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Notes on representing grain size distributions obtained by electron backscatter diffraction

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ABSTRACT

Grain size distributions measured by electron backscatter diffraction are commonly represented by histograms using either number or area fraction definitions. It is shown here that they should be presented in forms of density distribution functions for direct quantitative comparisons between different measurements. Here we make an interpretation of the frequently seen parabolic tales of the area distributions of bimodal grain structures and a transformation formula between the two distributions are given in this paper.

1. Introduction and Definitions

Electron Backscatter Diffraction (EBSD) is a powerful tool to study microstructures performing quantitative metallography [1]. One of the most important characteristics of microstructures of polycrystalline materials is its grain size distribution. The results of measurements are usually presented in histograms where the number of grains with their diameter D_i lying in an interval δD_i is counted as a function of grain size. δD_i is called a 'bin' and it is practical to chose the bin-size constant, thus, in the following, the index i is only used to identify a bin, it does not involve differences in size of the bin. Two kinds of representations are currently in use for 2D surfaces; the number fraction [2–4] and the area fraction definitions [5,6]. Even if applied for the same measurement, the two representations are quite different.

The number-fraction distribution $F_N(D_i)$ is defined by

$$N_i = F_N(D_i)N_{total} \tag{1}$$

where N_i is the number of grains in δD_i and N_{total} is the total number of grains. Similarly, the area fraction distribution $F_A(D_i)$ defines the sum of the areas A_i of grains that have their diameter D_i in the bin zone:

$$A_i = F_A(D_i)A_{total}. \tag{2}$$

Here A_{total} is the total area occupied by the grain, it is equal to the surface of the measurement if all pixels belong to grains in EBSD. It follows from the definitions above that the sum of

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the fraction-values added up for all the bins δD_i is equal to one (or 100% in percentage presentation):

$$\sum_{i=1}^{n} F_N(D_i) = 1, \quad \sum_{i=1}^{n} F_A(D_i) = 1. \tag{3a, b}$$

Here n is the total number of bins along the grains size axis.

Either using number-fraction or area-fraction distributions, the values of $F_N(D_i)$ and $F_A(D_i)$ depend on the length of the chosen bins δD_i which makes the results obtained with different bin incompatible to each other so any quantitative comparison of them is difficult. This incompatibility can be resolved by using normalized density distribution functions for both types of distributions:

$$f_N(D_i) = \frac{F_N(D_i)}{\delta D_i}, \quad f_A(D_i) = \frac{F_A(D_i)}{\delta D_i}. \tag{4a, b}$$

$f_N(D_i)$ and $f_A(D_i)$ are called density distribution functions. Then the following summations are satisfied:

$$\sum_{i=1}^{n} f_N(D_i)\delta D_i = 1, \quad \sum_{i=1}^{n} f_A(D_i)\delta D_i = 1. \tag{5a, b}$$

These density distribution functions can be continuous if $\delta D_i \rightarrow 0$ and the summations in Eq. (5a,b) become integrals:

$$\int_{d_{\min}}^{d_{\max}} f_N(D)dD = 1, \quad \int_{d_{\min}}^{d_{\max}} f_A(D)dD = 1. \tag{6a, b}$$

The meaning of the number-fraction density $f_N(D_i)$ and area-fraction density $f_A(D_i)$ distribution functions is as follows:

$$f_N(D_i)\delta D_i = \frac{N_i}{N_{total}}, \quad f_A(D_i)\delta D_i = \frac{A_i}{A_{total}}. \tag{7a, b}$$

The subject of the present work is to compare the two kinds of functions, to give a transformation formula between them and to explain a particular property of the area density distribution usually observed for bimodal grain structures. An experimental example is taken from EBSD maps measured after dynamic recrystallization of a Mg alloy in torsion (AM30, see more about the experiments in [7]).

2. Comparison of Number and Area-weighted Density Distributions

Fig. 1 shows the microstructure of a Mg AM30 alloy obtained by EBSD after torsion at 250 °C to a shear strain of 1.73 [7]. Due to partial dynamic recrystallization, there is a large population of small grains and another population of non-recrystallized grains in the measurement. The grain size distribution is displayed in Fig. 2 for both number and area density functions. The bimodal nature of the distribution appears in the area density representation as a large peak at small grain sizes and a nearly uniform distribution for grain sizes larger than about 10 μm (Fig. 2a). In the number-density representation there is only one peak because the small grains very much outnumber the large ones (Fig. 2b). The advantage of showing the area density distribution is clear for bimodal structures.

