On the Monte Carlo approach to texture determination

LETTER TO THE EDITOR

On the Monte Carlo approach to texture determination

K Krezhov†, T Vodenicharova‡ and P Konstantinov†

† Bulgarian Academy of Sciences, Institute of Nuclear Research and Nuclear Energy, 72 Tsarigradsko Chaussee Boulevard, Sofia 1784, Bulgaria
‡ Institute for Foreign Students, 27 A Veltchev Street, Sofia 1111, Bulgaria

Abstract. The feasibility of using the Monte Carlo (MC) approach to orientation distribution function (ODF) approximation from experimental pole figures (PFs) is demonstrated. The MC simulation is combined with the local projection method developed recently for generation of the PFs from a model ODF. First, a set of ideal orientations represented by a sum of Gaussians is assumed and the corresponding set of points describing the texture is located within the orientation space by means of the MC algorithm presented. Next, this set of data points is projected upon the PFs by means of the local projection technique. The validity of this procedure for texture simulation is tested on the example of cold-rolled steel.

It is well known that the interpretation of pole figures (PFs) obtained by diffraction methods on texturized polycrystalline samples is not straightforward and presents complicated problems. The appearance of false peaks (ghosts) in the distribution function of grain orientations $f(g)$ and the violation of its positivity are characteristic for the series expansion method of Bunge [1] and Roe [2] and related techniques [3] widely used for reconstruction of the ODF from experimental PFs. Series truncation is one cause but the loss of information on the odd part of the ODF is an inherent drawback, as shown in [4], due to the inversion symmetry of PFs, which is a consequence of the fact that the directions of the normals h_i and $-h_i$ to the set of the scattering microplanes $\{h_i, k_i, l_i\}$ cannot be fixed on the basis of the diffraction experiment.

In order to overcome the above-mentioned difficulties several authors have applied mathematical modelling of the ODF [5] or PFs [6]. Gaussians, Lorentzians [5] and more complex functions [7, 8] have been found useful in the already classical analysis by ODF and PF expansion in spherical harmonics. However, the use of model functions is especially appropriate in the discrete methods [9, 10, 11, 12, 13] developed recently in an effort to elaborate ghost-free techniques for quantitative texture analysis.

Following this line of study we have developed a local projection method (LPM) [14, 15] for the construction of the PFs on the basis of a model ODF. The method has been demonstrated using a superposition of spherical Gaussian-type functions. The present work is aimed at extending the theory and demonstrating the feasibility of using the Monte Carlo (MC) approach for approximating the ODF from experimental PFs of cold-rolled low-carbon-steel sheet.

Let us suppose that the true ODF is approximated by a constant background and a sum of spherical Gaussians, i.e.

$$f(g) = \sum_{i=1}^{l} f_i(g_{0i}, g).$$

Following Bunge [3] for the ith texture component centred at the point g_{0i} in the orientation space G we write

$$f(g_{0i}, g) = f_i(g_0, \tilde{\omega}) = S_{0i} \exp(-\tilde{\omega}^2/\varepsilon_i^2) \tag{1}$$

where $g_{0i}, g \in G$, $S_{0i} = (2\pi)/[b_i(1-\exp(-b_i^2/4))]$ is the maximum, and $\tilde{\omega}$ is the orientation distance between g_{0i} and the arbitrary point g in orientation space. Here $\varepsilon_i = b_i/2\sqrt{\ln 2}$, where $b_i = \Delta\tilde{\omega}$ is the full width at half-maximum. The orientation $g = \{\alpha, \beta, \gamma\}$ of the arbitrary microcrystalline grain is treated as a random variable defined through a triad of Eulerian angles $0 \leqslant \alpha, \gamma < 2\pi$ and $0 \leqslant \beta \leqslant \pi$ used to describe the mutual orientation of the coordinate system K_b fixed to the crystallite and the reference system K_a bound to the sample. In terms of the variables introduced by Matthies *et al* [16]

