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Grain shape and distribution of the grain-boundary density in polycrystalline materials

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A mathematical formalism using a series expansion in spherical surface harmonics is proposed to describe the grain shape and grain-boundary density distribution in polycrystalline materials. The mathematical treatment is compatible with existing descriptions of crystalline texture. Experiments on high strength steel show that expansion to second order suffices and measurements of grain size and grain-boundary density in three perpendicular directions characterize these aspects of the structure.

1. Introduction

The physical properties of polycrystalline materials can be influenced very strongly both by the character of individual grains and the statistical distributions characterizing them. As part of a programme to relate the magnetic and metallurgical properties of high strength steels, we have made extensive studies of the grain size and shape in such materials.

An understanding of the properties of materials will be much better founded if a full mathematical description is provided of the grain-orientation distribution, grain shape and grain relative orientation. The idea of an orientation distribution function of various structural elements of the polycrystalline materials has been put forward by Bunge [1]. This concept has been developed [1] and successfully applied not only to describe the texture but also to study the influence of texture on various properties of polycrystalline materials. For example, the macroscopic magnetic anisotropy of grain-oriented iron–silicon steel has been related to the intrinsic magnetocrystalline anisotropy via the orientation distribution function [2]. In addition, in permanent magnet manufacture partial alignment of elongated grains is induced and this has a decisive influence on the magnetic properties. The concept of particle orientation distribution functions can be used in calculating the anisotropy of these properties [3]. However, no attempts have been made to extend the concept of distribution functions to the description of grain shape. In this paper we present a mathematical description of the grain shape in terms of a grain-shape function $S(\mathbf{r})$ and a formalism for an analogous grain-boundary density distribution function $B(\mathbf{r})$. Examples of their use to characterize the microstructure of high strength steels are presented.

2. The grain-shape function (GSF)

Polycrystalline materials consist of a collection of grains which differ in size, shape and relative orientation and which may also have differing crystallographic structure. In a number of important applications, the concept of the mean grain shape suffices but this is not sufficient for materials in which varying and inhomogeneous grain structures are observed. To describe such microstructures we also need to introduce other functions which characterize the distribution of the grain dimensions.

In order to define a grain-shape function we define a Cartesian coordinate system in the frame of the specimen (Fig. 1). The three axes (x, y, z) may, for example, be chosen to correspond to specimen length, rolling direction or any other symmetry direction introduced during the specimen preparation process.

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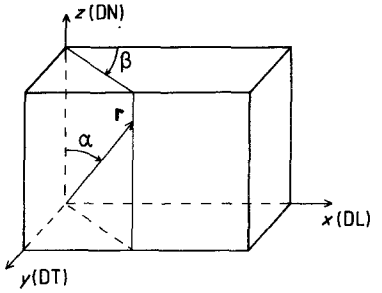

Figure 1 Illustration of the geometry of different cross-sections of the specimen as used for metallographic examination.

We define a unit vector **r** such that its direction (Fig. 1) is determined by polar coordinates α, β. The length of the mean grain $D(\alpha, \beta) = D(\mathbf{r})$ along this direction, and therefore the grain-dimension anisotropy, is known from experiment.

This dimension anisotropy of the mean grain may be complex, if the grain is very elongated or flattened and therefore we use a series expansion of spherical harmonics to represent the grain-dimension anisotropy function namely,

$$D(\alpha, \beta) = D(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{\nu=1}^{N(l)} \mathrm{d}_l^{\nu}(D) k_l^{\nu}(\mathbf{r}) \quad (1)$$

The series expansion coefficients $\mathrm{d}_l^{\nu}(D)$ are expressed in units of length and can be obtained by multiplying each side of Equation 1 by $k_l^{*\nu}(\mathbf{r})$ and integrating over all solid angle. This yields:

$$\mathrm{d}_l^{\nu}(D) = \oint D(\mathbf{r}) k_l^{*\nu}(\mathbf{r})\, \mathrm{d}\mathbf{r} \quad (2)$$

Often the description of the mean grain shape is needed and the above grain-dimension function (Equation 1) has to be normalized in order to compare the shape distribution of grains of various sizes. This grain-shape function (GSF) is defined as

$$\frac{D(\mathbf{r})}{D_0} = S(\mathbf{r}) \quad (3)$$

Where $D(\mathbf{r})/D_0$ is the relative dimension of a grain.

