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ACCURATE REPRESENTATIONS OF GENERAL TEXTURES BY A SET OF WEIGHTED GRAINS†

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INTRODUCTION

Texture information requires many numbers for a complete specification: only a few well-known cases can be described accurately enough by a few *components*, even when some specified spread around them is allowed, and even *fibers*, whose location and intensity profile must be specified, are restricted to special cases[1]. For general textures that are not sharp, have low symmetry, or are simply not known in advance, the complete orientation distribution (OD) is needed. It is typically described by intensities on a 5°x5°x5° grid in the three Euler angles. For polycrystals of cubic lattice symmetry and orthorhombic sample symmetry, this requires about 2000 numbers; for tetragonal crystals of monoclinic sample symmetry, about 12000; for arbitrary symmetry about 200000. With the advent of quantitative texture analysis as a routine tool in materials problems, cases of low symmetry arise frequently: e.g., arbitrary deformations must presume triclinic *sample* symmetry; and applications in geology usually relate to *crystal* symmetries lower than cubic.

The question then arises how one may reduce the number of necessary parameters and still retain sufficent accuracy. It is true that the number of coefficients in a series of generalized spherical harmonics, to some reasonable order, is much smaller, and that *tensor* properties can be derived from these exactly; however, for many problems, especially in plasticity and recrystallization, *simulation* is the only realistic approach to solving problems accurately enough, and this requires a set of *grains* of given orientations.

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It is for the purpose of having a standard, routine algorithm for deriving texture information to a prescribed accuracy that the method of *weighted grains* has been devised, which is the topic of this paper. Then arbitrary *measured* textures can be used as input to simulation codes such as the Los Alamos polycrystal plasticity (LApp) code[2].

The general principle is as follows. One starts with a number of grains and distributes both their location in Euler space and their weight such as to give a *uniform* density in orientation space to the desired accuracy. Then one multiplies the weight of each grain by the known intensity in the neighborhood of its location in orientation space. Finally, one may minimize the number of grains by discarding those that have less than a given weight, or contribute less than a certain fraction to the desired property. For sharp textures, one may therefore start with a large number of grains (so as not to miss sharp peaks) and then eliminate many of the grains in the sparsely covered areas. For weak textures, one must choose the initial number about equal to what one can afford. The judgment as to what is accurate enough can be made by comparing the original OD with one that is rederived from the weighted grains file.

In order to visualize the accuracy of OD representations, ODs should be plotted with minimum distortion. This is done by using *oblique sections*[3-5] in *polar* (not square), *equal-area* (not stereographic) projection[6], and so that the average of all sections corresponds to the inverse pole figure for axis 3. Orientation *densities* are plotted as gray-scales on a *logarithmic* scale (as the eye works); *discrete* orientations as crosses sized in proportion to the weight. (These software items are a part of popLA, the "preferred orientation package - Los Alamos"[7].)

GRAINS ON A LATTICE IN ORIENTATION SPACE

A 'lattice' in orientation space can in principle be chosen such that each point has the same weight for a uniform distribution (for example, by choosing the Θ-spacing proportional to $\sin\Theta$). This method produces an acceptable number of grains only when there are sufficiently many symmetry elements and one takes advantage of them. One such file has been proposed by Fortunier and Hirsch[8] for cubic crystal symmetry combined with orthorhombic sample symmetry; it contains 936 grains. We will use it for comparison with our present proposal below.

We have designed our file for tetragonal crystal symmetry and a diad in the sample Z-axis; then, our 3456 grains correspond to an average spacing of about 5° in orientation space. For cubic crystal symmetry, each set of three equivalent points in a quadrant can be averaged; then, you have 1152 points – still allowing for monoclinic sample symmetry.

