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DISCRETIZATION TECHNIQUES FOR ORIENTATION DISTRIBUTION FUNCTIONS

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Two methods for the discrete orientation representation of continuous orentation distribution functions (ODFs) are presented. The first one is based on the cumulative ODF, while the second one uses a minimum orientation distance criterion. The properties of these new techniques are discussed and contrasted with each other as well as with an earlier method which is based on cutting below certain limiting intensity. Four kinds of tests have been carried out on these techniques: i. their performance in reproducing the ODF, ii. prediction of physical parameters, as R and M values, iii. deformation texture predictions, iv. rediscretizations during deformation texture modelling. The results of these tests show the good applicability of the proposed two new discretization techniques for approximating the ODF, to calculate physical parameters and for deformation texture modelling, even at relatively low number of orientations. The cutting technique, however, found to be unprecise, even at large number of orientations. On the basis of the results obtained during the rediscretization tests, a new technique for modelling twinning in deformation texture codes has been proposed.

KEY WORDS Textures, Orientation distribution functions, Discretization, Modelling of twinning, *R* value predictions.

1. INTRODUCTION

Experimentally measured textures are usually represented by the series expansion method of Bunge (Bunge, 1982) in the form of continuous orientation distribution functions. The approximation of these ODFs by a discrete set of orientations is unavoidable when theoretical simulations for the given polycrystalline material are carried out (Dezillie *et al.* 1988, Kocks *et al.*, 1991). An important criterion is that the discrete distribution must be able to reproduce—as much as possible—the physical properties corresponding to an infinite number of orientations (continuous distribution). Another requirement is that the model ODF derived from the discrete set should display good fit to the experimental ODF. The latter one is more difficult to judge, as it strongly depends on the adopted value of the gaussian spread around an orientation.

For the purpose of theoretical simulations, the number of grain orientations is an important factor, as the calculation time is proportional to it. However, to reproduce the plastic properties satisfactorily, large number of discrete orientations are desired. A compromise is therefore necessary for the appropriate number of orientations.

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The output of an ODF software is usually a list of the intensities calculated at grid points of the Euler space, usually at every 5 degrees. It makes 6859 points in a $90 \times 90 \times 90$ degree space with 5° grid, which is used for cubic-orthorombic symmetry. For the case of monoclinic sample symmetry, this number is 13718. These ODF intensities can be converted into volume fractions which correspond to the boxes defined by the grid. These volume fractions then can be assigned to "grains" having their orientations at 6859 (or 13718) grid points in Euler space. A texture simulation is usually not feasible with such large number of grain orientations, therefore, a reduction in the number of orientations is necessary. Nevertheless, a discretization technique for such large number of orientations has also been suggested (Leffers and Jensen, 1986).

A method usually employed for this purpose is simply to leave out those grain orientations whose volume fraction is under a minimum value. This method will be referred to as the Cutting Technique (CUT method). Another, more sophisticated, way is to use an iterative technique with random grain orientations but with suitable weights (Kocks *et al.*, 1991).

Two alternative techniques are suggested in the present paper. The first one is based on statistical considerations and has extensively been used in our laboratory since 1985. It makes use of the so-called cumulative ODF and in short form will be referred to as the Statistical ("STAT") method hereafter. The other technique has been developed recently. It is based on a Limited Orientation Distance criterion and will be referred to as the "LOD"-method accordingly.

2. DISCRETIZATION ON THE BASIS OF THE "CUMULATIVE" ODF STATISTICAL (STAT) TECHNIQUE

When a physical property P is known as a function of the grain orientation $P = P(g)$, its average for the whole polycrystal is obtained by an integral over the whole orientation space using the orientation distribution function, $f(g)$:

$$P = \int P(g) f(g)\, \mathrm{d}g \tag{1}$$

In case of discrete grain orientations, P would be approximated by

$$P = \sum_{i=1}^{n} P_i v_i \tag{2}$$

where v_i is the volume fraction for the ith grain. v_i can be assumed to be constant as usually it is determined by the grain size and not by grain orientation ($v_i = 1/n$). It is therefore desirable to produce such a discrete grain orientation distribution in which each grain has the same volume fraction. Another requirement can be that the whole orientation distribution is taken into account in such a way that no region in orientation space would be totally ignored. The above conditions can be readily met by employing the cumulative ODF as described below.

The cumulative ODF can be defined as the function of the integral of the ODF along an arbitrary integration path that covers the whole orientation space:

$$F(G) = \int_{G_0}^{G} f(g)\, \mathrm{d}g \tag{3}$$

where G is a crystallite orientation. This definition must be regarded as "symbolic"; in view of our application of this cumulative distribution function (see below), it only makes sense if the integration is carried out in a discrete way over a number of "boxes" in Euler space. In a first stage, the 5°-grid in Euler space (19^3 points for cubic-orthorombic symmetry) is used to define N "boxes" in Euler space (18^3 for cubic-orthorombic symmetry). These boxes are given sequence numbers i ranging from 1 to N (the order is not relevant). The centre of such box is an orientation called g_i. f_i is the integral of the ODF in such box:

$$f_i = \int_{\text{box}\,i} f(g)\,\mathrm{d}g \tag{4}$$

Because of the definition for dg (Bunge, 1982), we have:

