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UNFOLDING THE BIVARIATE SIZE-ORIENTATION DISTRIBUTION

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ABSTRACT

A new stereological problem, unfolding the bivariate size-orientation distribution of platelike particles from vertical uniform random sections, is solved. While the theoretical double integral equation has been derived by Gokhale(1995), here we proceed by discretization. The input histogram of planar size-orientation parameters is transformed to the desired histogram of spatial quantities. The discretized equation is solved by means of an EM-algorithm.
Practical application when investigating the damage initiation process in metal matrix composites follows. The data measured by an image analyser are transformed and some important parameters are derived from the bivariate distribution.

Keywords: platelike particles, size-orientation distribution, unfolding.

INTRODUCTION

Modern stereological sampling techniques in biology since 1984 make use of three-dimensional probes. In material science up to exceptional cases, preparation of such probes is connected with a tremendous experimental effort. Therefore still classical methods based on an information from a single section plane are of interest. When estimating the geometry of phase particles the assumption of shape is then necessary. This is in practice often only an approximation, however, usually statistical methods are robust with respect to slight deviations of this assumption.
The unfolding problems in stereology connect geometrical parameters of random particles with those of planar particle sections. For specific shapes of particles, integral equations between corresponding spatial and planar probability distributions are known. When the geometry of particles is described by two parameters, equations for bivariate distributions are of interest. The problem of isotropic random spheroidal particles was solved by Cruz-Orive(1976), expressing the size-shape distribution of spheroids by means of the size-shape distribution of ellipses in the section plane. For polyhedral particles further methods (Ohser and Mücklich, 1995) were obtained by concerning the size-shape and size-number distribution, number denoting the number of edges. Even if sections of such particles are irregular and analytical equation is not available, an ingenious method using simulation of sections was suggested.
Here we solve a new type of bivariate unfolding problem of size and orientation for platelike particles with circular shape, where the spatial orientation is represented by colatitude from

a given axis. The method can be employed to anisotropic structures with dependent size and orientation of particles. The analytical solution derived by Gokhale(1995) was based on the planar information based on vertical uniform random sections. We observe that in this case sizes and orientations can be unfold in two subsequent steps and a discrete solution is presented which yields the desired bivariate histogram of spatial parameters.
The given axis (which is not called vertical in the following) corresponds in material science to situations where e.g. the specimen is deformed in one direction. When the structure presents rotational symmetry around this axis, than unfolding can be performed from a single section. An application to the study of damage initiation process in AlSi composites follows.

THEORETICAL SOLUTION

Let thin plates have random diameter d and orientation (θ, ϕ), θ being the colatitude and $\phi \in (0, 2\pi)$ the longitude. We denote $f(d,\theta) = \frac{1}{2\pi}\int_0^{2\pi} f_1(d,\theta,\phi)d\phi$ the joint probability density function of the diameter d and angle θ between the plate normal and the fixed symmetry axis. Let a symmetry section plane be such that contains the symmetry axis. In a random symmetry section plane particle sections are observed of length y and orientation angle α to the symmetry axis. Let $g(y,\alpha)$ be the corresponding probability density function. Further N_V, N_A are the mean number of particles per unit volume, particle sections per unit area, respectively. Gokhale(1995) derived an integral equation connecting f and g

$$N_A g(y,\alpha) = N_V \frac{4}{\pi}\int_y^\infty \int_{\pi/2-\alpha}^{\pi/2} \frac{y\cos\theta\sin\theta f(d,\theta)dd\,d\theta}{\sin^3\alpha\sqrt{(d^2-y^2)(\tan^2\theta-\cot^2\alpha)}}, \tag{1}$$