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

with $g_0 = \{\sigma_0, \beta_0', \delta_0\}$, $g = \{\sigma, \beta', \delta\}$ and $dg = 4\sin(2\beta')\,d\beta'\,d\delta\,d\sigma$, the orientation distance $\tilde{\omega}$ becomes

$$\cos\left(\frac{\tilde{\omega}}{2}\right) = \cos(\beta')\cos(\beta_0')\cos(\sigma - \sigma_0) + \cos(\beta')\cos(\beta_0')\sin(\delta - \delta_0). \tag{3}$$

The formulae (1), (2), (3) give the direct relationship between the spherical Gaussian-shaped model of the ODF and the ideal orientation $\{hkl\}\langle uvw\rangle$ introduced by Wasserman and Grewen [17] to describe the rolling texture of metals. Defined in terms of Miller indices the ideal orientation is a preferred orientation which involves the set of crystal microplanes $\{hkl\}$ parallel to the rolling plane and the crystal direction $\langle uvw\rangle$ parallel to the rolling direction.

In the case of cubic lattice symmetry, taken as an example, the ideal orientation can be expressed readily in terms of Eulerian angles:

$$
\begin{aligned}
\beta_0 &= \cos^{-1}\frac{l}{\sqrt{h^2 + k^2 + l^2}} \\
\alpha_0 &= \cos^{-1}\frac{k}{\sqrt{h^2 + k^2}} \\
\gamma_0 &= \sin^{-1}\left[\frac{w}{\sqrt{u^2 + v^2 + w^2}}\sqrt{\frac{h^2 + k^2 + l^2}{h^2 + k^2}}\right]
\end{aligned}
\tag{4}
$$

so we can determine the orientation distance $\tilde{\omega}$ by means of equation (3) and specify the component $f_i(g_0, \tilde{\omega})$ given by equation (1).

Now, as was shown in our previous paper [15], by means of the LPM we can generate in a straightforward manner the PF $P_{h_i}(y_i)$ where y and h_i correspond to h_i in K_a and K_b, respectively. Furthermore, it is easy to localize on $P_h(y)$ the reflections corresponding to the so-called unreduced PFs introduced by Imhof [9] in order to specify just one of the, all equivalent, $h_{i,e}$. For example there are six unreduced PFs corresponding to the direction $[h00]$ in a cubic structure: $(00h)$, $(0h0)$, $(h00)$, $(00\bar{h})$, $(0\bar{h}0)$ and $(\bar{h}00)$. The actual PF is an average over these unreduced PFs; this has been demonstrated in [15] for the PF (001) calculated from a Gaussian-shaped ODF centred at $g_0 = (0, 0, 0)$.

These considerations can be used in the MC calculations by postulating the Eulerian angles in orientation space to be the elementary events. In brief, we generate a random triad $(\alpha, \beta, \gamma) \in G$ and under the assumption that there is a set of k experimental PFs each of multiplicity M_j, $j = 1, 2, \ldots, k$, which should be the projection of the ODF represented by a sum of l Gaussian-shaped components, and we calculate the corresponding orientation

distances $\tilde{\omega}_k$, $k = 1, 2, \ldots, l$. Then, we localize the projection of the particular component $f_k(g_0, \tilde{\omega})$ on each unreduced PF, and if the calculated pole value is greater than the actual value we accept the event to contribute to the pattern; otherwise we reject it. Below we give more details on the simulation of the ODF from experimental PFs by means of the combined procedure.

Let N_0 and B be the *maximum overall intensity of the selected experimental* $P_{h_i}(y)$ and the estimated background intensity, respectively. N_0 is used as a total counter while B is the reference value.

Firstly, each $P_h(y)$ is partitioned into two-dimensional cells Δp_x, Δp_y chosen at equal distances in a square circumscribed around the PF with account taken of the experimental resolution. In principle, this partition is not mandatory but no experiment could yield enough information for all possible sample settings for a reasonable duration of the measurements. The centres $g_{0i} = (\alpha_{0i}, \beta_{0i}, \gamma_{0i})$ of the Gaussian components corresponding to the supposed ideal orientations are calculated using (4).