$$\sum_{i=1}^{N} f_i = 1 \tag{5}$$

Equation (4) is used to calculate the values of f_i with great care. The ODF is normally only known at the grid points surrounding the box. Negative values of f_i must be avoided at any prize. ODF-values which are strictly non-negative (obtained by means of the quadratic method (Van Houtte, 1983) or the exponential method (Van Houtte, 1991)) are used. Precision is enhanced by using correction terms in the formula for numerical integration. Also, it must be assured that Eq. (5) is exactly satisfied. A cumulative distribution function $F(j)$ is now constructed:

$$F(j) = \sum_{i=1}^{j} f_i \tag{6}$$

For non-integer values of j, $F(j)$ takes the value that it would have for the next lower integer. A kind of "staircase function" is created in this way (Figure 1). In order to discretise the ODF, a set of n numbers s_k, called "selectors", are generated in a range between 0 and 1. They can have a random distribution with a uniform probability, or a uniform distribution. One discrete orientation will be generated for each selector by using the inverse function $i = H(y)$ of the "staircase" function $y = F(j)$:

$$i_k = H(s_k) \tag{7}$$

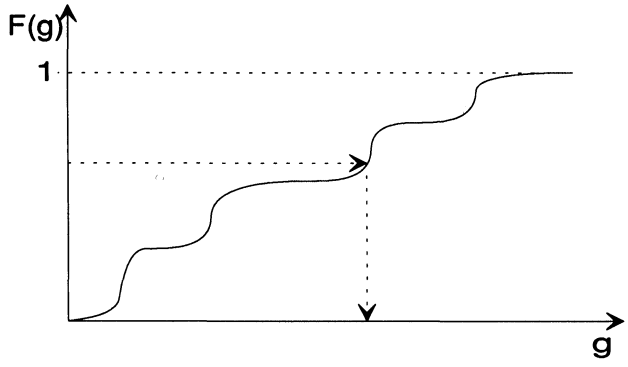

Figure 1 Schematic diagram for the cumulative ODF.

This can be achieved by marking the value s_k on the vertical axis of Figure 1, drawing a horizontal line, and then for i_k use the abscis of the intersection of this horizontal line with the staircase function. Let $p(i)$ be the probability that a particular value of i is obtained in this way. All possible s_k that lead to a particular i-value are situated within the range $F(i-1)\,..\,F(i)$ on the vertical axis. The length of that range is f_i, and the length of the total range of the vertical axis is 1. So

$$p(i) = f_i \tag{8}$$

since the probability distribution of the s_k is uniform. In this way, a set of n different i_k values is obtained. Each of them corresponds to a discrete orientation g_{i_k} where g_{i_k} is the centre of the box. The volume fraction v_k associated to all these orientations is the same, and equal to:[1]

$$v_k = \frac{1}{n} \tag{9}$$

Further details on the statistical properties of the STAT method are given in the Appendix.

3. LIMITED ORIENTATION DISTANCE (LOD) METHOD

It is well known that the orientation space as defined by Euler angles is distorted in two ways. Firstly, the unit volume depends on g ($\mathrm{d}V = \sin\phi\ \mathrm{d}\phi\ \mathrm{d}\phi_1\ \mathrm{d}\phi_2$). Secondly, orientations in the $\phi = 0$ section, for which $\phi_1 + \phi_2 = \text{constant}$, are equivalent. The consequence is that orientations in the vicinity of the $\phi = 0$ plane are much nearer to each other than at other places. Therefore, fewer orientations are necessary to represent the low ϕ value part of the ODF, compared to those regions where ϕ is near 90°. This requirement can be satisfied by selecting grain orientations on the basis of their relative orientation distance.

Before applying the limited orientation distance selection, the ODF is converted into volume fractions (v) of all the boxes which are defined by a 5° grid in Euler space. "Grains" are then assigned to these boxes with their orientations being in the center of each box.

It is practical to set a minimum value for the orientation distance between the selected grain orientations ($\omega_{\min}$). The seed of the selection procedure can be the point where v is maximum. Then the whole Euler space is scanned, and the orientation distances between the selected point and all other grid-points are calculated. The volume fraction of those orientations for which the orientation distance is under the minimum limit are composed into the selected grain orientation. These "neighbouring" grains are accounted for by a gaussian distribution function for which the spread is less or equal to the preset minimum limit distance. After their contribution is added to the selected grain's volume fraction, they are left out from the distribution. The next selected point is

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[1] In case m of the n discrete orientations would have the same g_{i_k}, then the computer program would combine these m orientations into a single one with volume fraction mv_k.

then again the one at which the now already reduced distribution displays its new maximum intensity (i.e. its maximum v). From this on, the procedure described above is repeated until the whole distribution is "consumed".

In the calculation procedure, the Eulerian matrices of the two selected grain orientations (a and b) are set up first (T_a and T_b). The matrix describing the rotation form a to b is then given by:

$$T_{\text{rot}} = T_a T_b^{-1}. \tag{10}$$

The angle of rotation can be obtained from:

$$\omega = \arccos((\text{trace}(T_{\text{rot}}) - 1)/2)) \tag{11}$$

where

$$\text{trace}(T_{\text{rot}}) = T_{aij} T_{bij}.$$

Because of the crystal and the sample symmetries, however, it is necessary to do all symmetry operations on T_a or T_b, then to look for the lowest absolute ω value. Because of this, and the scanning procedure over the whole orientation space, the calculation time can be lengthy, escially if low values of $\omega_{\min}$ are used. To avoid this, a standard data file can be calculated, once and for all, for the usual $\omega_{\min}$ value (between 5° and 10°). This data file contains the lists of those Eulerian grid-points which are nearer than $\omega_{\min}$, calculated for all grid points. Using such data file the calculation time is not significant.