For larger grains the area-density distribution has some interesting features because the intensity values are situated along some parabolic functions. First we make a quantitative description of these parabolic parts of the distribution. Let us consider such bins in the measurement in which there are the same number of grains denoted by n^*. The smallest number of n^* is 0 for which case there is no vertical bar in the histogram. For the case of area-density distribution, the total surface area of the grains with diameter values lying in a given bin can be approximated by using the equivalent circle area method:

$$A_i \cong \frac{n^* D_i^2 \pi}{4}. \tag{8}$$

Here D_i is the diameter value in the middle of the interval δD_i. Using this expression in Eq. (7a,b), we obtain the equation of such specific distribution:

$$f_A^{n^*}(D_i) = n^* \frac{\pi}{4A_{total}\delta D_i} D_i^2. \tag{9}$$

$f_A^{n^*}$ is the distribution function of those grains for which there is the same number n^* grain in a bin. As we can see, this is a simple parabolic function. Fig. 2a displays $f_A^{n^*}$ for increasing value of n^*. The large grain size part of f_A can be perfectly described by $f_A^{n^*}$ for $n^* = 1$, meaning that there is a maximum of only one grain in a bin. For increasing value of n^* there are also several parts of f_A which can be well described by $f_A^{n^*}$. Due to the nature of the construction of the histogram, any value in the distribution corresponds to a certain n^*, so the whole distribution can be described by a set of $f_A^{n^*}$ functions with varying n^*.

The function equivalent to $f_A^{n^*}$ in the number-density distribution is just a horizontal line defined by $N_i = n^*$ so we obtain using Eq. (7a,b):

$$f_N^{n*} = \frac{n^*}{N_{total}\delta D}. \tag{10}$$

(Here the subscript i is dropped from δD_i because δD_i is constant.) These horizontal lines are shown in the inset of Fig. 2b for large grain sizes. The largest value of n^* necessarily corresponds to the maximum value for the f_N distribution. However, this is not the case for the f_A distribution. The position of the maximum n^* in f_A is obtained from Eq. (9):

$$n^*_{\max} = \max\left[\frac{4A_{total}\delta D_i f_A(D_i)}{\pi D_i^2}\right]. \tag{11}$$

The position corresponding to Eq. (11) is identified in Fig. 2a, located at $D_i = 3.13$ μm with an $n^*_{\max}$ value of 1294. It is important to know that the maximum value does not correspond to the place which is most populated by the grains in an area-density distribution.

The average grain size is an important information that characterizes the microstructure. It is defined as follows:

$$\overline{D}_N = \frac{\sum_{i=1}^{n} f_N(D_i)D_i\delta D_i}{\sum_{i=1}^{n} f_N(D_i)\delta D_i} = \sum_{i=1}^{n} f_N(D_i)D_i\delta D_i = \sum_{i=1}^{n} F_N(D_i)D_i, \tag{12}$$

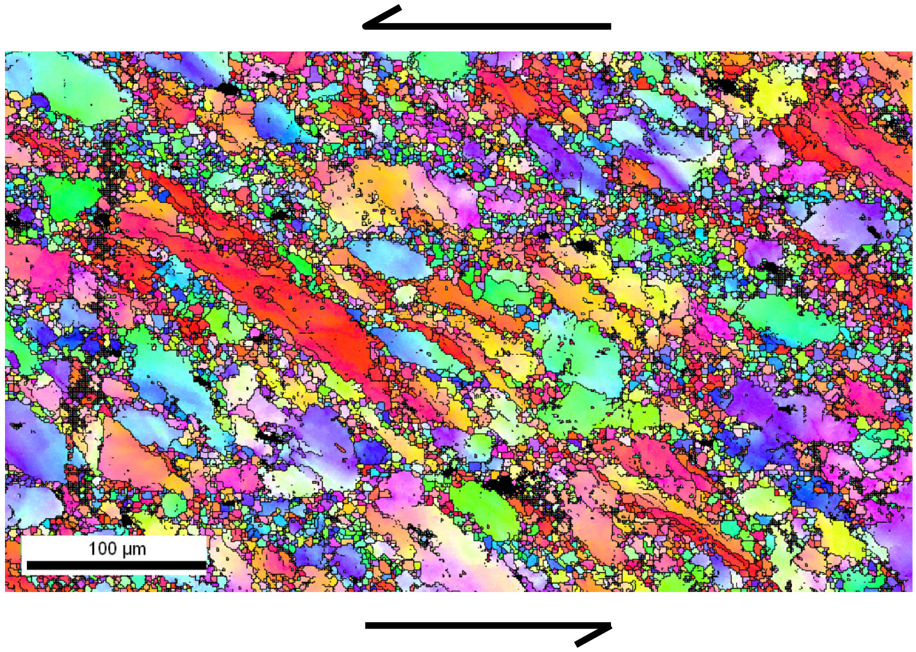

Fig. 1 – Inverse pole figure map of partially recrystallized Mg AM30 deformed at 250 °C to a shear of 1.73. Arrow indicates the direction of shear.

