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A combined test for randomness of spatial distribution of composite microstructures

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ABSTRACT

A new methodology is presented for characterizing the spatial distribution of second-phase particles in planar sections of multi-phase materials. It is based on the issue of statistically summarizing the results of independent tests against the hypothesis of randomness of the particles. The methodology was applied in multiple planar sections of an aluminium alloy reinforced with silicon carbide particles and leaded to a rejection of the hypothesis of randomness even when the tests from single planar sections were ambiguous.

Keywords: Particulate reinforced composite; spatial distribution; randomness; combined test.

1 INTRODUÇÃO

The improved material properties obtained with particulate metal matrix composite will depend on the spatial distribution of the particles in the matrix material [1, 2]. The basic methodology for characterizing the spatial distribution of second-phase particles in single planar sections of composite materials is now well-established [3]. In this context, during the last few years, statistical methods have been appearing, to a certain extent, in material literature to provide the analysis of spatial distribution of particles in composite materials. Methods such as quadrat counts [4], nearest neighbor distances [5], Dirichlet tessellation [6] and spatial pattern descriptors [7] have been applied to test departure against the hypothesis of randomness of the spatial distribution of the reinforcing particles.

A single sample rarely provides a definitive answer to research questions and, therefore there is an interest among material researchers to develop methods based on multiple samples for providing a more rigorous quantitative analysis of the spatial distribution of second-phase particles in two-dimensional multy-phase systems.

When multiple samples of composite material are available, in two or more experimental groups, parametric and non-parametric methods can be used to the analysis of data in the form of replicated spatial point patterns [8]. We are considering here the situation in which we have one experimental group that contains several planar sections of a composite material. The main aim of this paper is to present a method to combine *P*-values from several independent tests against the hypothesis of spatial randomness of the particles. The basic idea of the method is to test whether collectively they can reject the hypothesis of spatial randomness.

2 TESTING AGAINST SPATIAL RANDOMNESS FOR INDIVIDUAL SAMPLES

For practical purposes, each particle is treated as a point defined by its coordinates and, therefore the spatial data can be assumed a map of all particle locations in an essential planar region. Using some functional spatial pattern descriptors such as *F*, *G* and *K*-functions is a natural way to proceed with the statistical analysis of spatial distribution of particle centers in individual planar sections of composite materials [7].

In this paper, we use the *J*-function, introduced by LIESHOUT *et al.* [9], since it performs very well in detecting departure from randomness towards both regularity and clustering alternatives. For a stationary point process, the *J*-function is given by the equation:

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$$J(x) = \frac{1 - G(x)}{1 - F(x)} \qquad (1)$$

for all distances $x \geq 0$, such that $F(x) < 1$, where $F(x)$ is the distribution function of the distance from an arbitrary fixed point to the nearest particle center of the planar section and $G(x)$ is the distribution function of the nearest distance between two particle centers.

A suitable edge-corrected estimator for $F(x)$ is provided by the equation:

$$\hat{F}(x) = \frac{\sum_{i=1}^{m} I_x(x_i, r_i)}{\sum_{i=1}^{m} I_x(r_i)} \qquad (2)$$

where *m* is the number of sample points in the planar section, x_i denotes the distance from the *i*th chosen point to the nearest of the *n* particle centers in the analyzed pattern, $I_x(r_i)$ is an indicator function that takes the value 1 when x_i is less than or equal to *x*, r_i is the distance from each particle center the nearest point on the boundary of the planar section and $I_x(x_i, r_i)$ is an indicator function that takes the value 1 when x_i is less than or equal to *x* and r_i is greater than or equal to *x*. An estimator for $G(x)$ is provided by an equation analogous to equation (2), substituting the distance *x* by the nearest distance between two particle centers [10].

The simplest estimator for $J(x)$ is obtained by plugging into equation (1) the estimates of $F(x)$ and $G(x)$. It is easily seen that under the randomness hypothesis, $\hat{F}(x) = \hat{G}(x)$, so $\hat{J}(x) = 1$. Values of $\hat{J}(x)$ smaller than 1 indicate clustering while values larger than 1 indicate regularity.

