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FUNCTIONS DESCRIBING ORIENTATION CORRELATIONS IN POLYCRYSTALLINE MATERIALS

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Statistical functions are presented, which can be applied as characteristics of the polycrystalline microstructure when the parameters are the orientations at separate points of the sample. Basing on the formal definition of the ODF the corresponding definition of the two-point coherence function describing the orientation correlation is given. This immediately gives relations involving this function. Also a discretized form of such a two-point function is presented. Moreover, the relations of this function to other functions describing orientation correlation are considered.

KEY WORDS Individual grain orientations, two-point orientation correlation, coherence functions, series expansion, discretization.

INTRODUCTION

It is a well-known fact that the existence of correlations between orientations of spatially separated points in the polycrystalline sample influence the properties of a material. For example the determination of the effective properties of a polycrystal as heterogeneous continuum on the basis of statistical continuum theory requires the knowledge of many-point correlation functions of appropriate quantities (see e.g. Beran, 1971, Kröner, 1986). The coherence functions, which we are interested in, are the tools for the description of such correlations.

These functions are also useful from the view-point of description of microstructure and they play an essential role in analysis and modeling of processing polycrystalline materials (e.g. recrystalisation, deformation).

The growing interest in coherence functions follows the enormous progress of the experimental techniques for measuring individual grain orientations, which enables determination of such functions.

Throughout the paper statistical homogeneity of the sample and its infinite dimensions are assumed. These assumptions are necessary to the averaging procedure (over a suitably large area of the sample) used here.

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We shall present a new kind of formal definitions of the ODF and of the recently discussed (see e.g. Adams, Morris, Wang, Willden and Wright, 1987 or Adams,

Wang and Morris, 1988) two-point orientation coherence function (OCF) which complete their previous descriptive definitions. This will first be done for the intuitively clear case of the ODF determined on a discretized orientation space.

The ODF as a density function appears in expressions of the type $\int dg f(g)A(g)$ with A being an orientation dependent quantity. As we shall see, the function f can be written in such a form that the averaging process takes place in the specimen area.

Let G indicate the function which assigns the orientation of the crystallite to every point of the (homogeneous in large scale) area V cut out of infinite specimen

$$\mathsf{G}: \mathbb{R}^3 \supset V \ni \mathbf{r} \mapsto g \in \Omega. \tag{1}$$

The definition given above requires previous indication of the symmetrically equivalent area Ω in the orientation space; it is assumed here that this area is equal to the whole space of proper rotations. Let us define V as the volume of area V

$$\mathsf{V} = \int_V d_3\mathbf{r} \quad \text{and} \quad \int_\Omega dg = 1. \tag{2}$$

One can divide the orientation space into cells numbered by $i \in K \subset \mathbb{N}$ and having the volume Δg_i. Thus, we have the mapping

$$d_\Omega: \Omega \ni g \mapsto i \in K. \tag{3}$$

Let us define the function $\mathcal{D}: V \times K \mapsto \mathbb{R}$ as

$$\mathcal{D}(\mathbf{r}, i) = \frac{1}{\Delta g_i}\delta_{ij} \quad \text{where} \quad j = d_\Omega(\mathsf{G}(\mathbf{r})), \qquad j \in K. \tag{4}$$

By integrating it over the specimen area we get

$$\frac{1}{\mathsf{V}}\int_V d_3\mathbf{r}\mathcal{D}(\mathbf{r}, i) = \frac{1}{\Delta g_i}\frac{\Delta \mathsf{V}(i)}{\mathsf{V}} =: f(i) \tag{5}$$

where $\Delta\mathsf{V}(i)$ is the volume of all crystallites having the orientations belonging to $d_\Omega^{-1}(i)$. Therefore f in formula (5) is the discrete form of ODF.