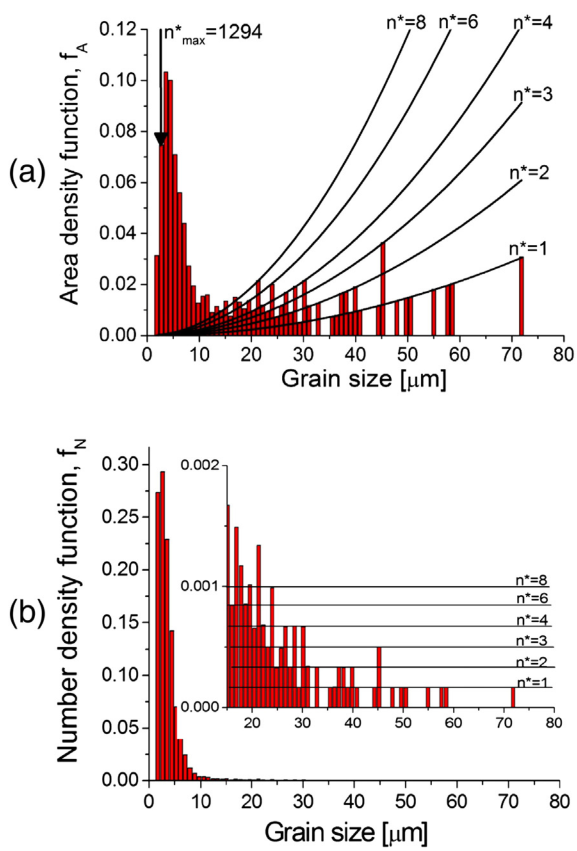

Fig. 2 – Area (a) and number (b) weighted grain size density distributions measured in Mg AM30 at 250 °C after a shear of 1.73. The parabolas in (a) and the horizontal lines in (b) correspond to a constant number of grains (n*) in the bins of the histograms.

$$\overline{D}_A = \frac{\sum_{i=1}^{n} f_A(D_i)D_i\delta D_i}{\sum_{i=1}^{n} f_A(D_i)\delta D_i} = \sum_{i=1}^{n} f_A(D_i)D_i\delta D_i = \sum_{i=1}^{n} F_A(D_i)D_i, \tag{13}$$

where Eqs. (5a,b) and (4a,b) were used. When a histogram is constructed from the measurement, care has to be taken that the trapezoidal integrals of $f_N(D_i)$ as well as $f_A(D_i)$ over the whole interval be 1, that is, the distribution functions have to be normalized. There is no need for such normalization for plotting $F_N(D_i)$ or $F_A(D_i)$. The average grain sizes obtained for the measurement in Fig. 2 are: $\overline{D}_N = 3.13$ μm, and $\overline{D}_A = 20.1$ μm. The difference between the two averages is significant.

When grain size distributions are presented, some authors use the number-weighted and others employ the area-weighted distributions. As the experimental example demonstrated above, they are not easily comparable. Therefore, it is useful to have a transformation formula between the two kinds of distributions. This formula can be obtained as follows.

As in a bin δD_i, corresponding to f_N or f_A, the number of grains N_i is equal, using Eqs. (7a,b) and (8) with N_i in place of n^*, we obtain:

$$f_A(D_i) = f_N(D_i)\frac{\pi N_{total}}{4A_{total}}D_i^2. \tag{14}$$

This relation permits to trace f_A directly from f_N as a function of D_i, or vice-versa. When $f_N(D_i)$ is known but the parameters in Eq. (14) are not all available, $f_A(D_i)$ can still be obtained from $f_N(D_i)$ using Eq. (14) by employing arbitrary values for the parameters (for example all equal to 1.0) and normalize the obtained $f_A(D_i)^*$ distribution so that its trapezoidal integral as a function of D_i and δD_i equals to 1.

3. Special Cases; the Uniform and Lognormal Distributions

Finally, two special cases will be examined as particular examples; the uniform and lognormal distributions.