In order to define a statistical test for detecting departure against randomness, it is usual to choose a measure of discrepancy that examines the degree of agreement between the observed and the expected empirical distribution functions under the null hypothesis of randomness. A sensible measure to evaluate these differences over a range of distances (x) is given by the equation:

$$u_i = \int_0^{x_0} \{\hat{J}_i(x) - 1\}^2 \, dx \qquad (3)$$

The statistic u_i does not have known sampling distribution. DIGGLE [10] suggests the use of the following Monte Carlo based method to perform the test against randomness. Let $\hat{J}_1(x)$ be the *J*-function of an observed point pattern with *n* events and $\hat{J}_2(x), \ldots, \hat{J}_s(x)$ the *J*-functions from *s* simulations of random patterns with *n* events. Calculate the statistic u_i for the observed and simulated patterns. Then, the value u_1 for the observed pattern is compared with values $u_2, \ldots, u_s$ for the simulated patterns. If u_1 ranks among the largest of $u_2, \ldots, u_s$, it indicates departure from randomness. Suppose $J_1 = J_{(j)}$ for some $j \in \{1, \ldots, s\}$ then reject the hypotheses of CSR if $P = \frac{(s + 1 - j)}{s} \leq \alpha$, where *P* is the one-tailed *P*-value. For example, based on 99 simulations (s = 100), rejection at the 5% level occurs if $J_{(96)} \leq J_1 \leq J_{(100)}$.

3 COMBINED TEST AGAINST SPATIAL RANDOMNESS

Since the individual *P*-values of each sample are available, we can carry out a combined test for a statistical generalization to be made with respect to the combined evidence of a random distribution of particles from all samples. For this, we consider each Monte Carlo test as an individual and independent study to test departure from randomness. Under this supposition, we advocate to use a technique for pooling results across different statistical tests against the hypothesis of randomness. This technique can provide one single *P*-value that allows us to decide the nature of the spatial distribution of the particles within the metal matrix.

When data come in the form of one-tailed *P*-values, FISHER [11] suggests that they can be combined by forming a statistic that is their product. If we have *k* independent studies that give P_i as the tail probabilities, the statistic summarizing the result is the product $P = P_1 P_2 ... P_k$.

If the null hypothesis is true, then P_i have uniform distribution on the interval from 0 to 1. FISHER [11] noted that if P_i is distributed according to the uniform distribution on the interval from 0 to 1, then consequently $-2\log_e P_j$ is distributed like a chi-square distribution with 2 degrees of freedom. If all of the null hypotheses of randomness the *k* tests are true, then the statistic:

$$\chi_o^2 = -2\sum_{j=1}^{k} \log_e P_j \tag{4}$$

will have a chi-square distribution with 2*k* degrees of freedom and so significance is tested by finding the probability of a larger value of the statistic χ_o^2 .

4 EXPERIMENTAL DATA

We have applied the combined test to eighteen metallographic samples of an aluminium silicon carbide composite material produced by the Department of Engineering of Materials, University of Sheffield, England, where silicon carbide second-phase particles had a volume fraction equal to 11%. The metallographic sample areas were $\cong 192 \times 288$ μm.

The eighteen metallographic samples were placed on a computer controlled optical microscope stage analyzer (Polyvar) which allowed fully automatic adjustment, focusing, positioning and scanning of the samples. The overall magnification used was 600 times, yielding a pixel size of 0.375 μm. Thus, the Polyvar produced eighteen digital images with area frame equal to 512 × 767 square pixels.

The two-dimensional digital images were analyzed by using image-processing techniques to extract the coordinates (centre) of each particle within the images. The actual images were 512 x 767 pixels, out of which we used only the particles located in the left top square of 512 x 512 pixels. The 512 x 512 images were transformed into patterns with unit square area to facilitate the spatial analysis.

