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Random geometrical structures: stereology, models, applications in metallography

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The random (geometrical) structure is a suitable mathematical model for material microstructures. Its quantitative characteristics (parameters and functions) describe microstructures. The general random structures are described quantitatively together with discussion of stereological questions. Special structures (the Poisson- and Matérn point field, as well as the Boolean- and Stienen model) are discussed in detail. This is followed by examples of practical application: the Fe_3C-dispersion in Fe-0.15%C and Fe-0.6%C steels were described by the Matérn point field and Stienen model, respectively.

Key words: *stochastic geometry, stereology, metallography, carbide dispersion in steel.*

1. Introduction

A metal material can be considered as a geometric object with internal structure, i.e., the microstructure [1, 2], Fig. 1. In metallography the microstructure is not accessible for direct observations, so its analysis is based on planar sections. The quantitative predictions about microstructure from sections are made by stereological methods [3]. Typical material microstructure is: irregular, extensive and isometric (i.e. homogeneous and isotropic). The irregularity is understood as opposite to ordered arrangement (e.g. the crystal structure) and indicates randomness of the microstructure. The extensiveness means that the size of spatial extension of the microstructure is much larger than its smallest typical part, so the microstructure can be considered as unbounded. The local properties of isometric microstructure are not dependent on position and direction in the space.

In general case, microstructure is a complex geometrical object in frame of which one can distinguish systems of simple geometrical objects (points, lines, surfaces, bodies). Such systems form geometrical structures, which preserve

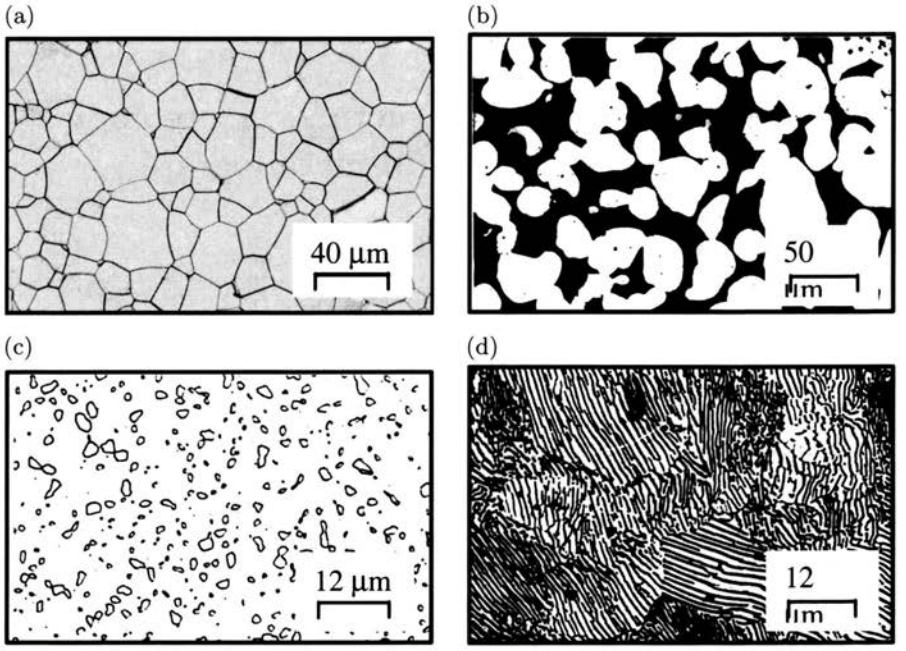

FIGURE 1. Microstructures of typical metal materials: (a) polycrystalline titanium, (b) bronze CuPb30, (c) disperse Fe_3C-phase in Fe-0.6%C steel, (d) pearlite (α+Fe_3C) in Fe-0.8%C steel.

the main properties of the microstructure (irregularity, extensiveness and isometry). From the stochastic geometry point of view a geometrical structure can be interpreted as realization of a random variable which is called: the *random geometrical structure* (abbreviated as *random structure*) [4, 5]. The random structure also can be considered as a random field (i.e., a stationary stochastic process in the Euclidean space) [6, 7].

The quantitative characteristics (parameters and functions) of a random structure also describe the geometric structures, which are their realizations. The stereology of a random structure is a simple and effective way for obtaining equations, which connect quantitative characteristics of the random structure and its planar sections [8]. In the stochastic geometry there are proposed special models, which can be used for approximation of real geometrical structures in order to make possible solving of more sofisticated statistical and stereological problems (see Chapter 4 of this article).

The aim of this article is to present the basic problems, which are connected to description of material microstructures by random geometrical structures.

2. Random structures and their stereology

In the Euclidean space $\mathbf{R}^d$ ($d = 2, 3$) which is equipped with Cartesian coordinates system, the object $x = (x_1, \ldots, x_d)$ is a point (or vector) with its coordinates $x_1, \ldots x_d$. In particular, $\mathbf{0} = (0, \ldots, 0)$ is the origin, $\mathbf{R}^2 = \{x : x = (x_1, x_2)\}$, $\mathbf{R}^3 = \{x : x = (x_1, x_2, x_3)\}$. In addition: (i) for a given real number α, $x + \alpha y = (x_1 + \alpha y_1, \ldots, x_d + \alpha y_d)$; (ii) for a subset A of $\mathbf{R}^d$, $A_x = A + x = \{y + x : y \in A\}$ is the translation of A by vector x.

A d-dimensional *closed* subset ξ of $\mathbf{R}^d$ ($d = 2, 3$) forms a geometrical structure. The d-dimensional structure ξ of $\mathbf{R}^d$ is the so-called full dimensional structure [9]. For a full dimensional structures ξ one can distinguish s-dimensional geometrical structures ($s = 0, 1, \ldots, d$): the boundary $\partial(\xi)$, edge $\kappa(\xi)$ (for $d = 3$), characteristic points $\varphi(\xi)$ (e.g., particle centers, grain vertices (for $d = 3$) and corners (for $d = 2$), etc.).

The structure ξ will be considered as realization of a random structure Ξ in $\mathbf{R}^d$ (i.e., a *random closed set* [4, 5]). The random structure Ξ is characterised by statistical parameters and functions.

