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SIMULATION OF DISPERSED MICROSTRUCTURE

1. INTRODUCTION

Stereological description of dispersed microstructure is not an easy problem and is constantly a subject of research [1–3]. From the practical point of view, the stereological description of this type of microstructures is essential in analyses of such processes as coarsening, spheroidization or in research of relationship between microstructure and mechanical properties (e.g. bearing steel).

The method of computer simulation is a very comfortable and useful way to test as well as to construct and verify stereological methods. There is a computer model of dispersed structure presented in this work and the assessment of correctness of its performance has been made. The demonstrated model can be used in examinations in scope of stereology of dispersed structures.

It should be mentioned in this place that computer models of such a type were already constructed and used in stereology of dispersed structures previously [4], from the works of Polish authors it is worth reminding the Adrian's [5] and Maliński's [6] studies.

2. STEREOLOGICAL DESCRIPTION OF DISPERSED MICROSTRUCTURE

In a dispersed microstructure one phase occurs in a form of small particles distributed randomly but homogeneously in the material space. Examples of dispersed microstructure: Fe_3C particles in steel (Fig. 1), spheroidal graphite in cast iron, etc. [7].

The basic quantitative characteristics of dispersed microstructure are: the particle density N_V and distribution function $N_V(D)$ ($N_V(D) = N_V f(D)$, $f(D)$ – density function of particle diameter D). The measurement of the N_V parameter and $N_V(D)$ function by stereological methods is an indirect procedure which is based on direct measurements of

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quantitative characteristics such as: particle section diameter (d), chord length (l), particle section area (a). The particle density N_V and distribution function $N_V(D)$ are most often achieved by the approximate methods i.e. Scheil – Schwartz – Saltykov method, Spektor method, Lord and Willis method, etc. [4, 7–10].



Fig. 1. Dispersed microstructure of Fe-0,6%C after isothermal annealing 715°C/600h (by courtesy P. Matusiewicz)

3. SIMULATION OF DISPERSED STRUCTURE – RULES

3.1. Model

Let's assume that particles of dispersed plane are spheres and are randomly distributed in the material space. The measure of the particle size is a diameter D ($0 \leq D \leq D_{\max}$; D_{\max} – the largest size of D ; maximum diameter). Diameter D is a continuous random variable defined by the density function $f(D)$.

The described microstructure is being cut by the random cutting plane on which we get particles sections. The measure of the particle section size is a diameter d ($0 \leq d \leq d_{\max}$; d_{\max} – the largest size of d ; maximum diameter d). Diameter d is a continuous random variable defined by the density function $f(d)$. We are interested in the relationship between densities $f(D)$ and $f(d)$.

3.2. Simulation

In the cartesian coordinate system there is a defined cube of a unit volume ($V = 1$). In the area of the cube the spheres are generated: (1) a sphere diameter D is subject to the given

distribution determined by a density function $f(D)$, (2) a position of the sphere is random; coordinates of the sphere center (x,y,z) in the considered space are subject to uniform distributions.

The considered cube with randomly distributed spheres is being cut by set of planes of determined position (to simplify – the cutting planes are parallel to the axis of a coordinate system). Relating to the spheres being cut by the cutting plane the diameter of a flat section is determined.

Input data for simulation are: (1) relative spheres density N_v , (2) the spheres volume fraction V_v , (3) distribution of spheres diameters determined of a density function $f(D)$ (of course $N_v(D) = N_v f(D)$); the parameters of the given distribution of diameters spheres are determined on the basis of the assumed earlier N_v and V_v .

The primary results of the simulation (1) the parameters: the relative area sections' fraction A_A , the relative sections density N_A , the empirical distribution of flat sections' diameters $N_A(d)$.

3.3. Random number generators, software environment

To generate random numbers of uniform distribution a linear congruential generator has been used [11–13]. In case of generating random numbers of other-than-uniform distributions an inverse cumulative distribution function (CDF) method or an acceptance/rejection method were used the most often [11–13].

In the framework of testing generators and selection of their first parameters the chi-square test of goodness of fit and test of runs have been carried out.

The calculations were carried out in the environment of the software Fortran 95 Lahey-Fujitsu with the application of the IMSL Library [14].

4. MODEL VERIFICATION

4.1. Rules

Before the application of model for proper tests (existing of approximate methods, construction and properties of estimators etc.) it has been verified for the sake of its correctness. To do this the analysis of two cases has been made for which relationships between distributions $f(D)$ and $f(d)$ are known and determinable by calculating.

