

CONSTRUCTION OF A PSEUDO-MATERIAL REPRESENTATIVE OF A REAL TEXTURED MATERIAL FROM ODF OR DIRECT POLE FIGURES.

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INTRODUCTION

The averaging of an orientation dependant physical quantity over a textured material is a classical operation which is often made directly with the help of the harmonic expansion method coefficients ⁽¹⁾. However, the use of a pseudo-material representing a real material is commonly found, for instance in the field of plastic deformation modelling ⁽²⁾ or elastic moduli calculation ⁽³⁾. In this representation, the material is considered as an aggregate of grains (or crystallites) characterized by their crystallographic orientation (among other characteristics which are beyond the purpose of the present paper). The property to be averaged is considered as constant throughout each grain; in such conditions, integral equations can be transformed into algebraic equations which make practical calculations much easier.

The orientation of a grain is described by three independant parameters corresponding to the three rotational degrees of freedom of a solid. The most commonly used are the three Euler angles as defined by Bunge convention. A pseudo-material is thus a set of triplets of Euler angles. For practical calculations, the number of crystallites of a pseudo-material varies around a few hundreds or a few thousands. In the modelization of texture development induced by plastic deformation, it is common to start with an isotropic pseudo-material ⁽²⁾. In the case of the study of X-ray elastic properties of textured materials, a pseudo-material has been generated according to an ideal fiber texture ⁽⁴⁾. However, it could be interesting to be able to build a pseudo-material representative of any given experimental texture and to determine how accurate this representation is. The purpose of the present paper is to show how this can be done either from the ODF of the specimen calculated with classical methods or directly from experimental pole figures.

CONSTRUCTION OF A PSEUDO-MATERIAL FROM THE ODF OF THE SPECIMEN.

Following an example given by Humbert ⁽⁵⁾, the ODF obtained from pole figures is a computation of information concerning some 10^4 grains, however, commonly used pseudo-materials contain much less crystallites (10^2 to 10^3) and must therefore be *statistically* representative of the ODF. The basic principle of such a fitting is to consider a pseudo-material as a particular sample taken randomly among an infinite

population distributed according to the ODF. This comes naturally, the ODF being by character a probability density distribution: if the ODF is normalized so that

$$\int_{\Omega} \text{ODF}(\Omega) \cdot d\Omega = 1, \text{ then } \text{ODF}(\Omega) d\Omega = \text{ODF}(\phi_1, \Phi, \phi_2) \cdot d\phi_1 \cdot \sin\Phi d\Phi \cdot d\phi_2 \text{ is the}$$

probability of a crystallite to have orientation $\Omega = (\phi_1, \Phi, \phi_2)$. Then, how is it possible to choose, say 100, values of Ω according to the ODF? If the material is isotropic (i.e. $\text{ODF}(\Omega)$ is constant), the three variables $\phi_1, \cos\Phi$ and ϕ_2 are uniformly distributed over $([0, \pi/2], [0, 1], [0, \pi/2])$ and a random number generator can then easily produce 100 times three values u, v, w ranging from 0 to 1. Then, setting $\phi_1 = u \cdot \pi/2$, $\cos\Phi = v$ and $\phi_2 = w \cdot \pi/2$, we obtain an isotropic pseudo-material. This procedure can be extended to any distribution with the help of ORIENTATION REPARTITION FUNCTIONS (ORF). Repartition Functions are statistical functions which can transform a given arbitrary distribution into a uniform distribution and can easily be inverted.

Let $\text{ODF}(\phi_1, \Phi, \phi_2)$ be the probability density for the Euler angles (ϕ_1, Φ, ϕ_2) ; the Margin Density Function of the couple (ϕ_1, Φ) is defined by:

$$\text{MDF}_{\phi_1\Phi}(\phi_1, \Phi) = \int_0^{\phi_2^{\max}} \text{ODF}(\phi_1, \Phi, \phi_2) \cdot d\phi_2$$

The density of crystallites along ϕ_2 depends on ϕ_1 and Φ , so we have to define the conditional density of ϕ_2 for given $\phi_1 = \phi_{10}$ and $\Phi = \Phi_0$ by:

