Probabilistic Engineering Mechanics 18 (2003) 139–149

PROBABILISTIC ENGINEERING MECHANICS

www.elsevier.com/locate/probengmech

Statistics of inhomogeneous media formed by nucleation and growth

M.T. Todinov

Reliability Engineering and Risk Management Centre, Building 56b, School of Industrial and Manufacturing Science, Cranfield University, Cranfield MK43 0AL, UK

Abstract

Important statistical properties of inhomogeneous microstructures formed by nucleation and growth are established using line transects. A fundamental time-dependent equation has been derived for the probability of sampling only matrix phase by a random line transect in a system containing growing Poisson-distributed spherical nuclei.

It is established that the probability of sampling matrix phase only measures simultaneously the product of two fundamental characteristics of inhomogeneity: the volume fraction of the matrix phase and the probability of existence in the matrix of a free path of specified minimum length. Increasing the number density of the nuclei and decreasing the size of the mean projection of the nuclei on a plane perpendicular to the line transect by the same factor does not change the mean and the variance of the free paths.

It is also demonstrated that the distribution of the intercepts from the weaker phase is an important indicator regarding the risk of poor properties. Accordingly, a new approach is suggested for setting MFFOP reliability requirements which minimise the risk from premature fracture.

Keywords: Statistics; Structure; Properties; Reliability; Inhomogeneous materials; Line transects; Strength distribution; MFFOP reliability requirements

1. Introduction

A common framework for predicting structural/mechanical reliability at a component level is the load–strength (demand–capacity) interference [1–3] which deals with the interaction of the upper tail of the load distribution with the lower tail of the strength distribution.

The strength variation is a complex function of the material properties, the design configuration and geometry. A long and thick lower tail in the material property distribution usually yields a long and thick lower tail of the strength distribution, which results in low reliability.

The variability of the material properties is often attributable to inhomogeneity of the microstructure [1]. The influence of the microstructural inhomogeneity is particularly strong for fracture properties as compared to other properties (e.g. the material's moduli) for which a smoothing effect appears. The reason, as pointed out in Ref. [4] is that the fracture criteria are particularly sensitive to microstructural heterogeneities which lead to local zones of weak resistance to crack extension. Often ahead of crack fronts in com7posite materials or in materials containing defects, the number density of the defects varies locally which is another manifestation of microstructural inhomogeneity. Depending on the microstructural constituents or the local number density of the defects ahead of the crack front, the local fracture toughness varies widely. As a result, the uncertainty (variability) of properties associated with inhomogeneous structures is intrinsic. It is not due for example to a measurement imprecision or inability to control the experiment and therefore cannot be reduced or eliminated.

The statistics of structure and properties of inhomogeneous materials is an interplay of Materials science and Applied statistics. The intersections defined by the key words 'statistics', 'structure' and 'properties', determine key research directions: 'statistics and structure', 'statistics and properties' and 'structure and properties'. An important topic from the research direction 'statistics and structure' is the spatial statistics of duplex structures in which only two structural components are present. For the purposes of investigating the average extension of the inhomogeneities the method of the two-point correlation functions was introduced in Ref. [5]. Further development of this technique (n-point correlation functions) for investigating disordered two-phase media can be found in Ref. [6].

An alternative powerful method of investigating inhomogeneous structures is based on random transects (point,

E-mail address: m.t.todinov@cranfield.ac.uk (M.T. Todinov).

0266-8920/03/$ - see front matter © 2003 Published by Elsevier Science Ltd.
PII: S0266-8920(02)00055-3

linear and areal). These have widely been used in the quantitative microscopy for estimating the volume fraction and surface area of various microstructural constituents [7–12]. In Refs. [13–16] a Monte Carlo simulation technique has been employed for collecting statistical information from inhomogeneous microstructures through sampling microstructural images by random line transects. A line transect (Fig. 1) is a segment AB of given length L cast in a random fashion over the microstructural image (with uniform distributions of the orientation angle and the coordinates of the mid point). The ratio L_β/L of the length of the transect L_β lying in one of the microstructural constituents (β) to the entire length L of the transect is referred to as 'intercept'. Its distribution is an important characteristic of duplex structures. One of the reasons is the fact that the distribution of phases along a notch or a crack front affects the behaviour of the surrounding material and from it, the micromechanism of crack extension.