4.2. Case I – the dispersed microstructure consists of spheres of equal size ($D = \text{const.}$)

In case of $D = \text{const.}$ the function of density of flat sections' diameters $f(d)$ takes the form [6, 15, 16]:

$$f(d) = \frac{d}{D\sqrt{D^2 - d^2}}; \quad 0 \leq d < D \quad (1)$$

The expected value $E(d)$ and variance $D^2(d)$ for the function (1) are adequately as follows:

$$E(d) = \frac{\pi D}{4} \quad (2)$$

$$D^2(d) = \frac{32 - 3\pi^2}{48} D^2 \quad (3)$$

The results of simulation are presented in Figure 2 and in Table 1.

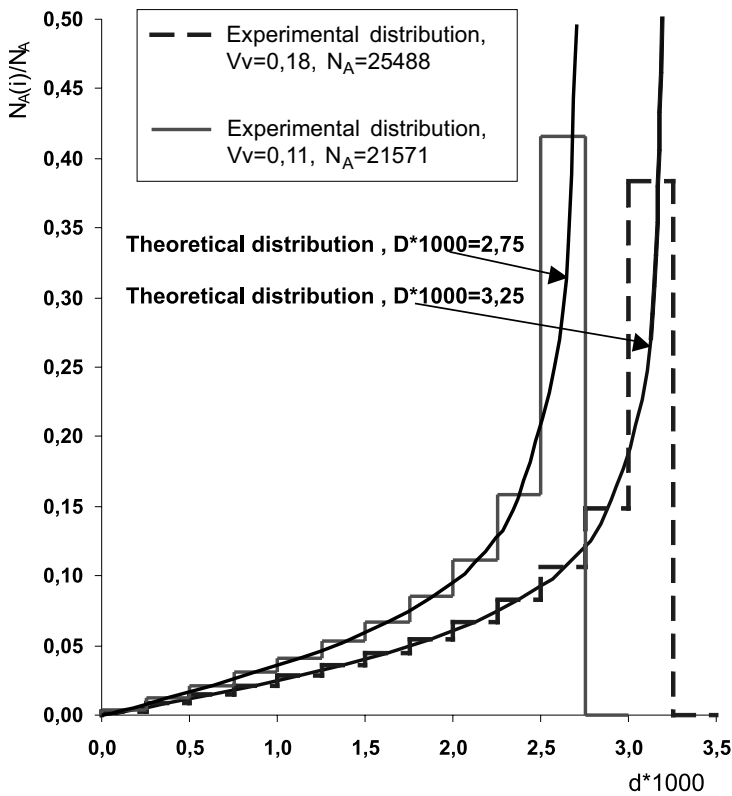


Fig. 2. Experimental and theoretical distributions of flat sections' diameters $d - D = const$

In the meaning of the performed chi-square test of goodness of fit [17] there is no basis for rejection of hypothesis that the achieved empirical distribution of flat sections' diameters (Fig. 1) corresponds to the density function (1) – ($Vv = 0.11$ – p-value = 0.698, $Vv = 0.18$ – p-value = 0.711).

Table 1. Simulation results

Parameter	Theoretical value	Simulation value	Parameter	Theoretical value	Simulation value
The dispersed microstructure consists of spheres of equal size (D=const)					
$V_v = 0.11, N_v=10000000, D*1000 = 2.75$					
$\bar{d} * 1000$	2,159 (Eq.2)	2.157	$\bar{d} * 1000$	2.551 (Eq.2)	2.549
$s_d * 1000$	0,618 (Eq.3)	0.619	$s_d * 1000$	0,730 (Eq.3)	0.733
The distribution of spheres' diameters is the Rayleigh distribution					
$V_v = 0.10, N_v=10000000, p = 0.169$					
$\bar{D} * 1000$	2,155 (Eq.5)	2.150	$\bar{D} * 1000$	2,467 (Eq.5)	2.461
$s_D * 1000$	1,128 (Eq.6)	1.134	$s_D * 1000$	1,291 (Eq.6)	1.296
$\bar{d} * 1000$	2,155 (Eq.5)	2.154	$\bar{d} * 1000$	2,467 (Eq.5)	2.460
$s_d * 1000$	1,128 (Eq.6)	1.130	$s_d * 1000$	1,291 (Eq.6)	1.292
<p><u>Note:</u> \bar{d}, \bar{D} – mean values s_d, s_D – standard deviations</p>					

4.3. Case II – the distribution of spheres' diameters is the Rayleigh distribution

We assume that the spheres' diameters in space D are subject to the Rayleigh distribution that is determined by the density function [17, 18] :

$$f(D) = 2pDe^{-pD^2}; \quad D > 0 \quad (4)$$

where: p – distribution parameter.