$\text{ODF}(\phi_2 | \phi_1 = \phi_{10}, \Phi = \Phi_0) = \text{ODF}(\phi_{10}, \Phi_0, \phi_2) / \text{MDF}_{\phi_1\Phi}(\phi_{10}, \Phi_0)$ and the conditional repartition function of ϕ_2 is therefore:

$$\text{ORF}(\phi_2 | \phi_{10}, \Phi_0) = \frac{\int_0^{\phi_2} \text{ODF}(\phi_{10}, \Phi_0, \phi_2) \cdot d\phi_2}{\text{MDF}_{\phi_1\Phi}(\phi_{10}, \Phi_0)}$$

In the same way, the Margin Density Function of ϕ_1 is:

$$\text{MDF}_{\phi_1}(\phi_1) = \int_0^{\Phi^{\max}} \text{MDF}_{\phi_1\Phi}(\phi_1, \Phi) \cdot \sin\Phi \cdot d\Phi$$

The Orientation Repartition Functions of Φ and ϕ_1 are:

$$\text{ORF}(\Phi | \phi_{10}) = \frac{\int_0^{\Phi} \text{MDF}_{\phi_1\Phi}(\phi_{10}, \Phi) \cdot \sin\Phi \cdot d\Phi}{\text{MDF}_{\phi_1}(\phi_{10})} \quad \text{ORF}(\phi_1) = \frac{\int_0^{\phi_1} \text{MDF}_{\phi_1}(\phi_1) \cdot d\phi_1}{\int_0^{\phi_1^{\max}} \text{MDF}_{\phi_1}(\phi_1) \cdot d\phi_1}$$

An Orientation Repartition Function thus enables to establish a correspondence between the domain of definition and the interval $[0,1]$. This ORF transforms the distribution defined by $MDF_{\Phi_1}(\phi_1)$ on $[\phi_{1\text{mini}}, \phi_{1\text{maxi}}]$ into a uniform distribution over $[0,1]$. The pseudo-material can thus be easily build with the following procedure:

- Generation of n triplets of reals $(u,v,w)_i$ uniformly spread over the range $[0,1]^3$.
- determination of ϕ_{10} so that $ORF(\phi_{10}) = u$.
- determination of Φ_0 so that $ORF(\Phi_0 | \phi_{10}) = v$.
- determination of ϕ_{20} so that $ORF(\phi_{20} | \phi_{10}, \Phi_0) = w$.

The n triplets $(\phi_{10}, \Phi_0, \phi_{20})_i$ are then distributed according to the ODF. The reliability of the method must of course be checked. However, a visual check such as that presented on figure (1) is not really satisfying. It is necessary to get quantitative information about the accuracy of the procedure. One way to perform this is to actually use the thus built pseudo-material to a practical calculation where the analytical solution is known. This has been done with good agreement in the case of elastic constants calculations for an isotropic material.

Another way to proceed, in the case of an arbitrarily textured material where no analytical solution is known, is to generate a pseudo-material of infinite number of grains, the statistical deviation being in this case equal to zero. This has been done in a previous work ⁽³⁾ in the case of elastic constants calculations for a cold rolled low carbon steel sheet.

But the most direct way is to compare the pseudo-material to the original ODF. The Khi-square test is commonly used to check the fitting of a sample (the pseudo-material) to a population whose distribution (the ODF) is known. The Euler space is discretized into classes, the number of crystallites in each class is N_{pseudo} and N_{odf} is the theoretical number in each class determined from the ODF. The quantity $R^2 = \sum (N_{\text{pseudo}} - N_{\text{odf}})^2 / N_{\text{odf}}$ is calculated and compared to a value R_s^2 calculated from the number of degree of freedom N_f of the distribution and the confidence interval (generally 95%). If $R^2 < R_s^2$ the Pseudo-Material can be considered as fitting the ODF. As the two distributions are experimental and cannot be expressed analytically, N_f is equal to the number of classes minus one. In order not to loose accuracy, the usual discretisation intervals of the ODF can be taken (e.g. $10^\circ \times 5^\circ \times 5^\circ$ in the Euler space). However, to perform the Khi-square test in good conditions, it is necessary that the number of crystallites in an interval is greater than five, so some intervals must be grouped to fulfil this condition.