The probability that a random transect of specified length will sample only matrix phase has been discussed in Refs. [17–21] where a lineal-path function $T(x)$ has been defined. $T(x)$ gives the probability of finding a line segment of length x wholly in the matrix phase α when randomly cast into the inhomogeneous structure. In the case of fully penetrable spherical nuclei with radii R, and a number density λ, the equation

$$T(x) = \exp(-\lambda v_Z) \quad (1)$$

has been applied, where v_Z was referred to as the volume of the 'exclusion region' and defined as $v_Z = (4\pi/3)R^3 + \pi R^2 x$ (sphero-cylinder) in the 3D case and $v_Z = \pi R^2 + 2Rx$ in the 2D case; x is the length of the cylinder (Fig. 4(a)). As stated in Ref. [21], the distribution of the chord lengths lying in the matrix phase has important applications in diffusion in porous media and transport problems involving 'free paths'. Accordingly, a problem related to

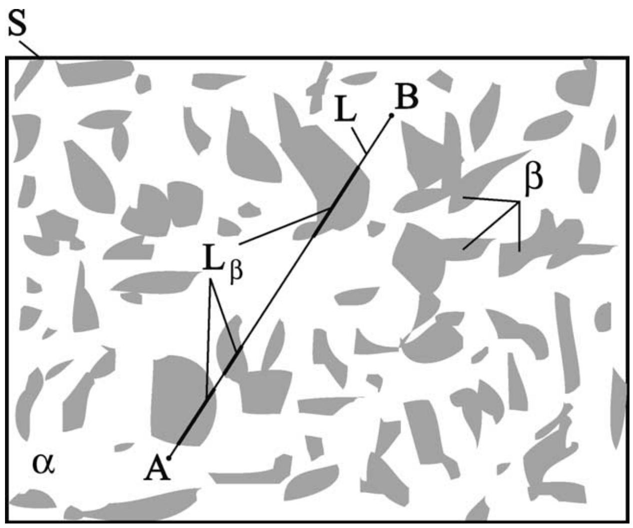

Fig. 1. Duplex structure containing two structural constituents α and β, sampled by a random line transect.

the chord-length distribution function for two-phase random media has been solved in Refs. [20,21]. The chords X have been defined by the intersection of a randomly cast line with the matrix phase α (Fig. 5(a)).

If the chord-length probability density function is denoted by $f(x)$, the mean chord (or intercept) length by l_a and the volume fraction of the matrix phase α by ξ_a, the link between the lineal path function $T(x)$ and $f(x)$ proposed in Refs. [20,21] is:

$$\frac{\mathrm{d}T(x)}{\mathrm{d}x} = -\frac{\xi_a}{l_a}\int_x^\infty f(v)\mathrm{d}v$$

where $l_a = \int_0^\infty v f(v)\mathrm{d}v$ and v is a dummy integration variable. The equation proposed can also be written as

$$\frac{\mathrm{d}T(x)}{\mathrm{d}x} = -\frac{\xi_a}{l_a}[1 - F(x)] \quad (2)$$

where $F(x)$ is the cumulative chord-length distribution function ($\mathrm{d}F(x)/\mathrm{d}x = f(x)$). An alternative simple link between $T(x)$ and $F(x)$ will be derived in the present work. In Refs. [13–16] it has been demonstrated that the variance and the empirical cumulative distributions of the intercepts from the microstructural constituents are important statistical fingerprints of an inhomogeneous microstructure, which contain valuable information regarding the risk of poor properties (e.g. fracture toughness). The power of the approach based on line transects has been demonstrated in Ref. [15] where the work focused on inhomogeneous structures, irrespective of the structural evolution. Since structures formed by nucleation and growth are very common, the present work focuses on the spatial statistics of duplex structures formed by nucleation and growth. In this case, time dependency is also present in the equations.

A typical feature of these structures is that they are formed by nuclei (β) arising and growing in a matrix (α), Fig. 5(c). It is assumed that the growth rate is isotropic and the growth stops at the contact zones of the growing nuclei (growth with impingement). Earlier work [13] demonstrated that for inhomogeneous microstructures formed by nucleation and growth the correlation between the sampling results of two points at a fixed distance from each other does not depend on the extent of inhomogeneity (the size of the aggregates from the second phase) no matter how many nuclei are present in the system and how large the nuclei aggregates are. The existence of a correlation depends only on the diameters of the nuclei and the distance L between the sampling points.