D_0 is the diameter of a spherical grain for which $D(\mathbf{r})/D_0 = 1$ and its value is calculated from the normalization condition:

$$D_0 = \frac{1}{4\pi} \oint D(\mathbf{r})\, \mathrm{d}\mathbf{r} \quad (4)$$

where $\mathbf{dr}$ is an element of solid angle given by

$$\mathbf{dr} = \sin\alpha\, \mathrm{d}\alpha\, \mathrm{d}\beta$$

Since the grain-shape function is normalized, i.e.

$$\oint S(\mathbf{r})\, \mathbf{dr} = 4\pi \quad (5)$$

we obtain the following formula for the grain shape series expansion coefficients

$$s_l^{\nu} = 4\pi \frac{\oint D(\mathbf{r}) k_l^{*\nu}(\mathbf{r})\, \mathbf{dr}}{\oint D(\mathbf{r})\, \mathbf{dr}} \quad (6)$$

Substituting Equations 2 and 4 into Equation 6 to obtain

$$s_l^{\nu} = d_l^{\nu}(D)/D_0 \quad (7)$$

and the GSF will be given as

$$S(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{\nu=1}^{N(l)} s_l^{\nu} k_l^{\nu}(\mathbf{r}) \quad (8)$$

Since the relation between grain-dimension coefficients and grain-shape coefficients is known (Equation 7), Equation 8 is formally equivalent to Equation 1 which describes the grain-dimension anisotropy.

The normalization constant, D_0, carries the dimension and therefore dimensionless expansion coefficients of the GSF (multiplied by D_0) can be used to express the actual anisotropy of dimensions of the average grain.

3. The grain-boundary density distribution function (GBDDF)

If the number of grain boundaries per unit length is measured in various directions **r** we may introduce the mean grain-boundary density function $B(\mathbf{r})$.

A similar mathematical formalism to that applied to the grain dimension description will be used. Thus, the grain-boundary density distribution can be written

$$B(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{\nu=1}^{N(l)} b_l^{\nu}(B) k_l^{\nu}(\mathbf{r}) \quad (9)$$

Series expansion coefficients can be calculated in the same way as those of Equation 2, that is

$$b_l^{\nu}(B) = \oint B(\mathbf{r}) k_l^{*\nu}(\mathbf{r})\, \mathbf{dr} \quad (10)$$

Since $B(\mathbf{r})$ expressed the number of grain boundaries per unit length, the $b_l^{\nu}(B)$ coefficients are not dimensionless.

The dimensionless function $A(\mathbf{r})$ which describes the anisotropy of grain-boundary density will be defined as the ratio of grain-boundary density in direction $\mathbf{r}$ to the mean grain-boundary density, B_0. Physically B_0 corresponds to an isotropic distribution of the grain-boundary density. Thus, we have

$$\frac{B(\mathbf{r})}{B_0} = A(\mathbf{r}) \tag{11}$$

Again, $A(\mathbf{r})$ can be expanded in surface spherical harmonics such that

$$A(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{\nu=1}^{N(l)} g_l^{\nu} k_l^{\nu}(\mathbf{r}) \tag{12}$$

The function $A(\mathbf{r})$ is normalized

$$\oint A(\mathbf{r})\, \mathbf{dr} = 4\pi \tag{13}$$

and the coefficients g_l^{ν} are related to the coefficients $b_l^{\nu}(B)$ through the relation,

$$g_l^{\nu} = b_l^{\nu}(B)/B_0 \tag{14}$$

B_0 can be calculated from

$$B_0 = \frac{1}{4\pi} \oint B(\mathbf{r})\, \mathbf{dr} \tag{15}$$

4. Series convergence

While the above formalism is quite general and has the advantage of being directly compatible with the standard description of crystallographic texture, if the series converges slowly, the description has little practical significance. In order to test the speed of convergence in typical engineering materials we have calculated the grain shape and grain-boundary density distribution functions for ferrite and pearlite in a typical constructional steel. We define the specimen coordinate system such that x is parallel to the rolling direction and z is perpendicular to the coupon surface.