The ODF of figure (1a) has been measured on a cold rolled, low carbon steel sheet on 3 uncomplete pole figures $\{110\}$, $\{200\}$, $\{211\}$ with $\text{MoK}\alpha$ radiation and calculated with the Harmonic Expansion Method and discretized on a grid of $10^\circ \times 5^\circ \times 5^\circ$ steps in (ϕ_1, Φ, ϕ_2) , i.e. 3610 elementary boxes, the negative values being artificially set to zero. A pseudo-material of 3000 grains has been generated from the ODF using the ORF method (fig.1b) and then a reconstructed ODF (fig.1c) has been calculated by mere counting. The reconstructed ODF is very similar in shape and intensity to the original one but it seems somewhat chaotic. However, this is not a problem for practical calculations: for bulk elastic constants, it has been shown that 1500 crystallites are enough to achieve 1% accuracy ⁽³⁾. The Khi-square test performed to compare this pseudo-material to the original ODF gives $R^2 = 407$ with 466 degree of freedom. The

threshold value $R_s^2(0.95, 466)$ is 517. As $R^2 < R_s^2$, one can conclude that the pseudo-material statistically fits the ODF with a confidence level of 95%.

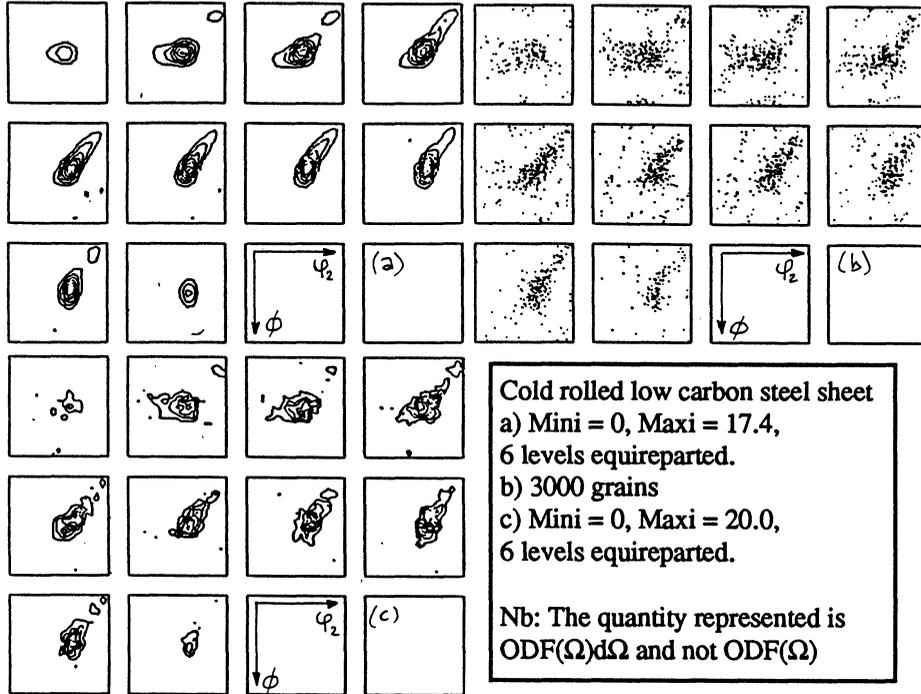


Figure 1: Pseudo-Material (b) generated from the ODF (a) and reconstructed ODF (c)

BUILDING OF A PSEUDO-MATERIAL FROM POLE FIGURES.

The method described above requires the knowledge of the ODF (obtained by any method), however, it is possible to work directly with two or more pole figures. The pole figures are transformed into Pole Density Functions by a pseudo-normalisation operation, then the Pole Repartition Functions can be calculated: $PRF(\Phi)$ and $PRF(\Psi | \Phi)$ or $PRF(\Psi)$ and $PRF(\Phi | \Psi)$ (the integration is performed on uncomplete Pole figures). The orientation of a crystallite is represented by three independent parameters. Two of them can be determined by the position of a pole on the first pole figure calculated from two random numbers and the Pole Repartition Functions. The third parameter is then determined with $PRF(\Psi)$ of the second pole figure which gives the position Ψ of another pole of the crystallite. From these three parameters, the Euler angles of the grain can easily be calculated. However, two problems arise in this method: first, though the family of the second plane is known, its particular permutation of $\{hkl\}$ indices is not (even if some of them can be eliminated for reasons of symmetry or geometrical impossibilities). Second, the use of the Pole Repartition Function of the second pole figure $PRF_2(\Psi)$ is not correct. It should be a conditional PRF, describing the repartition of Ψ_2 knowing Φ_1 and Ψ_1 , this function is of course not known. In order to solve these problems, an iterative procedure is executed until the orientation that fits the best the actual pole figures is found. The fitting function can be for instance, the R^2 quantity used to perform the Khi-square test. Iterations are stopped when the misfit is considered as due to random dispersion.