Indeed, the computer generated 'structure' shown in Fig. 2 containing a small number of equal sized nuclei with diameter D is characterised by a correlation between the sampling results from two sampling points if $L < D$. For the computer-generated structure in Fig. 3, however, the number of nuclei is large, large aggregates of nuclei are also present but no correlation exists if the distance L between

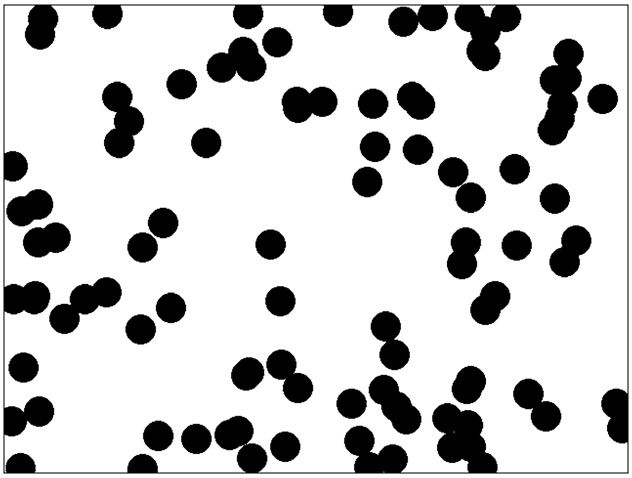

Fig. 2. Computer generated ‘duplex structure’ composed of 100 Poisson-distributed overlapping circles with equal diameters.

the sampling points is even slightly larger than the diameter d of the nuclei!

2. Intercepted fractions from the microstructural constituents by line transects

Assume (i) a duplex structure with finite volume V composed of (ii) interpenetrating spherical nuclei β the distribution of whose centres follows a homogeneous Poisson process. The nuclei arise with rate $I(\tau)$ and grow with a radial rate $r(\tau)$, where τ denotes time. The growth is isotropic, i.e. the growth rate is the same in any direction. According to Refs. [17,18], the probability that a randomly cast linear segment (line transect) with length x will sample only α is equal to the probability that the centres of all nuclei with radii $r(\tau)$ will lie outside the exclusion region Z with volume $v_Z(\tau) = \pi r^2(\tau)x + (4/3)$

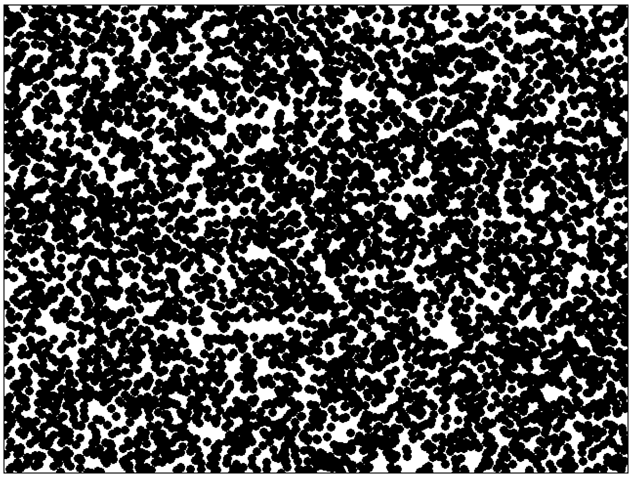

Fig. 3. Computer-generated ‘duplex structure’ composed of 6200 randomly distributed overlapping circles with equal diameters.