Ten specimens were cut, all with surfaces containing the z-axis and with values of β incremented in 10° intervals from 0° to 90°. Each specimen was polished and the grain boundaries etched and photographed. The number of intersections of grain boundaries with an array of parallel lines was counted. By rotating this array on the micrograph, measurements were made for values of α incremented in 10° intervals from 0° to 90°. From this we obtained the density of grain boundaries in 100 different directions. Measurements were carried out separately for ferrite and pearlite phases.

The data have been used to calculate the series expansion coefficients for the grain-shape function and the grain-boundary distribution function is both ferrite and pearlite structures. Table I shows the values of the coefficients of the grain-shape function obtained for expansion up to $l = 22$. It is evident that the expansion converges rapidly and beyond $l = 4$, no coefficient is above the statistical noise.

In order to test the internal consistency of truncation after two or three terms, the series expansion coefficients have been used to recalculate the mean shape of ferrite and pearlite grains. The maximum and minimum values of the grain length are shown in Fig. 2, for different numbers of expansion coefficients ranging from $l_{max} = 2$ to $l_{max} = 22$. For the specimen under investigation, truncation of the grain-shape function at $l_{max} = 4$ or $l_{max} = 6$ gives results which agree well with experimental data, while truncation at $l_{max} = 2$ gives a very reasonable approximation.

Fig. 2 also provides information on the grain-shape anisotropy and we note that the pearlite grains are more elongated than the ferrite grains.

TABLE I Exemplary series expansion coefficients characterizing the shape of pearlite grains

l	ν									
	1	2	3	4	5	6	7	8	9	10
2	−0.529	0.112								
4	0.074	0.034	0.128							
6	−0.020	−0.049	−0.038	0.050						
8	0.029	0.053	0.084	−0.025	−0.026					
10	−0.052	−0.027	−0.022	0.003	−0.014	−0.005				
12	0.018	0.047	0.023	0.032	−0.020	0.007	−0.038			
14	−0.016	−0.009	−0.009	0.022	0.019	0.035	−0.079	−0.010		
16	0.017	−0.001	0.018	0.011	−0.002	−0.019	−0.020	−0.003	−0.050	
18	−0.035	−0.004	0.008	−0.017	0.017	0.004	−0.023	0.022	0.052	−0.022
20	0.010	0.016	0.007	0.029	−0.017	−0.014	0.013	−0.006	0.013	0.018
22	−0.013	−0.018	−0.006	−0.003	−0.003	0.030	0.002	0.046	0.053	0.004

