

STATISTICAL ANALYSIS OF MISORIENTATION DISTRIBUTIONS FROM GROWTH SELECTION EXPERIMENTS IN IRON–3% Si

HELENA MAGNUSSON^{a,b,*} and NILS SANDBERG^a

^a*Theoretical Physics, Royal Institute of Technology, KTH, Sweden;*

^b*Swedish Institute for Metals Research*

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The frequency of occurrence of differently misoriented grain boundaries in growth selection experiments in silicon–iron was reported by Ibe and Lücke and has been the basis of many texture models. However, this pattern of behaviour bears much similarity to misorientation frequencies calculated from random textures. A comparison of the experimental and computed frequency distribution shows that there are statistically significant differences and therefore that some possibilities for growth selection do exist.

Keywords: Misorientation distribution function; Grain boundary mobility; Selective growth; Texture; Simulation

INTRODUCTION

The mobility of grain boundaries has been a subject for investigations for many years (Gottstein, Molodov and Shvindlerman, 1998). One often-debated question is how the misorientation associated with a grain boundary is related to its mobility, and to what extent selective growth exists during recrystallization or grain growth. A particular case in point concerns steels where the classical growth selection experiments of Ibe and Lücke (1968) indicated that high mobility is associated with boundary misorientations of 154° around $\langle 110 \rangle$ axes

*Corresponding author.

and also 96° around a $\langle 110 \rangle$ (see Fig. 1). These results have been utilised in numerous modelling attempts, *e.g.*, Dillamore (1965); Urabe and Jonas (1994); Köhler and Bunge (1996) and Gangli, Jonas and Urabe (1995), to explain the evolution of recrystallization textures in steels. However, Hutchinson *et al.* (1996) showed by means of simulations that a random set of grain boundaries may have some surprising similarities with these experimental data when analysed according to the same procedure.

It is the purpose of this paper to show how experimental data and simulated reference data, a 'zero hypothesis', can be compared in a quantitative way by applying a standard method in statistics.

We will practice the method on the well-known experiment by Ibe and Lücke (1968). They started with a single-crystal, lightly deformed to promote recrystallization, and deformed it heavily in one end. In that way a volume was introduced from which grains of all different kinds of orientations could start to nucleate and grow. One grain was more 'successful' and grew beyond all others in the single crystal matrix. By repeating the procedure many (257) times, Ibe *et al.*, formed an assembly of successful grain boundaries. The question now being asked is whether the successful grains actually had boundaries to the matrix which conferred higher mobility than for other grains, or whether some kind of instability, independent of misorientation, led to

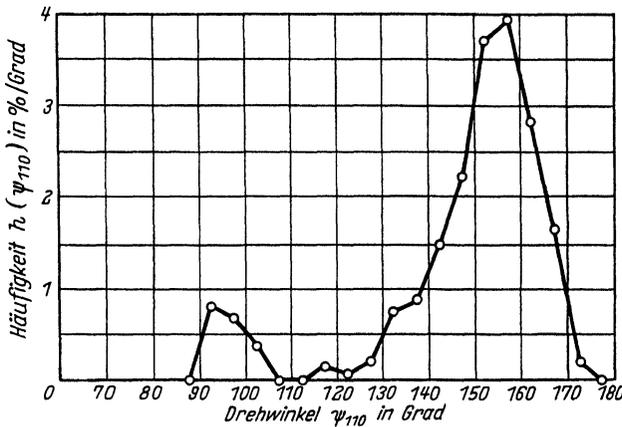


FIGURE 1 Experimental data from selective growth experiments by Ibe and Lücke (1968).

their dominance. In the latter case, if all orientations have an equal probability of winning, the distribution of misorientations should be that in a random case.¹

The misorientation between two grains, may be expressed as a rigid rotation g specified by three variables; the three Euler angles ($\varphi_1, \theta, \varphi_2$) or a rotation axis (\bar{n}) together with a rotation angle (ω) (Bunge, 1982). An assembly of grain boundaries thus constitutes a misorientation distribution, or a misorientation angle distribution (MAD) if only the angle ω is considered. However, in the latter case we have a certain freedom in presenting the data. For cubic symmetry there are 24 different axis/angle pairs that correspond to the same rotation g . The most common choice is to use the axis/angle pair that gives the smallest misorientation angle, sometimes called the disorientation. Another way is to use an axis close to a simple crystallographic direction common to both of the grains.