for $y \geq 0$, $\alpha \geq \frac{\pi}{2} - \theta$. It is a double Abelian equation the theoretical solution of which with respect to f is available, see Gokhale(1995).
Our aim is to develop and demonstrate a practical solution in the situation when the input is a bivariate frequency histogram of lengths and orientations measured in the section plane either manually or by an image analyser. In this case, the use of the analytical solution is not comfortable since it requires fitting of the bivariate density followed by numerical differentiation and integration. Therefore we develop a traditional approach of discretization of the integral equation (1) and evaluation of the bivariate histogram of spatial parameters. First denote

$$M(\theta,\alpha) = \frac{4}{\pi}\frac{\cos\theta\sin\theta}{\sin^3\alpha\sqrt{\tan^2\theta-\cot^2\alpha}} \tag{2}$$

and rewrite (1) as

$$N_A g(y,\alpha) = N_V \int_y^\infty \frac{y}{\sqrt{d^2-y^2}} \int_{\pi/2-\alpha}^{\pi/2} M(\theta,\alpha)f(d,\theta)d\theta\,dd. \tag{3}$$

We observe that (1) may be solved in two steps:
a) for each fixed α solve the "outer" problem

$$g(y,\alpha) = \frac{y}{\overline{h}}\int_y^\infty \frac{h(d,\alpha)}{\sqrt{d^2-y^2}}dd, \quad \overline{h} = \frac{N_A}{N_V}. \tag{4}$$

b) solve the "inner" problem

$$h(d,\alpha) = \int_{\pi/2-\alpha}^{\pi/2} M(\theta,\alpha)f(d,\theta)d\theta \tag{5}$$

w.r.t. f for each fixed $d > 0$.

In each step the discretization is applied to get finally the desired bivariate histogram of spatial size and orientation. We start with a) which is in fact the well-known Wicksell(1925) corpuscule problem. We briefly remind its discretization using the idea of Ohser, Mücklich(1995).
It starts from the integral equation (4) rewritten in terms of distribution fuctions H, G corresponding to h and g, we omitt the variable α:

$$N_A(1-G(y)) = N_V \int_0^\infty p(d,y)dH(d), \tag{6}$$

where the kernel function $p(d,y) = \sqrt{d^2-y^2}$, $d \geq y$, $p(d,y)=0$ else. In the discretization we simplify the situation assuming that the particle diameter is a discrete random variable with values $d_i = a^i$, $i \in Z$, $a > 1$ fixed. Then $N_V(i)$ denotes the mean number of particles of size d_i per unit volume. Next we classify the section lengths by putting $y_j = a^j$ and denoting $N_A(j)$ the mean number of sections with length y between $y_{j-1} \leq y < y_j$ per unit area of section plane. Let $j_0 \in Z$ corresponds to the class with smallest observed section length and $N_A(j) = N_A(G(y_j) - G(y_{j-1}))$, $j \in Z$. Then putting subsequently y_j and y_{j-1} into (6) and subtracting these two equations we obtain the desired discrete version of (6):

$$N_A(j) = \sum_{i=j}^{\infty} p_{ij} N_V(i), \quad j \in Z, \tag{7}$$

where $p_{ij} = p(d_i, y_{j-1}) - p(d_i, y_j)$. In fact only a vector of coefficients is desired since they have form $p_{ij} = a^i s_{j-i}$, where $s_j = \sqrt{1-a^{2(j-1)}} - \sqrt{1-a^{2j}}$. The solution of (7) is obtained by iterative EM-algorithm (Silvermann et al., 1990) which here takes a special form

$$N_V^{(m+1)}(i) = \frac{N_V^{(m)}(i)}{\sqrt{1-a^{2(j_0-i-1)}}} \sum_{j=j_0}^{i} \frac{N_A(j)s_{j-i}}{\sum_l N_V^{(m)}(l)p_{lj}}. \tag{8}$$