Next, by means of the randomly generated numbers ξ_1, ξ_2, ξ_3 subject to the condition $0 \leqslant \xi_1, \xi_3 < 2\pi$ and $0 \leqslant \xi_2 \leqslant \pi$ the triad of Eulerian angles $\alpha = \xi_1$, $\beta = \xi_2$, $\gamma = \xi_3$ is assigned. Thus, a random point corresponding to the orientation $g = (\alpha, \beta, \gamma)$ is specified in the orientation space.
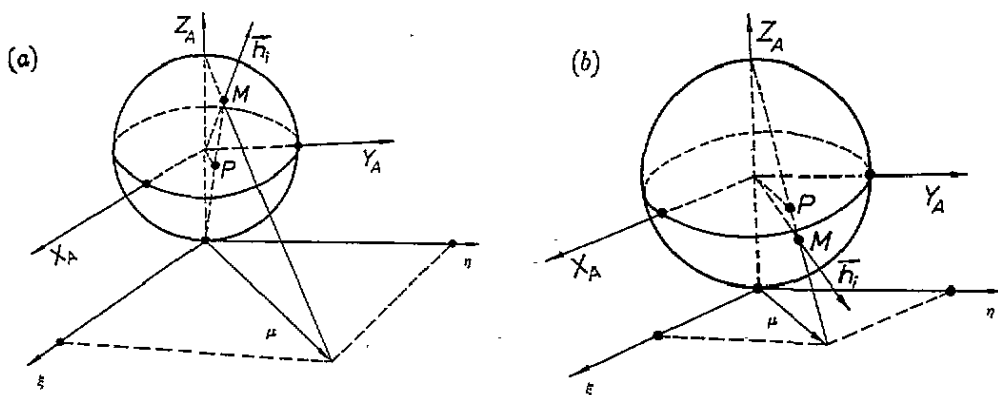

Figure 1. The projection of h_i on the plane ξ, η and projection p on the equatorial plane: (a) h_i is in the upper hemisphere; (b) h_i is in the lower hemisphere.

Now, we choose randomly one h_i with orthogonal coordinates of its intersection with the unit sphere x, y and z in K_a (see figure 1) from the set of equivalent $h_{i,e}$ of number M equal to the multiplicity. The rotation of K_a to K_b transforms the vector μ which is the stereographic projection of h_i onto a plane drawn through the south pole of the unit projection sphere

$$\mu = (x + iy)/(\tfrac{1}{2} - z) \tag{5}$$

in the form

$$\mu' = (a\mu + b)/(-b^*\mu + a^*) \tag{6}$$

where $a = \cos(\beta') \exp(-i\sigma)$ and $b = \sin(\beta') \exp(i\delta)$ are the Cayley–Klein symbols, and a^* and b^* are the corresponding complex conjugates. We calculate the vector μ' and determine the components p_x, p_y according to the direction of h_i with respect to the lower or upper

part of the sphere. For a known μ we get

$$p = \frac{2r^2}{\mu} \qquad p_x = \mathrm{Re}\left(\frac{2r^2}{\mu}\right) \qquad p_y = \mathrm{Im}\left(\frac{2r^2}{\mu}\right) \tag{7}$$

for h_i lying in the upper hemisphere (figure 1(a)) and

$$p = \frac{\mu}{2} \qquad p_x = \mathrm{Re}\left(\frac{\mu}{2}\right) \qquad p_y = \mathrm{Im}\left(\frac{\mu}{2}\right) \tag{8}$$

for h_i belonging to the lower hemisphere (figure 1(b)).