4. COMPARISON OF THE STATISTICAL, THE LIMITED ORIENTATION DISTANCE, AND THE CUTTING DISCRETIZATION METHODS

For the purpose of comparing the results of the different discretization techniques, an experimentally measured texture was chosen. The material was deep drawing steel, the texture was measured after hot rolling. From four pole figures, the ODF was computed by the series expansion method of Bunge (Bunge, 1982), up to $L = 22$. An iterative ghost correction procedure (exponential method: Van Houtte, 1991) was also applied. In this way, a strictly non-negative ODF has been obtained. This texture is displayed in the $\phi_1 = 0$ and $\phi_2 = 45°$ sections on top of Fig. 2. (In the following, in order to save space, all textures will be presented only by their $\phi_1 = 0$ and $\phi_2 = 45°$ sections.) This texture has been dicretized by the STAT, LOD and CUT techniques to obtain two sets of distributions in each case; 354 and 1970 orientations.

Four kinds of tests have been carried out on these distributions: I: the comparison of these orientation distributions themselves, II: R value and M value predictions, III: deformation texture predictions, and IV: rediscretizations during deformation texture modeling. The results are summarized as follows.

4.1. *Reproducibility of the ODF*

The first and most simple test for the quality of a discrete set is to recalculate its ODF. This can readily be done by assuming certain gaussian distributions around each orientation, then calculate the ODF with the series expansion method. Of

course, the result would very much depend on the assumed value for the spread in the gaussian distributions. Nevertheless, using the same value for each of the equivalent sets, the results can certainly be compared to each other. The textures obtained in this way for the three techniques and for two different grain numbers are shown in Figure 2.

It can be seen from Figure 2, that the texture derived by the Cutting technique differs the most from the experimental texture. Especially for the relatively low number of orientations. This is a simple consequence of the applied cutting limit; large low intensity regions are totally ignored. To obtain only 354 orientations, the ignored volume fraction is 60.7%, the same for 1970 orientations is still 15.6%.

The STAT and LOD techniques both perform well, even for the 354 grain case. The LOD technique seems to return more of the details of the original ODF. This is because there are no regions in orientation space which do not contribute to the final distribution. It should be noted, however, that grain orientations are all well separated in this method, at least by the limiting value, which is 10° for the 354, and 5° in the 1970 grain-number case. There is no such limitation in the STAT technique. In that case, more grain orientations are concentrated near the peak intensity locations, all having the same volume fraction. For the LOD method, the volume fraction is not constant, instead, it follows the ODF intensity variations. As a consequence, more information is concentrated in the same grain-number orientation distribution.

4.2. *R and M value predictions*

We have performed several imaginary Lankford tests on our distributions to obtain R-values. These were uniaxial tensile tests at different angles to the rolling direction. With the help of the Leuven-Taylor crystal plasticity code (Van Houtte, 1988), the plastic work (in other words Taylor, or M-factor) was calculated for a small increment of plastic deformation. The R value corresponds to the prescribed velocity gradient at which the plastic work is minimum (Van Houtte, 1987). This minimum was located by an iterative technique in case of the discrete sets to a precision of 0.005 in the R-value. For the continuous distribution, the minimization technique based on the series expansions of the Taylor factors (Van Houtte, 1987) has also been applied.

An additional simulation, in which all grain-orientations (6859) corresponding to the boxes of a 5° grid in Euler space, has also been carried out. The predicted R-values for this discrete distribution, obtained by the direct M-value minimization, were found to be identical (within the prescribed precision) to the results obtained by the Taylor factor-series expansion technique. Please note that for the latter, the calculation time was only 10 seconds, while for the 6859 grain orientation direct minimization, it was 12 hours on a Model 486 personal computer.

The Taylor factor-series expansion technique, unfortunately, is not appropriate to obtain R-values for the case of the discrete sets. Namely, for that purpose, the C-coefficients of the discrete set should be calculated, which is only possible if some gaussian spread is introduced around each orientation. This factor, however, affects the ODF intensities significantly, to the extent that the R-values obtained in this way are by far not as precise as those obtained by a direct