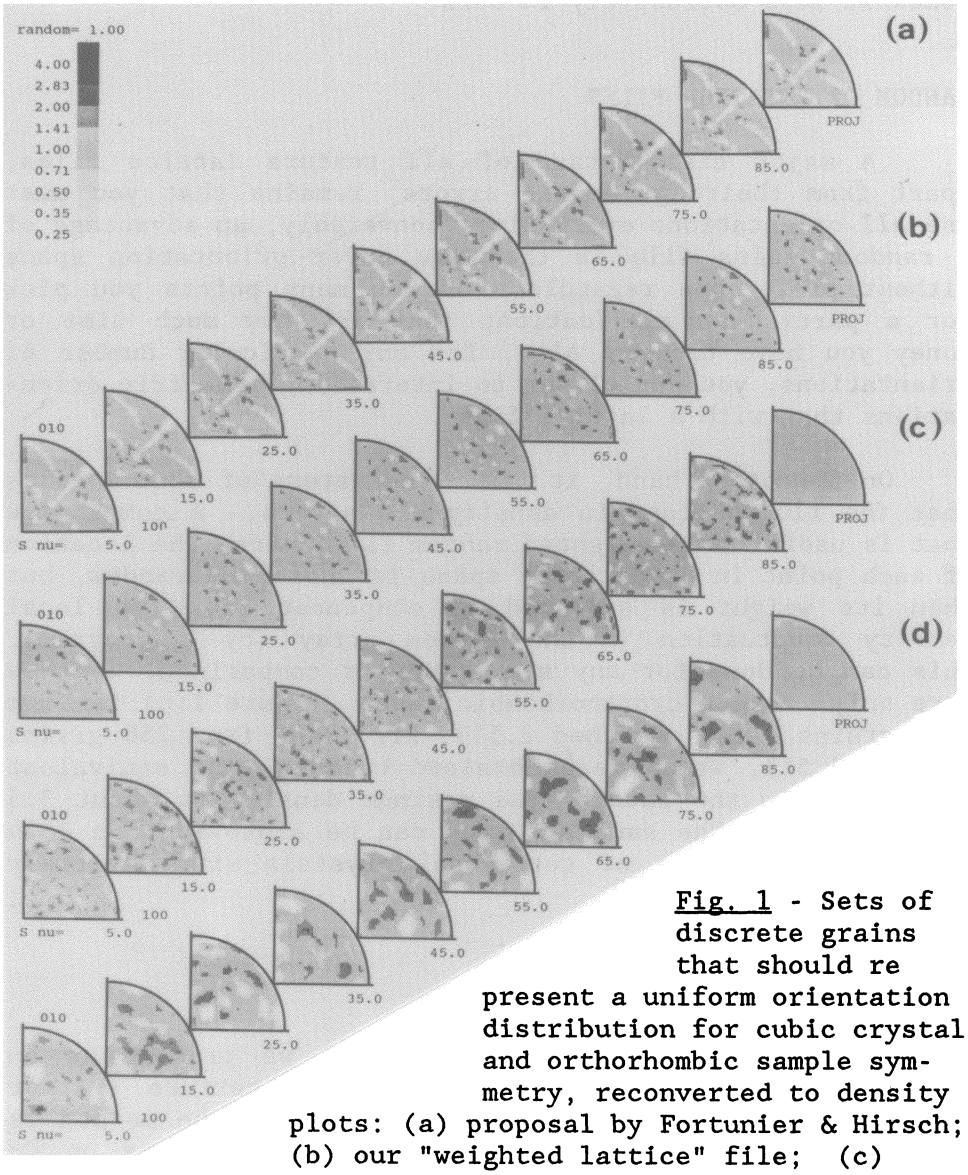

Fig. 1 - Sets of discrete grains that should represent a uniform orientation distribution for cubic crystal and orthorhombic sample symmetry, reconverted to density plots: (a) proposal by Fortunier & Hirsch; (b) our "weighted lattice" file; (c) a file of 1000 grains that are randomly placed but weighted to compensate for fluctuations; (d) as (c), but 256 grains, after triplet averaging.

Each grain is *weighted* in order to obtain as *uniform* a distribution as possible. Figures 1(a) and (b) show the recalculated density plots for the Fortunier/Hirsch set and ours, respectively, for cubic/orthorhombic symmetry. Both files were smoothed with a Gaussian filter with a decay angle of 2.5°. The range of significant intensities is between about 0.5 and 2.0 m.r.d. for both, but the distribution deviates from being uniform in a *systematic* way – somewhat less obtrusively in ours.

RANDOM ORIENTATION FILES

A major disadvantage of all texture *lattice* files, apart from their systematic errors, remains that you must use *all* orientations every time; conversely, an advantage of a *random* grains file is that you cover orientation space without preference regardless of how many points you pick for a particular application; that is, how much time or money you have today. Also, for any particular number of orientations, you get closer to interesting symmetric orientations than with a lattice file.

On the other hand, it is in the nature of random files that the fluctuations in density are severe. A compromise that is useful is a *weighted random* file: here, the location of each point in orientation space is chosen at random, but then its weight is adjusted to compensate for the local density fluctuation in the random array (by a program). This can be done for *any* symmetry; for comparison, we show here only the cubic/orthorhombic case. Figure 1(c) is from 1000 grains (also smoothed 2.5°), Fig. 1(d) from 256 grains (smoothed 5°), which were obtained by averaging equivalent triplets. In the latter, the maximum density is about 3.5 times random. The same accuracy can be achieved with 1024 grains for the case of tetragonal crystals with arbitrary sample symmetry.

AN APPLICATION

For comparison with other methods, we present as an example a well-known case, with a strong texture (rather than an unknown, low-symmetry case, for which the method is also applicable). Figure 5(a) is from experiments on Cu after channel-die compression to a von Mises strain of 1.1. It was represented first by the random weighted file of Fig. 1(d). Weights below 0.5 m.r.d. were discarded, which

resulted in a loss of a volume fraction of 0.13: only 87 grains remained. Fig. 5(c) shows the 87 grains discretely; Fig. 5(b) after re-binning them into a density file: the agreement is quite satisfactory. Finally, Fig.5(d) shows *lattice* points, again discarding weights below 0.5 m.r.d., which resulted in 364 grains.