Here m is the index of iteration, we put $N_V^{(0)}(i) = \frac{N_A(i)}{\bar{h}}$, where $\bar{h}$ is a rough estimator of the mean particle diameter.
Further we derive the discretization of the inner problem (5) including orientations. Omitting the size variable d we look for the relation between distribution functions $H(\alpha)$, $F(\theta)$ corresponding to densities h, f in (5). This is obtained by integration of formula (5):

$$H(\alpha) = C \int_{\pi/2-\alpha}^{\pi/2} \int_{\pi/2-\theta}^{\alpha} \frac{\cos\theta dF(\theta)dt}{\sin^3 t\sqrt{\tan^2\theta - \cot^2 t}}, \tag{9}$$

where C is a normalizing constant and $dF(\theta) = \sin\theta f(\theta)d\theta$. This equation is not yet ready for discretization, but using the substitution $\cot\theta\cot t = \sin\phi$, i.e. $d\phi = \frac{dt}{\sin^2 t\sqrt{\tan^2\theta-\cot^2 t}}$ and $\sqrt{1-\sin^2\theta\cos^2\phi} = \frac{\cos\theta}{\sin t}$, we get a form

$$H(\alpha) = C \int_{\pi/2-\alpha}^{\pi/2} \int_{\arccos D(\alpha,\theta)}^{\pi/2} \sqrt{1-\cos^2\phi\sin^2\theta}\, d\phi dF(\theta), \tag{10}$$

where

$$D(\alpha,\theta) = \frac{\sqrt{\sin^2\alpha - \cos^2\theta}}{\sin\theta\sin\alpha}.$$

The kernel function $p(\theta,\alpha)$ of (10) (i.e. $H(\alpha) = C\int p(\theta,\alpha)dF(\theta)$) is in fact the elliptic integral of the second kind denoted $E(\beta,k) = \int_0^\beta \sqrt{1-k^2\sin^2\phi d\phi}$, since

$$p(\theta,\alpha) = \int_0^{\arcsin D(\alpha,\theta)} \sqrt{1-\sin^2\phi\sin^2\theta d\phi} = E(\arcsin D(\alpha,\theta), \sin\theta).$$

Next we define discrete values $\theta_i,\ \alpha_j,\ i,j = 1,...,n$ and denote $H(j) = H(\alpha_j) - H(\alpha_{j-1}),\ F(i) = F(\theta_i) - F(\theta_{i-1})$. Then the discretized equation (10) is

$$H(j) = \sum_i p_{ij} F(i),\ j = 1,...,n, \tag{11}$$

where the coefficients

$$p_{ij} = p(\theta_i, \alpha_j) - p(\theta_i, \alpha_{j-1}) \tag{12}$$

for $j > n - i,\ p_{ij} = 0$ else. Numerical solution of this system by EM-algorithm is given by an iteration step formula:

$$F_i^{(m+1)} = \frac{F_i^{(m)}}{q_i} \sum_j \frac{H(j) p_{ij}}{\sum_l F_l^{(m)} p_{lj}}, \tag{13}$$

where $q_i = \sum_j p_{ij}$. As an initial iteration it is possible to put $F_i^{(0)} = H_i,\ i = 1,...,n$.
Natural choices of discrete values α_i, θ_j may lead to some difficulties because of the form of kernel function. Therefore we suggest the following. Consider the set of measured angles α. The subsample characterized by $\alpha = 0$ has to be tackled in a special way. In fact $\alpha = 0$ determines $\theta = \pi/2$ so for this subsample only the outer problem (4) has to be solved. In the remaining data we may assume that all measured angles α are greater than zero. We denote $\alpha_{\min}$ the minimal observed α, put $\theta_{\max} = \pi/2 - \alpha_{\min}$, $\triangle = \frac{\theta_{\max}}{n}$, $\theta_i = i\triangle$, $\alpha_i = \alpha_{\min} + (i-1)\triangle$, $i = 1,...,n$.
The normalizing constant C in (9) is known, but need not be evaluated. From (8) we in fact obtain by summing the estimator of N_V, then (13) is executed with input $N_V(i)$ from (8) instead of H_i. Finally, the solution F_i from (13) is normalized and multiplied by N_V to get the desired estimator.

