

Random material microstructures: methodical background

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The text below provides a brief introduction to modelling of complex, random material microstructures. It displays the basic principles and tools for the modelling and analysis of various types of micro-heterogeneous materials. In particular, it presents these results of random fields theory, which seem to be of prime importance for diverse applications. First, the random Poisson-type random fields are shortly discussed in order to indicate a potential tools for modelling of dispersed-type random microstructures. Then, the basic classes of continuous random fields (scalar, vectorial, tensorial) are presented to show their usefulness in modelling both the random morphology and properties of micro-heterogeneous media. In the last part, some our new results are shortly announced on reconstruction of the probability distribution of the basic features of polycrystalline microstructures (cf. Sobczyk, Trębicki, *Reconstruction of Random Material Microstructures: Patterns of Maximum Entropy*, Probabilistic Eng. Mech., Vol. 18, Nr. 4, 1993).

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sian ensembles, maximum entropy.*

1. Introduction: Complexity of material microstructure

Each piece of material has its internal structure, i.e. a specific arrangement of its morphological constituents along with their mutual relationships. The homogenous continuum (widely assumed in classical theories) is an idealization only valid on a certain particular scale. Microscopic examination, at well above the atomic level, reveals heterogeneity. Metals are, actually, polycrystals, i.e. aggregates of an immense number of anisotropic crystals, a key element of polymer structure is its crystalline molecule. Also, soils, rocks, and ceramics are examples of materials with very complex structures.

Although these heterogeneous media can be viewed differently in each of the examples given above, they share one common feature – the existence

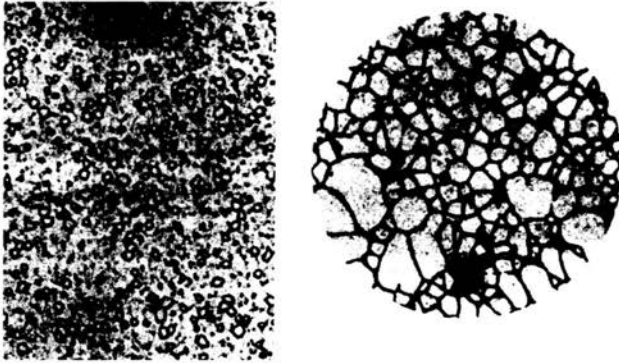


FIGURE 1. Microstructures of actual materials (AISI T15 tool steel and Zn-0.55Cu-0.12Ti die cast), after [23].

of an underlying structure at a scale small compared to the characteristic dimensions of the material specimen. This underlying structure is normally called the *microstructure* (cf. [1] and Fig. 1 displaying the microstructures of some actual materials).

There is no one aluminum, nor one steel. Depending on the thermomechanical processing history, the mechanical overall properties can be quite different. This is due to the fact that different processing histories yield different internal microstructures on various scales. Therefore, the basic paradigm indicating the origin of overall properties of material is: processing history \rightarrow microstructure \rightarrow properties.

It is clear that in order to obtain required macroscopic (engineering) properties (of the material in question) it is crucial to understand first a microstructure. This microstructure is in turn a direct consequence (a “final” state) of the processing history. Probably, the best known example of the coupling of microstructure and properties is the Hall-Petch relation between the yield stress (σ_y) and the metallurgical grain size (d): $\sigma_y \sim 1/\sqrt{d}$. This empirical law clearly indicate that not only structures at atomic level (e.g. the lattice defects, vacancies) are important but so too are the geometric structures at the higher (but still – micro) level. Macroscopic material properties depend heavily on the internal constitution of materials at various scales (from nanometers to millimeters). The internal constituents have *complex geometry*, their locations and orientations are usually nonuniform, and strong spatial correlation often exists among different types of features. Another factor is the apparent *randomness* of actual material microstructures.

From the point of view of material engineering and mechanics a question of a great importance is: *how may the various microstructures within material be tailored so as to yield desired properties?*

To make this challenging question really clear one has to *understand* first nature of true material microstructures. A way toward that end is mathematical characterization/modeling using the empirical data. The related problem consists in the reconstruction of random microstructural features on the basis of incomplete empirical information.

In modeling of random microstructures an important issue is that the properties of a material as a whole are determined not only by the properties (physical, mechanical) of the constituents, but also by their morphology, i.e. by their topological (concerning shape) and metric properties. In reality the material morphology has its origin in the processing history of the material. For example, the complexity of microstructure in metals is strongly connected with the grain growth mechanisms (cf. [2]). Grain growth in a polycrystalline aggregate differs fundamentally from the growth of a mass of separate particles. For the size of the average grain in an aggregate to increase, it is necessary that some grains should decrease in size or disappear from the system.

On the other hand, damage evolution and local fracture processes at lower scales are affected by the amount, size distribution and spatial arrangement of features at higher length scales and vice versa. For example (cf. [3]), for a typical microstructure of A356 cast alloy (an Al-Si-Mg base alloy) which contains nonuniformly distributed micropores an important damage mechanism is gradual fracture and debonding of silicon particles (of two order less magnitude than pores). The presence of micropores alters the local stress distribution around the Si particles, and affects the damage. However, the effect of micropores (on a higher length scale) on the damage evolution around Si particles depends on the volume fraction of micropores, their size distribution, and their spatial arrangement.

Although computational micro-mechanics based modelling and simulations of fracture has significant achievements, it usually ignores the complex morphological details of real microstructures; most of the simulations are performed on the idealized microstructures (having, e.g. uniformly distributed monosized microstructural constituents of simple shapes). Therefore, an important issue associated with complex material microstructures is: *how to incorporate the true size, shape and orientation distribution and spatial arrangements of the microstructural elements/features (at different length scales) in FE-based simulations?*

Another question (considered in [4]) is as follows: *what forms should the existing empirical equations (e.g. Hall-Petch relation) take if the more detailed information about the grain/particle size and shape is to be taken into account?*

One should also bear in mind, that the properties in 3-dimensions which we are interested in usually can not be measured directly. Most often they can be estimated from sectioned metallic samples, or projections of structure onto a screen or photographic plate. So, the serious question that arises is: *how can we extract the necessary information about the true spatial features on the basis of data gathered from plane sections?* Particles or grains of similar shape (in space) can produce quite heterogeneous profile shapes when randomly sectioned.

Various problems associated with the above question have been carefully studied in stereology – the field of science comprising methods for inferring spatial structure from partial information, usually lower-dimensional data that are in the form of sections or projections of the structure of interest. In recent years the “basic stereological principles” and the associated formulae have gained much wider and rigorous treatment within stochastic geometry and geometrical/spatial statistics (cf. [1], [5]). Another branch of mathematics playing a fundamental role in microstructural modelling and in the analysis of various physical/mechanical phenomena in random microstructures is the theory of random fields (cf. [1] and references therein).

2. Dispersed-type random microstructures: random Poisson point fields

In many situations we have to deal with a type of microstructure in which heterogeneity is distributed discretely and randomly. An example is a composite containing a random distribution of elements whose properties differ significantly from those of the surrounding material: these elements may be, for example, stress-free holes, pores, rigid inclusions and so forth.

Modelling of such complicated geometrical patterns is a challenging problem. Although a dispersed phase usually consists of particles of finite size (a situation, drastically different from that in statistical theory of gasses where particles can be treated as (dimensionless) points in the state space), it turns out that the random points fields can serve as an effective tool for building the models of microstructures with dispersed particles of other random phase. The simplest and basic model for random point pattern in space is the Poisson random fields.

2.1. Homogenous Poisson random field

The Poisson random field is a generalization of the concept of the Poisson distribution (and the Poisson random process) to random events in space. Like the Poisson process it is the simplest and most common model for

random point fields in space. The homogeneous Poisson field characterizes the “complete” randomness or the absence of any structure in the point pattern; in mutually disjoint sets the numbers of points are statistically independent. For this reason, the Poisson field is often used as the null hypothesis in statistical inference. Let $N(B)$ denote the random number of points contained in B , where B is a given bounded set in R^n

Definition 1: A random point field is a homogeneous Poisson field if:

- (i) for any integer number k and for disjoint Borel sets, B_1, \dots, B_k , in R^n the random variables are statistically independent;
- (ii) the number $N(B)$ of points in any Borel set B of finite measure $m(B)$ has the Poisson probability distribution with parameter $\lambda N(B)$ that is,

$$P\{N(B) = k\} = \frac{[\lambda m(B)]^k}{k!} \exp(-\lambda m(B)), \quad k = 0, 1, \dots \quad (2.1)$$

where $m(B)$ is the Lebesgue measure of B : it is the area of B when $n = 2$ and the volume of B for $n \geq 3$. The parameter λ is called the intensity of N and characterizes the mean density of points in B .

Similarly to the case of the Poisson process (on the time axis), the points of the Poisson field are, for any bounded Borel set, uniformly and independently distributed in B .

It can be shown directly from (i), (ii) that the joint n -dimensional distribution of the homogeneous Poisson field (for mutually disjoint sets B_k , $k = 0, 1, \dots, n$) is

$$\begin{aligned} P\{N(B_1) = k_1, \dots, N(B_n) = k_n\} \\ = \frac{[\lambda m(B_1)]^{k_1}}{k_1!} \dots \frac{[\lambda m(B_n)]^{k_n}}{k_n!} \exp\left[-\lambda \sum_{k=1}^n m(B_k)\right] \end{aligned} \quad (2.2)$$

Then clearly the *emptiness* (or the void) probability of the homogeneous Poisson process is

$$\nu_B = P\{N(B) = 0\} = e^{-\lambda m(B)} \quad (2.3)$$

Let B will be a bounded set with measure $m(B)$ such that the point $\mathbf{r} = 0$ belongs to B , then the following *contact-distribution function* (with respect to B) is defined as

$$H_B(q) = 1 - \nu_{qB} = 1 - P\{N(qB) = 0\}, \quad q \geq 0, \quad (2.4)$$

where qB denotes the dilation of B by a factor q , that is $qB = \{q\mathbf{r} : \mathbf{r} \in B\}$. If B is the unit ball, i.e. $B = \{\mathbf{r} : |\mathbf{r}| \leq 1\}$, we get the *spherical contact-distribution function*

$$H_S(q) = 1 - P\{N(S(\mathbf{0}, q)) = 0\} = 1 - e^{-\lambda \alpha_n q^n}, \quad (2.5)$$

where α_n is such that $\alpha_n q^n = \text{volume of the ball } S(\mathbf{0}, q) \text{ in } R^n$. For $n = 2$, $H_S(q) = 1 - \exp(-\lambda\pi q^2)$. It is clear that $H_S(q)$ is the distribution function of the distance from $\mathbf{0}$ to the nearest point of N . Because of the properties of the homogeneous Poisson field, the distance to the nearest point of the field N seen from an arbitrary location in space has the same distribution as the distance to the nearest neighbor of a randomly chosen point of the field (cf. [5]). This means that the nearest-neighbor distribution function $D(q)$ is equal to $H_S(q)$. Of course, the probability density $h_S(q)$ corresponding to (2.5) is

$$h_S(q) = n\lambda\alpha_n q^{n-1} e^{-\lambda\alpha_n q^n}. \quad (2.6)$$

The mean and variance of (2.6) for the Poisson field on the plane ($n = 2$) are obtained by integration of q and q^2 with respect to $h_S(q)$ with $n = 2$, $\alpha_n = \pi$; the result is

$$\langle h_S(q) \rangle = \frac{1}{2\sqrt{\lambda}}, \quad \text{var } h_S(q) = \frac{1}{\pi\lambda} - \frac{1}{4\lambda}. \quad (2.7)$$

The second order characteristics for the homogeneous Poisson process are especially simple, (cf. [5])

If B_1 and B_2 are *disjoint*, i.e. $B_1 \cap B_2 = 0$ then

$$\langle N(B_1)N(B_2) \rangle = \langle N(B_1) \rangle \langle N(B_2) \rangle = \lambda^2 m(B_1)m(B_2), \quad (2.8)$$

$$\text{var } N(B) = 0, \quad \text{cov}[N(B_1)N(B_2)] = 0. \quad (2.9)$$

If B_1 and B_2 are not disjoint, i.e. $B_1 \cap B_2 \neq 0$, then

$$\mu_2(B_1 \times B_2) = \langle N(B_1)N(B_2) \rangle = \lambda^2 m(B_1)m(B_2) + \lambda m(B_1 \cap B_2), \quad (2.10)$$

and therefore

$$\begin{aligned} \text{cov}[N(B_1)N(B_2)] &= \lambda m(B_1 \cap B_2), \\ \text{var}[N(B)] &= \lambda m(B). \end{aligned} \quad (2.11)$$

The factorial moment measure $\alpha_2(B_1 \times B_2)$ for the homogeneous Poisson process is

$$\alpha_2(B_1 \times B_2) = \lambda^2 m(B_1)m(B_2). \quad (2.12)$$

Therefore, from equation (3.11) in [1] we obtain the *second-order product density*

$$\zeta_2(\mathbf{r}_1, \mathbf{r}_2) = \lambda^2. \quad (2.13)$$

An important question in modelling real random point patterns is: how can one recognize that a given point pattern has the features of complete spatial randomness as embodied in a homogeneous random Poisson field?