Moreover, the following formulae hold:

$$\sum_{i\in K} \Delta g_i \mathcal{D}(\mathbf{r}, i) = 1 \tag{6}$$

and

$$\sum_{i\in K} \Delta g_i f(i) = \sum_{i\in K} \Delta g_i \frac{1}{\mathsf{V}}\int_V d_3\mathbf{r}\mathcal{D}(\mathbf{r}, i) = \frac{1}{\mathsf{V}}\int_V d_3\mathbf{r} \sum_{i\in K} \Delta g_i \mathcal{D}(\mathbf{r}, i) = 1. \tag{7}$$

The above given sequence of relations can be replaced by its compact form. For this purpose we shall assume that the volume $\Delta g := \max_{i\in K}\{\Delta g_i\}$ proceeds to zero and we shall replace $\delta_{ij}/\Delta g_i$ by the distribution $\delta(g', g)$ with $g' = \mathsf{G}(\mathbf{r})$ and the summation over the set K by integration over the orientation space

$$\mathcal{D}(\mathbf{r}, i) \xrightarrow[\Delta g\to 0]{} \delta(\mathsf{G}(\mathbf{r}), g), \qquad \sum_{i\in K} \Delta g_i(\cdot) \xrightarrow[\Delta g\to 0]{} \int_\Omega dg(\cdot). \tag{8}$$

Now, the ODF is determined on the continuous set Ω

$$f(i) \xrightarrow[\Delta g \to 0]{} f(g) = \frac{1}{V} \int_V d_3\mathbf{r}\, \delta(\mathbf{G}(\mathbf{r}), g). \tag{9}$$

Many of the known relations arise immediately from this definition as a result of the properties of δ-distribution, e.g. the procedure of averaging the orientation dependent quantity A is associated with averaging over the specimen area

$$\bar{A} = \int_\Omega dg f(g) A(g) = \frac{1}{V} \int_\Omega \mathrm{d}g \int_V d_3\mathbf{r}\, \delta(\mathbf{G}(\mathbf{r}), g) A(g)$$

$$= \frac{1}{V} \int_V d_3\mathbf{r} A(\mathbf{G}(\mathbf{r})). \tag{10}$$

In a similar way one can obtain an expression for the Fourier coefficients of the ODF

$$C_l^{mn} = (2l+1) \int_\Omega dg f(g) T_l^{*mn}(g) = \frac{(2l+1)}{V} \int_V d_3\mathbf{r} T_l^{*mn}(\mathbf{G}(\mathbf{r})). \tag{11}$$

Now consider the two-point orientation coherence function

$$c : \Omega \times \Omega \times \mathbb{R}^3 \to \mathbb{R} \tag{12}$$

defined in such a way that the value $c(g, g' \mid \mathbf{r}) dg dg'$ is equal to the probability that points separated by the vector $\mathbf{r}$ have orientations in the ranges $g \pm dg$ and $g' \pm dg'$, respectively. Now, the OCF can be expressed like the ODF in (9)

$$c(g, g' \mid \mathbf{r}) = \frac{1}{V} \int_V d_3\mathbf{r}'\, \delta(\mathbf{G}(\mathbf{r}'), g)\, \delta(\mathbf{G}(\mathbf{r}' + \mathbf{r}), g'). \tag{13}$$

The vectors $\mathbf{r}$, $\mathbf{r}'$ appear here as bound (fixed) vectors, but as a consequence of statistical homogeneity their initial point is free.

On the basis of the above definition one has immediately

$$\int_\Omega dg c(g, g' \mid \mathbf{r}) = \frac{1}{V} \int_V d_3\mathbf{r}' \left(\int_\Omega dg\, \delta(\mathbf{G}(\mathbf{r}'), g) \right) \delta(\mathbf{G}(\mathbf{r}' + \mathbf{r}), g') = f(g'). \tag{14}$$

Similarly

$$\int_\Omega dg' c(g, g' \mid \mathbf{r}) = f(g) \tag{15}$$

and

$$\frac{1}{V} \int_V d_3\mathbf{r} c(g, g' \mid \mathbf{r}) = f(g) f(g'). \tag{16}$$