Ibe *et al.*, chose to view the misorientations in their bcc material as a rotation around the axis closest to $\langle 110 \rangle$ and found the rotation angles clustering around a major peak at 154° and a minor one at 96° , see Figure 1. Since the $\langle 110 \rangle$ axis has a two-fold symmetry the angles can also be expressed as 26° and 84° respectively.² In fcc metals it has instead been found that many grain boundaries with a high mobility can be described by a $30^\circ - 40^\circ$ rotation around an axis close to $\langle 111 \rangle$ (Liebman, Lücke and Masing, 1956). The $\langle 111 \rangle$ axis has a three-fold symmetry, thus angles in the interval $120^\circ - 180^\circ$ can be transferred to the $0^\circ - 60^\circ$ interval.

SIMULATIONS

When we compute our reference “zero hypothesis” MADs, we make two assumptions regarding the underlying misorientation distribution. Firstly we assume that the texture of the material is random. Secondly we assume that all grains, irrespective of orientation, are equally

¹A misorientation is created by two different orientations, and for the misorientation to be random one of the orientations must be random, but not necessarily both.

²This is strictly true only if the axis is exactly parallel to $\langle 110 \rangle$; if there is a small deviation it can be shown that the axial deviation is smaller for the rotation lying in the range $90 - 180^\circ$ than that in $0 - 90^\circ$, hence the scale in Figures 1, 2 and 3.

probable of being next to a given grain, *i.e.*, spatial and orientational relations are non-correlated (Lee, Rollet and Adams, 1999). The first assumption can easily be relaxed to allow for texture in the material. The second assumption means that the misorientation distribution can be computed by pairing all grains in the texture with all other grains, which is mathematically expressed as a convolution integral.³ To compute the MADs, we sample randomly from the misorientation distribution, computing the minimum angle, near $\langle 100 \rangle$, near $\langle 110 \rangle$ and near $\langle 111 \rangle$ distributions, respectively. The results from a computation with $3 \cdot 10^6$ samples are shown in Figure 2. It should be noticed that the sampled minimum angle distribution agrees with high accuracy with the analytical solution for the angle distribution calculated by Mackenzie (1958).

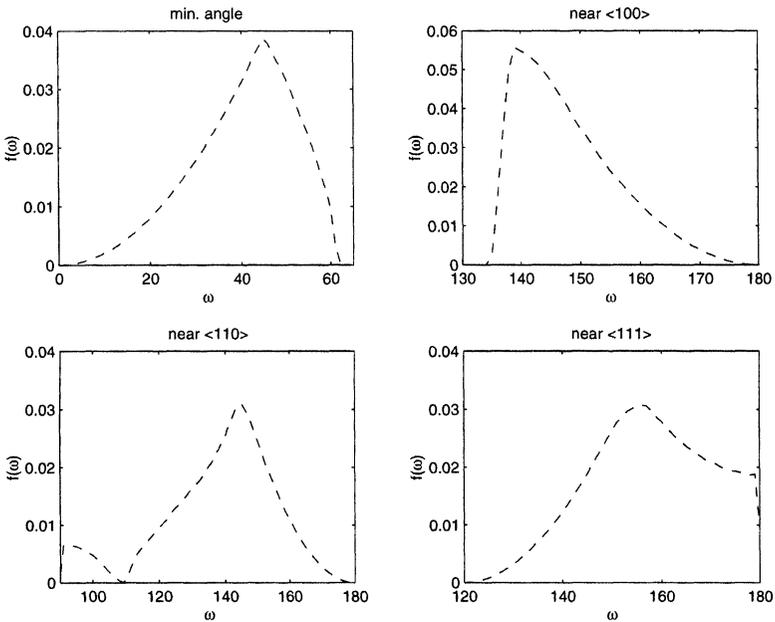


FIGURE 2 Misorientation angle distribution curves for random grain boundaries plotted as (a) minimum angle (Mackenzie distribution), (b) with rotation axis close to $\langle 100 \rangle$, (c) rotation axis close to $\langle 110 \rangle$, and (d) rotation axis close to $\langle 111 \rangle$.

³If the texture is expressed in generalised harmonics and C -coefficients, the convolution integral is computed by multiplying C -coefficients (8).

The near $\langle 110 \rangle$ distribution is centred around 90° and 145° , thus resembling the result by Ibe *et al.* The near $\langle 111 \rangle$ distribution is centred around 157° corresponding to 37° , which bears a resemblance to results reported for fcc-metals (Liebman, Lücke and Masing, 1956).