For a uniform distribution f_N = *constant* or f_A = *constant*. The value of the constant is the same and can be obtained from the condition of unit integral over the whole span of grain sizes (Eq. (6a,b) or (7a,b)): *constant* = $1/(D_{max} - D_{min})$. However, if one function is constant, the corresponding other function is not. When f_N = *constant*, using Eq. (14) we obtain for f_A the following expression:

$$f_A(D) = \frac{1}{D_{max} - D_{min}} \frac{\pi N_{total}}{4A_{total}} D^2 = \frac{1}{D_{max} - D_{min}} \frac{\pi}{4} BD^2, \quad \text{where } B = \frac{N_{total}}{A_{total}}. \tag{15}$$

The B value defined by the N_{total} and A_{total} quantities can be determined by applying again the normalization criterion (Eq. (6a,b)). After integrating, we obtain for f_A and for its maximum value:

$$f_A = \frac{3}{D_{max}^3 - D_{min}^3} D^2, \quad f_A^{max} = \frac{3D_{max}^2}{D_{max}^3 - D_{min}^3}. \tag{16}$$

The second possibility is to take f_A constant. Using again our transformation formula (Eq. (14)) and the normalization procedure in the way analogous to the preceding case, we obtain

$$f_N = \frac{D_{min} D_{max}}{(D_{min} - D_{max}) D^2}, \quad f_N^{max} = \frac{D_{max}}{(D_{min} - D_{max}) D_{min}}. \tag{17}$$

The obtained functions are displayed in Fig. 3 for an example where D_{min} = 2 μm, D_{max} = 20 μm. As can be seen, the 'uniform' distribution really depends on the choice of the distribution. When one is uniform, the other is varying between nearly 0 and a high maximum intensity. Comparing the case when f_A constant to the case for f_N constant, the variations obtained in the other distribution are much larger when f_A is constant because then f_N takes a very high maximum at the minimum grain size.

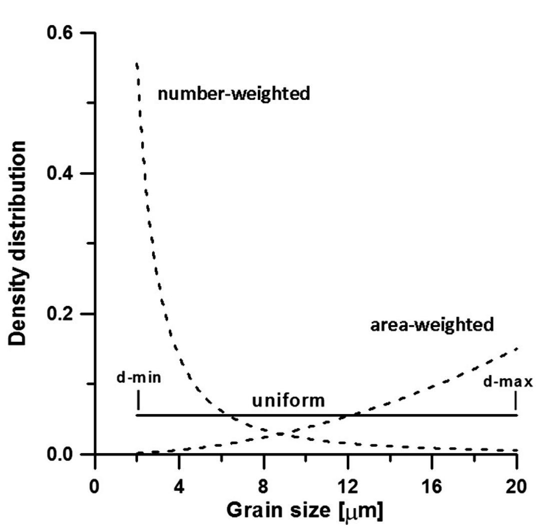

Fig. 3 – A comparison between number and area-weighted density distributions when one of them is uniform (the continuous line).

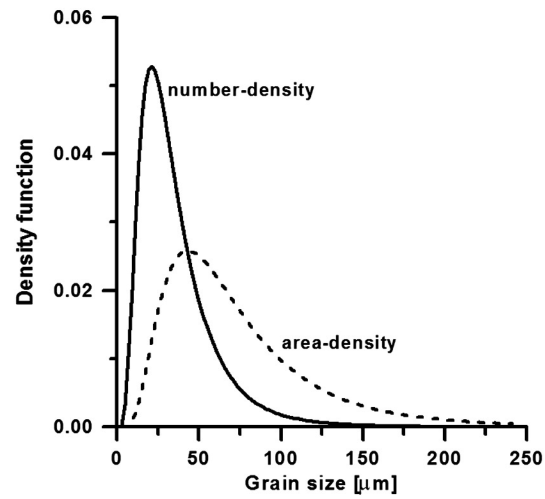

Fig. 4 – Comparison of number and area density functions corresponding to the same lognormal distribution.

Lognormal distributions are known to describe grain size distributions obtained by full recrystallization [8]. They are described by the following density function:

$$f_N = \frac{1}{D\sigma\sqrt{2\pi}} \exp\left[\frac{-(\ln D - \mu)^2}{2\sigma^2}\right] \tag{18}$$

where $\exp\left(\mu + \frac{\sigma^2}{2}\right)$ is called the mean, and e^{μ} is the median. Fig. 4 shows an example when mean = 36 μm and median = 30 μm in the expression of f_N. The corresponding area-weighted distribution is also displayed in Fig. 4 constructed with the help of Eq. (14). In this case, the differences between the two distributions are not so dramatic as for all the previous cases examined above. For example, the average grain sizes differ only by a factor of two.

4. Summary

In summary, an analysis has been carried out in the present paper concerning some particular properties of grain size distributions when they are presented in their number or area-weighted versions. Particular attention was made to bimodal grain structures, which was illustrated by a measurement on torsion of a Mg AM30 partially recrystallized alloy. A quantitative interpretation was given for the large strain part tales of the area-weighted density functions which can be described by parabolas that connect those points in the histogram which have equal number of grains in their corresponding bins. A transformation formula was developed that can be readily applied to convert an area or number density function into its corresponding counterpart function. Finally, the uniform and lognormal distributions were examined showing very specific features when their number and area versions are compared.

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