On the generation of pole figures from standard orientation distribution functions

1992 J. Phys.: Condens. Matter 4 L629

(http://iopscience.iop.org/0953-8984/4/48/001)

J. Phys.: Condens. Matter 4 (1992) L629–L632. Printed in the UK

LETTER TO THE EDITOR

On the generation of pole figures from standard orientation distribution functions

T Vodenicharova† and K Krezhov‡

† Institute for Foreign Students, 27 A Veltchev Strasse, 1111 Sofia, Bulgaria
‡ Bulgarian Academy of Sciences, Institute for Nuclear Research and Nuclear Energy, 1784 Sofia, Bulgaria

Received 17 August 1992

Abstract. A local projection technique for the mathematical construction of pole figures on the basis of a Gaussian-shaped orientation distribution function of microcrystallites in texture is presented. The relationship between this function and pole figures and some results from this technique are shown.

The direction of the normal h_i to the set of scattering microplanes $\{h_i\, k_i\, l_i\}$ cannot be fixed on the basis of a diffraction experiment with texturized samples. This drawback may lead to significant errors in the analysis of experimental pole figures (PF) by means of series expansion of the orientation distribution function (ODF) $f(g)$, defined through a set of Eulerian angles $g = (\alpha, \beta, \gamma)$ in the sense of [1], and corresponding determination of the series coefficients with the help of PF. This substantiates the use of standard distribution functions of orientations [1–3]. In general, published papers on this matter may be classified as using either the series expansion technique [4, 5], or discrete methods [6]. This work is an attempt to extend the known discrete methods that are pictorial, easier to interpret and involve simplified mathematics.

Examination of recently developed methods, e.g., the method of Imhof employing successive iterations [7, 8], or the maximum entropy method [9, 10], shows that a mathematical modelling of pole figures is useful. Therefore, as a first step in our investigation we consider the direct projection of PF from standard Gaussian ODF. Following the papers of Matthies, Helming and Kunze [11, 12], we substitute for the Eulerian angles used to describe the mutual orientation of the coordinate systems (K_b, fixed to an arbitrarily chosen microcrystallite and, K_a, fixed to the sample) with their linear combinations

$$\beta' = \tfrac{1}{2}(\beta) \qquad \sigma = \tfrac{1}{2}(\alpha + \gamma) \qquad \delta = \tfrac{1}{2}(\alpha - \gamma) \tag{1}$$

so that $g = [\sigma, \beta', \delta]$.

Let the centre of the Gaussian ODF be $g_0 = [\sigma_0, \beta'_0, \delta_0]$. Then the orientation distance between g_0 and an arbitrary point g is:

$$\cos(\tilde{\omega}/2) = \cos(\beta')\cos(\beta'_0)\cos(\sigma - \sigma_0) + \sin(\beta')\sin(\beta'_0)\cos(\delta - \delta_0). \tag{2}$$

We are going to use the angles σ, β', δ in order to determine the stereographic projection of an arbitrary direction of the normal $\boldsymbol{h}_i$ to the microplane $(hkl)_i$. Here we make use of a modification of the technique of Cartan [13]. Let us fix K_a, K_b and $\boldsymbol{h}_i$, as is usually done, to a common centre $g_0 = (0,0,0)$ so that only the mutual orientations are of interest. First allow K_a and K_b to coincide: the projection of $\boldsymbol{h}_i$ on the plane parallel to the equatorial plane but drawn through the south pole (see figure 1), will then be

$$\mu = (x + \mathrm{i}y)/(\tfrac{1}{2} - z) \tag{3}$$

with $R = \frac{1}{2}$ the radius of the sphere and x, y, z the coordinates of the intersection between $\boldsymbol{h}_i$ and the sphere. The rotation of K_b by angles α, β, γ leads to transformation of μ according to the expression

$$\mu' = (a\mu + b)/(-b^*\mu + a^*) \tag{4}$$

where

$$a = \cos(\beta')\exp(-\mathrm{i}\sigma) \qquad b = \sin(\beta')\exp(\mathrm{i}\delta) \tag{5}$$

where a and b are the Cayley–Klein symbols and a^* and b^* are the complex conjugates a and b, respectively. The relation between α, β and γ, and β', σ and δ is given by (1). The relation between μ and the pole p on the equatorial plane is

$$p = 2R^2/\mu \qquad p_x = \mathrm{Re}\,(2R^2/\mu) \qquad p_y = \mathrm{Im}\,(2R^2/\mu) \tag{6}$$

when the normal $\boldsymbol{h}_i$ lies in the upper hemisphere, and

$$p = \mu/2 \qquad p_x = \mathrm{Re}\,(\mu/2) \qquad p_y = \mathrm{Im}\,(\mu/2) \tag{7}$$

when the normal $\boldsymbol{h}_i$ is in the bottom part of the sphere.