Various tests are known to characterize types of point patterns. Early studies were primarily concerned with comparing area (or quadrat) counts to those of a Poisson distribution. Usually, quadrats of random location and orientation are sampled, the number of points in the quadrats are counted and statistics derived and computed and then compared with the corresponding statistics of the homogeneous Poisson field. Departure indicates that the pattern is not completely spatially random. The degree of departure is usually quantified through the values of some parameters (cf. Cressie [6] and references therein). Of course, the reduction of complex point patterns to counts of the number of points in randomly positioned quadrats and to one-dimensional indices leads to a considerable loss of information; for example, there is no consideration of the relative positions of points within quadrats.

Another type of statistic is based on distances between randomly sampled points and other points in a region B of interest. For example, mean distances to the first, second, third, etc. nearest neighbors may be estimated and compared to the corresponding distances under complete spatial randomness. Further insight into specific features of spatial random patterns can be gained by estimation and studying the pair-correlation function $d(q)$ defined by (3.12) in [1].

Figure 2 shows two realizations of a homogeneous Poisson random field for 100 points on the unit circle. Note that on average the distribution is uniform but particular realizations may show some nonuniformity and even some clustering.

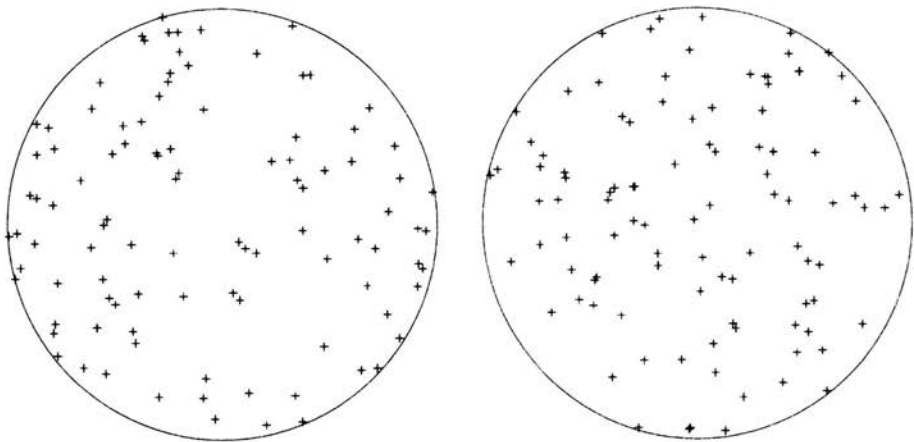


FIGURE 2. Two realizations of 100 points of a homogeneous poisson random field on the unit circle, after [1].

2.2. Inhomogeneous Poisson random field

A natural generalization of the homogeneous Poisson field is a field which while still being Poissonian has the potential to characterize spatial random patterns with variable point density. The mean measure of an inhomogeneous Poisson field is not proportional to the Lebesgue measure of the set B , but it is a general intensity measure $\mu(B)$ defined as

$$\mu(B) = \langle N(B) \rangle \quad (2.14)$$

for any Borel set B . If $\mu(B)$ is represented in the form

$$\mu(B) = \int_B \lambda(\mathbf{r}) d\mathbf{r}, \quad (2.15)$$

then the function $\lambda(\mathbf{r})$ is called the *intensity function*. If $\lambda(\mathbf{r}) = \lambda =$ a constant, then we have a homogeneous Poisson field.

Definition 2: A random point field N is an inhomogeneous Poisson field with mean measure μ if the number $N(B)$ of points in a bounded Borel set B has a Poisson distribution

$$P\{N(B) = k\} = \frac{[\mu(B)]^k}{k!} e^{-\mu(B)}, \quad k = 0, 1, \dots \quad (2.16)$$

The covariance and variance measures of the inhomogeneous Poisson process are, respectively

$$\begin{aligned} \text{cov}[N(B_1)N(B_2)] &= \mu(B_1 \cap B_2), \\ \text{var}[N(B)] &= \mu(B). \end{aligned} \quad (2.17)$$

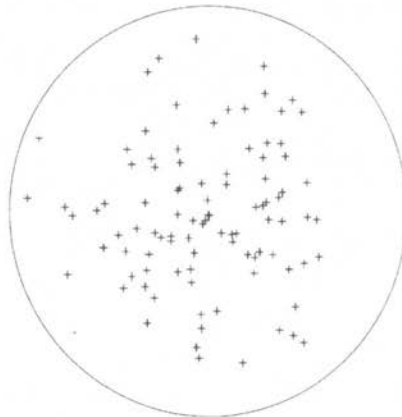


FIGURE 3. Realization of an inhomogeneous poisson random field, after [1].

The product density $\zeta_2(\mathbf{r}_1, \mathbf{r}_2)$ can be expressed in terms of the intensity function $\lambda(\mathbf{r})$. The probability that there is a point in each of two infinitesimally small regions (e.g. spheres) centered at \mathbf{r}_1 and \mathbf{r}_2 with volumes dV_1 and dV_2 is equal to

$$\zeta_2(\mathbf{r}_1, \mathbf{r}_2) = \lambda(\mathbf{r}_1)\lambda(\mathbf{r}_2)dV_1dV_2 \quad (2.18)$$

A realization of an inhomogeneous Poisson field on the unit circle is shown in Fig. 3. This assumes a radially symmetric intensity function $\lambda(r, \theta) = \lambda(r) = 1 - r$. The decreasing radial intensity is evident in the sample.

2.3. Doubly stochastic Poisson field

A useful generalization of a Poisson random field is obtained by randomizing the intensity measure, that is by assuming that the intensity measure is itself random.

Definition 3: *The random field N is a doubly stochastic Poisson field or Cox field with random intensity measure M if, conditional on $M = \mu$, the field N is an inhomogeneous Poisson process with mean measure μ .*

The above definition implies that a Cox field originates from a two-step random mechanism; the first (global) mechanism is governed by a Poisson-type distribution of points, whereas the second one is associated with randomness of the intensity measure. In this sense a Cox process can be viewed as a composite (or subordinated) random point field. In the literature this field (or process, if it is considered on the time axis) is sometimes referred to as a Cox field *directed* by the random measure M .

If the random intensity measure M of a doubly stochastic Poisson field N is distributed according to the probability distribution Q , then

$$P\{N(B) = k\} = \int \frac{[M(B)]^k}{k!} e^{-M(B)} dQ = \left\langle \frac{[M(B)]^k}{k!} e^{-M(B)} \right\rangle_Q. \quad (2.19)$$

In practice, when the intensity of an inhomogeneous Poisson field is characterized by the intensity function $\lambda(\mathbf{r})$, a Cox field is directed by the random function $\lambda(\mathbf{r}, \gamma)$. A wide class of Cox processes can be defined effectively by a random intensity function of the form

$$\lambda(\mathbf{r}, \gamma) = \lambda_0(\gamma)\lambda_1(\mathbf{r}), \quad (2.20)$$

where $\lambda_0(\gamma)$ is a non-negative random variable, and $\lambda_1(\mathbf{r})$ is a deterministic, non-negative function.

A particular case of (2.20) when $\lambda_1(\mathbf{r}) = 1$ yields the so called *mixed Poisson field* which is regarded as a homogeneous Poisson field with randomized

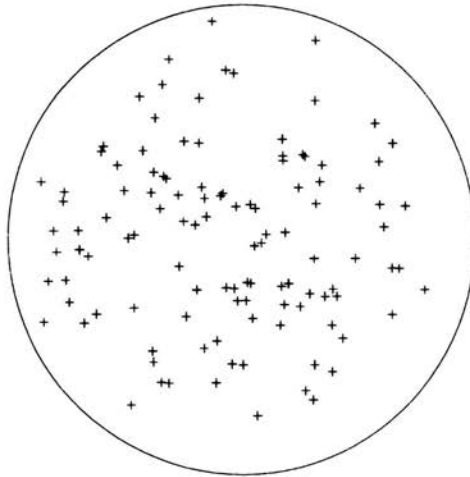


FIGURE 4. Realization of a Cox pattern or doubly-stochastic poisson random field, after [1].

intensity, i.e.

$$\lambda(\mathbf{r}, \gamma) = \lambda_0(\gamma). \quad (2.21)$$

It is clear that randomization of the intensity magnifies the overall randomness of the field. Hence, the variance of a number of Cox points in a bounded set B will exceed the variance of the number of points in the corresponding homogeneous Poisson field. A number of authors have studied Cox random fields in the context of statistics of spatial data (cf. Diggle [7], Lotwick [8]). Figure 4 shows a realization of a plane Cox pattern or doubly stochastic Poisson random field. This was generated by simulating an inhomogeneous Poisson random field using the same intensity function as in Fig. 3 ($\lambda(r, \theta) = \lambda(r) = 1 - r$). The field was then “thinned” by keeping points with probability $\lambda(r)$.

2.4. Poisson cluster field

If each point of a homogeneous Poisson field N is replaced by a cluster of points, random in number and scattered independently and with identical distribution, then we obtain a new random point field N_{cL} . This Poisson-induced field is called a Poisson cluster field or more often a *Neyman-Scott field*.

The parent points (belonging to N) are not the points of the field N_{cL} . The position of the k -th point of a cluster is characterized by a random vector \mathbf{Z} , where Z_i the components are identically and independently dis-

tributed with probability density $p(z)$. Most often it is assumed that the Z_i are isotropic, and therefore it is sufficient to determine the density function $p(r)$ of the distance of the points of N_{cL} from the cluster center.

Let us assume that the number of points per cluster has a Poisson distribution with intensity μ (the considered cluster field is a Cox field) and the points in the clusters are distributed uniformly and independently in the ball $b(0, R)$. In this case (known as the *Matern cluster field*) the intensity of the field N_{cL} is $\lambda_{cL} = \lambda\mu$. A detailed analysis of clustered fields can be found in an extensive literature (cf. [9], [10]); the problems of statistical inference for the Neyman-Scott processes are considered in the literature of spatial statistics.

A possible extension of the Poisson cluster field is concerned with multiple clusters of points. Points in generation k are assumed to be produced by a Poisson cluster field from “parents” in the generation $k - 1$. It is rational to assume that the number of points (“offspring”) of each parent is again governed by a Poisson distribution, and any discrete-type distribution may be used.

Figure 5 illustrates a Poisson cluster pattern of points. The locations of the centers of the clusters is a set of points (call these the cluster-center points) which are a realization of a homogeneous Poisson random field on the unit circle. Each cluster is itself a realization of a homogeneous Poisson random field of ten points on a circle of radius 0.1 centered at a cluster-center point.

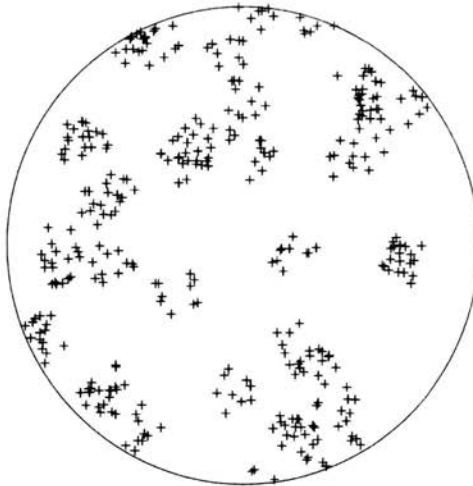


FIGURE 5. Realization of a Cox pattern or doubly-stochastic Poisson random field, after [1].

2.5. Poisson hard-core field

A *hard-core point field* is defined as a point field in which the points are not allowed to lie closer than at a certain specific distance. Let us denote this distance by h . It is clear that such fields may serve as possible models of a random distribution of non-overlapping spherical particles (of radius $h/2$) in space.

Let N be a homogeneous Poisson field R^n in with intensity λ . The hard-core field is formed by deleting all pairs of N points of that are separated by a distance of less than h . The remaining points form a spatial point field N_h which is called a Poisson hard-core field or the *Matern hard-core model* (Matern first described this type of field in 1960). This model is, in fact, produced by the operation of dependent thinning applied to the primary Poisson field N (cf. [1]).

The probability p_h that an arbitrary point of N is retained (the so-called retaining probability of a “typical point” of N) in the operation of thinning is

$$p_h = P\{N[S(\mathbf{r}, h)] = 0\} = \exp[-\lambda m(S(\mathbf{r}, h))] = \exp[-\lambda \alpha_n h^n], \quad (2.22)$$

where $\alpha_n = \pi^{n/2}/\Gamma(1 + n/2)$ is the volume of the unit sphere in R^n . This means that for $n = 2$ (point pattern on the plane) $p_h = \exp[-2\pi h^2]$, and for $n = 3$ $p_h = \exp[-4\lambda\pi h^3/3]$. The intensity of the hard-core field N_h is

$$\lambda_h = \lambda \cdot p_h. \quad (2.23)$$

If $h = 1$ then the maximum intensity λ_h is approximately 0.32 for a plane field, and 0.24 in the three-dimensional case.