From (7) or (8) and (6) we get the coordinates p'_x and p'_y of the pole $p' = p'(\alpha, \beta, \gamma) = p'(\sigma, \beta', \delta)$ and assign to this pole the value of $f(\sigma, \beta', \delta)$ calculated from equation (1). Thus, by means of the local projection method we find the point on the pole density map which corresponds to the projection of the arbitrarily chosen orientation g. In fact the ideal orientations are assumed on the basis of isolines of high-level intensity on the experimental PFs [18]. Now, if the value of the pole density is less than the value of the Gaussian function describing the ideal orientation, i.e. $p < f(g, g_{0,k}; \tilde{\omega})$, for all unreduced PFs the event g is neglected; otherwise g is accepted.

For g accepted the corresponding triad of Eulerian angles α, β, γ together with the calculated intensity are stored in a temporary file. Finally, both the value of the content of the cell Δp_x, Δp_y and the total counter N_0 are reduced by subtracting the value $f(g)$.

The above-described procedure is performed for each h_i from the set of $h_{i,e}$.

If the current reduced value $N'_0 = (N_0 - f(g)) \geq B$, the procedure is continued for the next supposed ideal orientation. After all supposed ideal orientations have been utilized the next random g is generated and the calculations are carried out until the current total counter value becomes less than B.

Finally, the distribution function of orientations found in this way is projected by means of the LPM in order to obtain the associated PF.

At this stage the comparison between experimental PFs and calculated PFs by means of the above-described combined procedure is based upon experience. Useful information on this subject can be found in the paper of Matthies *et al* [16] where the projection of the σ-section on the unit sphere is treated. The result of the comparison is accepted as being satisfactory in the case where the overall symmetry of PFs is preserved and the calculated local pole intensity is near to the measured value.

The quality of reproduction could be assessed using the reliability factor defined by

$$R = \left[\frac{1}{N} \sum_{i,j=1}^{N} \frac{\sqrt{(P_{ij}^{\mathrm{exp}} - P_{ij}^{\mathrm{calc}})^2}}{|P_{ij}^{\mathrm{exp}}|}\right] \times 100\% \tag{9}$$

where N is the total number of cells, and P_{ij}^{calc} and P_{ij}^{exp} are the recalculated and experimental pole values, respectively, in the cell i, j.