Parameters

A d-dimensional compact set $T \in \mathbf{R}^d$ of a $M^d(T) = M^d$ measure (which include the origin $\mathbf{0}$) will be assumed as a test set for analysis of structures in $\mathbf{R}^d$. Special T-sets are: d-dimensional cube and sphere. The set $\xi \cap T$ is a structure in T and the number $M^s(\xi \cap T)$, $s \leqslant d$, is the value of its s-dimensional parameter (i.e., parameter of a s-dimensional subset of a full d-dimensional set). For the random structure Ξ the number M^s is realization of a random variable, whose mean $\langle M^s \rangle$, is obtained for a sequence of realization of Ξ. If there exists such a number $M^s_{M^d}$ that for every T

$$\langle M^s \rangle = M^d M^s_{M^d} \quad \text{for } d = 2, 3;\ s = 0, 1, \ldots, d\,; \tag{2.1}$$

then $M^s_{M^d}$ is the M^s-parameter density of Ξ in $\mathbf{R}^d$ [1, 4]. The $M^s_{M^d}$ is a statistical (and also stereological) parameter of Ξ.

By using of the following stereological notation [3, 4]:

- $M^0 = P$ (P – number of points),
- $M^0 = N$ (N – particle number, which exists when ξ is a particle system),
- $M^1 = L$ (L – length of a line),
- $M^2 = S$ (S – surface area for $d = 3$),
- $M^2 = A$ and $M^3 = V$ (A – surface area for $d = 2$ and V – volume)

the particular parameters $M^s_{M^d}$, i.e., the point density P_{M^d}, the particle

TABLE 1. Parameters $M^s_{M^d}$ of random structure $\Xi \subset \mathbf{R}^d$.

d \ s	0	1	2	3
2	P_A, N_A	L_A	A_A	–
3	P_V, N_V	L_V	S_V	V_V

density N_{M^d}, the length density L_{M^d}, the surface area density A_A or S_V and the volume density V_V are given in Table 1.

In stereology, a two-dimensional ($d = 2$) structure is considered as a planar section of a three-dimensional ($d = 3$) structure. The fundamental stereological equations with the parameters presented in Table 1 are given below [3, 4, 10]:

$$V_V = A_A \,, \tag{2.2}$$

$$S_V = \frac{4}{\pi} L_A \,, \tag{2.3}$$

and

$$L_V = 2P_A. \tag{2.4}$$

Functions

The specification of statistical functions (and some additional parameters) is given below, firstly for random point field, $\Xi = \Phi$, and then for the full dimensional structure in $\mathbf{R}^d$, for which different particle system models are taken also into consideration.

2.1. Random point field [4]

A structure φ, ($\xi = \varphi$), in form of a system of isolated points $x_1, x_2, \ldots$ in $\mathbf{R}^d$, i.e.,

$$\varphi = \{x_1, x_2, \ldots, \} \subset \mathbf{R}^d \tag{2.5}$$

is a point field. It will be considered as realization of a random point field $\Phi \subset \mathbf{R}^d$ of point density $P_{M^d} = \lambda$, Fig. 2.

Probability function

For a fixed T, k is the number of points in $\varphi \cap T$ ($k = 0, 1, \ldots$). For the random set $\Phi \cap T$ the number k is realization of a discrete random variable X with the probability function (PF)

$$p\left(k; M^d\right) = \Pr\left(X = k; M^d\right). \tag{2.6}$$

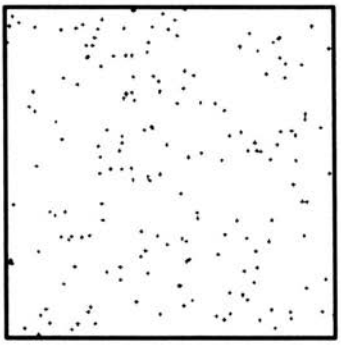

FIGURE 2. Two-dimensional ($d = 2$) point field.

Distance distribution

Let l be the distance between a given point $x_i \in \varphi$ and a point which is its nearest neighbour (NN) in φ, i.e.,

$$l = \Delta\left(x_i, \varphi \backslash x_i\right) , \tag{2.7}$$

where Δ denotes the distance between two sets.

For a random structure φ, the number l is realization of a continuous random variable X with probability distribution function (PDF)

$$Z(l) = \Pr(X < l). \tag{2.8}$$

It can be shown [4] that the NN distance $Z(l)$ – function is determined by the PF given by Eq. (2.6).

Let $T(x_i, l)$ be a sphere of radius l centred at $x_i \in \varphi$. The sphere volume is, $M^d = \omega_d\, l^d$ where

$$\omega_d = \begin{cases} \pi & \text{for } d = 2, \\ \frac{4\pi}{3} & \text{for } d = 3. \end{cases} \tag{2.9}$$

For a fixed l and random set $\Phi \cap T(x_i, l)$, $Z(l)$ obeys

$$Z(l) = 1 - p\left(k = 1; \omega_d l^d\right), \tag{2.10}$$

where $p(\cdot)$ gives the PF-function value at l for fixed $k = 1$ (i.e. the origin $\mathbf{0}$) in the sphere.

Pair correlation function

A possible form of the so-called pair correlation function (PCF) $g(r)$ for a point field Φ of point density λ is of the form

$$g(r) = \frac{\lambda(r)}{\lambda} , \tag{2.11}$$

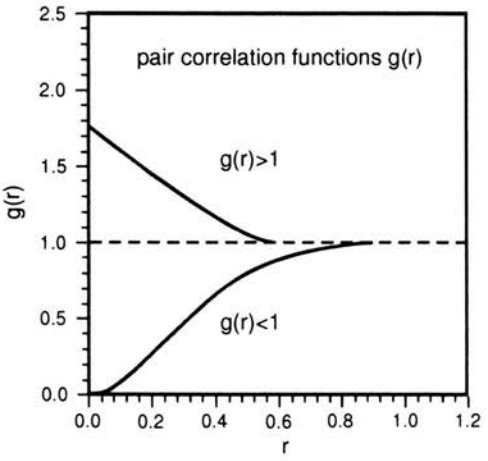

FIGURE 3. Typical PCF g(r) functions.

where $\lambda(r)$ is the point density of Φ at the distance r from a point of Φ. The PCF $g(r)$ describes a statistical relation between points in Φ. If $\lambda(r) = \lambda$, then $g(r) = 1$, which indicates a statistical independence and a lack of interaction between points in Φ. However, $g(r) \neq 1$ indicates points interaction in Ξ, i.e., points attraction ($g(r) > 1$) or points repulsion ($g(r) < 1$). Figure 3 shows the plots of typical PCF's.