Hard-core models are of great significance in many branches of physics and engineering. Random distributions of hard (i.e. non-overlapping) particles in R^3 arise in practice whenever inclusions, i.e. chunks of another substance are embedded in the matrix of a “basic” substance. Problems concerned with random distributions of particles have attracted much attention in studies of the structure of liquids (cf. Rice and Gray [11]).

3. Microstructural modeling via continuous random fields

There exists a class of problems in modelling of random microstructures and in micromechanical analysis of real material media which can be treated with use of continuous random fields. The term “continuous” is used here to distinguish this type of mathematical constructs from those discussed in the previous sub-section (and associated with discrete events in space). We

mean here random functions of a spatial variable which — in general, but not necessarily — vary smoothly in space.

Such random fields (under the appropriate assumptions) have been widely used in statistical turbulence theory (cf. [12]), in wave propagation in random media (cf. [13]) and in other fields. The possible realizations of such random fields, say $X(\mathbf{r}, \gamma)$, are hypersurfaces (surfaces, when $\mathbf{r} \in R^2$).

In order to give a rough idea about possible applications of random fields theory in modelling of complex heterogeneous material structures we mention briefly two problems.

- It is clear that such single geometrical objects as particles, nonmetallic inclusions, pores, grains (and many other) are constituents of actual microstructures and can be regarded as sets in R^3 . Most often these sets are random, i.e. such their features as shape, and size are random. By the way, the theory of random sets has a long history and an extensive literature (cf. [5]). It is interesting to note that in the thirties Kolmogorov already wrote on “regions . . . whose shape depends on chance”. Random sets can be characterized in various ways. A possible way of specifying random sets is through a section of a given continuous random field $X(\mathbf{r}, \gamma)$. If any random field is cut on some level u and looked at from above, then the boundary of the slice traces the boundary of random set. More specifically, this random set is defined as: let $D \in R^3$ be a specific subset of R^3 , then the excursion set of the field $X(\mathbf{r}, \gamma)$ above the level u in D is the following random set

$$B_u(D) = \{\mathbf{r} \in D : X(\mathbf{r}, \gamma) \geq u\}.$$

Such random sets have recently been used for modelling of random composites (the interface between the phases is characterized as a level cut of some Gaussian random field).

- Another natural application of continuous random fields is the characterization of the properties of the materials. For example, Young’s modulus of microheterogeneous material is a random variable that depends on spatial coordinates, i.e. it is a random field. Also, microstresses in random elastic solids are specified by (tensorial) random fields. In the investigation of contamination transport through underground formations and rocks random fields play a fundamental role.

In what follows we expound briefly the basic notions of random field theory and the associated modelling issues.

3.1. Basic concepts

In various applied problems one has to deal with quantities which are both random and dependent upon a parameter, and the “physical nature” of the parameter may be quite distinct in each particular situation. One of the best known examples of this type is Brownian motion; each coordinate of the Brownian particle is a random variable which changes in time. Such phenomena are modelled and studied using the theory of stochastic processes where families of random variables depending on a one-dimensional parameter (interpreted commonly as time) are considered.

However, we often encounter phenomena in which random variables depend on a multidimensional parameter. For example, the height of the surface of the sea, pollutant concentration in the ground, the velocity of a fluid particle in turbulent flow, Young’s modulus of micro-heterogeneous materials are random variables that depend on spatial coordinates. To study such phenomena one has to define and investigate random functions depending on an argument which is, in general, an element of n -dimensional Euclidean space R^n , where $n = 1, 2, \dots, N$. Such functions $X(\mathbf{r})$, $\mathbf{r} \in R^n$ are termed *random fields*. When $n = 1$, we have a random field defined on R^1 . The theory of such fields completely coincides with the theory of stochastic processes. In what follows we will deal with situations where $n \geq 2$. The cases $n = 3$, i.e. random fields $X(\mathbf{r})$ whose argument $\mathbf{r} = (x_1, x_2, x_3)$ belongs to physical three-dimensional space R^3 , and $n = 4$, i.e. random functions $X(\mathbf{r}, t)$ of \mathbf{r} and t where t is regarded as time will be of special concern.

Let D be a specified subset of n -dimensional space R^n or the space R^n itself. The points of D will be denoted by $\mathbf{r} = (x_1, x_2, \dots, x_n)$.

Definition 4: A random field $X(\mathbf{r})$ on D is a family of random variables $\{X_{\mathbf{r}}(\gamma), \mathbf{r} \in D, \gamma \in \Gamma\}$ depending upon $\mathbf{r} \in D$ and defined on the probability space (Γ, F, P) .

If random variables $X_{\mathbf{r}}(\gamma)$ forming a random field are for each $\mathbf{r} \in D$ one-dimensional (scalar), i.e. their sample values are real numbers, then the random field is termed a *scalar random field*. If the random variables $X_{\mathbf{r}}(\gamma)$ are multidimensional (e.g. k -dimensional) then the random field is a *vector random field*. Such a field takes the form:

$$\mathbf{X}(\mathbf{r}) = [X_1(\mathbf{r}), X_2(\mathbf{r}), \dots, X_k(\mathbf{r})], \quad \mathbf{r} \in D \subseteq R^n.$$

In Sections 3.1 – 3.5 we will discuss exclusively scalar random fields.

Definition 4 of a random field can equivalently be given as follows: a random field $X(\mathbf{r})$ is a function which maps the index set D into the space S of random variables defined on (Γ, F, P) .

Similarly to the case of stochastic processes, a random field is specified if for each finite set of \mathbf{r} -values, say $\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k\}$ a joint distribution function

$$F_{\mathbf{r}_1, \dots, \mathbf{r}_k}(x_1, \dots, x_k) = P\{X(\mathbf{r}_1) < x_1, \dots, X(\mathbf{r}_k) < x_k\} \quad (3.1)$$

(satisfying the consistency conditions) is given. The collection of these distributions is known as the *family of finite dimensional* distributions of the field $X(\mathbf{r})$. The Kolmogorov theorem (cf. [14]) gives a necessary and sufficient condition for the existence of a random field when the family of functions $F_{\mathbf{r}_1, \dots, \mathbf{r}_k}(x_1, \dots, x_k)$ is given.

For every fixed elementary event $\gamma \in \Gamma$, $X(\mathbf{r}, \gamma)$ is a deterministic function of \mathbf{r} , defined for all $\mathbf{r} \in D$. This function $x(\mathbf{r}) = X(\mathbf{r}, \gamma)$ for fixed $\gamma \in \Gamma$ describes a fixed realization of the random field $X(\mathbf{r})$. It is called a *realization* or *sample function* of the considered field. For example, if $X(\mathbf{r}, \gamma)$ describes the random surface of a road, then $\mathbf{r} = (x_1, x_2)$ and sample functions $x(\mathbf{r}) = X(\mathbf{r}, \gamma)$ are for each $\gamma \in \Gamma$ the actual surfaces of the considered class of roads.

It is worth noting that a significant class of random fields can be defined explicitly by analytical functions of a spatial variable $\mathbf{r} \in D$ and a collection of random variables $[\xi_1(\gamma), \xi_2(\gamma), \dots, \xi_N(\gamma)]$, that is

$$X(\mathbf{r}, \gamma) = g[\mathbf{r}, \xi_1(\gamma), \xi_2(\gamma), \dots, \xi_N(\gamma)], \quad (3.2)$$

where g is a specified (deterministic) function of \mathbf{r} and random variables $\xi_i(\gamma)$, $i = 1, 2, \dots, N$. The probability distributions of $X(\mathbf{r}, \gamma)$ can be determined in terms of the joint probability distributions of the random variables $\xi_i(\gamma)$, $i = 1, 2, \dots, N$. For example, a random harmonic wave field can be represented as

$$X(\mathbf{r}, \gamma) = \sum_{i=1}^N A_i(\gamma) \cos(\mathbf{k} \cdot \mathbf{r} - \omega t)$$

where $A_i(\gamma)$ are random variables and \mathbf{k} is the wave vector.

The simplest and most basic characteristics of a random field are the *mean*, or *average*, and the *covariance function*. The *mean* is defined as

$$m_X(\mathbf{r}) = E[X(\mathbf{r}, \gamma)] = \langle X(\mathbf{r}, \gamma) \rangle, \quad (3.3)$$

where averaging is performed with respect to γ , i.e. with respect to the probability distribution $F_{\mathbf{r}}(x)$. The *covariance function*,

$$K_X(\mathbf{r}_1, \mathbf{r}_2) = \left\langle [X(\mathbf{r}_1, \gamma) - m_X(\mathbf{r}_1)][\overline{X(\mathbf{r}_2, \gamma) - m_X(\mathbf{r}_2)}] \right\rangle, \quad (3.4)$$

where the overbar denotes the complex conjugate. For greater generality we have assumed that $X(\mathbf{r}, \gamma)$ is a complex-valued field, i.e. $X(\mathbf{r}, \gamma) = X_1(\mathbf{r}, \gamma) +$

$iX_2(\mathbf{r}, \gamma)$, where X_1 and X_2 are real fields. In particular, when $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}$ we obtain the *variance* of the random field $X(\mathbf{r}, \gamma)$

$$\nu_X(\mathbf{r}) = \sigma_X^2(\mathbf{r}) = \text{var } X(\mathbf{r}, \gamma) = |X(\mathbf{r}, \gamma) - m_X(\mathbf{r})|^2. \quad (3.5)$$

From the linearity of the expected value operator, it follows that

$$K_X(\mathbf{r}_1, \mathbf{r}_2) = \left\langle X(\mathbf{r}_1, \gamma) \overline{X(\mathbf{r}_2, \gamma)} \right\rangle - m_X(\mathbf{r}_1) m_X(\mathbf{r}_2). \quad (3.6)$$

A random field $X(\mathbf{r}, \gamma)$ is called a *second-order field* if $|X(\mathbf{r}, \gamma)|^2 < \infty$.

Without loss of generality we can assume that the random field under consideration has a zero mean value. Then the second-order moment $|X(\mathbf{r}, \gamma)|^2$ is the variance and $K_X(\mathbf{r}_1, \mathbf{r}_2)$ is the *correlation function* of the field. Furthermore, the Schwarz inequality implies that a second-order field always has a correlation function. Conversely, if there exists a finite $K_X(\mathbf{r}_1, \mathbf{r}_2)$ defined on the product $D \times D$, then $K_X(\mathbf{r}, \mathbf{r}) = |X(\mathbf{r}, \gamma)|^2 < \infty$. The properties of a random field expressed in terms of its second order moments are usually called *second-order properties*. Random variables with finite second order moments form a Hilbert space $L_2(\Gamma, F, P)$. A second order random field can thus be regarded as a function defined on $D \subset R^n$ and taking its values in $L_2(\Gamma, F, P)$. This implies that convergence of random variables in a mean square sense (being equivalent to convergence in the L_2 -norm) is a very natural mode of convergence in the theory of second-order random functions. This type of stochastic convergence also turns out to be very useful, since the basic properties of a random function defined in this way are analogous to the calculus of ordinary (deterministic) functions.

As with stochastic processes, the covariance function $K_X(\mathbf{r}, \mathbf{r})$ of a random field has the properties:

- a) $K_X(\mathbf{r}, \mathbf{r}) = \text{var } X(\mathbf{r}) \geq 0$
- b) $K_X(\mathbf{r}_1, \mathbf{r}_2)$ is a symmetric function, i.e. for all $\mathbf{r}_1, \mathbf{r}_2 \in D \subseteq R^n$

$$K_X(\mathbf{r}_1, \mathbf{r}_2) = \overline{K_X(\mathbf{r}_2, \mathbf{r}_1)}, \quad (3.7)$$

or in the case of real field

$$K_X(\mathbf{r}_1, \mathbf{r}_2) = K_X(\mathbf{r}_2, \mathbf{r}_1).$$

- c) every covariance function is *non-negative definite*, that is for arbitrary m , arbitrary finite sets of points $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_m$ belonging to R^n and arbitrary complex numbers z_1, z_2, \dots, z_m

$$\sum_{i,j=1}^m K_X(\mathbf{r}_i, \mathbf{r}_j) z_i \bar{z}_j \geq 0. \quad (3.8)$$

The properties a) and b) are clear from the definition. Property c) follows from the fact that the left hand side of (3.8) is equal to

$$\left\langle \left| \sum_{i=1}^m [X(\mathbf{r}_i) - m_X(\mathbf{r}_i)] z_i \right|^2 \right\rangle,$$

which must be real and non-negative. The property (3.8) is, in fact, a characteristic property of the class of all covariance functions; that is for any function $K(\mathbf{r}_1, \mathbf{r}_2)$ which is non-negative definite there always exists a random field whose covariance coincides with $K(\mathbf{r}_1, \mathbf{r}_2)$.

Higher-order moments of random fields are defined similarly as in the case of stochastic processes. In general, a moment (or moment function) of order $k = k_1 + k_2 + \dots + k_m$ is defined as follows:

$$m_{X|k_1, \dots, k_m}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_m) = \left\langle X^{k_1}(\mathbf{r}_1) \cdot X^{k_2}(\mathbf{r}_2) \cdot \dots \cdot X^{k_m}(\mathbf{r}_m) \right\rangle. \quad (3.9)$$

In particular, when $k = k_1 = k_2 = \dots = k_m = 1$ we obtain the common moment function of order m .