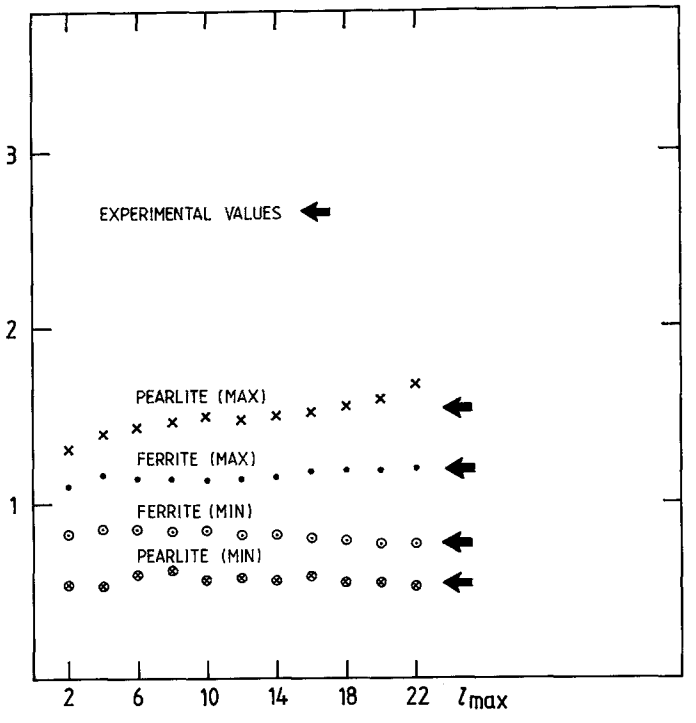

Figure 2 Maxima and minima of the grain-shape function calculated using different numbers of expansion coefficients.

The distribution of anisotropy is conveniently illustrated in stereographic projections of the grain-shape function on the plane of the specimen. These are shown in Fig. 3 for ferrite and pearlite, respectively. A value of unity corresponds to a spherical grain shape.

5. Ellipsoidal grains

Very often rolling treatments or recrystallization processes result in regular shapes of grains which can be approximated as ellipsoidal. Such an approximation corresponds to truncation of the series expansion at $l = 2$, retaining only two coefficients, and as seen in the last section, this procedure does not introduce unacceptable errors. In this case we need to measure the grain size D only in three perpendicular directions in order to determine the coefficients. Let us make measurements in x_0, y_0 and z_0 directions corresponding to the specimen length and directions normal and transverse to the coupon surface. These data can be obtained from measurements on two perpendicular surfaces. The spherical angular coordinates corresponding to these directions are

$$\begin{aligned} \text{DL} &= x_0 = (90°, 0°) \\ \text{DT} &= y_0 = (90°, 90°) \\ \text{DN} &= z_0 = (0°, 0°) \end{aligned} \tag{16}$$

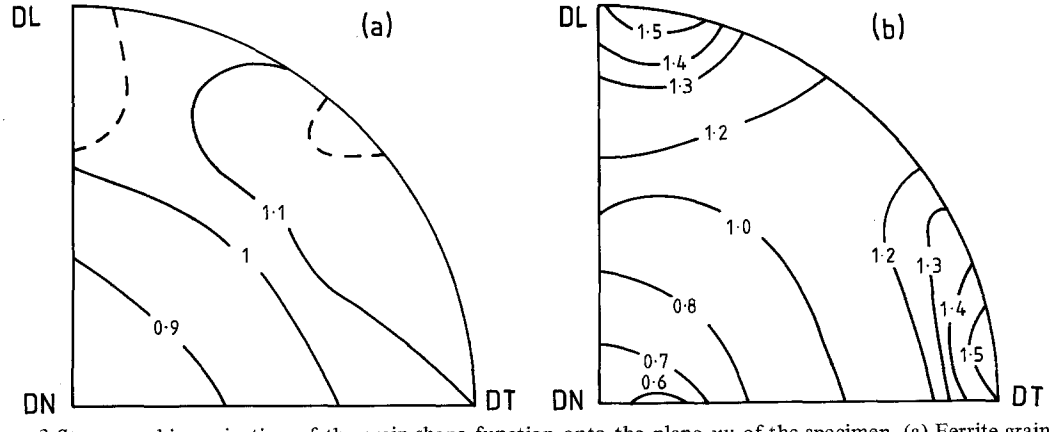

Figure 3 Stereographic projection of the grain-shape function onto the plane xy of the specimen. (a) Ferrite grain, (b) Pearlite grain. The dashed line refers to a GSF value of 1.15.

