_\lambda(\phi)$ are the associated normalized Legendre functions with the coefficients

$$F_\lambda(hkl) = \sqrt{\frac{2}{2\lambda + 1}} \sum_{\mu=1}^{M(\lambda)} C_\lambda^\mu \, \dot{K}_\lambda^\mu(hkl) \tag{22}$$

We introduce the analogous specialization to Eq. (2) and (3), that is we set

$$C_\ell^1 \neq 0, \qquad C_\ell^2 \neq 0 \tag{23}$$

with ℓ chosen out of the set (12, 16, 18, 20, 22) and

$$C_\lambda^\mu = 0 \text{ for } \lambda \neq \ell \tag{24}$$

We thus obtain the special distribution function (inverse pole figure)

$$R'(\phi\beta) = 1 + C_\ell^1 \, \dot{K}_\ell^1(\phi\beta) + C_\ell^2 \, \dot{K}_\ell^2(\phi\beta) \tag{25}$$

and the (hkl) pole figure writes

$$P'_{hkl}(\phi) = 1 + F_\ell(hkl) \, \bar{P}_\ell(\phi) \tag{26}$$

with the coefficient

$$F_\ell(hkl) = \sqrt{\frac{2}{2\ell + 1}} \left[C_\ell^1 \dot{\dot{K}}_\ell^1(hkl) + C_\ell^2 \dot{\dot{K}}_\ell^2(hkl) \right] \tag{27}$$

we now postulate that the (hkl) pole figure be random

$$P'_{hkl}(\phi) \equiv 1 \tag{28}$$

This requires

$$F_\ell(hkl) = 0 \tag{29}$$

which leads to the condition

$$C_\ell^2 = - \frac{\dot{\dot{K}}_\ell^1(hkl)}{\dot{\dot{K}}_\ell^2(hkl)} C_\ell^1 \tag{30}$$

If we substitute Eq. (30) for C_ℓ^2 in Eq. (25) we thus obtain

$$R'(\phi\beta) = 1 + C_\ell^1 \left[\dot{\dot{K}}_\ell^1(\phi\beta) - \frac{\dot{\dot{K}}_\ell^1(hkl)}{\dot{\dot{K}}_\ell^2(hkl)} \cdot \dot{\dot{K}}_\ell^2(\phi\beta) \right] \tag{31}$$

If C_ℓ^1 is not equal to zero this is a non-random orientation distribution function with a random pole figure according to Eq. (28). As in the case of general textures the condition of non-negativity

$$R'(\phi\beta) \geqslant 0 \tag{32}$$

imposes a restriction on the possible values of the coefficient C_ℓ^1. The upper bound of the cubic spherical harmonics may be estimated from the following relation

$$|\dot{\dot{K}}_\ell^\mu(\phi\beta)| = \sqrt{\frac{2\ell + 1}{4\pi}} \; |\dot{\dot{T}}_\ell^{\mu 0}(\varphi_1 \phi \varphi_2)| \leqslant \sqrt{\frac{2\ell + 1}{4\pi}} \tag{33}$$

from which one obtains the upper bound of the coefficient C_ℓ^1 in Eq. (31).

$$|C_\ell^1|_{max} = \sqrt{\frac{4\pi}{2\ell + 1}} \; \frac{|\dot{\dot{K}}_\ell^2(hkl)|}{|\dot{\dot{K}}_\ell^1(hkl)| + |\dot{\dot{K}}_\ell^2(hkl)|} = \sqrt{\frac{4\pi}{2\ell + 1}} \cdot |C_\ell^{10}|_{max} \tag{34}$$

where $|C_\ell^{10}|_{max}$ are the values given in Eq. (18). The same arguments as in the case of general textures then lead to the upper and lower limit for the orientation density

$$0 \leqslant R(\phi\beta) \leqslant 2 \tag{35}$$

while the (hkl) pole figure is random according to Eq. (28). (Other pole figures of the same texture, e.g. the (h'k'l') pole figure, will generally not be random.)

3. Non-random ODF with two random pole figures

The considerations of section 1 can be extended to the case that two random pole figures are required. If in this case the ODF is not to be zero then there must be at least three linearly independent coefficients of the order ℓ, i.e. $M(\ell) = 3$. We thus set

$$C_\ell^{1n} \neq 0, \quad C_\ell^{2n} \neq 0, \quad C_\ell^{3n} \neq 0 \tag{36}$$

with ℓ taken out of the set (24, 28, 30, 32, 34) and

$$C_\lambda^{\mu\nu} = 0 \qquad \text{for} \begin{cases} \lambda \neq \ell \\ \lambda = \ell, \ \nu \neq n \end{cases} \tag{37}$$

The general ODF Eq. (1) thus takes on the following form

$$f''(g) = 1 + C_\ell^{1n} \dot{\dot{T}}_\ell^{1n}(g) + C_\ell^{2n} \dot{\dot{T}}_\ell^{2n}(g) + C_\ell^{3n} \dot{\dot{T}}_\ell^{3n}(g) \tag{38}$$

The (hkl) and (h'k'l') pole figure of this texture are

$$P''_{hkl}(\phi\gamma) = 1 + F_\ell^n(hkl)\ \dot{K}_\ell^n(\phi\gamma) \tag{39}$$

$$P''_{h'k'l'}(\phi\gamma) = 1 + F_\ell^n(h'k'l')\ \dot{K}_\ell^n(\phi\gamma) \tag{40}$$

with the coefficients

$$F_\ell^n(hkl) = \frac{4\pi}{2\ell+1}\left[C_\ell^{1n}\dot{\dot{K}}_\ell^{*1}(hkl) + C_\ell^{2n}\dot{\dot{K}}_\ell^{*2}(hkl) + C_\ell^{3n}\dot{\dot{K}}_\ell^{*3}(hkl)\right] \tag{41}$$

$$F_\ell^n(h'k'l') = \frac{4\pi}{2\ell+1}\left[C_\ell^{1n}\dot{\dot{K}}_\ell^{*1}(h'k'l') + C_\ell^{2n}\dot{\dot{K}}_\ell^{*2}(h'k'l') + C_\ell^{3n}\dot{\dot{K}}_\ell^{*3}(h'k'l')\right] \tag{42}$$

We postulate that both pole figure Eq. (39) and (40) be random

$$P''_{hkl}(\phi\gamma) \equiv 1, \quad P''_{h'k'l'}(\phi\gamma) \equiv 1 \tag{43}$$