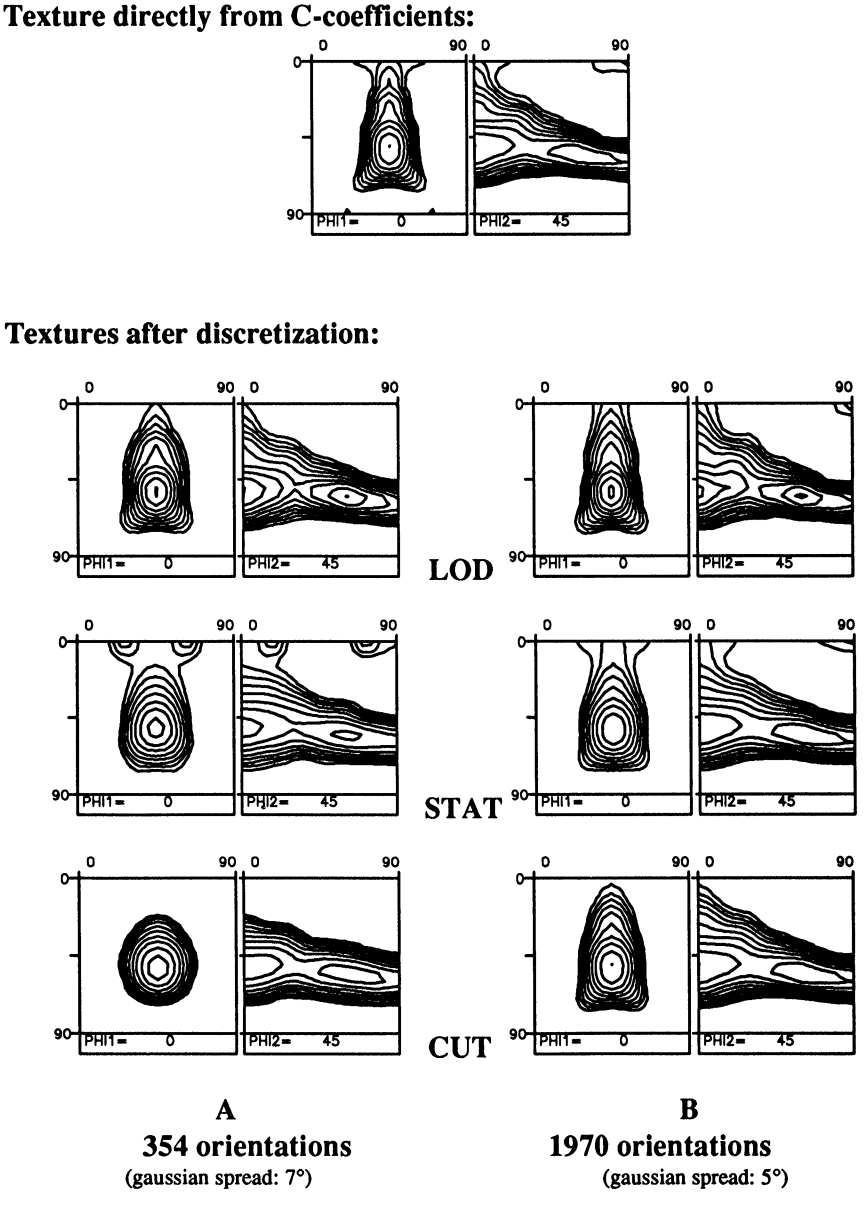


Figure 2 Comparison of the textures obtained by the 3 discretization techniques, LOD, STAT and CUT, with the starting continuous ODF, the latter plotted from *C*-coefficients. (Isovalues on all diagrams: 1, 1.3, 1.6, 2, 2.5, 3.2, 4, 5, 6.4, 8, except for the 354 grains CUT method, where these are: 0.7, 1, 1.4, 2, 2.8, 4, 5.6, 8, 11, 16.)

minimization of the plastic work, applied on the discrete set itself. This is because the plastic work function is very flat near its minimum, giving a large uncertainty in the R-values, if precision is limited. For example, to obtain R-value for a precision of 0.005, the plastic work has to be minimized to a precision about 6 numerical digits! Small deviations in the distribution can easily lead to higher than 10^{-6} order changes in the plastic work. This is exactly the reason why the R-value prediction is very suitable for testing the quality of a discrete set.

The predicted R and M values, using the direct minimization technique of the M factors on the different discrete sets, are plotted in Figures 3a–3d. The qualities of the discrete sets are well demonstrated by the deviations between R and M values obtained from the continuous distribution (broken lines). The