5 RESULTS AND DISCUSSION

The main aim of the present work has been to provide a statistical analysis of the spatial distribution of second-phase particle centers in two-dimensional distributed multi-phase materials. We have used eighteen samples of an aluminium silicon carbide composite material to answer the main scientific question: whether or not the composite material presents particles that are randomly distributed. We advocate that this question can be adequately answered by using a combined test from independent tests against the hypothesis of randomness.

The analysis start by performing a Monte Carlo test against the hypothesis of randomness of the particle centers in each planar section of the composite material. To carry out these tests, we used 99 simulations (*s* = 100) from a stationary Poisson process of intensity *n* (actual number of particles). As DIGLLE [10] points out *s* = 100 is usually sufficient since for greater *s* the power of the test increases only marginally with *s*. We use *m* sample points in a regular grid $v \times v$ to estimate the values of $\hat{F}(x)$ in equation (2), where $v \cong \sqrt{n}$. The integral in equation (3) was approximately calculated by a Riemann sum at 50 intervals between 0 and 0.05. Table 1 presents the results (one-tailed *P*-values) of the tests against randomness for the individual samples of the composite material.

Table 1: One-tailed *P*-values of the hypothesis tests against randomness of the particle centers for the eighteen samples of the aluminium alloy reinforced with silicon carbide particles

SAMPLE	1	2	3	4	5	6	7	8	9
P-value	0.04	0.03	0.60	0.69	0.03	0.12	0.02	0.61	0.40
SAMPLE	10	11	12	13	14	15	16	17	18
P-value	0.26	0.73	0.39	0.03	0.63	0.46	0.36	0.08	0.30

The one-tailed *P*-values provided in Table 1 show that it is not easy to decide whether the composite material presents evidence that the second-phase particles are randomly distributed. Observe that if one had chosen, for example, sample 2 for his analysis, he had rejected the hypothesis of randomness. Otherwise, if he had chosen sample 3, he had reached an opposite conclusion. Thus, we suggest combining the one-tailed *P*-values with the purpose of obtaining a summary overall *P*-value for testing the same hypothesis of randomness for the whole group of samples.

Applying equation (4) to the results presented in Table 1, we obtained χ^2_o = 61.31. Because there are eighteen independent tests, one for each sample, there are 36 degrees of freedom and χ^2_o = 61.31 is associated with P = 0.0054. Thus, the combined evidence from these eighteen samples indicates a strong rejection of the null hypothesis of a random distribution of particles in the composite material. Observe that the method leads to a rejection of the hypothesis of randomness even when the tests from single samples were ambiguous.

The combined test works well when the alternative distribution has a density that is, approximately, a reversed *J* shape because then it is likely that P_i fall near 0 and produce a small product, and we are likely to reject the null hypothesis. The strength of this approach is that it has good power against the randomness for reverse *J* shaped alternatives [12]. The more serious disadvantage of this combined test is that it treats large and small *P*-values asymmetrically. It is asymmetrically sensitive to small *P*-values compared to large *P*-values [13].

There are several other statistical methods available for combining *P*-values of independent studies. They range from various counting procedures to a variety of summation approaches involving either significance levels or weighted statistical tests such as *t* and *z* tests [12, 13]. Despite the available methods, the combined test presented here remains one of the best known and applied because it is the simplest and most asymptotically efficient of them [13].

One observation that is important to add to any discussion about the method for combining *P*-values is that it can be applied to ask whether the accumulative information among tests on similar null hypotheses can reject that shared null hypothesis. Thus, this procedure may be applied not only to spatial analysis of particle centers but also to any statistical analysis in materials research where there is an interest to test the significance of aggregate independent hypothesis tests.

6 CONCLUSION

The statistical analysis of the spatial distribution of particles can be improved by taking and analyzing multiple samples of composite materials. The goal of this paper has been to advocate the use of a combined test for providing an overall assessment against the hypothesis of spatial randomness of the distribution of particles in composite materials. We have demonstrated that the combined test is efficient to test spatial randomness of particles even when the tests from single planar sections were ambiguous.

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