STATISTICAL TEST

The second step, to determine whether a given experimental set of misorientation angles ω_i , $i = 1, 2, \dots, n$, may stem from a simulated distribution $f(\omega)$, can be cast in a general form, and carried out by use of standard methods in statistics. First, we compute the inverse of the cumulative distribution of $f(\omega)$; $Y = F^{-1}$. Given that the ω_i belong to $f(\omega)$, it can be shown that the points $Y_i = Y(\omega_i) = F^{-1}(\omega_i)$ will be evenly distributed between 0 and 1 (Morgan, 1984). Testing whether the Y_i are distributed "evenly enough", *i.e.*, if the deviations can be explained by mere chance, can be done in several ways. We use a standard test which is based on summing squares of the residuals (the deviation from the expected values of Y_i) resulting in a number that belongs to the χ^2 (chi-square) distribution, which can be found in mathematical tables. An unrealistically large (or small) value indicates that the ω_i do not originate from the distribution $f(\omega)$. Experimental data are often presented in histograms where the angles are summed in intervals. This does not change anything in principle, but the χ^2 test may be formulated in the following way;

$$X = \sum_{j=1}^N \frac{(O_j - E_j)^2}{E_j} \quad (1)$$

where O_j is the number of angles found in each interval j and E_j is the expected value. X will belong to the χ^2 -distribution under the zero hypothesis. However, since information is lost as we sum angles in intervals, the test becomes weaker.

Comparing Ibe *et al.*'s data with the random case (see Fig. 3a), and applying the χ^2 test as discussed above, results in a value of the sum X (see Eq. (1)) which is too large for the experimental MAD to be compatible with the random MAD. It can be concluded with a

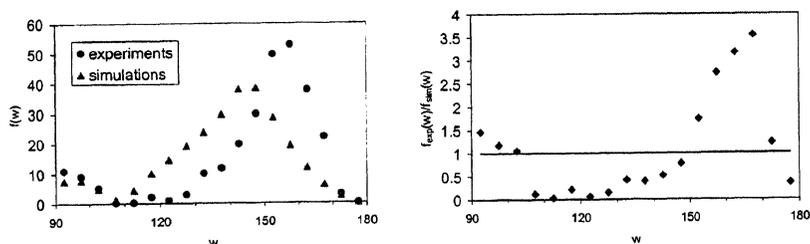


FIGURE 3 (a) The misorientation angle distribution curve published by Ibe and Lücke together with the random $\langle 110 \rangle$ curve for comparison. (b) The same data presented as the quotient between obtained (experimental) and expected (simulated) values. Misorientation angles in the interval $155-170^\circ$ are seen to be over represented in the experimental data, compared to the random case.

certainty of more than 99.95% that the experimental data did not come from a random distribution.

DISCUSSION

We have seen that random grain boundary MADs assume some rather peculiar forms, emphasising that selective grain growth cannot be proven simply by looking at the experimental results (“eye balling”). In particular, the random $\langle 110 \rangle$ distribution turns out to have a shape rather similar to the experimental MAD obtained by Lücke *et al.* (see Fig. 3). However, statistical tests as the χ^2 -test used in this article are very sensitive in probing dissimilarities between an assumed distribution and a set of experimental data. Thus, it is clear that the experimental MAD in Figure 1 did not emerge from a random distribution.

If this deviation is interpreted as a consequence of selective grain growth, we would conclude from Figure 3b that grain boundaries with misorientations of $155-170^\circ$ ($10-25^\circ$) around an axis near $\langle 110 \rangle$ have enhanced mobility, and may therefore confer a growth advantage. On the other hand, the statistical significance of these findings says nothing directly about the degree of variation in mobility of the grain boundaries. In such growth selection experiments a small advantage in velocity is all that is necessary for a grain to be ‘successful’.

The smaller peak near 90° is similar in magnitude in both distributions and is not believed to be of special relevance in terms of mobility although it, too, has been included in simulations of recrystallization previously (Köbler and Bunge, 1996).

The above analysis corresponds to an ideal situation, where grains of all orientations are perfectly lined up in the beginning of the experiment, corresponding to the zero hypothesis of no texture and no spatial-orientational correlation. This would result in a random assembly of winning grains if no growth selection occurred, and a deviation from this if growth selection did occur. However, other factors may have influenced the outcome as well. In the experiment it is obvious that the evolution from the initial condition is unstable; in each case one grain overtakes all the others. The grains evolving from the heavily deformed zone were measured to be close to random (and a deviation from this situation would not have been a problem from the simulational point of view). The other assumption, that grains are perfectly lined up, *i.e.*, have an equal probability to start growing, is more difficult to test. We believe it to be likely that the exact geometry of the deformed zone deviates from this ideal situation, thus giving some grains an initial advantage over the others. This is not enough though, to explain the result in Figure 3, since the initial deviation must be systematic, *i.e.*, only certain misorientations must be given an initial advantage, somehow, through the creation of the deformed zone. We do not see any reasons for such a situation to occur. Therefore, we conclude that the results of Ibe and Lücke strongly indicate the existence of selective grain growth, and that rotations of 10–25° around a $\langle 110 \rangle$ axis seem to be promoted.

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