This leads to an homogeneous system of two equations [the brackets in Eq. (41) and (42)] with three unknowns which has a solution of the form

$$C_\ell^{2n} = A\ C_\ell^{1n}, \qquad C_\ell^{3n} = B\ C_\ell^{1n} \tag{44}$$

with

$$A = -\frac{\dot{\dot{K}}{}^{*1}_{\ell}(h'k'l')\ \dot{\dot{K}}{}^{*3}_{\ell}(hkl) - \dot{\dot{K}}{}^{*1}_{\ell}(hkl)\ \dot{\dot{K}}{}^{*3}_{\ell}(h'k'l')}{\dot{\dot{K}}{}^{*2}_{\ell}(h'k'l')\ \dot{\dot{K}}{}^{*3}_{\ell}(hkl) - \dot{\dot{K}}{}^{*2}_{\ell}(hkl)\ \dot{\dot{K}}{}^{*3}_{\ell}(h'k'l')} \tag{45}$$

$$B = +\frac{\dot{\dot{K}}{}^{*1}_{\ell}(h'k'l')\ \dot{\dot{K}}{}^{*2}_{\ell}(hkl) - \dot{\dot{K}}{}^{*1}_{\ell}(hkl)\ \dot{\dot{K}}{}^{*2}_{\ell}(h'k'l')}{\dot{\dot{K}}{}^{*2}_{\ell}(h'k'l')\ \dot{\dot{K}}{}^{*3}_{\ell}(hkl) - \dot{\dot{K}}{}^{*2}_{\ell}(hkl)\ \dot{\dot{K}}{}^{*3}_{\ell}(h'k'l')} \tag{46}$$

Thus the ODF Eq. (38) becomes

$$f''(g) = 1 + C^{1n}_{\ell}\left[\dot{\dot{T}}{}^{1n}_{\ell}(g) + A\cdot\dot{\dot{T}}{}^{2n}_{\ell}(g) + B\cdot\dot{\dot{T}}{}^{3n}_{\ell}(g)\right] \tag{47}$$

The condition

$$f''(g) \geqslant 0 \tag{48}$$

leads then to the condition

$$|C^{1n}_{\ell}|_{max} = \frac{1}{1 + |A| + |B|} \tag{49}$$

The function f"(g) Eq. (47) is a non-random ODF with random (hkl) *and* (h'k'l') pole figures. If the coefficient C^{1n}_{ℓ} is chosen according to Eq. (49) then the maximum negative value of the second term in Eq. (47) does not exceed 1; hence Eq. (48) is fulfilled. If we may assume that in this case the maximum positive value is approximately of the same magnitude then f"(g) varies in the limits

$$0 \leqslant f''(g) \leqslant 2 \tag{50}$$

4. Non-random fiber texture with two random pole figures

In a similar way one obtains for fiber textures

$$R''(\phi\beta) = 1 + C^{1}_{\ell}\left[\dot{\dot{K}}{}^{1}_{\ell}(\phi\beta) + A\cdot\dot{\dot{K}}{}^{2}_{\ell}(\phi\beta) + B\cdot\dot{\dot{K}}{}^{3}_{\ell}(\phi\beta)\right] \tag{51}$$

with the values A and B of Eq. (45) and (46). The estimation of the maximum value of the symmetric spherical harmonics Eq. (33) yields the estimation of the maximum value of the coefficient C^{1}_{ℓ} in order that the function R" is not negative

$$|C^{1}_{\ell}|_{max} \leqslant \sqrt{\frac{4\pi}{2\ell + 1}} \cdot \frac{1}{1 + |A| + |B|} \tag{52}$$

The assumption that the maximum positive value of the expression in brackets of Eq. (51) be approximately the same as the maximum negative value leads thus to the estimation

$$0 \leqslant R''(\phi\beta) \leqslant 2 \tag{53}$$

while the (hkl) pole figure as well as the (h'k'l') pole figure both are random.

It is easily seen that these considerations can be extended to more than two pole figures. Indeed one can postulate that $M(\ell) - 1$ pole figures be random and at the same time the texture varies in the range from zero to about two according to Eq. (50) or (53).

5. Generalizations

In the case of $M(\ell) = 2$ and one random pole figure the indices ℓ and n could be chosen out of a set of values given in Eq. (2) and (3). Instead of the orientation distribution function f'(g) Eq. (13) we can sum up over all possible values of ℓ and n and still the (hkl) pole figure will be random.

$$f'''(g) = 1 + \sum_{\ell=12,16..22} \sum_{n=0}^{\ell} C_\ell^{1n} \left[\ddot{T}_\ell^{1n}(g) - \frac{\dot{K}_\ell^{*1}(hkl)}{\dot{K}_\ell^{*2}(hkl)} \ddot{T}_\ell^{2n}(g) \right] \tag{54}$$

The non-negativity condition

$$f'''(g) > 0 \tag{55}$$

leads to the following condition for the coefficients

$$\sum_\ell \sum_n |C_\ell^{1n}| \left[1 + \frac{|\dot{K}_\ell^{*1}(hkl)|}{|\dot{K}_\ell^{*2}(hkl)|} \right] \leqslant 1 \tag{56}$$

which defines a permitted range in the space of the coefficients C_ℓ^{1n}. Figure 1 shows a two-dimensional section of the multidimensional space defined by Eq. (56). The equality sign in Eq. (56) defines a straight line or in the multidimensional case an hyperplane in the space of the coefficients which intersects the coordinate axes at certain positive values. Because only the absolute value of C_ℓ^{1n} enters Eq. (56) the corresponding hyperplanes intersecting at negative values represent further boundaries of the permitted region in the space of coefficients. Every choice of coefficients C_ℓ^{1n} within this region represents a non-random texture with a random (hkl) pole figure.