The expected value $E(D)$ and variance $D^2(D)$ for the function (4) are adequately as follows:

$$E(D) = \frac{1}{2} \sqrt{\frac{\pi}{p}} \quad (5)$$

$$D^2(D) = \frac{4 - \pi}{4p} \quad (6)$$

Because the Rayleigh distribution (4) is invariant for the Wicksell's transformation, the distribution of flat sections' diameters will be also the Rayleigh distribution with the density function (4) and with the same parameter [4, 7, 18]. The results of simulation are presented in Figures 3, 4 and in Table 1.

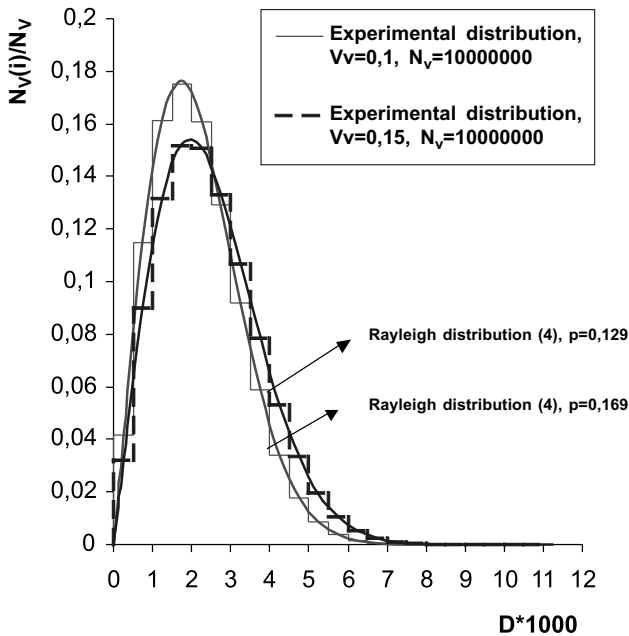


Fig. 3. Empirical and theoretical distributions of sphere diameters in space

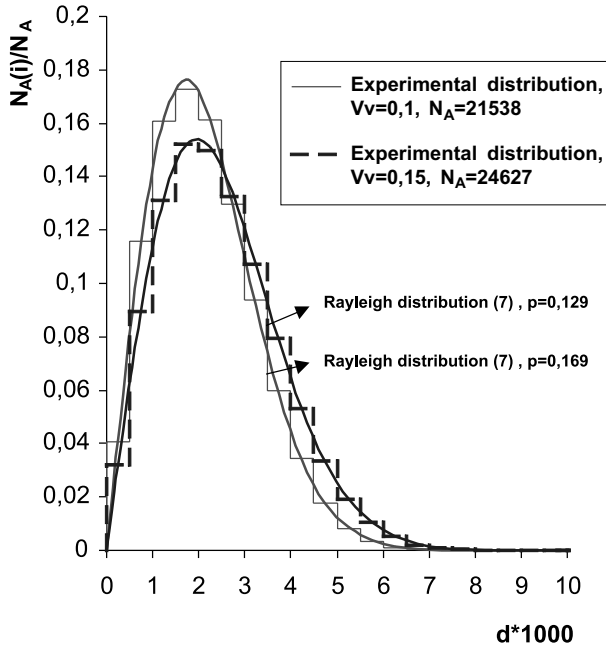


Fig. 4. Empirical and theoretical distributions of flat sections' diameters $d - D$ subject to Rayleigh distribution

In the meaning of the performed chi-square test of goodness of fit [17] there is no basis for rejection of hypothesis that all achieved empirical distribution of flat sections' diameters are conforming to the Rayleigh distribution with the same parameter p as distribution of spheres' diameters in space – ($V_v = 0.1 - p\text{-value} = 0.901$, $V_v = 0.15 - p\text{-value} = 0.588$)

5. SUMMARY

As it is resulted from the presented verification procedure the demonstrated model of dispersed microstructure operates correctly; the achieved empirical distribution of flat sections' diameters is conforming to the theoretical forecasting. Therefore, this model can be used in the analysis of performance of methods of approximate descriptions of the dispersed microstructure, in the comparative and construction analysis as well as testing the estimators.

The presented model can be also modified and developed for the sake of analyses connecting with the in-homogeneity analysis and evaluation.

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