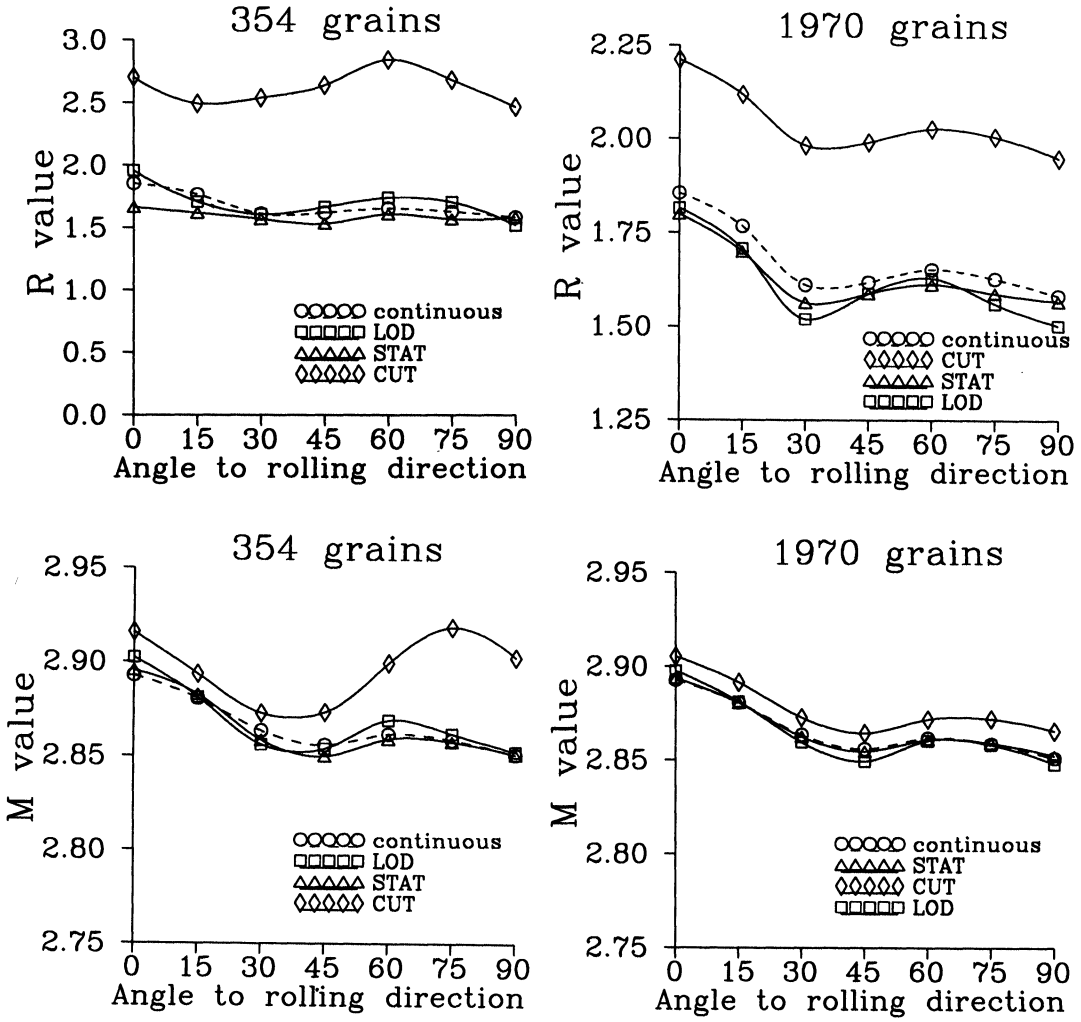


Figure 3 Predicted R and M values. A: R values, 354 grains, B: R values, 1970 grains, C: M values, 354 grains, D: M values, 1970 grains.

Table 1 Mean deviations of the R and M values between the results of the continuous distribution and the different sets of discrete orientations

Method	*STAT*		*LOD*		*CUT*	
Grain number	354	1970	354	1970	354	1970
S_R	0.0122	0.0024	0.0056	0.0043	1.07	0.157
$S_M \times 10^6$	13	0.98	36.61	15.67	1466	153.2

results obtained by the STAT or LOD methods are in good agreement with the continuous distribution, even for small number of grain orientations. The cutting method, however, results in systematically large deviations. Even for high number of grain orientation (1970 out of the maximum 6859), the deviations are considerably high. In order to quantify the observed differences between the results of the continuous and discrete methods, the mean differences are calculated and displayed in Table 1.

Concerning the R-values, the LOD technique seems to perform slightly better for the low number of grain orientations. At large numbers, however, the STAT method improves much more than the LOD technique. It is undoubted that this is because of the good statistical properties of the STAT technique.

4.3. *Tests on Deformation Texture Simulations*

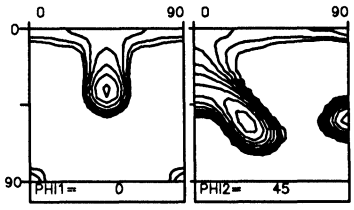
One possible use of a discrete set is to inject it into a crystal plasticity code and calculate deformation texture development. For this purpose, the rate sensitive crystal plasticity code (Tóth *et al.*, 1988, Neale *et al.*, 1990) was selected and simulations for $\varepsilon = 1$ rolling with "lath" relaxation in 20 increments have been carried out at a rate sensitivity exponent of $m = 0.05$. The reference texture in this case the one which is obtained by using all possible orientations, i.e. 6859 in the present case. This texture is plotted on the top of Figure 4. The textures obtained from the different discrete sets are also plotted in Figure 4.

It can be seen that the Cutting Technique leads to large differences at low grain number, but even for 1970 orientations, the low ϕ value region in the ODF is unprecise. By contrast, the LOD and STAT methods both are able to produce approximately the texture development compared to the 6859 grain number reference case. The results are slightly better in the Statistical Technique, they are acceptable even for the low grain number case. Obviously, as the development of the texture is very sensitive to the local nature of the rotation field, large number of grain orientations are necessary in regions where the rotation field is very much convergent or divergent. The LOD technique, however, selects orientations at a minimum limited orientation distance. As a consequence, only limited number of orientations are present in regions which may be decisive for the development of the texture.