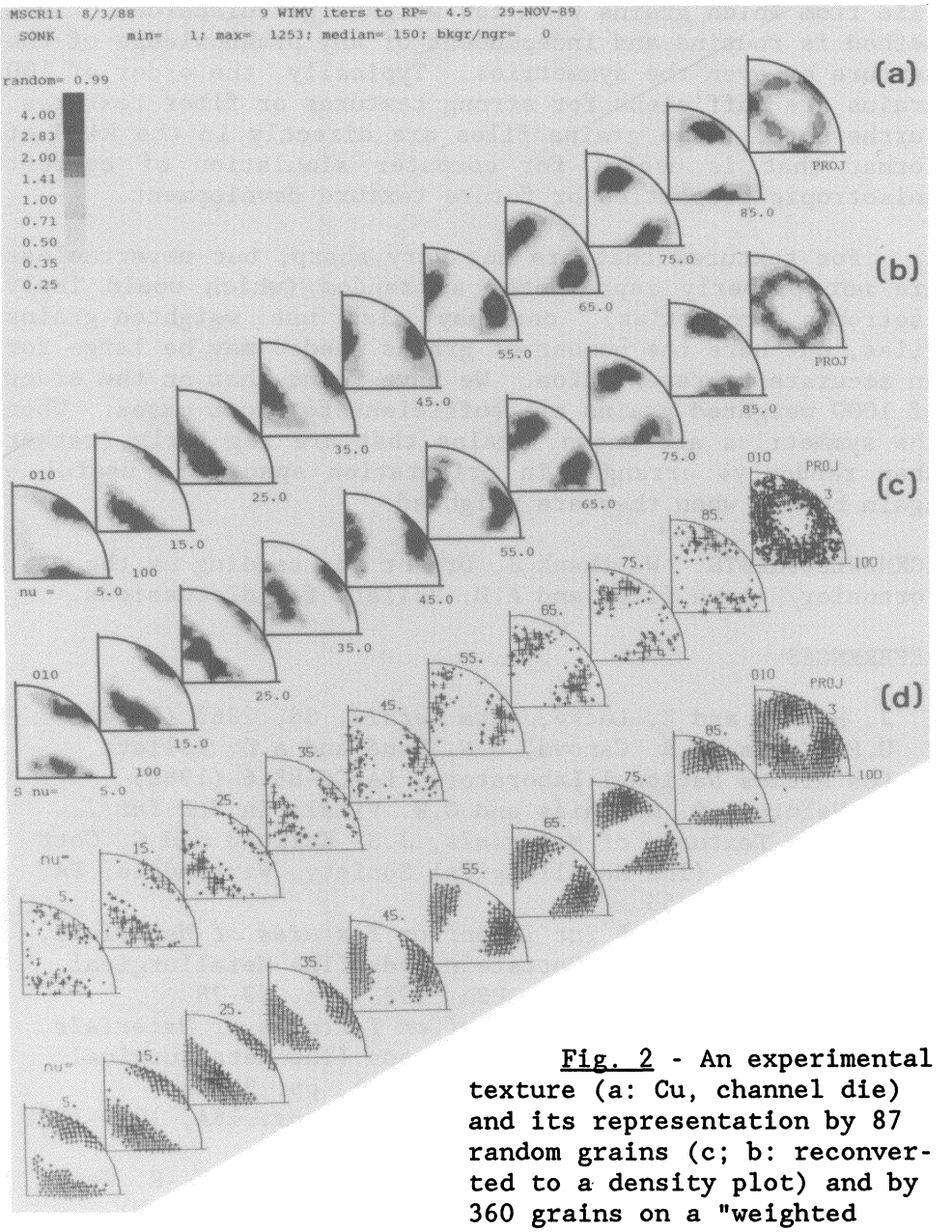

Fig. 2 - An experimental texture (a: Cu, channel die) and its representation by 87 random grains (c; b: reconverted to a density plot) and by 360 grains on a "weighted lattice" (d).

CONCLUSION

The most compact way of describing general texture information is by way of a file of weighted discrete grains. When the textures are strong, this results in a great saving of necessary parameters. The most efficient way is a random file from which grains with low weights get discarded. This method is routine and independent of any preknowledge of the texture or even the symmetries. Typically, the order of 100 grains are sufficient for strong textures or fiber textures. Furthermore, these grains files are directly in the kind of format that is useful for computer simulation of current anisotropic properties or future texture development.

For textures that are not very sharp, but nevertheless are not properly represented as random (which would imply isotropic properties), one may also use weighted-grains files, but here the number of grains needed may be large for an accurate representation. We have found that on the order of 1000 weighted grains are sufficient for most cases. When the symmetries are known, grains that are regularly (rather than randomly) arranged in orientation space are useful – again better when they are weighted.

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