An important class of random fields is the class of *Gaussian fields*. They constitute a straightforward extension of Gaussian stochastic processes to the multidimensional parameter (argument) space.

Definition 5: A random field $X(\mathbf{r})$ is said to be *Gaussian* if all its finite-dimensional probability distributions (3.1) are Gaussian.

It is clear that all finite-dimensional probability distributions of a real-valued Gaussian field have the exponential form, and they are completely determined by the mean $m_X(\mathbf{r})$ and covariance function $K_X(\mathbf{r}_1, \mathbf{r}_2)$. Most of the explicit results both in the theory and the application of random fields have been obtained for Gaussian fields.

3.2. Homogeneous random fields

As in the case of a one-dimensional argument (i.e. in the analysis of stochastic processes), we distinguish various classes of random fields. Particularly important is the class of random fields which satisfy certain conditions of statistical homogeneity in space and can be regarded as a generalization of stationary stochastic processes.

Definition 6: A random field $X(\mathbf{r})$ is strictly homogeneous if for any set of points $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k$ belonging to D and for any vector \mathbf{q} such that $\mathbf{r}_i + \mathbf{q} \in D$, for $i = 1, \dots, k$ the following equality holds

$$F_{\mathbf{r}_1, \dots, \mathbf{r}_k}(x_1, \dots, x_k) = F_{\mathbf{r}_1 + \mathbf{q}, \mathbf{r}_2 + \mathbf{q}, \dots, \mathbf{r}_k + \mathbf{q}}(x_1, \dots, x_k). \quad (3.10)$$

Therefore, the finite-dimensional distributions of a strictly homogeneous random field are invariant under translation of the points $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k$ by the vector \mathbf{q} . This implies directly that the mean function $m_X(\mathbf{r})$ is constant and the covariance function $K_X(\mathbf{r}_1, \mathbf{r}_2)$ is a function of the difference of \mathbf{r}_1 and \mathbf{r}_2 only.

Definition 7: A random field is weakly homogeneous, if

$$\begin{aligned} m_X(\mathbf{r}) &= m_X = \text{constant}, \\ K_X(\mathbf{r}_1, \mathbf{r}_2) &= K_X(\mathbf{r}_1 - \mathbf{r}_2) = K_X(\mathbf{q}), \quad \mathbf{q} = \mathbf{r}_1 - \mathbf{r}_2, \\ &\text{for arbitrary } \mathbf{r}_1, \mathbf{r}_2 \in D. \end{aligned} \quad (3.11)$$

Weakly homogeneous random fields play a fundamental role in theory and applications and they are commonly called simply *homogeneous random fields*. One should notice that instead of $2n$ variables as arguments of covariance function (the general case), the covariance function of a homogeneous field is a function of n variables only. Without loss of generality we will assume that the mean value m_X is zero (if this is not the case we can always consider a new field $Y(\mathbf{r}) = X(\mathbf{r}) - m_X$ whose mean is zero). Denote by q_1, q_2, \dots, q_n the coordinates of the vector \mathbf{q} . Then it follows from (3.11) that for real fields

$$K_X(\mathbf{q}) = K_X(q_1, q_2, \dots, q_n) = K_X(-q_1, -q_2, \dots, -q_n) \quad (3.12)$$

Notice however, that, for example, $K_X(-q_1, q_2, \dots, q_n) \neq K_X(q_1, q_2, \dots, q_n)$.

Again, as in the one-dimensional case, the covariance functions $K_X(\mathbf{q})$ of homogeneous fields in R^n belong to the class of positive definite functions of n variables and due to the Bochner theorem (if $K_X(\mathbf{q})$ is continuous) they have the following representation

$$K_X(\mathbf{q}) = \int_{R^n} e^{i(\mathbf{q} \cdot \mathbf{k})} dG(\mathbf{k}), \quad (3.13)$$

where \mathbf{k} is the wave vector (spatial counterpart of the frequency), i.e. $\mathbf{k} = (k_1, k_2, \dots, k_n)$, $(\mathbf{q} \cdot \mathbf{k}) = q_1 k_1 + q_2 k_2 + \dots + q_n k_n$ and $G(\mathbf{k})$ is a bounded, real-valued and nonnegative function. The function $G(\mathbf{k})$ is called a *spectral distribution function* of the field $X(\mathbf{r})$.

Concepts from the spectral representation of stationary stochastic processes can be extended to homogeneous random fields. The role of harmonic oscillations, $e^{i\omega t}$, is played by plane waves, $e^{i(\mathbf{k} \cdot \mathbf{r})}$, and the random function $\Phi(\Delta\omega) = \Phi([\omega_1, \omega_2]) = \Phi(\omega_2) - \Phi(\omega_1)$ is replaced by the function $\Phi(\Delta\mathbf{k}) = \Phi([\mathbf{k}, \mathbf{k} + \Delta\mathbf{k}]) = d\Phi(\mathbf{k})$, where $\Delta\mathbf{k} = \Delta k_1 \dots \Delta k_n$ is a volume ele-

ment of n -dimensional space R^n . Therefore, a spectral representation of a homogeneous random field $X(\mathbf{r})$ takes the form (it is assumed that $m_X = 0$),

$$X(\mathbf{r}) = \int_{R^n} e^{i(\mathbf{k} \cdot \mathbf{r})} d\Phi(\mathbf{q}), \quad (3.14)$$

where the integral is understood as a limit in the mean square sense of the appropriate integral sums, and $\Phi(\mathbf{k})$ is the field with orthogonal increments with the properties

$$\begin{aligned} \langle d\Phi(\mathbf{k}) \rangle &= 0, \\ \langle d\Phi(\mathbf{k}') d\Phi(\mathbf{k}'') \rangle &= \delta(\mathbf{k}' - \mathbf{k}'') g(\mathbf{k}') d\mathbf{k}' d\mathbf{k}'', \\ |d\Phi(\mathbf{k})|^2 &= dG(\mathbf{k}) = g(\mathbf{k}) d\mathbf{k} \geq 0. \end{aligned} \quad (3.15)$$

It is evident that substitution of the representation (3.14) into the expression for the covariance function $K_X(\mathbf{q})$ yields formula (3.13). Indeed,

$$\begin{aligned} K_X(\mathbf{q}) &= \langle \overline{X(\mathbf{r})} X(\mathbf{r} + \mathbf{q}) \rangle = \left\langle \left\langle \int e^{-i(\mathbf{k}_1 \cdot \mathbf{r})} d\overline{\Phi(\mathbf{k}_1)} \int e^{i(\mathbf{k}_2 \cdot (\mathbf{r} + \mathbf{q}))} d\overline{\Phi(\mathbf{k}_2)} \right\rangle \right\rangle \\ &= \iint e^{i(\mathbf{k}_2 \cdot \mathbf{q}) + i[(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{r}]} \langle d\overline{\Phi(\mathbf{k}_1)} d\Phi(\mathbf{k}_2) \rangle. \end{aligned}$$

Since the increments of $\Phi(\mathbf{k})$ are uncorrelated (orthogonal) on non-overlapping intervals of wave number \mathbf{k} (cf. the second equation of (3.15)) the last $2n$ -fold integral reduces to the n -fold integral (3.13).

Let us assume that the spectral distribution $G(\mathbf{k})$ is absolutely continuous. Then there exists a nonnegative function $g(\mathbf{k})$ such that

$$G(\mathbf{k}) = \int_{-\infty}^{k_1} \dots \int_{-\infty}^{k_n} g(\mathbf{k}) d\mathbf{k} \quad (3.16)$$

The function $g(\mathbf{k})$ is called the n -dimensional *spectral density* of a homogeneous random field $X(\mathbf{r})$. Equation (3.16) means that almost everywhere (with respect to the Lebesgue measure in R^k)

$$g(\mathbf{k}) = g(k_1, k_2, \dots, k_n) = \frac{\partial^n G(k_1, k_2, \dots, k_n)}{\partial k_1 \partial k_2 \dots \partial k_n}.$$

Therefore, the spectral representation of the correlation function (3.13) takes the form

$$K_X(\mathbf{q}) = \int_{R^n} e^{i(\mathbf{q} \cdot \mathbf{k})} g(\mathbf{k}) d^n \mathbf{k}, \quad (3.17)$$

where $d^n \mathbf{k} = dk_1 dk_2 \dots dk_n$. The spectral density $g(\mathbf{k})$, if it exists, can be obtained from the correlation function by use of the usual formula for the inversion of an n -dimensional Fourier integral,

$$g(\mathbf{k}) = \frac{1}{(2\pi)^n} \int_{R^n} e^{i(\mathbf{q} \cdot \mathbf{k})} K_X(\mathbf{q}) d^n \mathbf{q}. \quad (3.18)$$

The spectral density $g(\mathbf{k})$ of any homogeneous random field is a non-negative function of the wave number \mathbf{k} . Conversely, any non-negative integrable function $g(\mathbf{k})$ is the spectral density of some homogeneous random field. Therefore, any function $K(\mathbf{q})$ having a Fourier transform which is everywhere non-negative, is a possible correlation function of a homogeneous random field. For example, the function

$$K_X(\mathbf{q}) = K_X(q_1, \dots, q_n) = \sigma^2 \exp(-\alpha_1 |q_1| - \dots - \alpha_n |q_n|), \\ \alpha_i > 0, \quad i = 1, 2, \dots, n, \quad \sigma^2 > 0 \quad (3.19)$$

is the correlation function of a homogeneous random field in R^n ; its Fourier transform (i.e. spectral density) $g(\mathbf{k})$ takes the form

$$g(\mathbf{k}) = g(k_1, \dots, k_n) = \frac{\sigma^2}{\pi^n} \frac{\alpha_1}{(k_1^2 + \alpha_1^2)} \frac{\alpha_2}{(k_2^2 + \alpha_2^2)} \dots \frac{\alpha_n}{(k_n^2 + \alpha_n^2)} \quad (3.20)$$

and is everywhere positive.

Again, as in the case of stochastic processes, a notion of *spatial white noise* turns out to be useful. This is a random field (more exactly, a generalized random field) whose correlation function is defined as

$$K_\xi(\mathbf{q}) = K_\xi(q_1, \dots, q_n) = c \delta(q_1) \delta(q_2) \dots \delta(q_n), \quad (3.21)$$

where $\delta(q_i)$ is the Dirac function, and c is a positive constant. Making use of equation (3.18), we obtain the constant spectral density corresponding to (3.21)

$$g_\xi(\mathbf{k}) = \frac{c}{(2\pi)^n} \geq 0. \quad (3.22)$$

The spatial white noise field is a natural extension of an uncorrelated discrete parameter random field, i.e. a field defined for $\mathbf{r} \in Z^n$, where Z^n is the set of all points R^n with integer coordinates. The correlation function of such a field, say $E(\mathbf{r})$ is

$$K_E(\mathbf{q}) = \begin{cases} 1, & \text{for } \mathbf{q} = \mathbf{0} = (0, \dots, 0), \\ 0, & \text{for } \mathbf{q} \neq \mathbf{0}. \end{cases} \quad (3.23)$$

Remark 1. In applications we usually deal with real random fields. Then both the correlation function and the spectral density are symmetric functions about the origin of R^n . In this case they are related via the Fourier cosine transform, i.e.,

$$K_X(\mathbf{q}) = \int_{R^n} \cos(\mathbf{q} \cdot \mathbf{k}) g_X(\mathbf{k}) d\mathbf{k},$$

$$g_X(\mathbf{k}) = \frac{1}{(2\pi)^n} \int_{R^n} \cos(\mathbf{q} \cdot \mathbf{k}) K_X(\mathbf{q}) d\mathbf{q}. \quad (3.24)$$

3.3. Isotropic random fields

3.3.1. Definition and spectral analysis. A special class of homogeneous random fields is the class of isotropic fields.

Definition 8: A random field $X(\mathbf{r})$ is isotropic in the narrow sense (or, strictly isotropic) if all its finite-dimensional distributions do not change under arbitrary translation and rotation of points $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k$ around axes crossing the origin (of the coordinate system).

Most common in theory and application are isotropic fields in a broad sense (or, weakly isotropic) which are simultaneously assumed to be homogeneous.

Definition 9: A homogeneous random field $X(\mathbf{r})$ is said to be isotropic in a broad sense, or simply isotropic if its covariance function $K_X(\mathbf{q})$ depends only on the length $|\mathbf{q}| = q$ of the vector \mathbf{q} and it does not depend on its direction, that is

$$K_X(\mathbf{r}_1, \mathbf{r}_2) = K_X(\mathbf{q}) = K_X(q), \quad (3.25)$$

where $\mathbf{q} = \mathbf{r}_2 - \mathbf{r}_1$, $q = |\mathbf{q}| = (q_1^2 + q_2^2 + \dots + q_n^2)^{1/2}$.

Therefore, the covariance (and correlation) function of an isotropic random field depends only on one scalar variable $q = |\mathbf{q}|$. This means that for an isotropic random field in R^n all directions in space are equivalent.