The relevant spherical functions are [1]

$$k_2^1(r) = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\alpha - 1)$$
$$k_2^2(r) = \left(\frac{15}{16\pi}\right)^{1/2} \sin^2\alpha \cos 2\beta \quad (17)$$

Substituting Equation 17 into Equation 1 we obtain

$$D(x_0) = \frac{1}{N}\left\{1 + s_2^1\left[-\left(\frac{5}{16\pi}\right)^{1/2}\right] + s_2^2\left(\frac{5}{16\pi}\right)^{1/2}\right\}$$
$$D(y_0) = \frac{1}{N}\left\{1 + s_2^1\left[-\left(\frac{5}{16\pi}\right)^{1/2}\right] + s_2^2\left(\frac{5}{16\pi}\right)^{1/2}\right\}$$
$$D(z_0) = \frac{1}{N}\left\{1 + s_2^1\left[2\left(\frac{5}{16\pi}\right)^{1/2}\right]\right\} \quad (18)$$

Solving this system of equations for N, s_2^1 and s_2^2 yields

$$\frac{1}{N} = \frac{D(x_0) + D(y_0) + D(z_0)}{3}$$
$$s_2^1 = \frac{1}{\left(\frac{5}{16\pi}\right)^{1/2}}\left[\frac{3D(z_0)}{D(x_0) + D(y_0) + D(z_0)} - 1\right]$$
$$s_2^2 = \frac{3}{\left(\frac{15}{16\pi}\right)^{1/2}}\left[\frac{2D(x_0) + D(z_0)}{D(x_0) + D(y_0) + D(z_0)}\right] \quad (19)$$

The grain shape can be thus expressed by

$$S(\mathbf{r}) = 1 + s_2^1 k_2^1(\mathbf{r}) + s_2^2 k_2^2(\mathbf{r}) \quad (20)$$

and the grain size function is then

$$D(\mathbf{r}) = \frac{1}{N}[1 + s_2^1 k_2^1(\mathbf{r}) + s_2^2 k_2^2(\mathbf{r})] \quad (21)$$

Similarly, we can obtain the grain-boundary density distribution coefficients by measurements of the number of grain boundaries per unit length B in three orthogonal directions. Using a simplified expression, as for the grain-shape function, one obtains

$$\frac{1}{M} = \frac{B(x_0) + B(y_0) + B(z_0)}{3}$$
$$b_2^1 = \frac{1}{2\left(\frac{5}{16\pi}\right)^{1/2}}\left[\frac{3B(z_0)}{B(x_0) + B(y_0) + B(z_0)} - 1\right] \quad (22)$$
$$b_2^2 = \frac{3}{2\left(\frac{15}{16\pi}\right)^{1/2}}\left[\frac{2B(x_0) + B(z_0)}{B(x_0) + B(y_0) + B(z_0)} - 1\right]$$

Thus the grain boundary density distribution function $B(\mathbf{r})$ is given by

$$B(\mathbf{r}) = \frac{1}{M}[1 + b_2^1 k_2^1(\mathbf{r}) + b_2^2 k_2^2(\mathbf{r})] \quad (23)$$

Tables IIA to IIC show the coefficients of another typical steel obtained using the simplified method of analysis.

It is important to note that a variety of descriptions are possible for the grain-boundary density in two-phase materials. Large segregations of pearlite or ferrite structure require a definition of GBDDF which has only local meaning and characterizes the grain boundary density separately for ferrite and pearlite phases. Alternatively, a global function may be defined for the whole specimen which therefore represents the mean value of the grain-boundary density. All grain boundaries are counted regardless of the difference in phase and distribution of phases. The coefficients characterizing the grain-density distribution function defined in both manners are given in Table II. The maximum grain-boundary density obtained from the latter definition is higher than that for the ferrite but lower than that for the pearlite structure, since the pearlite grains are smaller than the ferrite grains. In relating magnetic and metallurgical properties of the high-strength steels such as used as an example here, there will be an additional complication due to the fact that the pearlite is itself a two-phase mixture. This additional complexity does not in any way invalidate the mathematical model developed but it should be noted that extra parameters may be necessary to specify the distribution of the grain boundaries in the pearlite grains themselves if correlation between physical parameters is attempted.