Moreover, it holds

$$c(g, g' \mid \mathbf{r}) = \frac{1}{V}\int_V d_3\mathbf{r}'\, \delta(\mathsf{G}(\mathbf{r}'), g)\, \delta(\mathsf{G}(\mathbf{r}' + \mathbf{r}), g')$$
$$= \frac{1}{V}\int_V d_3\mathbf{r}''\, \delta(\mathsf{G}(\mathbf{r}'' - \mathbf{r}), g)\, \delta(\mathsf{G}(\mathbf{r}''), g')$$
$$= c(g', g \mid -\mathbf{r}). \tag{17}$$

The OCF can be expressed in the form of a Fourier series (Morris, Wang and Adams, 1988). Assuming that

$$c(g, g' \mid \mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m,n=-1}^{l} \sum_{l'=0}^{\infty} \sum_{m',n'=-l'}^{l'} D_{ll'}^{mm'nn'}(\mathbf{r}) T_l^{mn}(g) T_{l'}^{m'n'}(g') \tag{18}$$

analogously to (12) one can write

$$D_{ll'}^{mm'nn'}(\mathbf{r}) = \frac{(2l+1)(2l'+1)}{V}\int_V d_3\mathbf{r}'\, T_l^{*mn}(\mathsf{G}(\mathbf{r}'))\, T_{l'}^{*m'n'}(\mathsf{G}(\mathbf{r}' + \mathbf{r})). \tag{19}$$

The relations (14), (15) between OCF and ODF and the normalization condition expressed by Fourier coefficients take the following form:

$$D_{l0}^{m0n0} = D_{0l}^{0m0n} = C_l^{mn}, \qquad D_{00}^{0000} = 1. \tag{20}$$

Formulae (16) and (17) lead to the relations

$$C_l^{mn} C_{l'}^{m'n'} = \frac{1}{V}\int_V d_3\mathbf{r} D_{ll'}^{mm'nn'}(\mathbf{r}), \tag{21}$$

$$D_{ll'}^{mm'nn'}(\mathbf{r}) = D_{ll'}^{m'mn'n}(-\mathbf{r}). \tag{22}$$

One should emphasize that relations (14–22) follow directly from the definition (13).

DISCRETIZED FORM OF THE TWO-POINT COHERENCE FUNCTION

In a common experiment individual orientations are measured at points arranged in uniform grids. Thus, the specimen area is treated as a discrete set. On the other hand, because of computational difficulties, the orientation space often has also to be discretized, i.e. one assumes that the functions over the rotation space have constant values in defined cells.

Therefore, let the orientation space be divided in the same way as in the first paragraph and moreover, let the specimen be represented by a discrete structure (grid).

If the ODF is available in continuous form one can get the components of the texture vector by assuming that the value of its ith component is equal to the mean value of the texture function over the ith cell

$$f_i = \frac{1}{\Delta g_i}\int_{d\bar{\Omega}^1(i)} f(g)\, dg. \tag{23}$$

Let the points of the grid (numbered by Greek indices) form the set M containing $\mathbf{M}$ elements. The function $\mathbf{G}$ is re-defined now as $\mathbf{G}: M \to K$. Analogously to (3) one can write

$$d_v : V \ni \mathbf{r} \mapsto \mu \in M \tag{24}$$

Moreover, when $i = d_\Omega(g)$ and $j = d_\Omega(g')$ we shall write $d_\Omega(gg') = i \cdot j$. Similarly, when $\mu = d_V(\mathbf{r})$, $\nu = d_V(\mathbf{r}')$ we shall write $d_V(\mathbf{r} + \mathbf{r}') = \mu + \nu$.

The formulae from the first paragraph can be written in the discrete form. In particular we have

$$f_i = \frac{1}{\mathbf{M}} \sum_\mu \frac{1}{\Delta g_i} \delta_{i,\mathbf{G}(\mu)}, \qquad c_{ij}^\mu = \frac{1}{\mathbf{M}} \sum_\nu \frac{1}{\Delta g_i \, \Delta g_j} \delta_{i,\mathbf{G}(\nu)} \, \delta_{j,\mathbf{G}(\nu+\mu)} \tag{25}$$

and

$$\sum_i c_{ij}^\mu \, \Delta g_i = f_j, \qquad \sum_j c_{ij}^\mu \, \Delta g_j = f_i, \qquad \frac{1}{\mathbf{M}} \sum_\mu c_{ij}^\mu = f_i f_j. \tag{26}$$