Now we will discuss the implications of the isotropy property on the covariance and spectral density. Recall first the following identity

$$\int_0^\pi e^{iqk \cos \theta} \sin^{n-2} \theta d\theta = \frac{J_{(n-2)/2}(qk)}{(qk)^{(n-2)/2}}, \quad (3.26)$$

where $J_m(x)$ is the Bessel function of the first kind of order m . This function

is defined as follows

$$J_m(x) = \sum_{k=0}^{\infty} (-1)^k \frac{(x/2)^{m+2k}}{k! \Gamma(m+k+1)} \quad (3.27)$$

where $\Gamma(x)$ is the gamma function.

Therefore, we can now formulate the *Bochner theorem for isotropic random fields* (cf. [1], [14]).

A continuous function $K_X(q)$, $0 \leq q < \infty$ is the covariance function of an isotropic random field if and only if it has the representation

$$K_X(q) = A_{n-2} \int_0^{\infty} \frac{J_{(n-2)/2}(qk)}{(qk)^{(n-2)/2}} dG(k) \quad (3.28)$$

where $G(k)$ is a bounded, nondecreasing function of k and the constant A_{n-2} is the total surface area of S_{n-2} – the $(n-2)$ dimensional sphere in R^n .

The representation of $K_X(q)$ in the form (3.28) is called a *spectral representation of an n -dimensional correlation function*.

If the constant A_{n-2} is shown explicitly then equation (3.28) takes the form

$$K_X(q) = 2^{(n-2)/2} \Gamma\left(\frac{n}{2}\right) \int_0^{\infty} \frac{J_{(n-2)/2}(qk)}{(qk)^{(n-2)/2}} dG(k). \quad (3.28a)$$

Now consider the spectral density of an isotropic random field. If the correlation function $K_X(q)$ decreases rapidly enough as $q \rightarrow \infty$ then the isotropic field $X(\mathbf{r})$ will have a spectral density $g_X(k)$ which can be determined from the given correlation function by formula (3.18). However, since $K_X(\mathbf{q})$ depends only on $|\mathbf{q}| = q$ we can perform the integration with respect to angular variables (after transforming to spherical coordinates). As a result we obtain, $g_X(\mathbf{k}) = g_X(k)$, $k = |\mathbf{k}|$ and

$$g_X(k) = \frac{1}{(2\pi)^{n/2}} \int_0^{\infty} \frac{J_{(n-2)/2}(qk)}{(qk)^{(n-2)/2}} q^{n-1} K_X(q) dq. \quad (3.29)$$

The corresponding formula for the correlation function is

$$K_X(q) = (2\pi)^{n/2} \int_0^{\infty} \frac{J_{(n-2)/2}(qk)}{(qk)^{(n-2)/2}} k^{n-1} q_X(k) dk. \quad (3.30)$$

The functions $g_X(k)$ and $K_X(q)$ given above are called the *n -dimensional spectral density* and *n -dimensional correlation function*, respectively.

Remark 2. The reader will notice that, in contrast to the one-dimensional case (stochastic processes), the representation (3.30) of $K_X(q)$ in terms of the spectral density $g_X(k)$ for $n > 1$ includes the additional factor k^{n-1} and a different constant in front of the integral. This is due to the fact that in the multidimensional case

$$G(k) = \int \dots \int_{|\mathbf{k}| < k} dG(\mathbf{k}) = A_n \int_0^k \kappa^{n-1} g_X(\kappa) d\kappa, \quad (3.31)$$

where $A_n = 2(\pi)^{n/2}/\Gamma(n/2)$ is the total area of the unit sphere in R^n .

3.3.2. Special cases. $n = 2$. If a random isotropic field is defined on the plane, that is $\mathbf{r} = (x_1, x_2)$, then in equations (3.28) through (3.30) one should take $n = 2$.

Equations (3.29) and (3.30), that are found frequently in applications, take the form

$$g_X(k) = \frac{1}{2\pi} \int_0^\infty J_0(qk) q K_X(q) dq, \quad (3.32)$$

$$K_X(q) = 2\pi \int_0^\infty J_0(qk) k g_X(k) dk. \quad (3.33)$$

$n = 3$. In many applications random isotropic fields in the three-dimensional space are of interest. In this particular case $\mathbf{r} = (x_1, x_2, x_3)$ and $J_{(n-2)/2}(qk) = J_{1/2}(qk)$ where

$$J_{1/2}(qk) = \left(\frac{2}{\pi x}\right)^{1/2} \sin x.$$

Then we get

$$g_X(k) = \frac{1}{2\pi^2 k} \int_0^\infty \sin(qk) q K_X(q) dq, \quad (3.34)$$

$$K_X(q) = \frac{4\pi}{q} \int_0^\infty \sin(qk) k g_X(k) dk. \quad (3.35)$$

The function $g_X(k)$ must be nonnegative. Therefore, the class of possible correlation functions of isotropic fields (defined in general by representation

(3.28)) is determined by the requirement that the integral (3.29) is nonnegative for all $k \geq 0$. In the particular cases $n = 2, n = 3$, this condition refers to integrals (3.32) and (3.34), respectively.

The 3-dimensional spectral density $g_X(k)$ is a basic characteristic of the isotropic field $X(\mathbf{r})$. However, statistical inference leading to estimation of $g_X(k)$ from observations of $X(\mathbf{r})$ is difficult. Therefore, measurements of $X(\mathbf{r})$ are very often taken at points along some straight line in R^3 , e.g. at the points of the first coordinate axis; i.e. along $X(x_1, 0, 0)$. In this way we obtain a homogeneous random field on the straight line (i.e. a stationary process in the variable x_1 having the correlation function $K_X(q)$, where $q = x_1'' - x_1'$). In particular, defining $K_X(q)$ for $q < 0$ as $K_X(-q) = K_X(q)$ we have

$$g_X(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ikq} K_X(q) dq = \frac{1}{\pi} \int_0^{\infty} \cos(kq) K_X(q) dq, \quad (3.36)$$

$$K_X(q) = \int_{-\infty}^{+\infty} e^{-ikq} g_1(k) dk = 2 \int_0^{\infty} \cos(kq) g_1(k) dk. \quad (3.37)$$

The function $g_1(k)$ is called the *1-dimensional spectral density* (or *1-dimensional spectrum*) of the isotropic field $X(\mathbf{r})$.

It is natural to inquire about the relationship between the 1-dimensional spectrum and the 3-dimensional spectrum $g_X(k)$ of the given isotropic field.

Differentiation of formula (3.36) with respect to k and comparison of the result with (3.34) yields

$$g_X(\mathbf{k}) = g_X(k) = -\frac{1}{2\pi k} \frac{dg_1(k)}{dk}. \quad (3.38)$$

The above relation expresses the 3-dimensional spectral density $g_X(k)$ of the isotropic random field in terms of its 1-dimensional spectral density $g_1(k)$. It is seen that if $g_1(k)$ is non-negative, it does not imply that $g_X(k)$ is non-negative. This observation is a manifestation of the more general fact that a given function $g(k)$ of one variable k can be a spectral density of a homogeneous field on the straight line (of a stochastic process), but it may not be a spectral density of an isotropic field in n -dimensional space. An analogous assertion holds for the correlation functions.

We now consider a few examples of correlation functions and the corresponding spectral densities of isotropic random fields.

1. The exponential correlation

$$K_X(q) = Ce^{-\alpha q}, \quad q = |\mathbf{q}|, \quad \mathbf{q} = \mathbf{r}_1 - \mathbf{r}_2, \quad (3.39)$$

where $C > 0$, $\alpha > 0$, $q \geq 0$.

In the case $n = 1$ the function given by (3.39) is one of the most common examples of a correlation function for stationary processes (where $q = |\tau| = |t_2 - t_1|$). This function is also a correlation function of an isotropic random field in R^n for any integer n .

Using the identity:

$$\int_0^\infty e^{-\alpha x} J_m(kx) x^{m+1} dx = \frac{2\alpha(2k)^m \Gamma(m + 3/2)}{\pi^{1/2}(\alpha^2 + k^2)^{m+3/2}},$$

and equation (3.29) we obtain the n -dimensional spectral density

$$g_X(k) = \frac{C\alpha\Gamma((n + 1)/2)}{\pi^{(n+1)/2}(\alpha^2 + k^2)^{(n+1)/2}}, \tag{3.40}$$

which is nonnegative for any integer n .

For $n = 2$, and $n = 3$ we have

$$g_X(k) = \frac{C\alpha}{2\pi(\alpha^2 + k^2)^{3/2}}, \quad n = 2, \tag{3.41}$$

$$g_X(k) = \frac{C\alpha}{\pi^2(\alpha^2 + k^2)^2}, \quad n = 3. \tag{3.42}$$

The one-dimensional spectral density $g_1(k)$ is

$$g_1(k) = \frac{C\alpha}{\pi^2(\alpha^2 + k^2)}. \tag{3.43}$$

Of course, substituting equation (3.43) into (3.38) yields equation (3.42)

2. The “exponential-Gaussian” correlation

$$K_X(q) = Ce^{-\alpha q^2}, \quad C > 0, \quad \alpha > 0, \quad q \geq 0. \tag{3.44}$$

In order to evaluate the n -dimensional spectral density via equation (3.29) the following equality is used

$$\int_0^\infty e^{\alpha x^2} J_m(kx) x^{m+1} dx = k^m (2x)^{-m-1} \exp(-k^2/4\alpha).$$

The result is

$$g_X(k) = \frac{C}{2^n(\pi\alpha)^{n/2}} \exp(-k^2/4\alpha). \tag{3.45}$$

The above spectral density is everywhere positive for any n and α . It can also be obtained by use of the 1-dimensional spectral density (corresponding to (3.44) and equation (3.38)).

3. The triangular correlation

$$K_X(q) = \begin{cases} C(1 - \alpha q), & q \leq 1/\alpha \\ 0, & q > 1/\alpha \end{cases} \quad (3.46)$$

Using equation (3.36) yields the following (positive) expression for the 1-dimensional spectral density

$$g_1(k) = \frac{4C\alpha \sin^2(k/2\alpha)}{\pi k^2}. \quad (3.47)$$

However, equation (3.38) implies that the 3-dimensional spectral density may also assume negative values. Therefore, (3.46), being a correlation function on the line, cannot be a correlation function of an isotropic random field in R^3 . It can be shown that the function defined in (3.47) cannot be an isotropic correlation function in the plane either.

4. The "damped -oscillatory" correlation

$$K_X(q) = Ce^{-\alpha q} \cos k_0 q, \quad (3.48)$$

where $C > 0$, $\alpha > 0$, $k_0 > 0$, $q \geq 0$. It can be easily shown that the spectral density $g_1(k)$ corresponding to (3.48) is

$$g_1(k) = \frac{C\alpha}{2\pi} \left[\frac{1}{\alpha^2 + (k + k_0)^2} + \frac{1}{\alpha^2 + (k - k_0)^2} \right], \quad (3.49)$$

or, in abbreviated form

$$g_1(k) = \frac{A(k^2 + b^2)}{k^4 + 2ak^2 + b^4},$$

where $A = C\alpha/\pi$, $a = \alpha^2 - k_0^2$, $b = (\alpha^2 + k_0^2)^{1/2}$.

Making use of equation (3.32) and evaluating the two-dimensional spectral density $g_X(k)$ corresponding to the correlation function (3.48) indicates that this $g_X(k)$ is nonnegative only if $\alpha \geq k_0$. Looking more carefully at the behavior of $g_1(k)$ given by (3.49) with respect to k , it can be shown that $g_1(k)$ is monotonically nonincreasing on the positive half-axis $k > 0$ only if $\alpha \geq \sqrt{3}k_0$. Hence, equation (3.38) implies that $g_X(k)$ will be nonnegative only for $\alpha \geq \sqrt{3}k_0$. Therefore, the function given in (3.48) can be a two-dimensional correlation function of an isotropic field only if $\alpha \geq k_0$, and it can be a three-dimensional correlation function only if $\alpha \geq \sqrt{3}k_0$.

3.4. Vector-valued random fields

3.4.1. Basic concepts. In the previous sections we discussed scalar random fields, i.e. fields whose values for each $\mathbf{r} \in D \subseteq R^n$ are one-dimensional random variables. However, in numerous applications there is a need for analyzing vectorial random fields. For example, the velocity field in a turbulent medium and the electromagnetic field propagating in a random medium are modeled as vectorial random fields. The theory of vector random fields (when both the arguments and values are multidimensional) is geometrically more complicated than the theory of scalar-valued random fields. The presentation below should be regarded as only an introduction to more systematic and advanced analysis of vector-valued random fields.

Definition 10: A random field $X(\mathbf{r})$ with vectorial values, that is a field of the form

$$X(\mathbf{r}) = [X_1(\mathbf{r}), X_2(\mathbf{r}), \dots, X_n(\mathbf{r})], \mathbf{r} \in D, \quad (3.50)$$

where $X_i(\mathbf{r})$, $i = 1, 2, \dots, n$ are scalar random fields is called a vector-valued random field defined on the domain $D \subseteq R^n$.

In general $\mathbf{r} = (x_1, x_2, \dots, x_m)$; here we restrict ourselves to the most important case where $\mathbf{r} = (x_1, x_2, x_3)$.