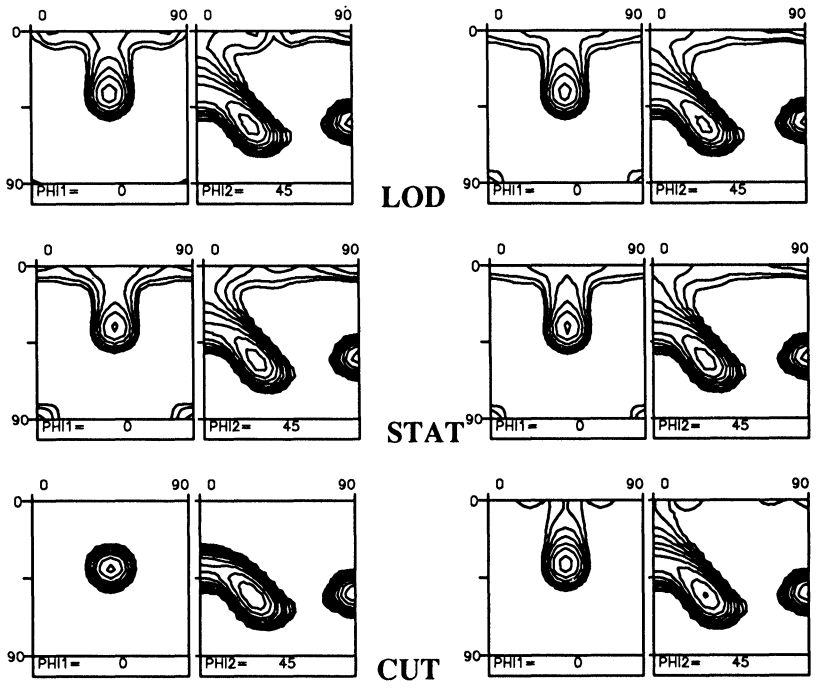
4.4. *Rediscretization During Deformation Texture Modeling*

The most severe test on a discretization method is to apply the technique during a deformation texture simulation. After a certain number of strain-increments, the

Simulated texture from 6859 orientations:



Simulated textures from discretized distributions:



A **B**

354 orientations **1970 orientations**

Figure 4 Comparison of the simulated textures obtained by the 3 discretization techniques, LOD, STAT and CUT, with the simulated texture obtained by using all grain orientations (6859). Rolling, $\varepsilon = 1$, lath model with rate sensitive slip, $m = 0.05$. (Isovalues on all diagrams: 1, 1.4, 2, 2.8, 4, 5.6, 8, 11, 16, 22. Gaussian spread: 7°.

discrete set is made continuous by using Gaussian distribution. This continuous set is then discretized, and the deformation is continued with the new distribution. The result obtained in this way can be compared with the one which is computed without subsequent rediscretization. Such tests have been carried out on all the techniques in question, using the 354 grain orientation distributions. An additional test, using the 1970 grain number set with the STAT technique, has also been performed. Results are not presented here for the Cutting Method, as this technique did not perform satisfactorily for the previous tests, see above, and also did not meet our expectations for the present rediscretization tests.

The results obtained for the 354 grain number case are presented in Figure 5 for the LOD and STAT methods. In this figure the textures on top (A) were obtained without rediscretizations during the simulation. These are therefore considered now as the basis for comparisons. The textures displayed in the middle (B) on Figure 5 are obtained by continuing the deformation for 5 steps with the initial set, then a rediscretization was applied, followed by 5 continuous steps again, etc. Finally, after 4 rediscretizations, the same deformation was achieved for the B textures as it was in the A case. In the C case in Figure 5, rediscretization was applied after every strain-incerement, i.e. 20 times.

By comparing the B and C textures to the A in Figure 5, we can conclude that the simulated textures are still acceptable in the B case, but not for the C. It can also be observed that the LOD technique works better for the high intensity regions, while the STAT method is more precise in regions where the intensity is low. In general, as a result of the rediscretizations, there is a weakening in the textures. This effect is less strong for the LOD technique.

The results obtained for the larger number of grain-orientation (1970), computed using the STAT technique, are displayed in Figure 6. The results are significantly better than those obtained for the 354 grain-number case. The weakening of the texture is still relevant, especially when rediscretization has been carried out after every strain increment. This, however, can partly be accounted for the gaussian spread which is used to generate the continuous distribution.

5. A POSSIBLE APPLICATION: MODELING OF DEFORMATION TWINNING DURING TEXTURE DEVELOPMENT

The results above obtained from the rediscretization tests suggest a possible application for the present discretization technique, namely; a new way of modeling twinning in deformation texture development. The basic difficulty treating twinning is that the twinned volume fractions in each grain are in different orientations from the parent crystal. The presence of twinning therefore increases the number of orientations. After a number of increments, the number of orientations are not feasible for the computer codes. To solve the problems, two different techniques have been proposed in the past. i; the random choice Monte Carlo method (Van Houtte, 1978), ii; the Volume Transfer Technique (Lebensohn and Tome, 1991, Tome *et al.*, 1992). These techniques have successfully been applied for predicting texture development in the presence of twinning. Both, however, suffer from certain limitations.