Thus far we have considered special orientation distribution functions with only such values of ℓ that $M(\ell)$ was constant, and we postulated that $M - 1$ pole figures be random. We now look at the specific case $M(\ell) = 3$ and we postulate that *one* pole figure be random. This leaves two degrees of freedom for every choice of ℓ and n. We assume a texture with coefficients according to Eq. (36) and (37) but we postulate that only $F_\ell^n(hkl)$ of Eq. (41) be zero [and not $F_\ell^n(h'k'l')$ of

Eq. (42)]. This leads to the condition

$$C_\ell^{3n} = -\frac{\dot{\dot{K}}{}_\ell^{*1}(hkl)}{\dot{\dot{K}}{}_\ell^{*3}(hkl)} \cdot C_\ell^{1n} - \frac{\dot{\dot{K}}{}_\ell^{*2}(hkl)}{\dot{\dot{K}}{}_\ell^{*3}(hkl)} \cdot C_\ell^{2n} \tag{57}$$

The function Eq. (38) can then be written

$$f''(g) = 1 + C_\ell^{1n}\left[\dot{\dot{T}}{}_\ell^{1n}(g) - \frac{\dot{\dot{K}}{}_\ell^{*1}(hkl)}{\dot{\dot{K}}{}_\ell^{*3}(hkl)} \cdot \dot{\dot{T}}{}_\ell^{3n}(g)\right] + C_\ell^{2n}\left[\dot{\dot{T}}{}_\ell^{2n}(g) - \frac{\dot{\dot{K}}{}_\ell^{*2}(hkl)}{\dot{\dot{K}}{}_\ell^{*3}(hkl)} \cdot \dot{\dot{T}}{}_\ell^{3n}(g)\right] \tag{58}$$

If C_ℓ^{1n} and C_ℓ^{2n} are not zero at the same time then Eq. (58) represents a non-random texture with a random (hkl) pole figure. The non-negativity condition together with the estimation of the maximum values of $\dot{\dot{T}}{}_\ell^{\mu n}$ according to Eq. (15) leads to the condition for the coefficients

$$|C_\ell^{1n}|\left[1 + \frac{|\dot{\dot{K}}{}_\ell^{*1}(hkl)|}{|\dot{\dot{K}}{}_\ell^{*3}(hkl)|}\right] + |C_\ell^{2n}|\left[1 + \frac{|\dot{\dot{K}}{}_\ell^{*2}(hkl)|}{|\dot{\dot{K}}{}_\ell^{*3}(hkl)|}\right] \leqslant 1 \tag{59}$$

which is very similar to Eq. (56). If we set

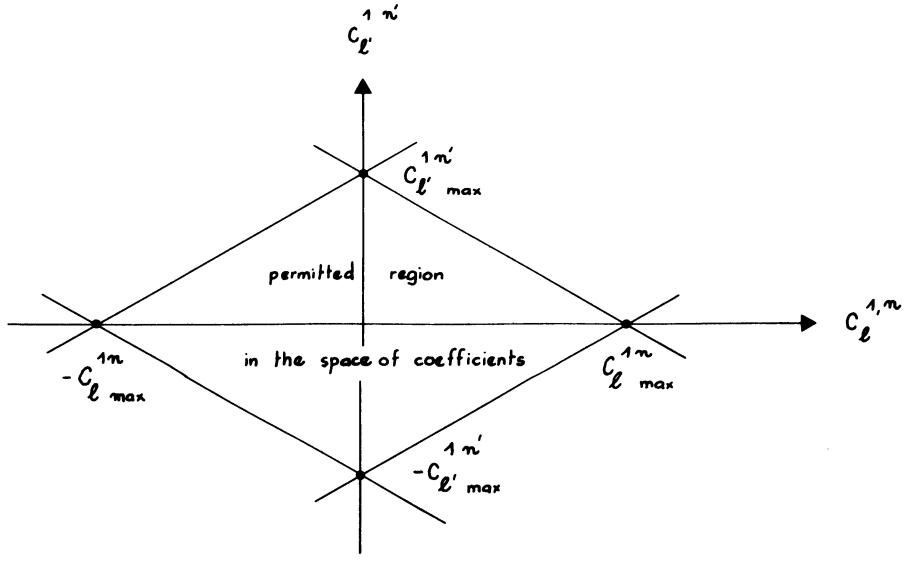


Figure 1. Two-dimensional section of the multi-dimensional coefficient space defined by Eq. (56).

$$|C_\ell^{in}|_{max} = \frac{|\dot{\dot{K}}_\ell^{*3}(hkl)|}{|\dot{\dot{K}}_\ell^{*i}(hkl)| + |\dot{\dot{K}}_\ell^{*3}(hkl)|} \tag{60}$$

then Eq. (59) reads

$$\frac{|C_\ell^{1n}|}{|C_\ell^{1n}|_{max}} + \frac{|C_\ell^{2n}|}{|C_\ell^{2n}|_{max}} \leqslant 1 \tag{61}$$

which defines a permitted region for the coefficients similar to that one shown in Figure 1.

6. The general case of a non-random texture with one random pole figure

Finally we consider an orientation distribution function according to Eq. (1) and we do not introduce the restrictions Eq. (2) and (3) to the coefficients. The (hkl) pole figure is postulated to be random according to Eq. (9). Equation (10) introduced in Eq. (6) thus leads to the condition

$$C_\lambda^{M\nu} = - \sum_{\mu=1}^{M(\lambda)-1} \frac{\dot{\dot{K}}_\lambda^{*\mu}(hkl)}{\dot{\dot{K}}_\lambda^{*M}(hkl)} C_\lambda^{\mu\nu} \tag{62}$$

with this condition the distribution function Eq. (1) takes on the following form

$$f(g) = 1 + \sum_{\lambda=12}^{\infty} \sum_{\mu=1}^{M(\lambda)-1} \sum_{\nu=0}^{\lambda} C_\lambda^{\mu\nu} \left[\dot{\dot{T}}_\lambda^{\mu\nu}(g) - \frac{\dot{\dot{K}}_\lambda^{*\mu}(hkl)}{\dot{\dot{K}}_\lambda^{*M}(hkl)} T_\lambda^{M\nu}(g) \right] \tag{63}$$

where λ runs over all those values for which

$$M(\lambda) \geqslant 2 \tag{64}$$

That is,

$$\lambda = 12,\ 16,\ 18,\ \ldots.(2)\ldots.\ \infty \tag{65}$$

The non-negativity condition together with the estimation Eq. (15) leads to the condition for the coefficients

$$\sum_{\lambda=12,16..}^{\infty} \sum_{\mu=1}^{M(\lambda)-1} \sum_{\nu=0(2)}^{\lambda} \frac{|C_\lambda^{\mu\nu}|}{|C_\lambda^{\mu\nu}|_{max}} \leqslant 1 \tag{66}$$

where

$$|C_\lambda^{\mu\nu}|_{max} = \frac{|\dot{K}_\lambda^{*M}(hkl)|}{|\dot{K}_\lambda^{*M}(hkl)| + |\dot{K}_\lambda^{*\mu}(hkl)|} \tag{67}$$

Equation (66) defines a permitted region in the space of the coefficients which is limited by several hyperplanes defined by the equality sign in Eq. (66). All functions in Eq. (1) with coefficients $C_\lambda^{\mu\nu}$ satisfying Eq. (66) are non-random textures with a random (hkl) pole figure.