As in the case of a scalar random field a complete probabilistic characterization of a vector random field can be given by its finite-dimensional probability distributions. The simplest characteristics are *mean value vector*:

$$\mathbf{m}_X(\mathbf{r}) = \langle \mathbf{X}(\mathbf{r}) \rangle = [m_{X_1}(\mathbf{r}), \dots, m_{X_n}(\mathbf{r})], \quad (3.51)$$

and the *covariance tensor* $K_X(\mathbf{r}_1, \mathbf{r}_2)$ with elements $K_{ik}(\mathbf{r}_1, \mathbf{r}_2)$

$$K_{ik}(\mathbf{r}_1, \mathbf{r}_2) = \langle [\mathbf{X}_i(\mathbf{r}_1) - m_{X_i}(\mathbf{r}_1)][\mathbf{X}_k(\mathbf{r}_2) - m_{X_k}(\mathbf{r}_2)] \rangle, \quad (3.52)$$

$i, k = 1, 2, \dots, n$. Of course, one can also consider the covariance tensors $K_{ikl}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ or in general, $K_{i_1 i_2 \dots i_n}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n)$.

A vector-valued random field $\mathbf{X}(\mathbf{r})$ is said to be *homogeneous* if

$$\mathbf{m}_X(\mathbf{r}) = \mathbf{m}_X = \text{constant}, \quad K_{ik}(\mathbf{r}_1, \mathbf{r}_2) = K_{ik}(\mathbf{q}), \quad \mathbf{q} = \mathbf{r}_2 - \mathbf{r}_1 \quad (3.53)$$

for all $i, k = 1, 2, \dots, n$ and all possible $\mathbf{r}_1, \mathbf{r}_2$ from the domain of definition of $\mathbf{X}(\mathbf{r})$. In what follows we assume that $\mathbf{m}_X = 0$. Since all the component fields $X_i(\mathbf{r})$, $i = 1, 2, \dots, n$ of the vectorial homogeneous $\mathbf{X}(\mathbf{r})$ are homogeneous scalar fields they have spectral representation of the form (3.13), whereas all the elements $K_{ik}(\mathbf{q})$ of the correlation tensor of the field $\mathbf{X}(\mathbf{r})$ can be represented as

$$K_{ik}(\mathbf{q}) = \int e^{i(\mathbf{q} \cdot \mathbf{k})} dG_{ik}(\mathbf{k}) \quad (3.54)$$

where $G_{ik}(\mathbf{q}) = G_{ik}(k_1, \dots, k_n)$ are the cross-spectral distribution functions of the field $\mathbf{X}(\mathbf{r})$.

3.4.2. Isotropic vector random fields.

a. Definition

Let us now consider the concept of an isotropic vector-valued random field. The simplest possible definition is as follows. The vector field $\mathbf{X}(\mathbf{r})$ is *isotropic* if its mean is constant and all the elements of the correlation matrix $K_{ik}(\mathbf{r}_1, \mathbf{r}_2)$ depend only on the distance $|\mathbf{r}_2 - \mathbf{r}_1|$ between \mathbf{r}_1 and \mathbf{r}_2 , that is

$$K_{ik}(\mathbf{r}_1, \mathbf{r}_2) = K_{ik}(q), \quad q = |\mathbf{r}_2 - \mathbf{r}_1|. \quad (3.55)$$

It is clear that all component fields $X_i(\mathbf{r})$, $i = 1, 2, \dots, n$ of such a field are isotropic scalar fields, and that $X_i(\mathbf{r})$ and $X_j(\mathbf{r})$, $i \neq j$ are jointly isotropic (or, isotropically correlated). The pressure and temperature fields of a turbulent flow are commonly regarded as jointly isotropic.

The concept of isotropy defined above is too restrictive and is not very useful in applications. It is thus necessary to more closely examine the concept of an isotropic vector random field. In the case of an isotropic scalar field, the correlation $\langle X(\mathbf{r}_1)X(\mathbf{r}_2) \rangle$ does not depend on the orientation of the vector $\mathbf{q} = \mathbf{r}_2 - \mathbf{r}_1$. In the case of a vector-valued field the situation is different. Consider, for example, the element $K_{11}(\mathbf{q})$ of the correlation matrix, that is $K_{11}(\mathbf{q}) = \langle X_1(\mathbf{r}_1)X_1(\mathbf{r}_2) \rangle$. It is clear that here $X_1(\mathbf{r}_k)$ is a projection of the vector $X(\mathbf{r}_k)$ on the x_1 axis. Assume that points \mathbf{r}_1 and \mathbf{r}_2 lay along the x_1 axis. In this case $K_{11}(\mathbf{q})$ characterizes the correlation of the longitudinal components (with respect to the vector $\mathbf{q} = \mathbf{r}_2 - \mathbf{r}_1$) of the vector \mathbf{X} . Now perform a 90° rotation of \mathbf{q} about the point \mathbf{r}_1 so that the vector $\mathbf{r}_2 - \mathbf{r}_1$ will be parallel to the x_2 axis. In this case $X_1(\mathbf{r}_1)$ and $X_1(\mathbf{r}_2)$ are still the projections of the vector \mathbf{X} on the x_1 axis, however the vector \mathbf{q} is now perpendicular to the x_1 axis and therefore $K_{11}(\mathbf{q})$ characterizes the correlation of the transverse components (with respect to \mathbf{q}) of the vector \mathbf{X} . Hence, it is clear that if we wish to have an applicable concept of isotropy we should not require equality of $K_{11}(\mathbf{q})$ in these two cases, since the mutual position (with respect to \mathbf{q}) of the components $X_1(\mathbf{r}_1)$ and $X_1(\mathbf{r}_2)$ of the vector field has changed.

The above reasoning indicates that in an isotropic vector random field each element $K_{ik}(\mathbf{q})$ of the correlation tensor should depend on the direction of the vector \mathbf{q} . Isotropy of a random vector field consists in the invariance of the probabilistic characteristics of the field $X(\mathbf{r})$ whose components are

specified in the coordinate system rigidly connected with the observation points \mathbf{r}_i . A more rigorous definition follows.

A vector-valued random field $X(\mathbf{r})$ is called an *isotropic field* if the probabilistic characteristics (probability distributions, or, in a broad sense, the elements of the correlation tensor) of the field for any fixed collection of points $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$ are invariant under arbitrary parallel translations, rotations and reflections of these points performed simultaneously with translation, rotation and reflection of the coordinate system with respect to which the components of the field $X(\mathbf{r})$ are specified.

Notice that since an isotropic vector field is homogeneous, its mean $\langle \mathbf{X}(\mathbf{r}) \rangle = \mathbf{m}$ is a constant vector. However, due to isotropy this vector should be invariant under all possible rotations; therefore, it must be a zero vector.

b. General form of correlation tensor

An important problem is concerned with the general form of the correlation tensor of vector isotropic random fields. In what follows we shall briefly discuss this problem (cf. [15] and also [1]).

The function $K_{ik}(\mathbf{q})$ is a tensor function of the vector \mathbf{q} , which is invariant under all rotation and reflection transformations. In this case, for arbitrary unit vectors \mathbf{a} and \mathbf{b} , the quadratic form

$$K(\mathbf{q}, \mathbf{a}, \mathbf{b}) = K_{ik}(\mathbf{q})a_ib_k \quad (3.56)$$

is a scalar depending on three vectors $(\mathbf{q}, \mathbf{a}, \mathbf{b})$ and dependence on \mathbf{a} and \mathbf{b} is linear. Using the results of group invariant theory we conclude that the scalar K can be expressed in terms of the basic invariants of the vectors $\mathbf{q}, \mathbf{a}, \mathbf{b}$, that is by and the scalar products $(\mathbf{q} \cdot \mathbf{a}) = q_ia_i$, $(\mathbf{q} \cdot \mathbf{b}) = q_ib_i$ and $(\mathbf{a} \cdot \mathbf{b}) = a_ib_i$ and (note that $|\mathbf{a}| = |\mathbf{b}| = 1$). Therefore, the general form of the function $K(\mathbf{q}, \mathbf{a}, \mathbf{b})$ which depends linearly on \mathbf{a} and \mathbf{b} is

$$K(\mathbf{q}, \mathbf{a}, \mathbf{b}) = A_1(q)q_ia_iq_kb_k + A_2(q)a_ib_i. \quad (3.57)$$

This means that *the general form of the correlation tensor of an isotropic vector random field* is

$$K_{ik}(\mathbf{q}) = A_1(q)q_ik + A_2(q)\delta_{ik}, \quad (3.58)$$

where $A_1(q)$ and $A_2(q)$ are real-valued functions of the scalar argument $q = |\mathbf{q}|$ and δ_{ik} is the unit, Kronecker's tensor.

In the general case a tensor of second order has nine independent components, and a symmetric tensor six components. Equation (3.58) shows that

the conditions of isotropy reduce the number of components of the correlation tensor to two independent components. This is very important for application of the theory.

Now direct the x_3 axis of the basic coordinate system along the vector \mathbf{q} , taken to be of unit length. In this case the components of \mathbf{q} are $[0, 0, 1]$. Taking the indices in equation (3.58) equal to 1, 1; 2, 2; or 3, 3 we obtain

$$K_{11} = K_{22} = A_2, \quad K_{33} = A_1 + A_2.$$

Hence, the transverse components K_{11} , K_{22} are the same. Denote them by $K_N(q)$, i.e. $K_N(q) = K_{11}(q) = K_{22}(q)$. The longitudinal component $K_L(q)$ is equal to $A_1(q) + A_2(q)$. So equation (3.58) takes the form

$$K_{ik}(q) = [K_L(q) - K_N(q)]n_i n_k + K_N(q)\delta_{ik}, \quad (3.59)$$

where n_i are the components of the unit vector \mathbf{q}/q , and

$$K_L(q) = \langle X_L(\mathbf{r})X_L(\mathbf{r}') \rangle, \quad (3.60)$$

$$K_N(q) = \langle X_N(\mathbf{r})X_N(\mathbf{r}') \rangle, \quad (3.61)$$

and X_L , X_N , are the projections of the vector \mathbf{X} onto a line along the direction of the vector \mathbf{q} and on any line perpendicular to \mathbf{q} , respectively.

The function $K_L(q)$ is called a *longitudinal correlation function* of the isotropic vector field $X(\mathbf{r})$, whereas $K_N(q)$ is called its *transversal correlation function*. These two functions specify uniquely the correlation tensor $K_{ik}(\mathbf{q})$.

According to equation (3.59) the correlation tensor $K_{ik}(\mathbf{q})$ is specified if functions $K_L(q)$ and $K_N(q)$ are given. Since each of these functions is the correlation function of a homogeneous random field on a straight line ($K_L(q)$ on the line: $x_1 = x_2 = 0$ and $K_N(q)$ on any line in the plane $x_3 = 0$) they are both of non-negative definite type and can be characterized by their spectral measures (longitudinal $G_L(q)$ and transversal $G_N(q)$, respectively). If the functions $K_L(q)$ and $K_N(q)$ decrease rapidly enough as $q \rightarrow \infty$, then the spectral distributions $G_L(q)$ and $G_N(q)$ can be characterized by their spectral densities.

The results concerning isotropic vector random fields presented above simplify in situations when we know *a priori* that the field under consideration is *solenoidal* (its divergence vanishes) or *potential* (it is a gradient of a scalar isotropic field). For such specific fields there exist simple relationships between longitudinal and transversal correlation functions and as a result the correlation tensor $K_{ik}(\mathbf{q})$ is determined by only one scalar function.