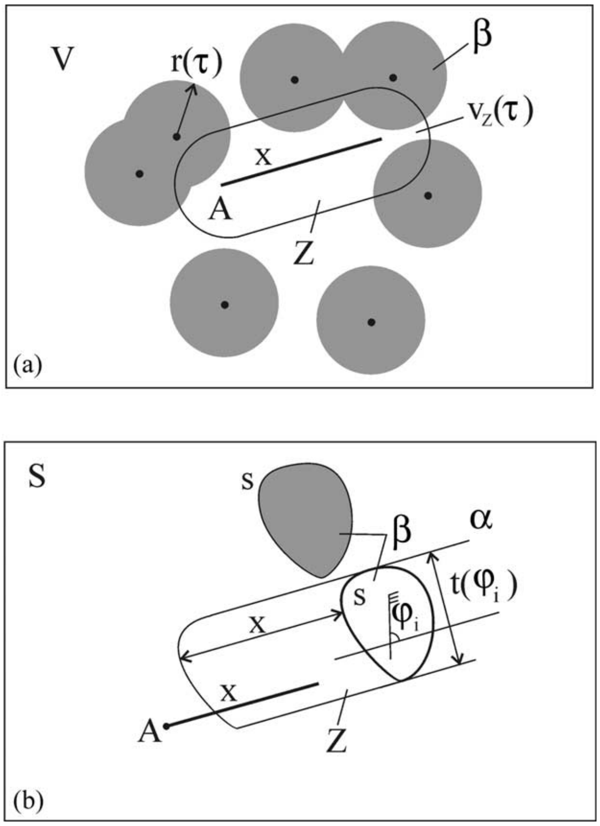

Fig. 4. (a) Exclusion zone Z for a random transect with length x and equal-sized circular nuclei; (b) exclusion zone Z for a random transect with length x and equal-sized convex nuclei for a particular orientation angle φ_i.

$\pi r^3(\tau)$, $(s_Z(\tau) = 2r(\tau)x + \pi r^2(\tau))$ in the two-dimensional case (Fig. 4(a)). The probability that none of the nuclei with radii $r(\tau)$ that have arisen in the infinitesimal time interval $\tau - \nu$, $\tau - \nu + \mathrm{d}\tau$ will intersect the line transect is given by

$$\{1 - [\pi r^2(\tau - \nu)x + (4/3)\pi r^3(\tau - \nu)]/V\}^{VI(\tau-\nu)\mathrm{d}\nu}$$
$$= \exp\{VI(\tau - \nu)\mathrm{d}\nu \ln[1 - (x\pi r^2(\tau - \nu) + (4/3)\pi r^3(\tau - \nu))/V]\}$$

$(\exp\{VI(\tau - \nu)\mathrm{d}\nu \ln[1 - (2xr(\tau - \nu) + \pi r^2(\tau - \nu))/V]\}$ in the two-dimensional case), where $I(\tau - \nu)$ is the nucleation rate at the instant $\tau - \nu$ and $r(\tau - \nu)$ is the radius of the nuclei that have nucleated at the instant $\tau - \nu$ (ν is a time increment). The probability that none of the nuclei that have appeared in the time interval $(0,\tau)$ will intersect the line transect is a product of the probabilities of ‘non-intersection’ characterising all portions of nuclei that have arisen in the time interval $(0,\tau)$. Hence, the probability $T(x)$ that the line transect with length x will sample only α-phase is

$$T(x) = \exp\left(\int_0^\tau VI(\tau - \nu)\ln\{1 - [x\pi r^2(\tau - \nu) + (4/3)\pi r^3(\tau - \nu)]/V\}\mathrm{d}\nu\right) \quad (3)$$

in the three-dimensional case where V is the finite volume of the system and the time increment ν acts as a dummy integration variable.

If the ratio of the exclusion volume Z in Fig. 4(a) to the system volume V is small then $\ln\{1-[x\pi r^2(\tau-\nu)+(4/3)\pi r^3(\tau-\nu)]/V\} \approx -[x\pi r^2(\tau-\nu)+(4/3)\pi r^3(\tau-\nu)]/V$ and Eq. (3) becomes

$$T(x)=\exp\left(-\int_0^\tau I(\tau-\nu)[x\pi r^2(\tau-\nu)+(4/3)\pi r^3(\tau-\nu)]\mathrm{d}\nu\right) \tag{4}$$

In the two-dimensional case, the equation corresponding to Eq. (3) is

$$T(x)=\exp\left(\int_0^\tau SI(\tau-\nu)\ln\{1-[2xr(\tau-\nu)+\pi r^2(\tau-\nu)]/S\}\mathrm{d}\nu\right) \tag{5}$$

where S is the finite area of the system where the nucleation takes place. Similarly, if the ratio of the exclusion area to the system area S is small, $\ln\{1-[2xr(\tau-\nu)+\pi r^2(\tau-\nu)]/S\}\approx -[2xr(\tau-\nu)+\pi r^2(\tau-\nu)]/S$ and Eq. (5) becomes

$$T(x)=\exp\left(-\int_0^\tau I(\tau-\nu)[2xr(\tau-\nu)+\pi r^2(\tau-\nu)]\mathrm{d}\nu\right) \tag{6}$$