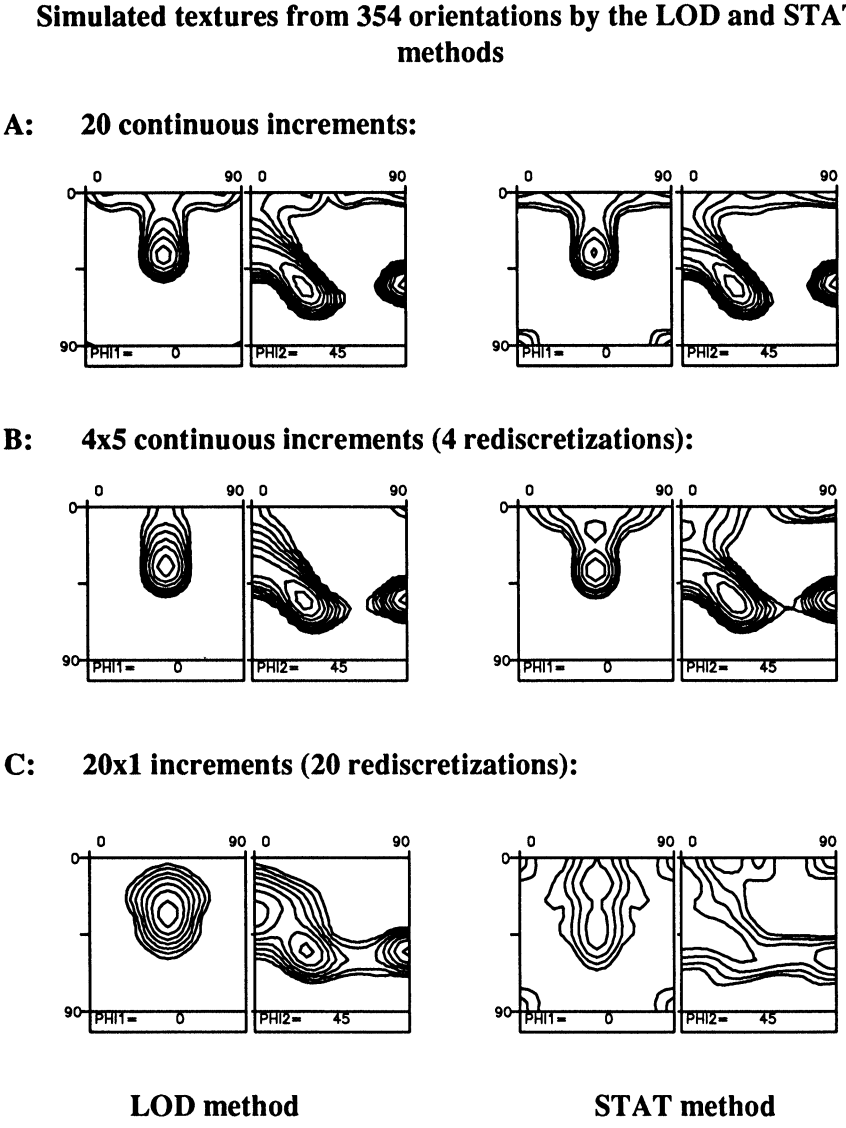


Figure 5 Effect of rediscretization during the simulation of texture development. The simulated textures obtained by the LOD and STAT methods are compared. Rolling, $\varepsilon = 1$, lath model with rate sensitive slip, $m = 0.05$. (Isovalues on all diagrams: 1, 1.4, 2, 2.8, 4, 5.6, 8, 11, 16, 22. Gaussian spread: 7°.)

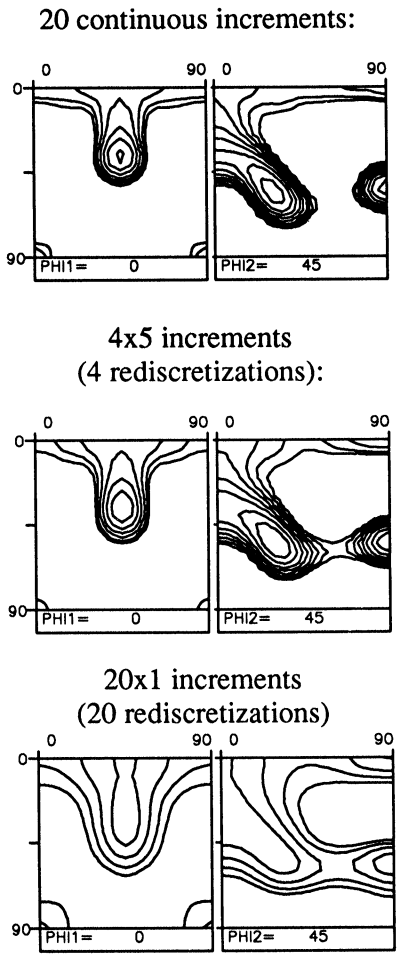


Figure 6 The effect of rediscretization during texture development using the Statistical Technique with 1970 grain orientations. Rolling, $\varepsilon = 1$, lath model with rate sensitive slip, $m = 0{\cdot}05$. (Isovalues on all diagrams: 1, 1.4, 2, 2.8, 4, 5.6, 8, 11, 16, 22. Gaussian spread: 7°).

We propose here the following procedure for the modeling of twinning. During the simulation of deformation texture development, twinning is allowed in each crystal, and the new twin orientations with their precise orientations and the computed volume fractions are treated as new grains. In this way, after approximately 3–5 increments, the number of orientations can increase up to a couple of thousand if the initial set was around 300–500. When a critical large number of orientations are accumulated, the distribution is made continuous by putting a Gaussian distribution on each orientation. Then a rediscretization of the continuous distribution is performed. By using the LOD or the STAT technique, as we demonstrated in the previous sections, satisfactory new distributions can be obtained. With this new distribution, the deformation is continued and re-

discretization is again applied when the grain number becomes too large. In this way, large strains can be achieved.