2.2. Full dimensional random structure [4]

Ξ is a d-dimensional random structure in $\mathbf{R}^d$.

Size distribution

Let $u \subset \mathbf{R}^d$ be a fixed unit vector. The local size of a d-dimensional structure ξ at the point x in direction u is the chord length $D(x,u) = D$, Fig. 4, (usually $x = \mathbf{0}$). For Ξ, the chord length is a random variable with PDF $F(D)$ and mean $\langle D \rangle$.

In stereology the size PDF $F(D)$ is independent of the structure dimension d. As a consequence, the following stereological equation exists [3]

$$\langle D \rangle = w_d \frac{M^d_{M^d}}{M^{d-1}_{M^d}}\,, \tag{2.12}$$

where

$$w_d = \begin{cases} \pi & \text{for } d = 2\,, \\ 4 & \text{for } d = 3. \end{cases} \tag{2.13}$$

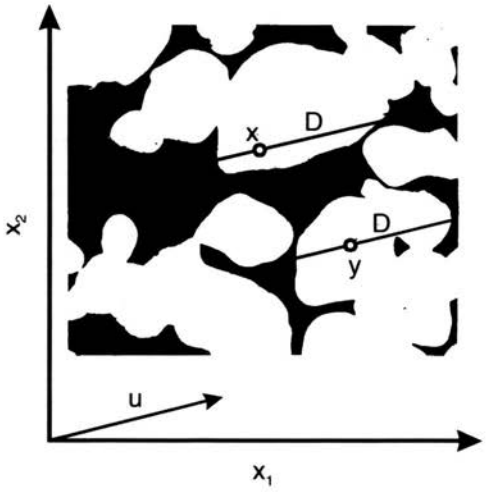

FIGURE 4. Local size D (chord length) of the ξ-structure (in points: x and y, for the u-direction).

Covariance

Let $h \in \mathbf{R}^d$ be a point at the distance r from the origin $\mathbf{0}$ (or a vector of r-length). The points x and $x+h$ are at the distance r.

The covariance $C(r)$ of a random structure Ξ is equal to the probability, that the points x, $x+h$ belong to Ξ, i.e.,

$$C(r) = \Pr(x \in \Xi \quad \text{and} \quad x+h \in \Xi). \tag{2.14}$$

The covariance $C(r)$ describes the spatial distribution of Ξ in $\mathbf{R}^d$. The basic properties of the $C(r)$-function are as follows

$$C(0) = M^d_{M^d} \tag{2.15}$$

and

$$C'(0) = -\frac{\omega_{d-1}}{d\omega_d} M^{d-1}_{M^d} \tag{2.16}$$

where ω_d is given in Eq. (2.9) and $\omega_1 = 2$.

It should be noticed that from the independence of the covariance of the space dimension d and from Eqs. (2.15) and (2.16) result the stereological equations (2.2) and (2.3).

Let $C_1(r)$ and $C_2(r)$ denote the probability that the points x, $x+h$ belong to the same part of the structure and to different parts, respectively. It follows that: (i) for $r = 0$, $C_1(0) = C(0)$ and $C_2(0) = 0$; (ii) for $r = \infty$, $C_2(\infty) = C(\infty)$ and $C_1(\infty) = 0$. The covariance $C(r)$ can be written [11] as:

$$C(r) = C_1(r) + C_2(r). \tag{2.17}$$

The C_1-function characterizes the local properties of the Ξ-structure; however, the C_2-function characterizes the spatial distribution of Ξ. The C_1 is of the form

$$C_1(r) = C'(0) \int_r^\infty (D - r) dF(D). \tag{2.18}$$

Equation (2.18) connects the covariance $C(r)$ with the PDF $F(D)$.

2.2.1. Particle system. Let $\xi(x_i) \subset \mathbf{R}^d$ be a particle centred at the point x_i (e.g. center of the mass). The structure

$$\xi = \{\xi(x_1), \xi(x_2), \ldots, \} \subset \mathbf{R}^d, \quad \xi(x_i) \cap \xi(x_j) = \emptyset \quad \text{for } i \neq j \tag{2.19}$$

is a particle system, Fig. 1a, c. The structure ξ is realization of a random set Ξ; however, the particle centers of ξ are realization of a point field Φ of point density λ. The particle density N_{M^d} of Ξ is given by

$$N_{M^d} = \lambda. \tag{2.20}$$

The particle size distribution function

Let D be the size of a particle. For the structure ξ, $D \in [0, D_m]$, D_m is the maximal size. For a fixed D, $N_{M^d}(D)$ is the density of particles of the size smaller than D. The cumulative particle size distribution function $N_{M^d}(D)$ for $D \in [0, D_m]$ is non-decreasing and

$$N_{M^d}(D) = \begin{cases} 0 & \text{for } D = 0, \\ N_{M^d} & \text{for } D = D_m. \end{cases} \tag{2.21}$$

The PDF $F(D)$ can be written as follows

$$F(D) = N_{M^d}^{-1} N_{M^d}(D). \tag{2.22}$$

Convex particle system in $\mathbf{R}^3$

Let $\Xi \subset \mathbf{R}^3$ be a random set of convex particles with particle density N_V and mean size $\langle D \rangle$.

Let h be a unit vector and E, E_r be a pair of parallel planes at a distance r and perpendicular to h.

For a fixed r, $N_A(r)$ is the particle sections density in $\mathbf{R}^2 = E$ for the particles, which also form a section with E_r. For variable r, the monotonically decreasing function $N_A(r)$ is specified by

$$N_A(r) = \begin{cases} N_A & \text{for } r = 0, \\ 0 & \text{for } r = D_m, \end{cases} \tag{2.23}$$

where D_m is the maximal particle thickness in the h-direction.