The probability that the transect with length x will be intersected by at least a single nucleus is $1-T(x)$. For a transect with zero length $x=0$ (a single-point transect), the expression $T(x)$ will give the probability of sampling matrix phase α by a randomly cast point. This probability is equal to the volume fraction ξ_a of the α-phase. Thus

$$\xi_a=T(0) \tag{7}$$

Substituting $x=0$ in Eq. (4) gives:

$$T(0)=\xi_a=\exp\left(-\int_0^\tau I(\tau-\nu)(4/3)\pi r^3(\tau-\nu)\mathrm{d}\nu\right) \tag{8}$$

As a result, expression (4) characterising the three-dimensional case can also be presented as:

$$T(x)=\xi_a\exp\left(-x\int_0^\tau I(\tau-\nu)\pi r^2(\tau-\nu)\mathrm{d}\nu\right) \tag{9}$$

Similarly, Eq. (6) characterising the two-dimensional case can be presented as

$$T(x)=\xi_a\exp\left(-x\int_0^\tau I(\tau-\nu)2r(\tau-\nu)\mathrm{d}\nu\right) \tag{10}$$

Since $\xi_a+\xi_\beta=1$, $\xi_\beta=1-T(0)$. Substituting $x=0$ in Eq. (3) and taking $V=1$ gives

$$\xi_\beta(\tau)=1-\exp\left\{\int_0^\tau \ln[1-(4/3)\pi r^3(\tau-\nu)]I(\tau-\nu)\mathrm{d}\nu\right\} \tag{11}$$

which is an equation describing kinetics of phase transformation with constant radial growth rate [22].

It has been demonstrated [22] that there exists equivalence between the kinetics of a phase transformation of the type nucleation and growth with constant radial rate and the process of continuous coverage of space by overlapping spheres growing with constant radial rate [22]. The special case equation (11) from the general equation (3) can also be confirmed by the probabilistic argument presented in Appendix A.

2.1. Probability of sampling only matrix phase for a structure containing convex nuclei with irregular shape

If the shape of the nuclei is irregular but convex (Fig. 4(b)), the probability that a transect with length X will intercept α-phase only, can be deduced from the following argument. Assume that the transect is fixed and the nuclei are introduced (cast randomly) one-by-one. For a specified relative orientation angle of a particular nucleus regarding the line transect with length x, the nucleus is 'cast' in such a way so that the relative orientation angle φ_i remains the same (Fig. 4(b)). For each specified orientation angle φ_i, the probability of non-intersection of the nucleus with the transect is equal to the probability that the end A of the transect will not be covered by the exclusion zone Z of the nucleus (Fig. 4(b)). Since the area of the exclusion zone is equal to $xt(\varphi_i)+s$, where s is the area of the nucleus, the probability of non-coverage for a number of nuclei oriented at the same angle φ_i is $[1-(xt(\varphi_i)+s)/S]^{\lambda_i S}$ where λ_i is the number density of all nuclei oriented at an angle φ_i and $t(\varphi_i)$ is the calliper diameter of the nuclei with orientation angle φ_i (Fig. 4(b)). The probability of non-intersection for an arbitrary orientation of the nuclei can be determined as a sum of the probabilities of non-intersection for all nuclei oriented at different angles regarding the line transect. Suppose that the angle of rotation of the nuclei is uniformly distributed, with probability density $1/(2\pi)$ (all orientation angles being equally likely). Then, the probability of non-intersection for nuclei with orientation angles in the small interval φ, $\varphi+\Delta\varphi$ is $[1-(xt(\varphi)+s)/S]^{\lambda\Delta\varphi S/2\pi}$, where $\lambda(\Delta\varphi/2\pi)$ is the number density of the nuclei whose orientation angles are in the interval $(\varphi, \varphi+\Delta\varphi)$. The probability of non-intersection for all nuclei (oriented at arbitrary angles) is then

$$T(x)=\exp\left\{\lambda S\frac{1}{2\pi}\int_0^{2\pi}\ln[1-(xt(\varphi)+s)/S]\mathrm{d}\varphi\right\} \tag{12}$$