APPLICATION

The developed method was used for the unfolding of particle size and orientation in two series of specimens. A chill cast Al-1 wt%Si composite has been heat treated in two different ways in order to obtain precipitation of platelike Si particles. By dissolution annealing at 540°C for 6 hours and slow cooling (18°C/hour) to 20°C the specimen denoted by 2 has been obtained. By dissolution annealing at 540°C for 6 hours, annealing at 440°C for 12 hours and slow cooling (18°C/hour) to 20°C the specimen denoted by 3 has been obtained.

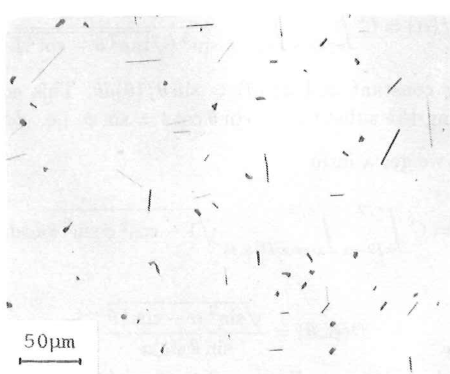

Fig.1: Micrograph of polished metallographic sample, specimen 2.

Uniaxial tensile tests using cylindrical specimens of diameter 8 mm and length 60 mm were carried out. Brittle silicon particles embedded in ductile aluminium matrix do not deform

plastically and particle cracking has been expected to occur during deformation. In order to study the damage of Si particles metallographic samples were prepared from specimens deformed up to fracture. The corresponding strain of specimen 2, 3 was 22.7%, 27.7%, respectively. The deformation axis is here the symmetry axis. The samples (symmetry planes) were cut uniformly randomly parallel to this axis. Therefore the sampling assumptions of the presented method are fulfilled. The angle from the symmetry axis (colatitude) is of interest only. The micrograph of a sample cut from specimen 2 is in Fig. 1, the deformation axis is horizontal.
Quantitative metallographic analysis has been performed by image analysis technique using IBAS-Kontron analyser connected to light microscope. Two sets of data were obtained from each sample: a) the set of data for all particle sections observed (denoted iL, i=2,3); b) the set of data for particle sections with observed cracks (denoted iLC, i=2,3). The size of Si particle section was assessed by the parameter DMAX, representing the maximum length of the section. The orientation of the section was characterized by ANGLEDMAX, the planar angle α from the deformation axis. Since IBAS software allows the measurement of discrete angles in 32 directions only, we obtain a subsample of angles $\alpha = 0$, at least among all particles. For this subsample we have directly $\theta = \frac{\pi}{2}$ as discussed in the previous section.