If $F_3(D)$ denotes the PDF of particle thickness D in the h-direction, then the functions $N_A(r)$ and $F_3(D)$ satisfy the equation

$$N_A(r) = N_V \int_r^{D_m} (D - r)\, dF_3(D). \tag{2.24}$$

From Eq. (2.24) result further properties of the $N_A(r)$-function. For $r = 0$, $N_A(r) = N_A$ and

$$N_A = N_V \int_0^{D_m} D\, dF_3(D). \tag{2.25}$$

Because for isometric Ξ the integral in Eq. (2.25) is independent of the h-vector direction, it gives the mean particle breadth $\langle D \rangle$. Then, the first derivatire of $N_A(r)$ may be expressed as follows

$$N'_A(r) = N_V \left[F_3(D = r) - 1\right]. \tag{2.26}$$

Because for $r = 0$, $F_3(0) = 0$, from Eq. (2.26) it results

$$N_V = -N'_A(0). \tag{2.27}$$

Taking into account Eq. (2.27), Eq. (2.26) can be written in the form

$$F_3(D = r) = 1 - \frac{N'_A(r)}{N'_A(0)}. \tag{2.28}$$

Equations (2.27) and (2.28) are of importance in the stereology of convex particles, because they determine the measurement method of the parameter N_V and the $F_3(D)$-function as well [10]. Additionally, Eq. (2.27) can be used as a basis for N_V – measurement in a system of convex particles by means of the so-called disector method [4, 12].

System of spheres

For a random system of spheres and its planar section, with diameter distribution functions $F_3(D)$ and $F_2(D)$, respectively, the function $C_1(r)$ in

Eq. (2.17) is of the form [4, 10]:

$$C_1(r) = \begin{cases} \frac{1}{2}\int_r^\infty D^2 \arccos\left(\frac{r}{D}\right) - \frac{r}{d}\sqrt{1-\left(\frac{r}{D}\right)^2}\, dF_2(D) & \text{for } d=2, \\ \frac{\pi}{12}\int_r^\infty (D-r)^2(2D+r)\, dF_3(D) & \text{for } d=3. \end{cases} \tag{2.29}$$

From the $C_1(r)$ – independence on d and from Eq. (2.29) a possible form of the Wicksell equation results [1, 10]:

$$F_2(D) = 1 - \frac{N_V}{N_A}\int_0^{D_m} \sqrt{x^2 - D^2}\, dF_3(x). \tag{2.30}$$

It is possible to transform Eq. (2.30) to an Abel type integral equation, which has analytical solution with respect to the unknown $F_3(D)$, [1].

PCF's, $g_3(r)$ and $g_2(r)$ for sphere- and circle centers, respectively, satisfy a stereological equation, which in a general case is of complex form [4]. In the simplest case with random non-overlapping spheres of equal diameters there exists the following equation [1]:

$$g_2'(r) = 2D^{-2}\int_0^D (D-x) g_3\left(\sqrt{x^2-D^2}\right)\, dx \quad \text{for } r \geqslant 0. \tag{2.31}$$

3. Models

The following models will be taken into account: 1. the Poisson point field, 2. the Matérn cluster point field, 3. the Boolean model, and 4. the Stienen model.

3.1. Poisson point field [4]

A random point field $\Phi \subset \mathbf{R}^d$ of point density λ is a Poisson point field (P-field), Fig. 2, when:

(i) for a given test set $T \subset \mathbf{R}^d$ of measure M^d the PF is of a form

$$p\left(k; M^d\right) = \frac{\left(\lambda M^d\right)^k}{k!} \exp\left(-\lambda M^d\right) \quad \text{for } k = 0, 1, \ldots, \tag{3.1}$$

(ii) for every pair of disjoint test fields T_1, $T_2 \subset \mathbf{R}^d$, the numbers of points of the random sets $\Phi \cap T_1$ and $\Phi \cap T_2$ are independent random variables.

From Eqs. (2.10) and (3.1) follows the *NN* distance PDF $Z(l)$ in the form:

$$Z(l) = 1 - \exp\left(-\lambda \omega_d l^d\right), \tag{3.2}$$

where ω_d is given in Eq. (2.9). According to Eq. (3.2) for a P-field the PDF $Z(l)$ is of the Weibull type.

From (ii) it follows that $\lambda(r) = \lambda$ and consequently $g(r) = 1$, which indicates a lack of interaction between points in a P-field.

3.2. Matérn cluster point field [4]

The Matérn cluster point field is formed on the basis of a homogeneous P-field of point density λ_0, in $\mathbf{R}^d$.

Every point of the P-field is assumed to be the center of spheres $s(x_i, R)$ of radius R. $\varphi(x_i, R)$ is cluster of points in sphere $s(x_i, R)$. The number of cluster points is a random variable of Poisson distribution with mean $m(R)$. The $\varphi(x_i, R)$-cluster points are independently and uniformly distributed in the sphere $s(x_i, R)$. The union of clusters $\varphi(x_i, R)(i = 1, 2, \ldots)$

$$\varphi = \bigcup_{i=1}^{\infty} \varphi(x_i, R) \tag{3.3}$$

is realization of a random point field $\Phi \subset \mathbf{R}^d$, i.e., the Matérn cluster point field, Fig. 5. Its point density λ may be expressed as follows

$$\lambda = \lambda_0 m(R). \tag{3.4}$$

The PCF $g(r)$ is of the form

$$g(r) = \begin{cases} 1 + \frac{f(r;R)}{\lambda_0 d \omega_d r^{d-1}} & \text{for } 0 \leqslant r \leqslant 2R, \\ 0 & \text{otherwise,} \end{cases} \tag{3.5}$$

where

$$f(r;R) = \begin{cases} \frac{4r}{\pi R^2}\left(\arccos\frac{r}{2R} - \frac{r}{2R}\sqrt{1 - \left(\frac{r}{2R}\right)^2}\right) & \text{for } d = 2, \\ \frac{3r^2}{2R^6}\left(R - \frac{r}{2}\right)^2\left(2R + \frac{r}{2}\right) & \text{for } d = 3, \end{cases} \tag{3.6}$$

for $0 < r < 2R$; otherwise $f(r;R) = 0$. The $f(r;R)$ function is the probability density for the distance between two independent random cluster points.