In the case where the ratio $(xt(\varphi)+s)/S$ is small, $\ln[1-(xt(\varphi)+s)/S] \approx -(xt(\varphi)+s)/S$ and Eq. (12) becomes

$$T(x)=\exp[-\lambda(\bar{t}x+s)] \tag{13}$$

where $\bar{t}=(1/2\pi)\int_0^{2\pi} t(\varphi)\mathrm{d}\varphi$ is the mean calliper diameter of a single 2D-nucleus. Similarly, in the three-dimensional case, for a small ratio of the nuclei volume and the volume of the system, the probability of non-intersection will also be given by Eq. (13) where

$$\bar{t}=\frac{1}{4\pi}\int_{\varphi,\theta} t(\varphi,\theta)\mathrm{d}\varphi\,\mathrm{d}\theta \tag{14}$$

is now the mean projection area of a single 3D-nucleus on a plane perpendicular to the direction of the transect. $t(\varphi, \theta)$ in Eq. (14) is the area of the projection of the nucleus on a plane perpendicular to the direction of the transect, for a specified orientation of the nucleus, given by the spherical angular coordinates φ and θ; s in Eq. (13) is now the volume of the nucleus.

3. Probability distribution of the free-paths in the matrix

Another important question is related to the probability of existence of a α-phase free path. The α-phase free path is a segment which starts either in α-phase (Fig. 5(c)) or at a border of a nucleus (Fig. 5(b)) traverses α-phase only and ends at an α/β interface.

Let us denote the cumulative probability distribution function of the α free-paths by $F(x)$. In other words, $F(x)$ is the probability that a free path X will not be greater than x: $F(x) = P(X \leq x)$. The probability density function will be denoted by $f(x)(f(x) = F'(x))$. Let us consider a particular α-phase free path (Fig. 5(a)) where X is a α-phase free path, which starts from the point A (Fig. 5(b) and (c)). If A is a border point (Fig. 5(b)) or a point in α-phase (Fig. 5(c)), there will be no centres of nuclei inside the circular exclusion zone with the centre point A and radius equal to the radius R of the nuclei (Fig. 5(b), the dashed circle). Otherwise, point A will be a point inside β-phase.

The probability that the free path X will be smaller than x is equal to unity minus the probability that the free path will be larger than x which in turn equals the probability that there will be no nuclei centres residing inside the exclusion zone Z (Fig. 5(b)). Since the area of this zone is $s_Z = 2Rx$ (Fig. 5(b)), the probability is equal to $(1 - 2Rx/S)^{\lambda S}$. The probability that the free path will be smaller than x then becomes

$$F(x) = 1 - (1 - kx)^n \tag{15}$$

where $n = \lambda S$ is the expected number of nuclei in the system with area S and $k = 2R/S$ is a constant. Differentiating the cumulative distribution function (15) regarding x gives the probability density function

$$f(x) = nk(1 - kx)^{n-1} \tag{16}$$

Distribution (16) has x mean

$$\bar{x} = \frac{1}{k(n+1)} \tag{17}$$

and variance

$$V = \frac{n}{k^2(n+1)^2(n+2)} \tag{18}$$

If the ratio $2Rx/S$ is small, distribution (15) can be approximated by the exponential distribution

$$F(x) = 1 - \exp(-2\lambda Rx) \tag{19}$$

Indeed $F(x) = 1 - (1 - 2Rx/S)^{\lambda S} = 1 - \exp(\lambda S \ln[1 - 2Rx/S]) \approx 1 - \exp(-2\lambda Rx)$, and after differentiation, the exponential probability density

$$f(x) = \beta \exp(-\beta x) \tag{20}$$

is obtained, where $\beta = 2\lambda R$. The mean and the variance of the exponential density (20) are $1/\beta$ and $1/\beta^2$, respectively. Thus, for a small areal ratio $2xR/S$, the probability density (16) transforms into the exponential probability density Eq. (20), with mean $\bar{x} = 1/(\lambda D)$ and variance $V = 1/(\lambda D)^2$ where $D = 2R$ is the diameter of the nuclei.