In order to test the combined method described above our first step was to use as input data for the MC simulation the unreduced PFs (100), (010), ($\bar{1}$00) and (0$\bar{1}$0) constructed by means of the local projection method for a Gaussian centred at $g_0 = (0, 0, 45°)$ as a model. Then we checked three ideal orientations [15] {001}⟨100⟩, {001}⟨010⟩ and {001}⟨110⟩ for which the corresponding model ODF is in each case a single Gaussian, centred at $g_1 = (0, 0, 0)$, $g_2 = (0, 45°, 0)$ and $g_3 = (0, 0, 45°)$ respectively, and perform the MC simulation. The resulting four-dimensional array $\{\alpha, \beta, \gamma, f(g)\}$ is projected by the LPM onto the basis set of unreduced PFs again. Both the resulting maxima and their locations $(g_0 = g_3)$ [19] unambiguously proved the validity of the MC method described.
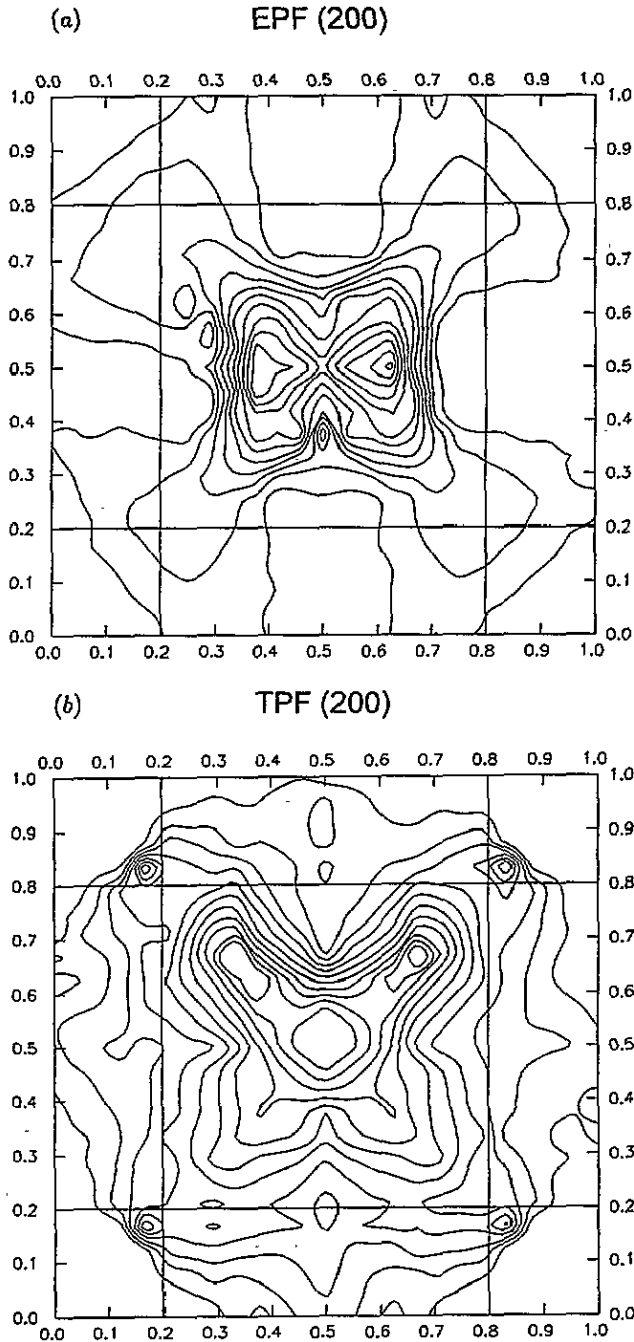
(a) EPF (200)

TPF (200)

Figure 2. (a) An experimental incomplete PF, EPF (200), of Fe–Si cold-rolled steel sheet (see the text). The levels are equidistant, in steps of 120 from 450 to 1800; additional vertical and horizontal lines limit the square within which experimental data are available. (b) A theoretical PF, TPF (200), obtained with a Gaussian-shaped ODF ($g_0 = (0, 0, 45°)$, $b = 20°$). The calculations are with Eulerian angles in steps of $\Delta\alpha = \Delta\beta = \Delta\gamma = 5°$. The levels are equidistant, with steps of 120 from 120 to 1700.