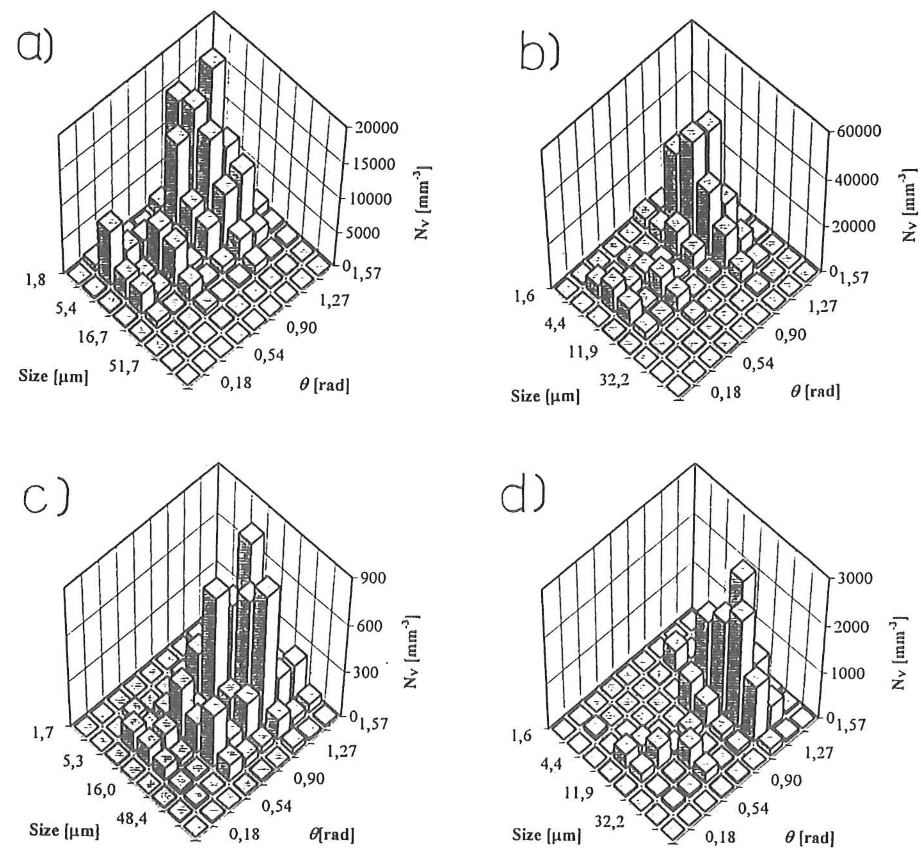

Fig.2: Estimated spatial size-orientation histograms from samples $2L$ (a), $3L$ (b), $2LC$ (c), $3LC$ (d).

The total area included in the analyses for the specimen 2, 3 was 3.72 mm^2, 1.86 mm^2, respectively. The evaluation of bivariate size-orientation distribution according to the developed methods leads to histograms presented in Fig. 2. Due to small sample size only $m = 8$ classes were used for discretization, the ninth orientation class corresponds to $\theta = \frac{\pi}{2}$. It should be noted that not all cracks are observed in the section plane. $N_V(i,j)$ for cracked particles should be corrected in histograms (c), (d) in Fig.2 by $N_V = 2\hat{N_V}$, where $\hat{N_V}$ is the basic estimator obtained by the unfolding. The correction factor 2 is based on the assumption that there is at most one crack in a particle, otherwise it could be smaller in practice.
The total number n of measured particle sections is in Table 1 together with estimated expectations and variances Ed [μm], $E\theta$ [rad], $var\ d$ [μm^2], $var\ \theta$ [rad^2] of particle diameter d, orientation θ, respectively. Clearly (see Ed values) larger particles initiate more frequently cracks. The dependence between spatial size and orientation of particles can be investigated by the correlation coefficient $\varrho_{d\theta}$. Larger positive values of $\varrho_{d\theta}$ for samples iLC in Table 1 are caused by the fact that bigger particles tend to be cracked with increasing θ, i.e. being nearly parallel to the deformation axis.

	n	Ed	$E\theta$	$vard$	$var\theta$	$\varrho_{d\theta}$	λ_n
2L	3335	4.825	1.015	21.42	0.124	0.087	
2LC	454	12.36	0.945	107.94	0.161	0.688	1.257
3L	3018	5.074	1.043	15.51	0.124	0.008	
3LC	397	12.31	1.080	59.87	0.169	0.352	1.614

Table 1: Spatial parameters of the structure estimated from measured data.

The statistics $\lambda_n = \sqrt{n}\, max_{j\leq m}|F(\theta_j) - F_c(\theta_j)|$, where F, F_c are marginal distribution functions of θ corresponding to samples iL, iLC, is another measure of dependence of particle damage on orientation. Approximately, comparing λ_n in Table 1 with critical value $\lambda_n^* = 1.52$ of the Kolmogorov-Smirnov goodness-of-fit test (on significance level 0.05) we have got an evidence of the dependence from 3LC only. Larger samples are desired for a more precise analysis.

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