The permitted region Eq. (66) is so chosen that the non-negativity condition is necessarily fulfilled.

There may however be coefficients corresponding to points outside the region Eq. (66) that do not violate the non-negativity condition, that is to say, that the maximum permitted region may be larger than that defined by Eq. (66). Hence Eq. (66) is a sufficient but not a necessary condition for non-negativity of the distribution function.

In the special cases with only very few coefficients $C_\lambda^{\mu\nu}$ different from zero, e.g. Eq. (2) and (3), it was assumed that the term in brackets in Eq. (13) takes on maximum positive values of the same order as the maximum negative values. This condition holds for every single function $\dot{\dot{T}}_\lambda^{\mu\nu}(g)$. Hence we obtained the upper bound Eq. (19) for the function f'(g). If the series expansion of a distribution function contains however a large number of terms the upper bound of the assumed positive values may be much higher than that of the negative values. Hence a special choice of coefficients $C_\lambda^{\mu\nu}$ may exist [certainly outside the region defined by Eq. (67)] such that for the function Eq. (63) the condition holds

$$0 \leqslant f(g) < f_{max} \tag{68}$$

with $f_{max} > 2$.

A function of this type can be constructed if in Eq. (63) the coefficient $C_\lambda^{\mu\nu}$ is given the same sign as the function in brackets takes on at a certain orientation g_0. Thus we may set for example

$$C_\lambda^{\mu\nu} = B(2\lambda + 1)\left[\dot{\dot{T}}_\lambda^{\mu\nu}(g_0) - \frac{\dot{K}_\lambda^{*\mu}(hkl)}{\dot{K}_\lambda^{*M}(hkl)}\,\dot{\dot{T}}_\lambda^{M\nu}(g_0)\right] \tag{69}$$

Then all the terms in the sum Eq. (63) are positive at the orientation g_0 whereas they will take on positive and negative values at other orientations thus leading to smaller (positive or negative) values. If we put

$$\frac{1}{B} = -\left[\sum_{\lambda=12}^{\infty}\sum_{\mu=1}^{M(\lambda)-1}\sum_{\nu=0}^{\lambda} C_\lambda^{\mu\nu}\left[\dot{\dot{T}}_\lambda^{\mu\nu}(g) - \frac{\dot{K}_\lambda^{*\mu}(hkl)}{\dot{K}_\lambda^{*M}(hkl)}\,\dot{\dot{T}}_\lambda^{M\nu}(g)\right]\right]_{Min} \tag{70}$$

then the maximum negative value of the sum in Eq. (63) will remain above -1 everywhere so that the non-negativity condition Eq. (68) is not violated whereas f_{max} will be larger than 2 according to Eq. (68). At the same time the (hkl) pole figure is random as was assumed.

In the case of fiber textures, Eq. (20), with one random pole figure we obtain similarly

$$R(\phi\beta) = 1 + \sum_{\lambda=12}^{\infty} \sum_{\mu=1}^{M(\lambda)-1} C_\lambda^\mu \left[\dot{K}_\lambda^\mu(\phi\beta) - \frac{\dot{K}_\lambda^\mu(hkl)}{\dot{K}_\lambda^M(hkl)} \dot{K}_\lambda^M(\phi\beta) \right] \tag{71}$$

In order that the function takes on a high value at the orientation $\phi_0\beta_0$ we put

$$C_\lambda^\mu = B\ 4\pi \left[\dot{K}_\lambda^\mu(\phi_0\beta_0) - \frac{\dot{K}_\lambda^\mu(hkl)}{\dot{K}_\lambda^M(hkl)} \dot{K}_\lambda^M(\phi_0\beta_0) \right] \tag{72}$$

where

$$\frac{1}{B} = -\left[\sum_{\lambda=12}^{\infty} \sum_{\mu=1}^{M(\lambda)-1} C_\lambda^\mu \left[\dot{K}_\lambda^\mu(\phi\beta) - \frac{\dot{K}_\lambda^\mu(hkl)}{\dot{K}_\lambda^M(hkl)} \dot{K}_\lambda^M(\phi\beta) \right] \right]_{Min} \tag{73}$$

For this function a variability range will be obtained

$$0 < R(\phi\beta) < R_{max} \tag{74}$$

with $R_{max} > 2$ (75)

These considerations have shown that it is possible to construct orientation distribution functions with a considerable range of variation according to Eq. (68) or at least according to Eq. (19) which have one or even more random pole figures. If $f^{(n)}(g)$ is a so constructed non-random function with n random pole figures then

$$\Delta f(g) = f^{(n)}(g) - 1 \tag{76}$$

is a non-random function with n pole figures which are identically zero. [Of course, $\Delta f(g)$ will generally not obey the non-negativity condition.] If f(g) is a certain orientation distribution function then the function

$$f'(g) = f(g) + \Delta f(g) \tag{77}$$

has exactly the same n pole figures as the function f(g) which we started with. The two functions cannot be distinguished from the n pole figures under consideration. The function $\Delta f(g)$ thus describes the ambiguity of the orientation distribution determined from n pole figures. The variability range of the function $\Delta f(g)$ may be restricted to a certain degree since the non-negativity condition must hold for f'(g).

c

The restriction is however the smaller the less f(g) deviates from 1 (the random distribution).

These considerations must be kept in mind when an orientation distribution function f(g) is calculated from pole figure data by methods not based on series expansion such as the methods described by Williams,[2] Ruer[3] or Imhof.[4] In these methods a solution f(g) is constructed from pole figures.

There is however no way of estimating the ambiguity range of the obtained solution.

The three methods have been described with one or two pole figures as the starting experimental data.