Defining

$$\bar{f}_i = f_i \, \Delta g_i, \qquad \bar{c}_{ij}^\nu = c_{ij}^\nu \, \Delta g_i \, \Delta g_j \tag{27}$$

one can re-write (26) in the simpler form

$$\sum_i \bar{c}_{ij}^\nu = \bar{f}_j, \qquad \sum_j \bar{c}_{ij}^\nu = \bar{f}_i, \qquad \frac{1}{\mathbf{M}} \sum_\mu \bar{c}_{ij}^\nu = \bar{f}_i \bar{f}_j. \tag{28}$$

Because the coherence matrices $\bar{c}^\nu$ are non-negative we conclude that if $\bar{f}_i$ vanishes, the ith row and ith column of arbitrary coherence matrix vanish, too. We shall assume below that $\bar{f}_i \neq 0$ for all $i \in K$.

One can define stochastic matrices $s_{ij}^\nu := \bar{c}_{ij}^\nu / \bar{f}_i$ corresponding to the conditional probability that the point situated at the distance $\mathbf{r}$ from the arbitrary point having the orientation g has the orientation g': $c(g' \mid g, \mathbf{r}) := c(g, g' \mid \mathbf{r})/f(g)$. In the simple one-dimensional case, assuming that the orientation at point a correlates with the orientation at point c only through point b (—a—b—c—) one can write

$$s_{ij}^{\nu+\nu} = \sum_k s_{ik}^\nu s_{kj}^\nu. \tag{29}$$

It can be shown (using the Perron–Frobenius theorem), that

$$\lim_{n \to \infty} (s^\nu)^n = \omega, \quad \text{where} \quad \omega_{ij} = \bar{f}_j \tag{30}$$

and from the definition of the s^ν matrix one gets the particular case of the statement that $c(g, g' \mid \mathbf{r}) = f(g) f(g')$ for large $|\mathbf{r}|$

$$\lim_{n \to \infty} \bar{c}_{ij}^{\overbrace{\nu+\nu+\cdots+\nu}^{n}} = \bar{f}_i \omega_{ij} = \bar{f}_i \bar{f}_j. \tag{31}$$

The last result expresses the fact that the orientations of remote points are not correlated.

RELATIONS BETWEEN THE OCF AND OTHER CORRELATION FUNCTIONS

The disorientation distribution function $w(g)$ (textural orientation correlation after Pflege, 1987) is defined as the density function of the probability that the difference of orientations of two arbitrarily chosen points of the specimen is in the range $g \pm dg$. Keeping in mind the fact that $\int dg' c(g', gg' \mid \mathbf{r})$ corresponds to the probability that the difference of orientations of two points separated by the vector $\mathbf{r}$ is in the range $g \pm dg$ we find

$$w(g) = \frac{1}{\mathsf{V}} \int_V d_3\mathbf{r} \int_\Omega dg' c(g', gg' \mid \mathbf{r}). \tag{32}$$

On the basis of (16) one gets

$$w(g) = \int_\Omega dg' f(g') f(gg') \tag{33}$$

and from this the relation $w(g) = w(g^{-1})$.

It is easy to write (32) in the discrete form

$$\bar{w}_i = \frac{1}{\mathsf{M}} \sum_\nu \sum_j \bar{c}^\nu_{ji \cdot j} = \sum_j \bar{f}_j \bar{f}_{i \cdot j}, \tag{34}$$

where with $\bar{w}_i$ related to the continuous w function by $\bar{w}_i = \int_{d\bar{\Omega}^1(i)} w(g)\, dg$.

The problem of the association of the OCF with the misorientation distribution function $m(g)$ (Pospiech, Sztwiertnia and Haessner, 1986) defined as the density function of the probability that neighbouring grain orientations differ by $g \pm dg$ is more complicated.