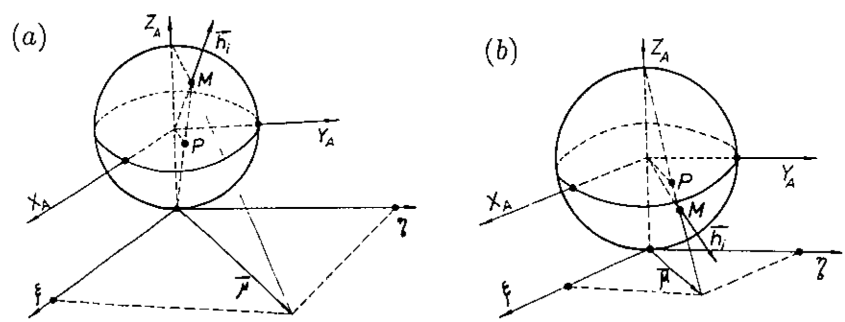

Figure 1. The projection of $\boldsymbol{h}_i$, μ, on the plane ξ, η and PF projection p on the equatorial plane: (a) $\boldsymbol{h}_i$ is in the upper hemisphere; (b) $\boldsymbol{h}_i$ is in the lower hemisphere.

By substituting (6) or (7) in (4) we get $p' = \mathrm{PF}(\sigma, \beta', \delta)$. Now we use the Gauss ODF [2]:

$$f(g) = f(b, \tilde{\omega}) = S_0 \exp(-\tilde{\omega}^2/\varepsilon^2) \tag{8}$$

with

$$S_0(b) = 2\pi/[\varepsilon(1 - \exp(-\varepsilon^2/4))]. \tag{9}$$

Here $\varepsilon = b/2\sqrt{\ln 2}$ where $b = \Delta\tilde{\omega}$ is the full width at half maximum (FWHM) of the model ODF. It should be noted here that there is no need to introduce any modifications in the ODF taken in the form (8) since we do not apply the series expansion technique. We simply calculate the coordinates p'_x and p'_y of the pole $p' = p'(\alpha, \beta, \gamma) = p'(\sigma, \beta', \delta)$ by means of (6), (7) and (4) and assign to this point the value of $f(\sigma, \beta', \delta)$ calculated from (8). This way we can easily construct the pole figure $P_{h_i}(y)$ where y and h_i correspond to h_i in K_a and K_b, respectively.

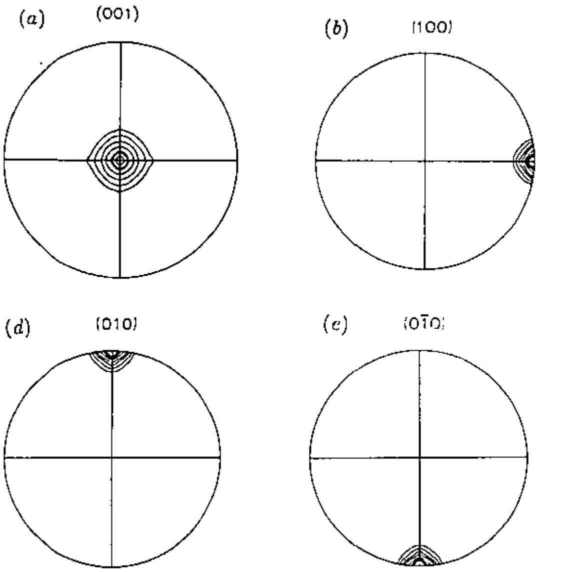

Figure 2. Using Gaussian-shaped ODF in the G-space with $g_0 = (0,0,0)$, $b = 5°$, $S_0 = 10.0$, the unreduced PFs (001) and (100), ($\bar{1}$00), (010), and (0$\bar{1}$0), obtained by the local projection technique, are shown. The steps $\Delta\alpha, \Delta\beta, \Delta\gamma$ are 5°. For (100), (010), ($\bar{1}$00) and (0$\bar{1}$0), $-85° \leqslant \alpha, \gamma \leqslant 85°$ and $0 \leqslant \beta \leqslant 85°$ For (001) $0° \leqslant \alpha, \gamma < 360°$ and $0° \leqslant \beta \leqslant 85°$. The levels are: 20; 30; 40; 50; 70; 100; 200; 300; 320; 350; 380.

Some details of the projection technique described above were treated in [14]. Below, your attention is drawn to some aspects related to the positive answer to the question regarding the possibility of constructing mathematically the so-called unreduced PF. Following Imhof [7] an unreduced PF is just one of the, all equivalent, $h_{i,e}$. In the case of cubic structures there are six unreduced PFs corresponding to the direction [001]: (001), (010), (100), (00$\bar{1}$), (0$\bar{1}$0) and ($\bar{1}$00). By means of our method for local projection we succeed in localizing the reflections from these equivalent directions.