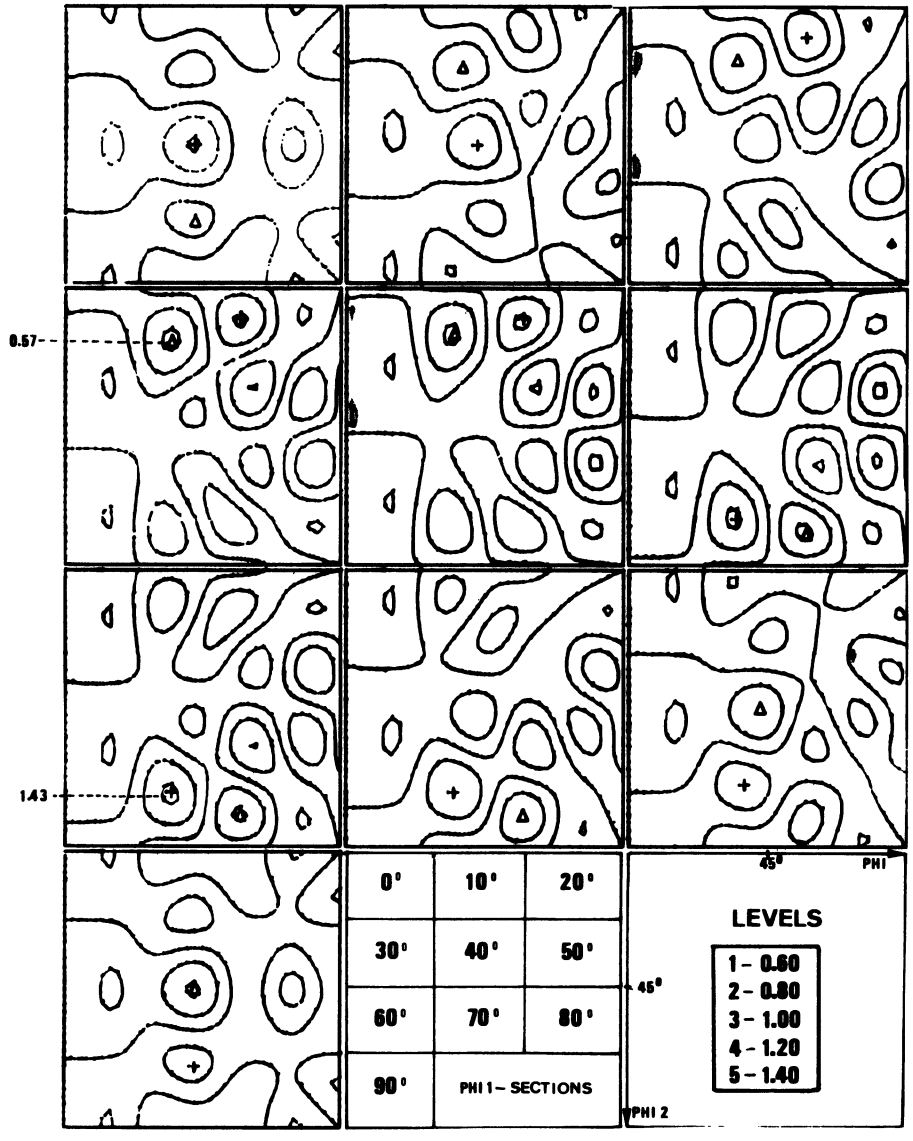
If these pole figures are random the solution according to the methods[2-4] is a random distribution function. As has been shown however in this paper the solution can equally well be one of the functions f'(g) or f"(g) constructed above which can vary at least in the region from zero to twice the random density.

7. Numerical examples

In order to get an impression of the shape of non-random orientation distribution functions with random pole figures according to the above formulae some numerical examples have been calculated and have been graphically represented in the following Figures 2-4. All the examples correspond to *one* random pole figure respectively.

The particular case of functions of one rank ℓ only has been considered in section 1. They consist of two generalized spherical harmonics Eq. (4) the coefficients of which are determined according to Eq. (17) and (12). Table I gives the numerical calculation of these coefficients starting with the values $\dot{K}^1_\ell(hkl)$ and $\dot{K}^2_\ell(hkl)$ of cubic spherical harmonics for the cases (hkl) = (100), (110), (111), where (hkl) are the indices of the pole figure which is assumed to be random. The so obtained coefficients $|C^{1n}_\ell|_{max}$ were already given in Eq. (18). The choice of the index n is deliberate. Figure 2a shows a distribution function of this type of the rank $\ell = 12$ with n = 2 the (100) pole figure of which is random. The function varies between its minimum value 0.57 and the maximum value 1.43 thus showing that the estimation of the maximum value of the coefficient $|C^{1n}_\ell|$ which does not violate the non-negativity condition Eq. (14) was very much on the safe side. Really the coefficients C^{1n}_ℓ and C^{2n}_ℓ could have been chosen considerably larger than the ones given in Table I (about twice as large) and still Eq. (14) would not have been violated. Figure 2b shows a function of rank $\ell = 22$ with n = 2 and a randon (100) pole figure. Here the maximum and minimum values are 1.33 and 0.67 respectively.