$2R$ in Eq. (19) is the projection of the nuclei on a plane (line) perpendicular to the direction of the transect. In the three-dimensional case, the distribution of the free paths in the matrix phase is also given by Eqs. (15) and (16), where

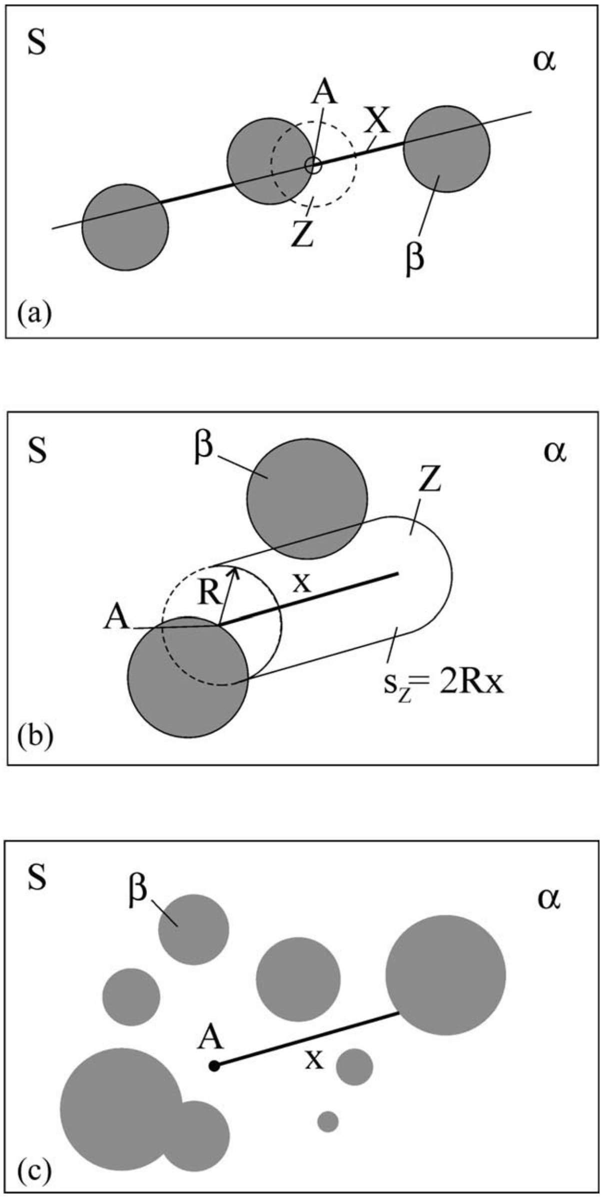

Fig. 5. (a) Segments X which an infinitely long line intercepts from the matrix (the α-phase); (b) if A is a border point, then no nuclei centres reside inside the circular exclusion zone with centre the point A and radius R; (c) a free path of length x in the matrix phase.

$n = \lambda V$ and $k = \pi R^2/V$. Similarly, in case of convex nuclei with arbitrary shape, and a small volume ratio, the distribution of the free paths is also exponential

$$f(x) = \lambda \bar{t} \exp(-\lambda \bar{t} x) \tag{21}$$

with mean $\bar{x} = 1/(\lambda \bar{t})$ and variance $V = 1/(\lambda \bar{t})^2$, where $\bar{t}$ is the mean projection area of the nucleus on a plane perpendicular to the direction of the transect.

Eqs. (15) and (16) can be generalised for nuclei arising with rate $I(\tau)$. Suppose that the nuclei with different sizes are partitioned into groups comprising nuclei with approximately the same size. Then the probability that the free path will be larger than a specified value x is equal to the product of the probabilities that the centres of the different size nuclei will lie outside the corresponding to their sizes exclusion zones. If the distribution of the nuclei follows a Poisson process, the probability that all nuclei with radii $r(\tau - \nu)$ that have arisen in the infinitesimal time interval $\tau - \nu, \tau - \nu + d\tau$ will not intersect the line transect is given by $\exp(VI(\tau - \nu)d\nu \ln[1 - \pi x r^2(\tau - \nu)/V])$, where $I(\tau - \nu)$ and $r(\tau - \nu)$ are the nucleation rate at the instant $\tau - \nu$ and the radii of the nuclei that have nucleated at that instant, respectively. Since the probability that no nucleus will intersect the line transect is a product of the probabilities of non-intersection characterising all portions of nuclei that have arisen in the time interval $(0,\tau)$, the probability of a free path with length larger than x becomes

$$\exp\left(\int_0^\tau VI(\tau - \nu)\ln[1 - \pi x r^2(\tau - \nu)/V]d\nu\right),$$

where ν is a dummy integration variable. The probability that the free path X will be smaller than or equal to x is then

$$F(x) = 1 - \exp\left(\int_0^\tau VI(\tau - \nu)\ln[1 - \pi r^2(\tau - \nu)x/V]d\nu\right) \tag{22}$$