For a Gauss ODF centred at $g_0 = (\sigma_0, \beta'_0, \delta_0) = (0,0,0)$ the reflections (001) and (00$\bar{1}$) coincide, but the remaining four reflections are well spaced and therefore distinguishable (see figure 2). This implies that the actual PF is an average over these reflections, which are expected to appear, summed together. Our results are in good agreement with the PFs given in [15].

This may prove to be useful in reconstructing the ODF by its representation as a result of summation of Gauss functions.

We have carried out a detailed analysis of the influence of the location of the centre g_0 and the FWHM in the PF. We did not encounter any probiems of principle in modelling the PF by mixed Gaussian ODFs. An example is shown in figure 3 which

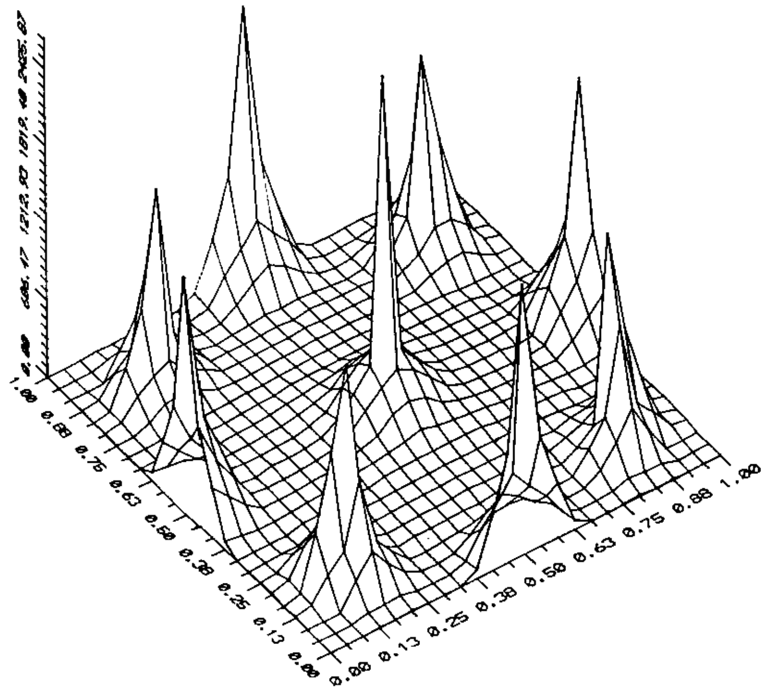

Figure 3. Three-dimensional image of the reduced PF (001), corresponding to a model with two Gaussian-shaped ODFs with $b = 5°$, $S_0 = 10.0$ and centred at $g_0 = (0, 0, 0)$, $g_1 = (0, 0, 45°)$.

illustrates a reduced pole figure constructed from a model with two Gaussian-shaped orientation distribution functions. We next intend to apply the Monte Carlo technique for determining the set g_{0i}, and then to obtain the corresponding maximum values of the Gauss functions S_{0i}, and FWHMs b_i with the help of an appropriate iteration method or by a direct scaling method the in case where rigorous criteria are found.

References

[1] Matthies S, Vinel G and Helming K 1987 *Distribution in Texture Analyses* (Berlin: Springer)
[2] Bunge H 1969 *Mathematische Metoden der Texturanalyse* (Berlin: Springer)
[3] Savelova T 1984 *Zavodskaia Laboratoriia* **50** 48 (in Russian)
[4] Bunge H 1965 *L. Mettallj* **56** 12
[5] Roe R 1965 *J. Appl. Phys.* **36** 6
[6] Ruer D and Baro J 1984 *J. Appl. Crystallogr.* **10** 458
[7] Imhof J 1983 *Phys. Status Solidi* b **119** 693
[8] Imhof J 1983 *Phys. Status Solidi* b **120** 321
[9] Schaeben H 1988 *Phys. Status Solidi* b **148** 63
[10] Schaeben H, Siemes H and Auerbach S 1990 *Phys. Status Solidi* b **158** 407
[11] Matthies S, Helming K and Kunze K 1990 *Phys. Status Solidi* b **157** 71
[12] Matthies S, Helming K and, Kunze K 1990 *Phys. Status Solidi* b **157** 489
[13] Cartan E 1966 *The Theory of Spinors* (Cambridge: MIT)
[14] Vodenicharova T and Krezhov K 1992 *Bulg. J. Phys.* at press
[15] Nicolaev D and Savelova T 1986 *MIFI (Moscow) Preprint* 060-86 (in Russian)