Let $q(\mathbf{r} \mid 1)$ be the density function of the probability that two points of neighbouring crystallites are separated by the vector $\mathbf{r}$. From the formula for the total probability one finds that $\int_V d_3\mathbf{r} c(g', gg' \mid \mathbf{r}) q(\mathbf{r} \mid 1)$ corresponds to the probability that two neighbouring grains have the orientations g' and gg' and from this one has

$$m(g) = \int_\Omega dg' \int_V d_3\mathbf{r} c(g', gg' \mid \mathbf{r}) q(\mathbf{r} \mid 1). \tag{35}$$

Assuming that the distribution of the chord lengths in an established direction n is described by a γ-distribution

$$\gamma(x) = (\beta^\alpha \Gamma(\alpha))^{-1} x^{\alpha-1} \exp(-x\beta^{-1}) \tag{36}$$

one obtains

$$q(rn \mid 1) = \frac{1}{\beta(\alpha-1)} \left(\frac{r}{\beta(\alpha-1)} - \frac{2r}{\beta(\alpha-1)} \Gamma_{r/\beta}(\alpha-1) + 2\Gamma_{r/\beta}(\alpha) + \int_0^r \gamma(r-x) \frac{2x-r}{r-x} \Gamma_{x/\beta}(\alpha-1)\, dx \right) \tag{37}$$

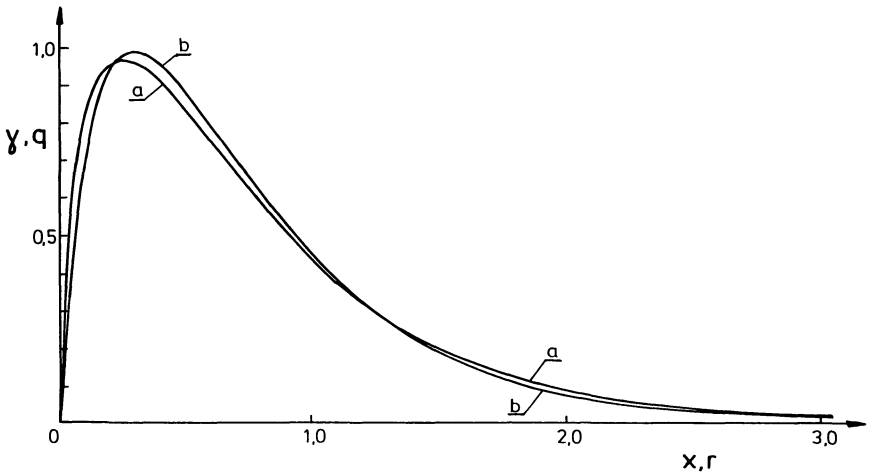

Figure 1 The γ distribution (a) and corresponding $q(rn \mid 1)$ distribution (b) for $\alpha = 1.5$ and $\beta = 0.5$.

where α and β depend on n and Γ_y indicates incomplete Euler Γ-function i.e.

$$\Gamma_y(\alpha) = (\Gamma(\alpha))^{-1} \int_0^y x^\alpha \exp(-x)\, dx. \tag{38}$$

Figure 1 shows an example for the γ distribution and the corresponding $q(rn \mid 1)$ distribution.

Formula (35) can be written in the discrete form as

$$\bar{m}_i = \sum_j \sum_\nu \bar{c}^\nu_{ji\cdot j} q(\nu \mid 1) \tag{39}$$

with $\bar{m}_i$ defined analogously to $\bar{w}_i$.

FINAL REMARKS

Among the functions describing correlations between orientations the n-point (in particular two-point) coherence functions are most universal. But the usage of them is influenced by calculation and experimental restrictions. From the view-point of economy of data storage the best way of dealing with two-point coherence function is to calculate the Fourier coefficients

$$D^{mm'nn'}_{ll'}(\mu) = \frac{(2l+1)(2l'+1)}{\mathsf{M}} \sum_\nu T^{*mn}_l(\mathsf{G}(\nu)) T^{*m'n'}_{l'}(\mathsf{G}(\nu+\mu)). \tag{40}$$

For a quantitative analysis of various aspects of the polycrystalline microstructure some other functions describing orientation correlations are of interest. Those of them, which are discussed in the present paper, contain less information than the two-point coherence function.

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