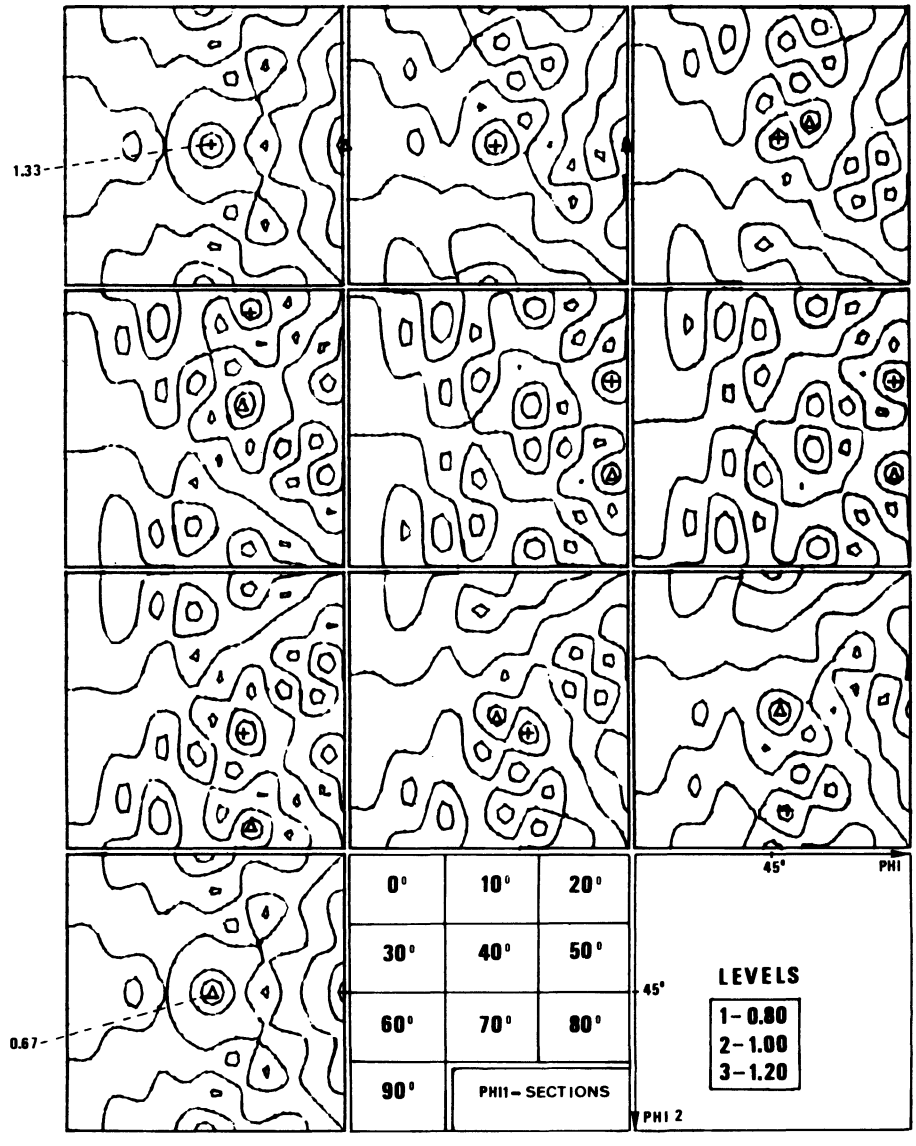
The case of axially symmetric distribution functions (inverse pole figures) of one rank ℓ only has been considered in section 2. They consist of two spherical harmonics Eq. (25)



(a)

Figure 2. Non-random orientation distribution functions having random (100) pole figures according to Eq. (4) with coefficients defined by Eq. (17) and Eq. (12). a) $\ell = 12$, $n = 2$; b) $\ell = 22$, $n = 2$.

the coefficients of which are to be chosen according to Eq. (34) and (30). The coefficients correspond to the ones of the non-axially symmetric case but for the factor $\sqrt{\frac{4\pi}{2\ell+1}}$.



(b)

These coefficients are also given in Table I. Figure 3 shows four examples of distribution functions of this type corresponding to the ranks ℓ = 16, 18 and 22 respectively. The random pole figures being (100), (110) and (111) respectively. The maximum and minimum values indicated in the figures show that in all cases the coefficients could have been chosen larger than the ones of Table I without violating the non-negativity condition.

In section 6 distribution functions containing terms of several ranks ℓ have been considered. In this case, the coefficients were so chosen that the functional value $R(\phi\beta)$ (in

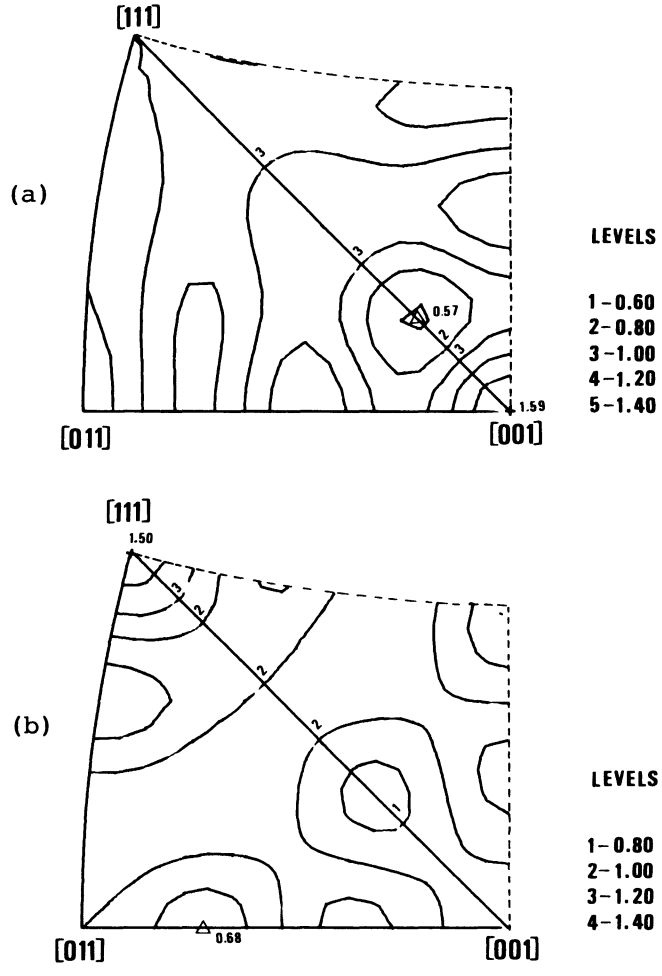
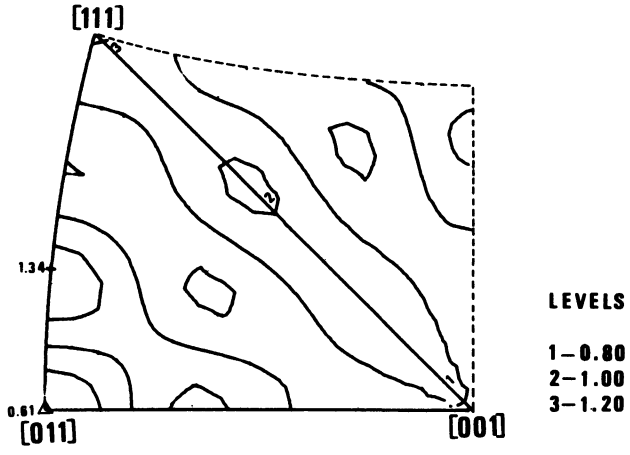