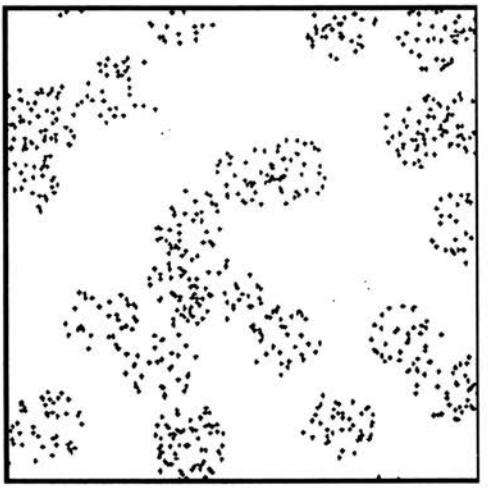

FIGURE 5. Two-dimensional ($d = 2$) Matérn cluster point field.

A graph of the PCF $g(r)$ is given in Fig. 3 for $g(r) > 1$. From Eq. (3.5) and Fig. 3 a point attraction results, which is limited to the distance of $r = 2R$. The Matérn cluster field is characterized by three parameters: λ_0, R and $m(R)$.

3.3. Boolean model [4]

The Boolean model is formed on the basis of a homogeneous P-field of point density λ, in $\mathbf{R}^d$.

Let a compact d-dimensional set, i.e., the figure $\xi_0 \subset \mathbf{R}^d$, characterized by a parameter M^s, be realization of a random figure Ξ_0 of definite distribution and the mean $\langle M^s(\Xi_0)\rangle$ $(s = d, d-1)$. The $\Xi_i \subset \mathbf{R}^d, i = 1, 2, \ldots$ is a sequence of independent identical distributed random figures of the same distribution as Ξ_0. The d-dimensional figure $\xi(x_i)$, i.e., a realization of Ξ_i, has the center at $x_i \in \varphi$. The structure

$$\xi = \bigcup_{i=1}^{\infty} \xi(x_i) \tag{3.7}$$

is a realization of a random structure $\Xi \subset \mathbf{R}^d$, the so-called Boolean model, Fig. 6.

The fundamental stereological parameters are as follows

$$M^d_{M^d} = 1 - \exp\left[-\lambda \left\langle M^d(\Xi_0)\right\rangle\right], \tag{3.8}$$

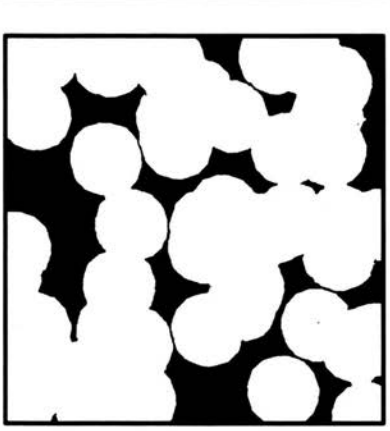

FIGURE 6. Two-dimensional ($d = 2$) Boolean model for identic circles.

and

$$M_{M^d}^{d-1} = \lambda \left\langle M^d(\Xi_0) \right\rangle \exp\left[-\lambda \left\langle M^d(\Xi_0) \right\rangle\right]. \tag{3.9}$$

The covariance $C(r)$ is of the form

$$C(r) = 2M_{M^d}^d - 1 + \left(1 - M_{M^d}^d\right)^2 \exp\left[\lambda \gamma_{\Xi_0}(r)\right], \tag{3.10}$$

where

$$\gamma_{\Xi_0}(r) = \left\langle M^d(\Xi_0 \cap (\Xi_0 - r)) \right\rangle. \tag{3.11}$$

We observe that a planar section of spatial Boolean model is a two-dimensional Boolean model.

3.4. Stienen model [13]

The Stienen model is formed on the basis of a homogeneous P-field of point density λ, in $\mathbf{R}^d$.

For the P-field the *NN* distance PDF $Z(l)$ is given by Eq. (3.2). Let $\xi(x_i, D(x_i))$ be a sphere centred at the point $x_i \in \varphi$ and of the diameter

$$D(x_i) = \alpha l(x_i)^{\frac{d}{m}} \quad \text{for } \alpha, m > 0; \tag{3.12}$$

where $l(x_i)$ is given by Eq. (2.7). The structure

$$\xi = \bigcup_{i=1}^{\infty} \xi(x_i, D(x_i)) \tag{3.13}$$

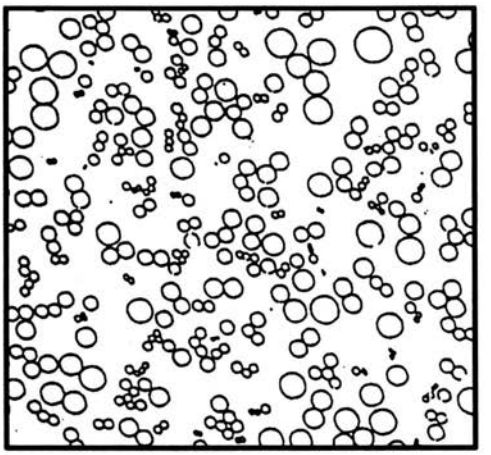

FIGURE 7. Two-dimensional ($d = 2$) Stienen model ($m = 2$, $\alpha = 1$).

is realization of a random structure $\Xi \subset \mathbf{R}^d$, the so-called Stienen model of particle density $N_{M^d} = \lambda$. Figure 7 shows realization of a two-dimensional Stienen model ($d = 2$, $m = 2$, $\alpha = 1$).

From Eq. (3.12) it results that for given α and m the diameter D is a monotone function of l, i.e., $D(l)$. If $l(D)$ is the reciprocal function of $D(l)$, then the properties of the PDF determine the following identity for the diameter and NN distance PDF's:

$$F(D) = Z\left[l(D)\right]. \tag{3.14}$$

Taking into account Eqs. (3.2) and (3.12) in (3.14) results in

$$F(D) = 1 - \exp\left[-\frac{\omega_d N_{M^d}}{\alpha^m} D^m\right]. \tag{3.15}$$

The obtained PDF $F(D)$ is of a Weibull type. The k-th moment $\langle D^k \rangle$ for the Weibull distribution is of the form

$$\left\langle D^k \right\rangle = \alpha^k \Gamma\left(\frac{k}{m} + 1\right) (\omega_d N_{M^d})^{-\frac{k}{m}} \quad \text{for } k = 1, 2, \ldots. \tag{3.16}$$