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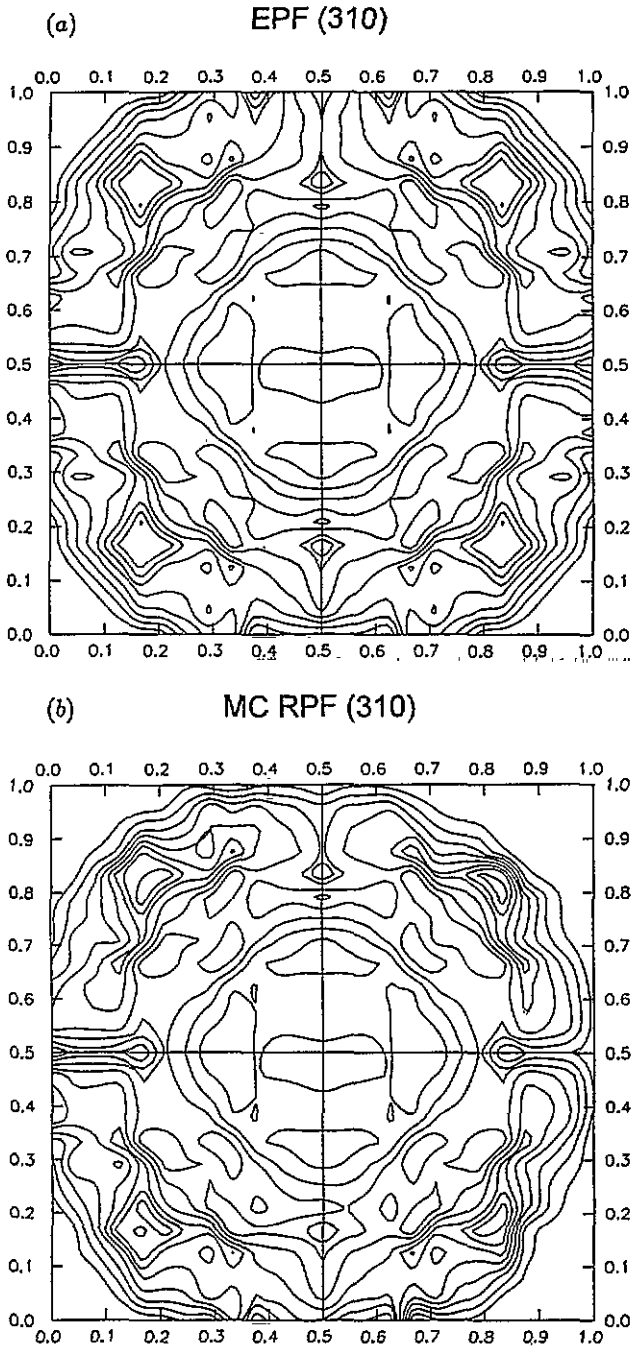
(a)   EPF (310)

(b)   MC RPF (310)

Figure 3. (a) An experimental TOF PF, EPF (310), of Fe–Si cold-rolled steel sheet. The levels are equidistant, in steps of 800 from 800 to 7200. (b) The MC-recalculated PF (310), from a model ODF composed of two Gaussians ($g_{01} = (0, 0, 45°)$ and $g_{02} = (0, 35.3°, 45°)$, $b = 29°$) corresponding to ideal orientations {001}⟨110⟩ and {112}⟨110⟩. The levels are equidistant, in steps of 800 from 800 to 7100.

The next step was to apply the technique to results of texture measurements on a thick specimen of cold-rolled low-carbon steel by means of neutron diffraction. The experimental conditions and the other details can be found elsewhere [20]. An incomplete reduced PF (200) for which the data for the central and the peripheral parts are missing (figure 2(*a*)), is presented in order to illustrate the possibility of drawing correct conclusions to some extent, even in the case of limited information availability. The distribution of isolines with a remote resemblance to a four-leaved clover provides grounds for supposing a texture orientation {001}⟨110⟩ to be present, which in terms of Gaussian representation corresponds to $(0, 0, 45°)$. Obtained with the help of LPM, the theoretically calculated PF based upon this model ODF is given in figure 2(*b*). The result confirms the validity of the assumption of the texture orientation {001}⟨110⟩. However, the PF data make plausible the presence of a second texture component, but separating it out would require additional information.

Figure 3(*a*) shows the complete reduced PF (310) measured on the same specimen. The resulting MC-simulated PF (310), which has been recalculated from a model ODF composed of two spherical Gaussians of equal halfwidth $b = 29°$ centred at $g_1 = (0, 0, 45°)$ and $g_2 = (0, 35.3°, 45°)$ corresponding to ideal orientations {001}⟨110⟩ and {112}⟨110⟩, is given in figure 3(*b*). The number of unreduced PFs for $(hk0)$ is 24. The good agreement between experimental and recalculated PFs is evident. The reliability factor according to equation (9) is $R \approx 10\%$.

In conclusion the authors feel that they have demonstrated the applicability of the MC approach for the reconstruction of the orientation distribution function (ODF) from experimental PFs. At present the MC simulation is combined with the local projection method developed recently for generation of the PFs from a model ODF, but other discrete methods may also be found to be appropriate.

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