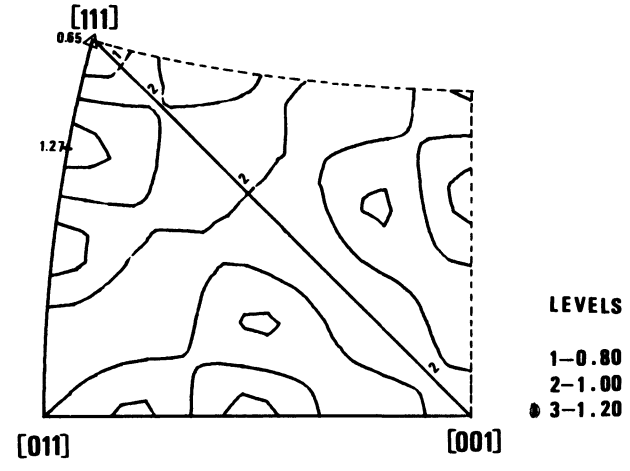
Figure 3. Non-random orientation distribution functions (inverse pole figures) for axial symmetry (fiber textures) having random (hkl) pole figures according to Eq. (25) with coefficients defined by Eq. (34) and Eq. (30). a) $\ell = 16$, (hkl) = (111); b) $\ell = 16$, (hkl) = (110); c) $\ell = 18$, (hkl) = (100); d) $\ell = 22$, (hkl) = (110).

the case of axially symmetric functions) takes on a large value at the point $[\phi_0 \beta_0]$ which also can be described by the Miller indices [uvw]. Coefficients C_λ^μ which correspond to this assumption may be obtained according to Eq. (72) where the factor B takes care of the non-negativity condition. Coefficients obtained this way for $\lambda \leqslant 22$ are given in Table II for random pole figures of the type (100), (110) and (111) the orientation of maximum value [uvw] being [100], [110] and [111] respectively. The quantity B was so chosen that the minimum functional value is equal to zero. It is obvious that

(c)



(d)



a function of this type with (hkl) = [uvw] does not exist. Figure 4 shows four examples of functions of this type with various combinations of (hkl) and [uvw]. According to the different combinations of (hkl) and [uvw] different maximum values were obtained. The largest value occurs in Figure 4a which corresponds to a random (111) pole figure. The maximum functional value of 4.17 is being taken on at the orientation [100].

The degree of the series expansion in Figure 4 was restricted to $\lambda \leqslant 22$. One can easily estimate that distribution functions with one random pole figure (or even several ones) can be obtained with unlimited maximum functional values. As is shown in Figure 5a the value of the (hkl) pole figure at the angle ϕ (in the case of axially symmetric textures) can be obtained from the inverse pole figure by taking the mean value of this figure along a small-circle of radius ϕ about the point [hkl]. In Figure 5a this is shown for the (111) pole figure and a texture having its maximum value at the

MAXIMUM ORIENTATION DENSITY AT [uvw]

RANDOM POLE FIGURE (hkl)

(hkl)	[uvw] / ℓ	[100] C^1_ℓ	[100] C^2_ℓ	[100] B	[110] C^1_ℓ	[110] C^2_ℓ	[110] B	[111] C^1_ℓ	[111] C^2_ℓ	[111] B
(100)	12				- 2.467096	6.935814	0.011296	- 1.732720	4.871244	0.011248
	16				0.273104	- 0.552818		2.045969	- 4.141455	
	18				- 2.332967	5.717430		1.259641	- 3.087017	
	20				- 1.389649	2.354321		- 1.850775	3.135554	
	22				0.095496	- 0.159915		- 1.695784	2.839727	
(110)	12	1.129160	0.703748	0.019545				0.235435	0.146735	0.005507
	16	- 1.197681	5.357444					4.451188	-19.910979	
	18	- 0.841849	- 0.324256					0.327589	0.126178	
	20	1.671169	1.699093					1.067212	1.085044	
	22	0.241731	- 0.532853					- 2.148393	4.735748	
(111)	12	0.994087	0.211142	0.047920	- 0.295120	- 0.062683	0.047920			
	16	1.018792	0.060102		0.505416	0.029816				
	18	- 1.137735	- 1.572234		0.819969	1.133114				
	20	1.059963	0.026753		- 0.508244	- 0.012828				
	22	- 0.905691	- 0.280940		0.453288	0.140607				

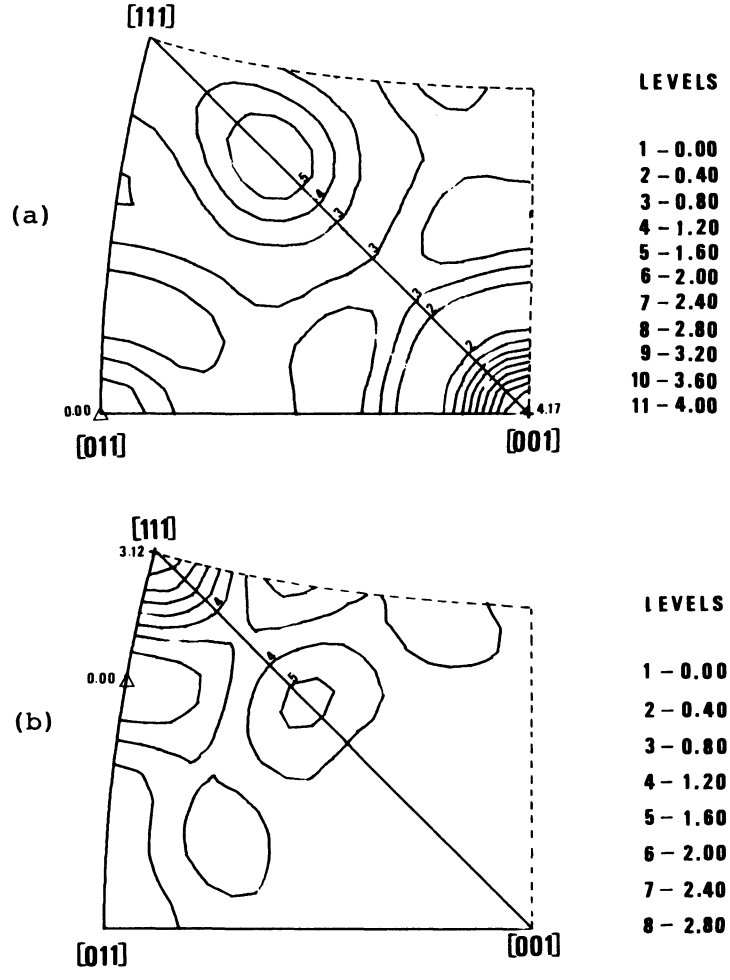
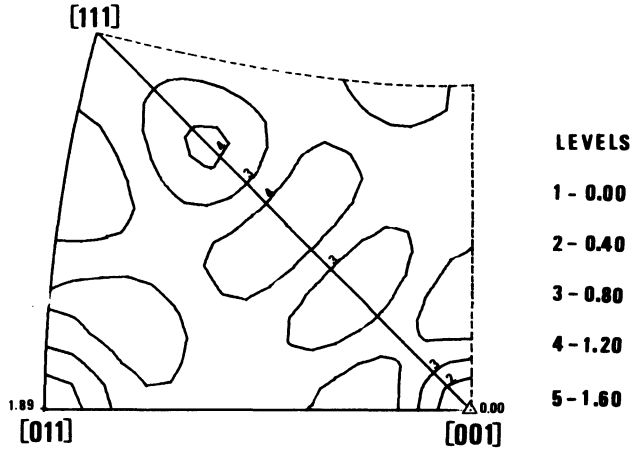