Finally we note that the present formalism is well suited to the use of computer graphics for production of two-dimensional diagrams of the anisotropy of the grain-boundary density. An example of this is shown in Fig. 4 where the length of the line for a given polar coordinate α, β represents the difference between the grain-boundary density at α, β and the minimum grain-boundary density.

TABLE IIA Exemplary coefficients characterizing GSF

GSF	Experimental data			Coefficients of expansion			Calculated maximum value of function (μm)	Calculated minimum value of function (μm)
	$D(x_0)$ (μm)	$D(y_0)$ (μm)	$D(z_0)$ (μm)	N	s_2^1	s_2^2		
Ferrite	6.5	6.3	5.2	6.0	−0.29	0.03	6.5	5.2
pearlite	5.3	4.2	4.0	4.5	−0.18	0.22	5.3	4.0

TABLE IIB Exemplary coefficients characterizing GBDDF

GBDDF (local meaning)	Experimental data			Coefficients of expansion			(no mm^{-1})	(no mm^{-1})
	$B(x_0)$ (no mm^{-1})	$B(y_0)$ (no mm^{-1})	$B(z_0)$ (no mm^{-1})	M	b_2^1	b_2^2		
Ferrite	154	153	192	168	0.22	−0.03	159	154
pearlite	188	238	250	225	0.17	−0.20	250	188

TABLE IIC Exemplary coefficients characterizing GBDDF

GBDDF (characterizing bulk specimen)	Experimental data			Coefficients of expansion			(no mm^{-1})	(no mm^{-1})
	$B'(x_0)$ (no mm^{-1})	$B'(y_0)$ (no mm^{-1})	$B'(z_0)$ (no mm^{-1})	M^S	$b_2'^1$	$b_2'^2$		
Ferrite + pearlite	168	189	205	187	0.15	−0.10	205	168

6. Conclusions

A series expansion method has been developed to describe the anisotropy of grain shape and grain-boundary density in polycrystalline materials. The method is compatible with the standard mathematical treatment of crystallographic texture. Already, the formalism has been used to extend the Stoner and Wohlfarth theory [3] for the magnetic properties of single domain, non-interacting, ellipsoidal, ferromagnetic particles to the case of an arbitrary distribution of particle orientations [4]. While in many practical cases a simplified formalism can be used which requires only measurements of the grain size or grain-boundary density in three perpendicular directions use of a series expansion of spherical surface harmonics permits expansion to higher order if experiments indicate that the mean shape of the grains is complex or the grain-boundary density is highly anisotropic. We suggest that the description could have many applications in the treatment of magnetic, electrical, acoustic, thermal and plastic properties of polycrystalline materials.

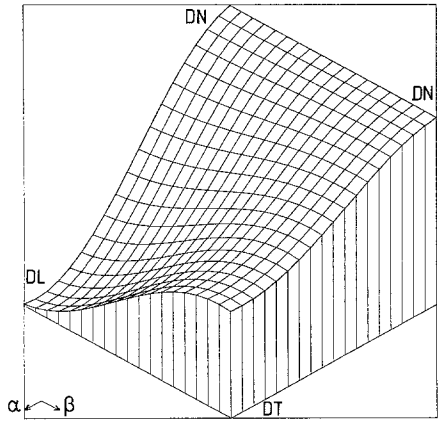

Figure 4 Graphical representation of the GBDDF. Only the differences between minimum and maximum grain-boundary density are displayed. Maximum density is 205 boundaries per mm and minimum 168 boundaries per mm.

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References

1. H. J. BUNGE, "Texture Analysis in Materials Science" (Butterworths, 1982).
2. J. SZPUNAR and M. OJANEN, *Met. Trans. AIME* **6A** (1975) 561.
3. E. C. STONER and E. P. WOHLFARTH, *Phil. Trans. Roy. Soc.* **A240** (1948) 599.
4. B. SZPUNAR and J. SZPUNAR, *J. Magn. Magn. Mater.* (in press).

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