For $k = 1$, Eq. (3.16) gives the mean diameter $\langle D \rangle$. Taking into account $\langle D \rangle$ in Eq. (3.15) results in

$$F(D) = 1 - \exp\left[-\Gamma^m\left(\frac{1}{m} + 1\right)\left(\frac{D}{\langle D \rangle}\right)^m\right]. \tag{3.17}$$

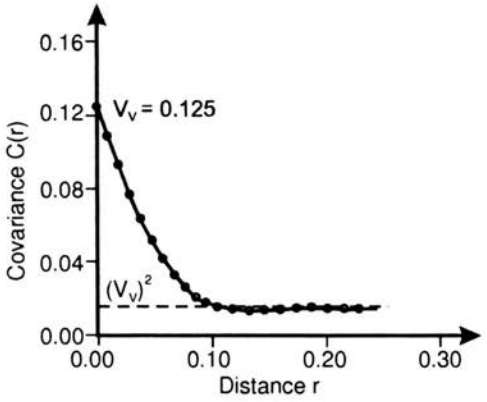

FIGURE 8. Covariance $C(r)$ of the Stienen model ($d = 3$, $m = 3$, $\alpha = 1$).

The Stienen model involves three parameters, i.e., N_{M^d}, m and α. A particular case ($d = 3$, $m = 3$, $\alpha = 1$) is the classical model [14]. A model ($d = 3$, $m = 3$, $\alpha \leqslant 1$) was analysed in [15].

The fundamental stereological parameters $M^s_{M^d}$ for $s = d - 1$, d, are as follows

$$M^{d-1}_{M^d} = \pi \left\langle D^{d-1} \right\rangle N_{M^d} \tag{3.18}$$

and

$$M^d_{M^d} = \frac{\omega_d}{2^d} \left\langle D^d \right\rangle N_{M^d}. \tag{3.19}$$

The expression of the moments $\langle D^{d-1} \rangle$ and $\langle D^d \rangle$ in Eqs. (3.18) and (3.19), respectively, by Eq. (3.16) gives the relation between stereological and model parameters.

The analytical form of the covariance $C(r)$ for the Stienen model is not known. Figure 8 shows the function $C(r)$ for a model ($d = 3$, $m = 3$ and $\alpha = 1$) obtained by simulation [11].

Other properties of Stienen model are:

(i) the sphere centers PCF $g_3(r) = 1$;

(ii) a planar section of spatial model does not form a two-dimensional Stienen model.

Planar section

From simulation it results that the PF for point field of circle centers in a planar section of the Stienen model is of the form:

$$p(k; A) = \binom{N(A)}{k} p^k (1-p)^{N(A)-k}, \quad k = 0, 1, \ldots, N(A), \tag{3.20}$$

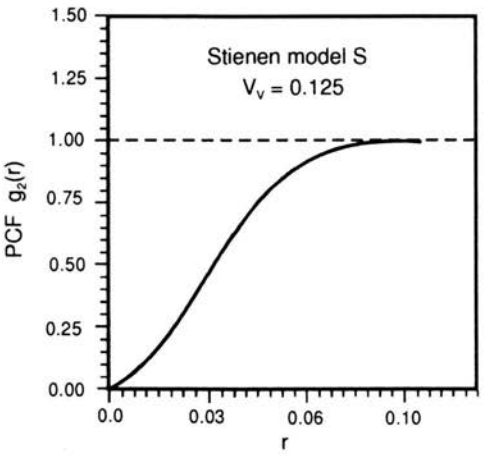

FIGURE 9. Pair correlation function $g_2(r)$ for circle centers on planar section of the Stienen model (S) ($d = 3$, $m = 3$, $\alpha = 1$).

where $p \in [0; 0.5]$ and $N(A)$ denote the greatest number of the points in T [16]. From Eq. (3.20) it results, that circle centers form a binomial point field in bounded T.

Fig. 9 shows the circle centers PCF $g_2(r)$ for a planar section of the Stienen model ($d = 3$, $m = 3$, $\alpha = 1$), [17]. For a small distance r, $g_2(r) < 1$, repulsion of points occurs.

4. Applications in metallography

4.1. Arrangement of particles in planar section of Fe_3C-dispersion in steel [18]

The aim of the investigations was the model description of particles arrangement of a non-uniform Fe_3C-dispersion in Fe-0.15%C carbon steel.

The qualitative metallography shows that the Fe_3C-dispersion structure is isometric, but when compared to a uniform spheroidite (Fig. 1c) it is non-uniform with areas having quite different fractions of particles, Fig. 10a.

In order to perform the quantitative description of particles distribution, the Fe_3C-dispersion was represented by a two-dimensional point field in the plane $\mathbf{R}^2$, which is formed by the particle center points, Fig. 10b. Its fundamental quantitative characteristics are: the point density λ (it is equal to the particle density N_A) and the PCF $g(r)$. The co-ordinates of the points were measured (at $\times 1340$ microstructure magnification) by an image analyser for $N = 6431$ particles in 8, 150×215 mm test rectangles T. The empirical point

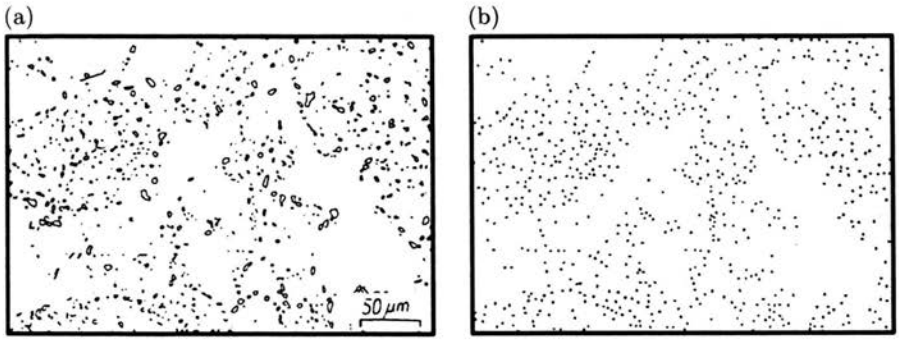

FIGURE 10. Disperse Fe_3C-phase in Fe-0.15%C steel: (a) microstructure; (b) point field of particle section centers.

density is, $\lambda = 4.5 \times 10^4\,\mathrm{mm}^{-2}$. The PCF $g(r)$ was determined by an edge corrected kernel estimator [4].