Consider first a homogeneous vector random field which is *solenoidal*, i.e.

$$\operatorname{div} \mathbf{X}(\mathbf{r}) = \sum_{i=1}^n \frac{\partial X_i(\mathbf{r})}{\partial x_i} \equiv \frac{\partial X_i(\mathbf{r})}{\partial x_i} = 0, \quad (3.62)$$

where $\mathbf{r} = (x_1, x_2, x_3)$ and in the last equality the summation convention is used which means that a repeated index implies summation over the range of the index. By definition, the components of the correlation tensor of $\mathbf{X}(\mathbf{t})$ with zero mean are

$$K_{ik}(\mathbf{r}_2 - \mathbf{r}_1) = \langle X_i(\mathbf{r}_2)X_k(\mathbf{r}_1) \rangle. \quad (3.63)$$

Differentiation of (3.63) with respect to the coordinates of $\mathbf{r}_2 = (x_{2,1}, x_{2,2}, x_{2,3})$ and subsequent summation over the indices $i, j = 1, 2, 3$ accounting for (3.62) yields

$$\frac{\partial K_{ik}(\mathbf{r}_2 - \mathbf{r}_1)}{\partial x_{2,i}} = \left\langle \frac{\partial X_i(\mathbf{r}_2)}{\partial x_{2,i}} X_k(\mathbf{r}_1) \right\rangle = 0. \quad (3.64)$$

Since differentiation of K_{ik} with respect to the coordinates of \mathbf{r}_2 is equivalent to differentiation with respect to $\mathbf{q} = \mathbf{r}_2 - \mathbf{r}_1$, the correlation tensor of a homogeneous solenoidal vector random field satisfies the conditions

$$\frac{\partial K_{ik}(\mathbf{q})}{\partial x_i} = 0, \quad \frac{\partial K_{ik}(\mathbf{q})}{\partial x_k} = 0. \quad (3.65)$$

If the field $\mathbf{X}(\mathbf{r})$ is isotropic, the components of the correlation tensor are represented by equation (3.59) where $q = |\mathbf{q}| = |\mathbf{r}_2 - \mathbf{r}_1|$. Substitution of (3.59) into (3.65) and making use of the following relations

$$\begin{aligned} \frac{\partial q}{\partial x_i} &= \frac{\partial}{\partial x_i} \sqrt{x_1^2 + x_2^2 + x_3^2} = \frac{x_i}{q} = n_i, \\ \frac{\partial n_k}{\partial x_i} &= \frac{\partial}{\partial x_i} \left(\frac{x_i}{q} \right) = \frac{\delta_{ik}q - x_k n_i}{q^2} = \frac{\delta_{ik} - n_i n_k}{q}, \\ \frac{\partial n_i}{\partial x_i} &= \frac{\delta_{ii} - n_i n_i}{q} = \frac{2}{q}, \quad n_i \frac{\partial n_k}{\partial x_i} = 0, \end{aligned} \quad (3.66)$$

(where $\delta_{ii} = 3$ and $n_i^2 = 1$), yields the equation

$$\frac{dK_L}{dq} n_k + (K_L - K_N) \frac{2}{q} n_k = 0, \quad (3.67)$$

which can be represented in either of two equivalent forms:

$$\begin{aligned} K_N(q) &= K_L(q) + \frac{q}{2} \frac{d}{dq} K_L(q) \\ &= \frac{1}{2q} \frac{d}{dq} [q^2 K_L(q)]. \end{aligned} \quad (3.68)$$

The above relation between $K_N(q)$ and $K_L(q)$ is known in statistical turbulence theory as the *Karman equation*. An analogous relationship holds for

the longitudinal and transverse spectral densities of the solenoidal random field.

Assume now that $\mathbf{X}(\mathbf{r})$ is a *potential* homogeneous random field, i.e. its components are of the form

$$X_k(\mathbf{r}) = \frac{\partial A(\mathbf{r})}{\partial x_k}, \quad (3.69)$$

where $A(\mathbf{r})$ is a scalar random field with zero mean and correlation function

$$K_A(\mathbf{r}_2 - \mathbf{r}_1) = \langle A(\mathbf{r}_2)A(\mathbf{r}_1) \rangle. \quad (3.70)$$

Differentiation of the above function with respect to the coordinates of \mathbf{r}_1 and \mathbf{r}_2 gives

$$\begin{aligned} K_{ik}(\mathbf{q}) &= \langle X_i(\mathbf{r}_2)X_k(\mathbf{r}_1) \rangle \left\langle \frac{\partial A(\mathbf{r}_2)}{\partial x_{2,i}} \frac{\partial A(\mathbf{r}_1)}{\partial x_{1,k}} \right\rangle \\ &= \frac{\partial^2 K_A(\mathbf{r}_2 - \mathbf{r}_1)}{\partial x_{2,i} \partial x_{1,k}} = -\frac{\partial^2 K_A(q)}{\partial x_i \partial x_k}. \end{aligned} \quad (3.71)$$

Performing the differentiation of $K_A(q)$ as indicated in (3.71) with use of the relations (3.66) we obtain

$$K_{ik}(q) = - \left[\frac{d^2 K_A(q)}{dq^2} - \frac{1}{q} \frac{dK_A(q)}{dq} \right] n_i n_k - \frac{1}{q} \frac{dK_A(q)}{dq} \delta_{ik}. \quad (3.72)$$

Comparison of the above expression for $K_{ik}(q)$ with the general representation (3.59) of the correlation tensor of an isotropic field yields the following relationship between the longitudinal and transverse components of a potential isotropic random field

$$K_L(q) = \frac{d}{dq} [qK_N(q)]. \quad (3.73)$$

The above equation is associated with the names of Obukhov and Yaglom.

3.5. Tensor-valued random fields

In the investigation of solid media the need for analysis using tensor random fields often arises. For example, if a deformable solid is subjected to a random load, or if such a solid has randomly varying properties then the stress tensor σ_{ij} should be regarded as a tensor random field $\sigma_{ij}(\mathbf{r}, \gamma)$. Such random fields can be analyzed along the same lines as shown in the previous section for vector random fields but, as one might expect, the analysis and the associated mathematical transformations are much more complicated.

Definition 11: A random field $\mathbf{T}(\mathbf{r})$, $\mathbf{r} \in D \subseteq R^3$ with tensorial values (of the second rank), that is a field of the form

$$\mathbf{T}(\mathbf{r}, \gamma) = \{T_{ij}(\mathbf{r}, \gamma)\}, \quad \mathbf{r} \in D, \quad \gamma \in \Gamma, \quad i, j = 1, 2, 3, \quad (3.74)$$

where $T_{ij}(\mathbf{r}, \gamma)$ for each (i, j) are scalar random fields is called a tensor-valued random field defined on the domain $D \subseteq R^3$. We assume here that such objects which obey all the usual transformation rules required by the definition of a second-order or second-rank tensor.

A complete probabilistic characterization of a random tensor field $\mathbf{T}(\mathbf{r}, \gamma)$ is given if for each finite set of \mathbf{r} -values, say $\{\mathbf{r}_1, \dots, \mathbf{r}_k\}$, $k = 1, 2, \dots, n$, joint $N \cdot k$ -dimensional probability distributions of the random variables $T_{ij}(\mathbf{r}, \gamma)$ are specified, where N denotes the number of elements of the tensor $\mathbf{T}(\mathbf{r}, \gamma)$. For an unsymmetric, second-order tensor $N = 9$, and for a symmetric, second order tensor (i.e. when $T_{ij} = T_{ji}$) $N = 6$.

As in all previous situations (scalar and vector fields) the simplest characteristic of the tensor random field $\mathbf{T}(\mathbf{r})$ is its mean value $\langle \mathbf{T}(\mathbf{r}) \rangle$, or in terms of components, $\langle T_{ij}(\mathbf{r}) \rangle = m_{ij}(\mathbf{r})$, $i, j = 1, 2, 3$. Define the fluctuation of $\mathbf{T}(\mathbf{r})$ as

$$\begin{aligned} \Theta(\mathbf{r}) &= \mathbf{T}(\mathbf{r}) - \langle \mathbf{T}(\mathbf{r}) \rangle, \\ \theta_{ij}(\mathbf{r}) &= T_{ij}(\mathbf{r}) - m_{ij}(\mathbf{r}). \end{aligned} \quad (3.75)$$

An important characteristic of the tensor random field $\mathbf{T}(\mathbf{r})$ is its n -point moment function:

$$m_{i_1 j_1 \dots i_n j_n}^{\mathbf{T}}(\mathbf{r}_1, \dots, \mathbf{r}_n) = \langle \theta_{i_1 j_1}(\mathbf{r}_1) \cdot \dots \cdot \theta_{i_n j_n}(\mathbf{r}_n) \rangle. \quad (3.76)$$

The moment defined in (3.76) is a tensor-valued function of $3n$ independent variables x_s^k , $s = 1, 2, 3$; $k = 1, 2, 3$. Another basic characteristic of a tensor-valued random field $\mathbf{T}(\mathbf{r})$ is its correlation tensor:

$$K_{ijkl}(\mathbf{r}_1, \mathbf{r}_2) = \langle \theta_{ij}(\mathbf{r}_1) \theta_{kl}(\mathbf{r}_2) \rangle. \quad (3.77)$$

If the tensor field $\mathbf{T}(\mathbf{r})$ has symmetric components, then $\theta_{ij} = \theta_{ji}$, and

$$K_{ijkl} = K_{jikl} = K_{ijlk} = K_{jilk}. \quad (3.78)$$

We will now consider homogenous tensor fields.

Definition 12: A random tensor field $\mathbf{T}(\mathbf{r})$ is said to be strictly homogeneous in R^3 if for any finite set of points $\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k\}$ belonging to R^3 and for any vector $\mathbf{q} \in R^3$ all the joint probability distributions of $T_{ij}(\mathbf{r})$ are invariant under the shift transformations

$$\mathbf{r}_i^1 = \mathbf{r}_i + \mathbf{q}, \quad i = 1, 2, \dots, k. \quad (3.79)$$

The above definition implies that the finite dimensional probability distributions of a strictly homogeneous tensor field depend only on the relative location of the points \mathbf{r}_k , $k = 1, 2, \dots, n$, to each other but they do *not* depend on the absolute location of these points in space. The moment functions (3.76) depend in this case on $(n - 1)$ vectors which define the spatial configuration of points \mathbf{r}_k . Definition 12 also implies that:

$$\langle \mathbf{T}(\mathbf{r}, \gamma) \rangle = \mathbf{m}(\mathbf{r}) \equiv \{m_{ij}(\mathbf{r})\} = \text{constant}, \quad (3.80)$$

$$K_{ijkl}(\mathbf{r}_1, \mathbf{r}_2) = K_{ijkl}(\mathbf{q}), \quad \mathbf{q} = \mathbf{r}_2 - \mathbf{r}_1, \quad (3.81)$$

where $\mathbf{q} = (q_1, q_2, q_3)$.

Random tensor fields satisfying the invariance conditions (3.80), (3.81) are called *weakly homogeneous tensor fields*, and like weakly homogeneous vector fields, are of prime interest. A weakly homogeneous random tensor field is characterized by six constants m_{ij} and eighty-one functions K_{ijkl} of three variables (q_1, q_2, q_3) . In the case when the tensor \mathbf{T} is symmetric and the relations (3.78) hold, the number of functions $K_{ijkl}(q_1, q_2, q_3)$ reduces to twenty-one. In addition, it can be shown that

$$K_{ijkl}(\mathbf{q}) = K_{ijkl}(q_1, q_2, q_3) = K_{ijkl}(-q_1, -q_2, -q_3). \quad (3.82)$$

Definition 13: A random tensor field $\mathbf{T}(\mathbf{r}) \equiv \{T_{ij}(\mathbf{r})\}$ is isotropic in a narrow sense if it is strictly homogeneous and all its finite-dimensional distributions (in the coordinate system rigidly connected with the points $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k$) are invariant under rotations and reflections of the configuration of points $\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k\}$.

Isotropy restricts the class of tensor random fields as potential models of real physical fields, however it allows a more effective representation of the correlation tensor $K_{ijkl}(\mathbf{q})$. If the field $\mathbf{T}(\mathbf{r})$ is isotropic and, in addition, it has symmetric components satisfying (3.78), (3.82) yields the following representation (cf. [16]) holds

$$\begin{aligned} K_{ijkl}(\mathbf{q}) = & a_1 \delta_{ij} \delta_{kl} + a_2 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \\ & + a_3 (q_j q_k \delta_{ij} + q_i q_l \delta_{jk} + q_i q_k \delta_{jl} + q_j q_l \delta_{ik}) \\ & + a_4 (q_i q_j \delta_{kl} + q_k q_l \delta_{ij}) + a_5 q_i q_j q_k q_l \end{aligned} \quad (3.83)$$

where $a_i = a_i(\mathbf{q})$, $i = 1, 2, \dots, 5$, $q^2 = q_j q_j$, and δ_{ik} is the unit, second-rank Kronecker tensor.

Analogous to the meaning of longitudinal and transverse components K_L and K_N of isotropic vector fields, the functions $a_i(q)$ here characterize the components of the correlation tensor K_{ijkl} in specified directions. To see this,

define a coordinate system with the center at point \mathbf{r}_1 and with the axis x_1 directed to the point \mathbf{r}_2 and denote the components of K_{ijkl} in this system by K_{ijkl}^1 and taking $K_1 = K_{1111}^1$, $K_2 = K_{2222}^1$, $K_3 = K_{1122}^1$, $K_4 = K_{2233}^1$, $K_5 = K_{1212}^1$, $K_6 = K_{2323}^1$ we obtain from (3.83)

$$\begin{aligned} K_1 &= a_1 + 2a_2 + 2q^2(2a_3 + a_4) + q^4 a_5, \\ K_2 &= a_1 + 2a_2, \quad K_3 = a_1 + a_4 q^2, \quad K_4 = a_1, \\ K_5 &= a_2 + a_3 q^2, \quad K_6 = a_2. \end{aligned} \quad (3.84)$$

Additionally we have the relation

$$K_4 + 2K_6 - K_2 = 0. \quad (3.85)$$

Solving the above system of equations for the a_i and then substituting the results into (3.83) with $q_i/q = n_i$ we obtain the representation:

$$\begin{aligned} K_{ijkl}(\mathbf{q}) &= K_4(q)\delta_{ij}\delta_{kl} + K_6(q)[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] \\ &+ [K_5(q) - K_6(q)][n_j n_k \delta_{il} + n_i n_l \delta_{il} + n_i n_k \delta_{jl} + n_j n_l \delta_{ik}] \\ &+ [K_3(q) - K_4(q)][n_i n_j \delta_{kl} + n_k n_l \delta_{ij}] \\ &+ [K_1(q) + K_2(q) - 2K_3(q) - 4K_5(q)]n_i n_j n_k n_l. \end{aligned} \quad (3.86)$$

Equation (3.86) can be regarded as the counterpart of the (3.59) for isotropic vector fields.