No simulations have been carried out yet with the above technique. It is one of the purpose of the present paper to suggest this new possibility. It is expected, however, that this new technique can handle twinning more precisely than the methods available so far.

6. SUMMARY

In this paper, we have presented two new techniques for the discretization of continuous orientation distribution functions: the Statistical and the Limited Orientation Distance procedures. A frequently utilized third technique, known as the Cutting Method, has also been examined for comparison purposes. Four tests have been carried out on the generated discrete distributions:

I. their performance to reproduce the ODF,
II. R and M-value predictions,
III. simulation of deformation texture development,
IV. rediscretizations during deformation texture modeling.

The results of the above tests have demonstrated that the STAT and LOD techniques are capable to generate discrete distributions which represent the texture and the physical parameters in good agreement with the continuous distribution. Even relatively small grain-number distributions (e.g. 354) can produce satisfactory results. It was found, however, that the Cutting Method is not suitable for such low number of grain orientations, but even for larger number (e.g. 1970) some of the results (i.e. R and M values) are not satisfactory.

The results obtained from the rediscretization tests, carried out by the STAT and LOD techniques, have shown that by rediscretizing after every 5 step during deformation texture modeling, the texture is still well reproduced. On the basis of this result, a new technique has been suggested to account for twinning during deformation texture development.

APPENDIX

Statistical Properties of the STAT-Method

In this Appendix, we will use the classical statistical concept of the *expected value operator,* to be applied to a random variable y:

$$E(y) = \int_{-\infty}^{\infty} yp(y)\,\mathrm{d}y \tag{A-1}$$

in case of a continuous random variable ($p(y)$ is its probability distribution function), and

$$E(y) = \sum_{i=1}^{N} y_i p(i) \tag{A-2}$$

for random variables with N discrete values. $p(i)$ is the probability of y_i. In both cases, the expected value is the true average μ_y of the population of all y, i.e. the average of all y if an infinite number of y-values would be produced. It is shown in handbooks on statistics that the $E(y)$-operator is distributive over the terms of a sum.

Let $M(g)$ be some physical property which is a function of the crystal orientation, for example (but not necessarily) a Taylor factor. The average of $M(g)$ for the polycrystal is:

$$M_m = \int M(g)f(g)\,\mathrm{d}g \tag{A-3}$$

the integral to be taken over the entire Euler space. A good approximation of M_m would be the following value:

$$\mu_M = \sum_{i=1}^{N} M(g_i)f_i \tag{A-4}$$

which is an estimate of the integral based on the N discrete boxes in Euler space (f_i is defined in Eq. (4)). Eq. (8) and (A-2) show, that it also is the expected value of the M-function calculated for an orientation g_{i_k} obtained by the STAT-discretization method described above. The N different $M(g_i)$-values used in Eq. (A-4) can be seen as statistical values in their own right. They form a set, or *population,* of which μ_M is the mean and σ_M^2 the variance:

$$\sigma_M^2 = \sum_{i=1}^{N} [M(g_i) - \mu_M]^2 f_i \tag{A-5}$$

which can be readily calculated.

THEOREM The expected value of the average $\bar{M}$ of the M-functions of a set of n discrete orientations, derived from the ODF by the STAT-method, is equal to μ_M, and hence is a good estimate of M_m.

Proof

$$\bar{M} = \sum_{k=1}^{n} M(g_{i_k})v_k \tag{A-6}$$

in which v_k is defined by Eq. (9). So, since the expected value operator is distributive,

$$E(\bar{M}) = \sum_{k=1}^{n} v_k E[M(g_{i_k})] \tag{A-7}$$

Because of the fact that the expected value of the M-function calculated for an orientation g_{i_k} obtained by the STAT discretization method is μ_M (as explained above), and because of Eq. (9), this becomes

$$E(\bar{M}) = \sum_{k=1}^{n} v_k \mu_M = \mu_M \tag{A-8}$$

So this means that the average of the $\bar{M}$-values obtained from all possible discretizations in n orientations by the STAT method, is indeed equal to μ_M and

hence very close to M_m. In statistical languague, one would say that $\bar{M}$ is an *unbiased estimator* of μ_M. The authors do not know any other discretization method for which such a property can be proved. Note that all this becomes at once clear if one regards the n values of $M(g_i)$ (obtained from the n discrete orientations) as a set in their own right. They then can be seen as a sample of size n taken from the population of the N values $M(g_i)$. It is well known in statistics that M, the mean of such sample, is an unbiased estimator of μ_M, the mean of the population $M(g_i)$. According to the central limit theorem, the variance $\sigma^2_{\bar{M}}$ of the $\bar{M}$-distribution is equal to σ^2_M/n. The distribution moreover becomes Gaussian if n is large enough. This makes it possible to establish a confidence range for μ_M: e.g. $\bar{M} + 1.96\,\sigma_{\bar{M}}$ for a confidence level of 95%. So it is possible to estimate the error induced by statistical type discretisations on the average values of physical properties.

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