Let x_i $(i = 1, 2, \ldots, n)$ denote points of the analysed point field in T. The kernel estimator is of the form

$$g(r) = \frac{1}{2\pi\lambda^2} \sum_{i=1}^{n} \sum_{(j\neq i)=1}^{n} \frac{k_h(r - r_{ij})}{r_{ij} A(T_x \cap T_y)}. \tag{4.1}$$

The summation runs over all points $x_i, i = 1, \ldots, n$, in the window of observation T; r_{ij} is the distance between points x_i, x_j; T_x is the set of all points of the plane having the form $z = w + x$ for $w \in T$; $A(\cdot)$ is the area and $k_h(\cdot)$ is the kernel function. A possible kernel function is of the form

$$k_h(t) = \begin{cases} \frac{3}{4h}\left(1 - \frac{t^2}{h^2}\right) & \text{for } |t| < h, \\ 0 & \text{otherwise,} \end{cases} \tag{4.2}$$

where h is a band-width parameter ($h \approx c\lambda^{-1/3}$ for $0.1 < c < 0.2$ [1]).

Figure 11 shows the empirical PCF $g(r)$, which was determined by using Eqs. (4.1) and (4.2).

Its form is different from that of the Poisson point field, i.e., for $r < 0.016\,\mathrm{mm}$, $g(r) > 1$, and is similar to a PCF of cluster point fields (Fig. 5). Therefore, the empirical point field was described by the Matérn cluster point field. For the measured characteristics of the empirical point field, i.e., the parameter λ and the PCF $g(r)$, the model parameters R and λ_0 were determined. From Eqs. (3.5) and (3.6) for $d = 2$ it results that R and λ_0 may be expressed as follows

$$R = \frac{2}{\pi} \frac{g(0) - 1}{g'(0)}, \tag{4.3}$$

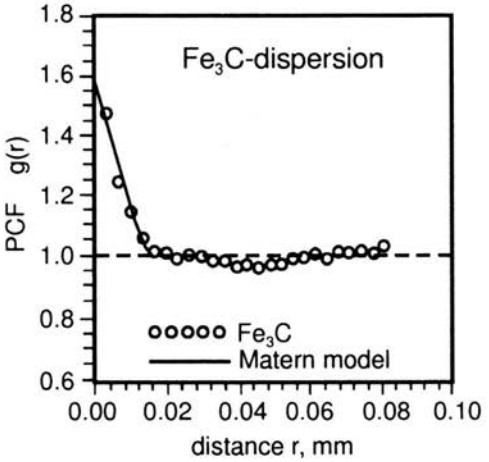

FIGURE 11. Pair correlation function $g(r)$ for the point field of Fe_3C-particle section centers of Fe-0.15%C steel compared to PCF of the Matérn cluster point field.

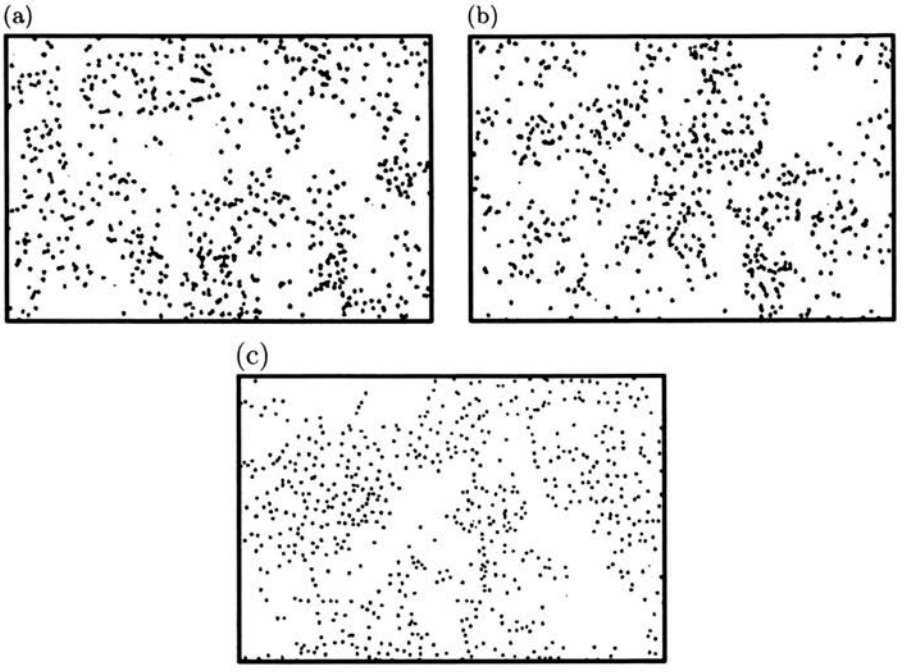

FIGURE 12. Images: (a), (b) Matérn cluster point field, (c) Fe_3C-particle centers.

and

$$\lambda_0 = \frac{1}{\pi R^2 [g(0) - 1]}, \tag{4.4}$$

where $g'(0)$ denotes the first derivative of the PCF $g(r)$ with respect to the r-variable at $r = 0$.

The model parameters are as follows: $R = 7.6 \times 10^{-3}$ mm and $\lambda_0 = 8.9 \times 10^3\,\mathrm{mm}^{-2}$. Then $m(R)$ was calculated with Eq. (3.4), $m(R) = 5$. For the obtained parameters R and λ_0, the model PCF $g(r)$ was calculated with Eqs. (3.5) and (3.6) for $d = 2$. Figure 11 shows the $g(r)$ -graph compared to the empirical function, giving an acceptable agreement.

As an example, Fig. 12a,b presents two simulated images of the model which approximates the empirical point field. It indicates that, in principle, the structure of the model approximation is similar to the empirical point field (Fig. 12c) in the meaning that there exist some features of a distinct non-uniformity. However, in the approximation image the recognition of separate clusters is not feasible. It means that the relatively simple model, i.e., the Matérn cluster point field, is flexible and enables the description of point systems of quite different structures.

4.2. Description of a disperse Fe_3C-phase in steel by Stienen model [13]

A hardened specimen of Fe-0.6%C carbon steel was annealed in vacuum at 700°C for 600h, [13, 19-20]. Figure 13 presents a typical microstructure.