4. Reconstruction of probability distribution of polycrystalline microstructures

4.1. Statistical physics of Voronoi tessellations

According to the spirit of classical statistical physics the phase probability density should be selected in such a way that it “agrees” with external conditions of the system and empirical macroscopic information. A key role is played by the Gibbsian statistical ensembles. Each element of such an ensemble “contributes” to realization of a required macrostate. For example, for the canonical ensemble (closed system with fixed N and V , exchanging the energy) the probability density of microscopic states is given by the following canonical Gibbs distribution

$$f(\mathbf{p}, \mathbf{q}) = \frac{1}{Q(\theta, V, N)} \exp\left(-\frac{E(\mathbf{p}, \mathbf{q})}{\theta}\right), \quad (4.1)$$

where θ is a parameter playing a role of temperature and Q , the statistical integral, is determined from the normalization condition for $f(\mathbf{p}, \mathbf{q})$. It is

interesting that the canonical distribution (4.1) can be obtained from maximization of the Shannon/Gibbs entropy under constraints representing the available information in the form of average energy of the system considered (θ is then the inverse of the Lagrange multiplier associated with the constraint of mean energy). This observation indicates how the underlying probability distributions of microscopic states can be constructed from "macroscopic" data. It is, therefore, tempting to extend this fruitful idea to more complex systems, such as random material microstructures.

Various possible configurations of random tessellation aggregates are characterized by a number of parameters (topological and metric) of the constituent polyhedral. These parameters (positive real numbers) denoted symbolically as $(X_1, X_2, \dots, X_k) \equiv \mathbf{X}$ define a *microstate* of the system. The *macrostates* (or *mesostates*) are characterized by appropriate averaged values over microscopic states (and the correlations between them), which are integrals over the probability distribution of microscopic states. According to the spirit of classical statistical mechanics these averages, regarded as observables, will be used here as a prior information (constraints) on unknown probability distribution of microstates. Miles (cf. [19]) distinguishes seven quantities being the fundamental variables of random polyhedral tessellations; namely $X_1 = C$ - the number of corners (vertices), $X_2 = E$ - the number of edges, $X_3 = F$ - the number of faces (topological characteristics) and $X_4 = L$ - the total edge length, $X_5 = M$ - the length of orthogonal projection of a polyhedron onto an isotropic random line, X_6 - the polyhedron area, X_7 - the polyhedron volume (metric characteristics).

Topological randomness of the aggregate means that (X_1, X_2, X_3) are random variables satisfying self-consistency relations. These variables are related to each other by the Euler formula

$$C - E + F = 2, \quad (4.2)$$

for one isolated polyhedron, and for any subdivision of a domain into a finite number of polyhedrals (Moller [20])

$$C - E + F + N = 1, \quad (4.3)$$

where N is a number of polyhedrals (grains) in an aggregate; the above is valid irrespective of the number of edges connected at each corner (vertex).

However, since the coordination number of the polyhedral aggregate $Z = 4$, i.e. four edges meet at each corner (vertex) and each edge connects two vertices, we have $C = 2(E/4)$, or $E = 2C$. Therefore, the topological shape state (X_1, X_2, X_3) is fully specified by only one characteristic, which is commonly taken as being the number of faces F . Metric characteristics

(X_4, \dots, X_7) are independent of topological properties, and the grain volume V is regarded as the most informative one.

4.2. Probability distribution of “sidedness” of grains

As we have shown in the previous section, the main characteristic of a random polyhedral aggregate is the sidedness of a randomly selected polyhedron, i.e. the number of its faces F . The problem concerns a possible probability distribution of F , which is a discrete random variable taking on the integer values k , where $k = 4, 5, \dots, K$ where K is the largest possible number of faces per grain in real grain aggregates. The probability distribution of interest is

$$\{P\} = \{p_4, \dots, p_K\}, \quad p_k \geq 0, \quad \sum_k p_k = 1, \quad (4.4)$$

where $p_k = P(F = k)$. The distribution $\{P\}$ defines a distribution of the microscopic shape states.

Let us assume that given data concerning the aggregate are in the form of average value of m functions $G_r(k)$ ($r = 1, 2, \dots, m$; $m < K - 3$) defined on the shape states $\{k\}$, that is

$$g_r \equiv \langle G_r(k) \rangle = \sum_{k=4}^K G_k p_k, \quad r = 1, 2, \dots, m. \quad (4.5)$$

The values of $G_r(k)$ for various shapes k can characterize the appropriate physical/mechanical observables (e.g. Young modulus, hardness, etc); analogously to the energy in statistical physics, the quantities G_r depends on the microstates $\{k\}$.

It is clear that information about the distribution $P = \{p_4, \dots, p_K\}$ contained in (4.4) and (4.5) is not sufficient to determine P exactly. In this situation we ask: *which of many possible distributions satisfying (4.4), (4.5) is best suited to describe P ?* This is a problem of reconstructing P on the basis of incomplete information. According to the spirit of classical statistical mechanics (Gibbsian ensembles) and the maximum entropy principle, the “most rational” approximation P^* of P which satisfies (4.4) and (4.5) is that one which maximizes the Shannon/Gibbs entropy. The variational method of Lagrange multipliers gives the result

$$P^* = \{p_k^*\} = \frac{1}{Z(\lambda)} \exp(-\lambda \mathbf{G}_k), \quad k = 4, 5, \dots, K, \quad (4.6)$$

where $\lambda = [\lambda_1, \dots, \lambda_m]$, $\mathbf{G}(k) = [G_1(k), \dots, G_m(k)]$, $\lambda \mathbf{G}_k = \lambda_1 G_1(k) + \dots$

$+\lambda_m G_m(k),$

$$Z(\lambda) = \sum_k \exp(-\lambda \mathbf{G}(k)). \quad (4.7)$$

The unknown Lagrange multipliers λ_r , $r = 1, \dots, m$ are determined by substitution of (4.6) into constraints (4.5), (4.4). This yields the following system of m equations

$$g_r \equiv \langle G_r \rangle = -\frac{\partial}{\partial \lambda_r} \ln Z(\lambda), \quad r = 1, \dots, m. \quad (4.8)$$

It is generally accepted on the basis of empirical studies (cf. Kumar et al. [21]) that in real metallic and ceramic materials the number of faces F of polyhedral grains varies from $F = 4$ to 36, i.e. $K = 36$, whereas the mean of F is around 14–15. On the other hand, the analysis within stochastic geometry has given for the Poisson–Voronoi tessellations (cf. Miles [19])

$$\langle F \rangle = \bar{k} = 2 + \frac{48\pi}{35} = 15.5355. \quad (4.9)$$

It is clear that our “canonical” shape distribution depends on the form of given data (since it has been constructed to be consistent with observables). If the data $G_r(k)$ are such that $r = 1, 2$ and $G_1(k) = k$, $G_2(k) = k^2$ then

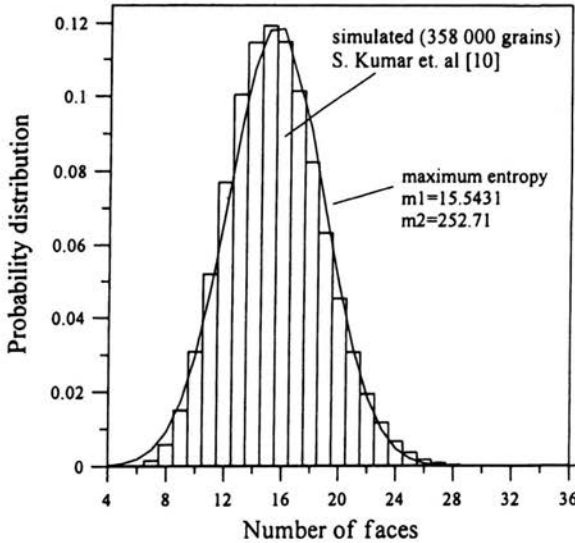


FIGURE 6. Probability distribution of the number of faces in spatial P-V tessellation.

$g_1 = \langle k \rangle$, $g_2 = \langle k^2 \rangle$. In this case the shape distribution (4.6) is

$$P^* = \{p_k^*\} = \frac{1}{Z(\lambda_1, \lambda_2)} \exp(-\lambda_1 k - \lambda_2 k^2), \quad k = 4, \dots, K. \quad (4.10)$$

Figure 6 shows distribution (4.10) for given $g_1 = 15.5431$ and $g_2 = 252.71$ and its comparison with simulations of P-V tessellations by Kumar et al. [21]. If $r = 1, 2$ and $G_1(k) = k$, $G_2(k) = \ln k$ then $g_1 = \langle k \rangle$, $g_2 = \langle \ln k \rangle$, the shape distribution (4.6) is a “discretized” gamma distribution with parameters $a = 1/\lambda_1$, $b = 1 - \lambda_2$.

4.3. Probability distribution of grain volume

Among the metric characteristics of grains in microstructural polyhedral aggregate the grain volume V is the most basic one. For example, the size of a regular polyhedral grain has been often characterized via the equivalent spherical diameter defined as

$$D_V = \left(\frac{6V}{\pi} \right)^{1/3}, \quad (4.11)$$

where V is the actual volume of the grain. Having characterized the variability of V we can quantify (more properly than via stereological formulae) the grain size. The grain size of a polycrystalline solids has an important effect on its properties. The so called grain-size effect is commonly known. Many properties of materials such as the yield stress, ductility, hardness and fatigue limit show very pronounced and simple dependence on the grain size, namely (grain size) $^{-1/2}$, cf. [4] and references therein.

Let us assume, in general, that V is a continuous random variable and our available information about V is in the form of given few moments $\langle V^r \rangle$, $r = 1, 2, \dots, R$. For some specific models the mean value and variance of V has been derived; however, to date no closed-form representation has been found for the probability distribution of V . This can be obtained by using the maximum entropy principle. Like in classical statistical mechanics this principle allows one to make unbiased estimate on the probability distribution of microscopic metric (here, volume) characteristic of our system when only certain averaged observables are known. Therefore, we are looking for the probability density $f(v)$ of the random polyhedral grain V which satisfies

the moment constraints and the normalization condition, i.e.,

$$\int_0^{\infty} v^r f(v) dv = m_r, \quad r = 1, 2, \dots, R, \quad (4.12)$$

$$\int_0^{\infty} f(v) dv = 1,$$

and maximizes entropy functional

$$H(f) = - \int f(v) \ln f(v) dv. \quad (4.13)$$

The result is

$$f^*(v) = C \exp \left(- \sum_{r=1}^R \lambda_r v^r \right), \quad (4.14)$$

where λ_r , the Lagrange multipliers, and constant C are determined from the system of algebraic equations resulting from substitution of (4.14) into constraints (4.12). It has been shown (Gilbert [22]) that for P-V tessellation generated by the Poisson point field with intensity ρ we get

$$\begin{aligned} m_1 &= \langle V \rangle = \rho^{-1}, \\ m_2 &= \langle V^2 \rangle = 1.180 \rho^{-2}. \end{aligned} \quad (4.15)$$

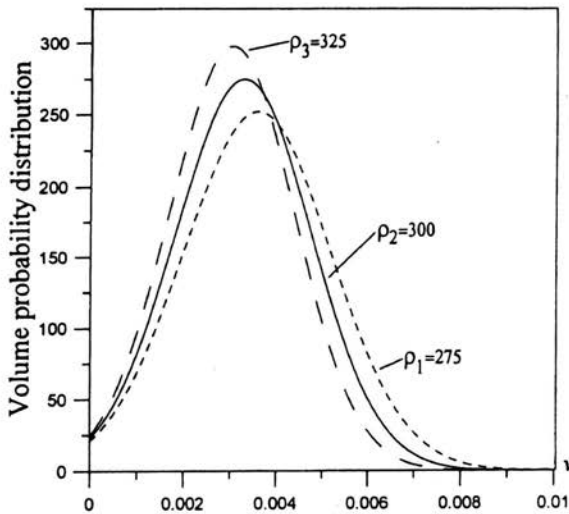


FIGURE 7. The maximum entropy probability density of grain volume obtained for two first moments given and for different values of intensity of Poisson points.

Therefore, the most probable probability distribution satisfying (4.12) takes the form of the truncated normal distribution

$$f^*(v) = C(\lambda_1, \lambda_2) \exp(-\lambda_1 v - \lambda_2 v^2), \quad v, \lambda_2 \geq 0 \quad (4.16)$$

5. Closing remarks

Once the morphology and properties of a random microheterogeneous medium are described and its basic morphological parameters estimated, various physical phenomena taking place in it can then be investigated. The physical phenomena can be, for example, diffusion type processes, deformation due to mechanical forces and damage evolution, wave propagation, and so forth. Very often the physical phenomenon under consideration is governed by partial differential equations with coefficients which include the appropriate random fields. In the last decades a significant amount of attention has been devoted to the determination of the properties of solution of such stochastic differential equations (cf. [13, 17, 18]).

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