COMPARISON OF ODFs OR POLE FIGURES WITH A χ^2 TEST.

The Chi-square test is commonly used in statistics to determine the fitting of samples and distributions. The test gives a quantitative value R^2 characteristic of the distance between two distributions and, given a threshold value, a yes/no answer to the question "Are these two distributions significantly different?". This procedure can be extended to the comparison of two ODFs or two pole figures; the method described below refers to the latter case but the treatment of the former is very similar.

The two pole figures to compare are discretized identically and transformed into Pole Distribution Functions. The Pole Repartition Functions are then calculated and the poles occurrences in every classes of both pole figures are determined. The quantity R^2 can then be computed and compared to the threshold value and it can be decided whether the two pole figures are alike or not. The distance between the two pole figures being constant, the value of R^2 will depend on the total number of poles. The greater this number, the more significant the distance. An example is shown on figure (2), where the two pole figures {200} have been measured on the same specimen, one with $\text{CrK}\alpha$ radiation and a position sensitive detector and the other with $\text{CoK}\alpha$ radiation and a scintillation detector. The specimen is the same than for figure (1). For 3000 poles generated from the Pole figures, R^2 is equal to 157, the number of degree of freedom is $N_f = 139$ and $R_s^2(0.95, 139) = 166$, the two pole figures cannot thus be considered as different; For 5000 poles, $R^2 = 268$, $N_f = 162$ and $R_s^2(0.95, 162) = 191$, the two pole figures are significantly different. This can be considered in two ways:

- given the accuracy of the calculation to perform on the pseudo-material, e.g. 1% for calculation of Bulk Elastic Constants, the number of crystallites in the pseudo-material can be determined as was shown in a previous work (3). Once the total number of crystallites and poles is known, the comparison can be performed and the two ODFs or pole figures will be said to be identical (or different) relatively to the accuracy of the calculation.

- In the second way the two pole figures are considered as identical under a critical number of poles N_c and different beyond this number. N_c can be taken as a semi-quantitative measure of the distance between the two pole figures (or ODFs). In the example of figure (2), N_c is equal to 3250 poles.

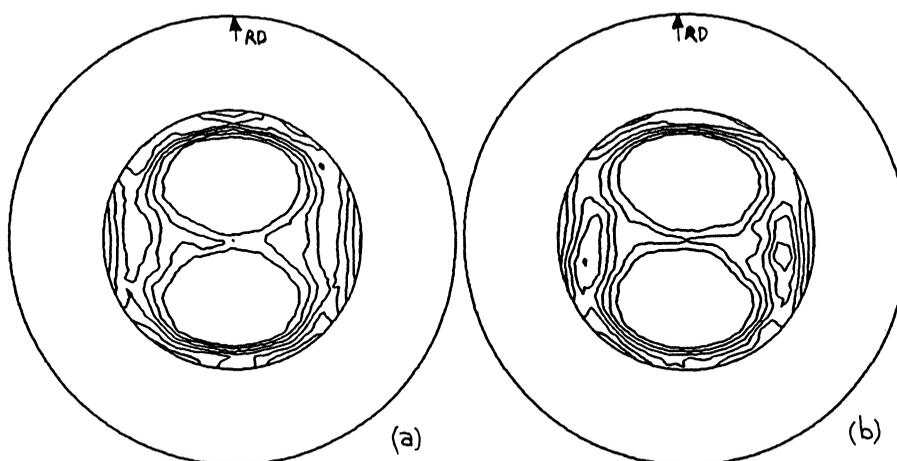


Figure 2: {200} pole figure with $\text{CrK}\alpha$ (a) and $\text{CoK}\alpha$ (b) radiation

CONCLUSION

The present study showed how it is possible to build a pseudo-material representative of the texture of a specimen using Repartition Functions. It can be constructed either from the ODF of the material obtained by classical methods or directly from two or more pole figures. The reliability of the method has been checked with the help of a Khi-square test. This test can also be used to compare two pole figures and ODF and lead to a meaningful concept of distance between the two distributions.

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