Quantitative analysis of the microstructure was performed in 80×80 mm squares on images at $\times 2000$ magnification. For 1540 particle sections the

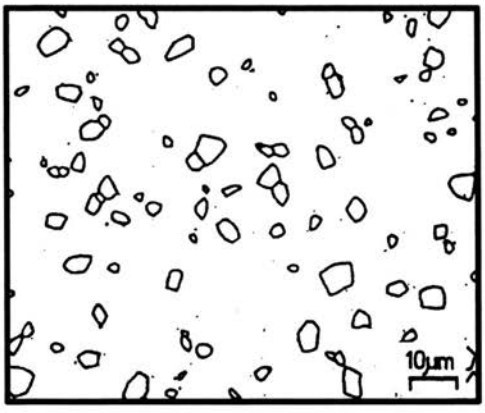

FIGURE 13. Fe-0.6%C steel microstructure with Fe_3C-dispersion.

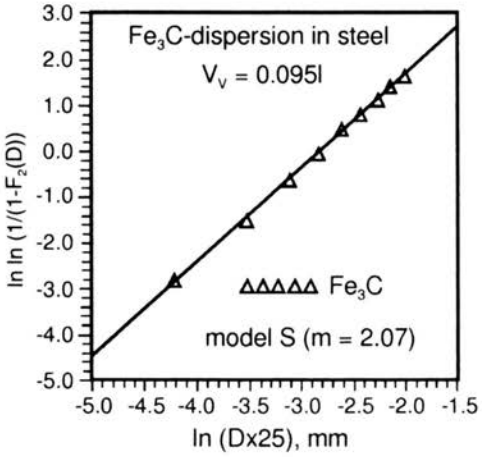

FIGURE 14. Fe_3C-particle section diameters PDF $F_2(D)$ in logarithmic co-ordinates.

diameter D was measured and the particle center was marked by the TGZ-3 (Opton) particle size analyser.

Figure 14 shows the PDF $F_2(D)$ for Fe_3C-particle sections (in logarithmic co-ordinates) in comparison with the Rayleigh PDF given by Eq. (3.17) for $m = 2$ in the form

$$F_2(D) = 1 - \exp\left[-\frac{\pi}{4}\left(\frac{D}{\langle D\rangle}\right)^2\right]. \tag{4.5}$$

It can be assumed that the empirical function coincides approximately with the Rayleigh one. Because the Rayleigh PDF is invariant due to the Wicksell transformation Eq. (2.30), it follows that

$$F_3(D) = F_2(D). \tag{4.6}$$

The parameters of the Fe_3C phase are: $N_V = 9.5 \times 10^6\,\mathrm{mm}^{-3}$ and $\langle \mathrm{D}\rangle = 2.3 \times 10^{-3}\,\mathrm{mm}$.

The circle centers in a planar section of the Fe_3C-dispersion form the empirical point field of the point density $\lambda = N_A = 2.2 \times 10^4\,\mathrm{mm}^{-2}$. Figure 15 shows the empirical PCF $g_2(r)$ (determined by using Eqs. (4.1) and (4.2)) compared to the PCF of Stienen model for $m = 2$, giving an acceptable agreement.

We conclude that: (i) the empirical PDF $F_3(D)$ for sphere diameters follows the Rayleigh PDF; (ii) the particle sections PCF $g_2(r)$ is similar to the circle section PCF of the Stienen model for $m = 2$; (iii) the point fields of Fe_3C-particle section centers are of a binomial type [21].

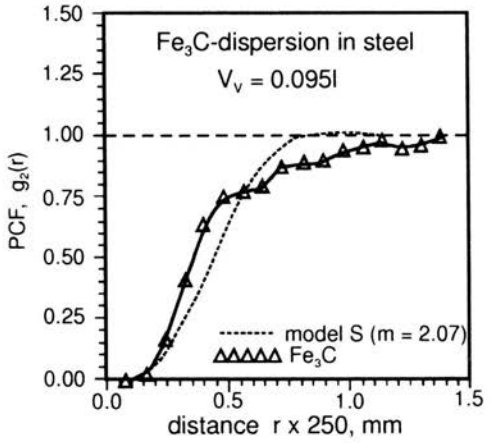

FIGURE 15. Pair correlation function $g_2(r)$ for the point field of Fe_3C-particle section centers of Fe-0.6% C steel in comparison with PCF for planar section of the Stienen model (S) .

As a result, one can assume that the Fe_3C-dispersion follows the Stienen model for $m = 2$, i.e., the particle centers form a Poisson field (they are arranged at random in space, the PCF $g_3(r) = 1$), while the particle sizes are statistically dependent and determined by the nearest neighbour distances.

As an example, Fig. 16 shows simulated planar section of the Stienen model compared to the Fe_3C-sections in a circle approximation.

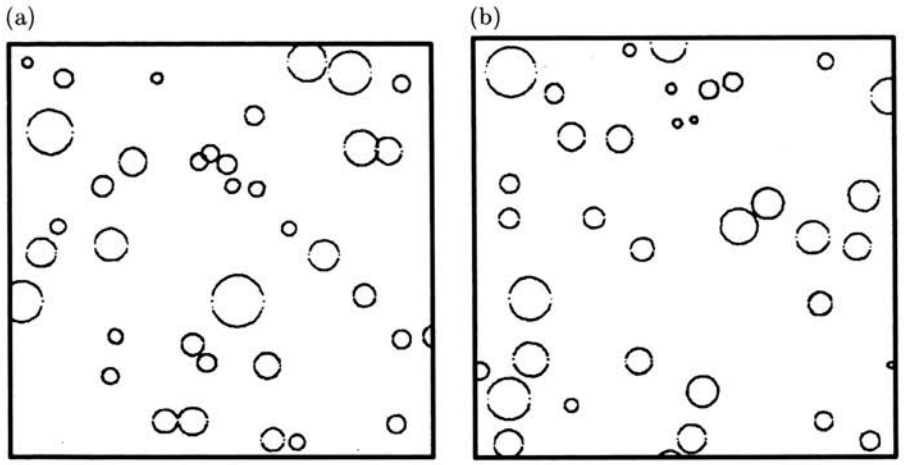

FIGURE 16. Planar section of the: (a) Fe_3C-dispersion in circle approximation; (b) Stienen model for $m = 2$.

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