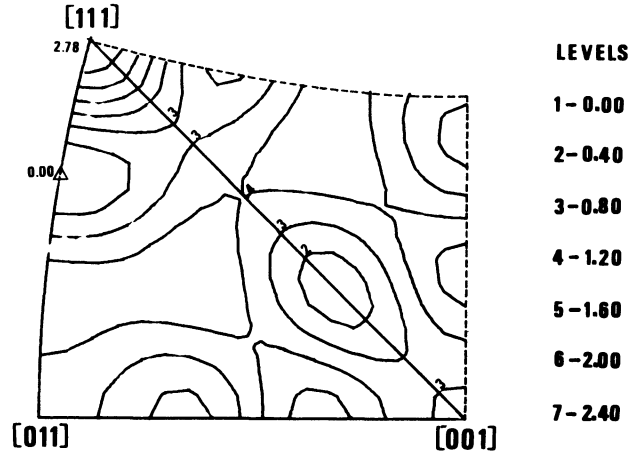
Figure 4. Non-random orientation distribution functions (inverse pole figures) for axial symmetry (fiber textures) having maximum density at the orientation [uvw] and a random (hkl) pole figure. The functions are defined according to Eq. (71) with $\lambda \leqslant 22$. The coefficients defined by Eq. (72) and Eq. (73) are given in Table II. a) [uvw] = [100], (hkl) = (111); b) [uvw] = [111], (hkl) = (100); c) [uvw] = [110], (hkl) = (111); d) [uvw] = [111], (hkl) = (110).

orientation [100] corresponding to the situation of Figure 4a. Figure 5b is a schematic representation of the functional values of the distribution function along the circle ϕ. The mean value of this distribution is the value of the (111) pole figure at the angle ϕ (from the axis of symmetry). If this pole figure is to take on the value 1 at all angles ϕ (random pole figure) then the maximum value f_m may roughly be estimated by the condition

(c)

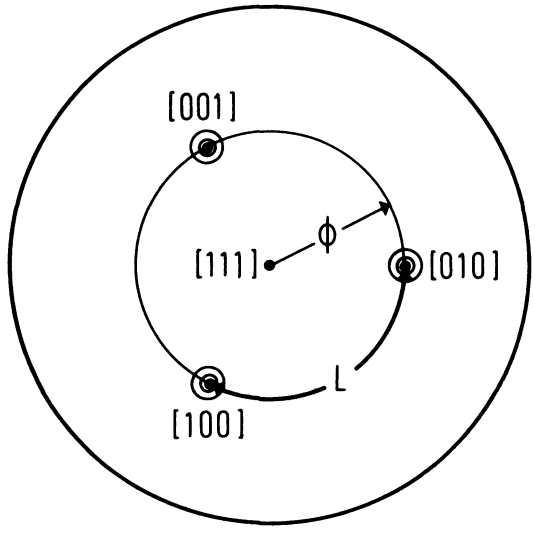


(d)

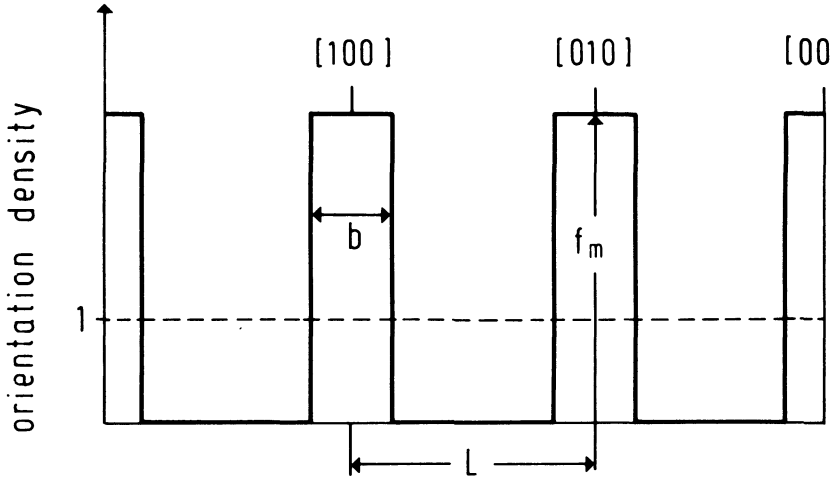


$$b \cdot f_m = l \cdot L, \quad \text{or} \quad f_m = \frac{L}{b} \tag{78}$$

Here the length of the path L is determined by the number of equivalent directions of the type [uvw] (in this case three directions of the type [100]) and the angle ϕ between these directions and the normal to the reflecting lattice plane of the (hkl) pole figure [in this case (111)]. If the distribution function is represented by a series expansion, b may be taken as the half-value-width of a peak represented by a series of maximum degree ℓ. This was called the angular resolving power corresponding to the series degree ℓ. As was shown in Ref. 1, p. 109, b decreases to zero if ℓ is increased to infinity. Hence, it is obvious from Eq. (78) that non-random distribution functions with infinitely high peak values can be constructed which have one (or even more) random pole figures.



(a)



(b)

Figure 5. An inverse pole figure having peaks at [100]. The mean value of this function along a small circle of radius ϕ about the [111] direction corresponds to the value of the (111) pole figure at the angle ϕ.

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