For a small volume ratio $\pi r^2(\tau - \nu)x/V$ the probability that the free path will be smaller than or equal to x becomes

$$F(x) = 1 - \exp\left(-x\int_0^\tau I(\tau - \nu)\pi r^2(\tau - \nu)d\nu\right) \tag{23}$$

After differentiating Eq. (23) regarding x the exponential distribution (20) is obtained, where $\beta = \int_0^\tau I(\tau - \nu)\pi r^2(\tau - \nu)d\nu$.

3.1. A link between the probability of a minimum free path in the matrix and the probability of sampling only matrix phase by a random transect

For an arbitrary two-phase microstructure formed by Poisson-distributed nuclei, there exists a link between the probability $P(x) = 1 - F(x)$ that the free path will be greater or equal than a specified length x and the probability $T(x)$ of sampling only matrix phase by a line transect of length x. The link between the two probabilities can be found using the following probabilistic argument.

The probability $T(x)$ is a product of the probabilities of two events. The first event: 'a particular selected end of the transect (e.g. the end A in Fig. 5(c)) samples α' is characterised by probability ξ_α where ξ_α is the volume fraction of α phase. The probability of the second event 'the continuation of the transect will be longer than x given that the end A samples α phase' is in fact the probability $P(x)$ of existence of a free path of minimum length x. As a result:

$$T(x) = \xi_\alpha P(x) \tag{24}$$

Indeed, consider the case where the second phase β is formed by overlapping equal-sized circular nuclei with radii r on a plane. From Eq. (19) it follows that the probability $P(x)$ for a path starting in α, being longer than x (Fig. 5(b)) is given by $P(x) = 1 - F(x) = \exp(-2\lambda x r)$. The probability $T(x)$ is given by $T(x) = \exp[-\lambda(2xr + \pi r^2)]$ (Eq. (1)). The latter expression can also be rearranged as $T(x) = \exp(-2\lambda x r)\exp(-\lambda \pi r^2) = \xi_\alpha \exp(-2\lambda x r) = \xi_\alpha P(x)$, which is exactly Eq. (24).

The same link (Eq. (24)) can be derived for nuclei of different size directly growing in a system of finite volume V by comparing Eqs. (9) and (23).

From Eq. (24) it follows that $T(x = 0) = \xi_a P(x = 0)$. Since $P(x = 0) = 1$, from Eq. (24) it follows that $T(0) = \xi_a$ confirming Eq. (7). Eq. (24) then can be presented as

$$P(x) = \frac{T(x)}{T(0)} \tag{25}$$

giving a link between three fundamental characteristics of inhomogeneity, which is an alternative to the link given by Eq. (2) discussed in the Introduction section.

4. Monte Carlo simulations

The validity of the equations derived has been established by Monte Carlo simulations on computer-generated 'microstructures' (similar to those from Figs. 2 and 3) where all parameters of the inhomogeneous microstructure (shape and size of the nuclei and number density) are controlled and known.

The validity of Eq. (4) was confirmed through Eq. (11) which is a special case of Eq. (4). Eq. (11) in turn has been validated by numerous Monte Carlo simulations published in a previous work [23].

Computer simulations on real microstructures have also been carried out. In the general case of microstructures including nuclei with irregular shape, the distributions of the intercepted fractions and the probabilities that the transect will lie entirely in α or β phase can only be obtained through Monte Carlo simulations. The simulations consist of numerous random placements of the line transect over images of the microstructure and registering the intercepted fractions from the second microstructural constituent.

The intercepted fractions are ratios of the segment lengths intercepted from one of the phases to the total length of the transect (Fig. 1). The microstructural image remains static throughout the simulations.

For the real microstructural section in Fig. 6, for example, the probability of sampling only α phase (white patches), only β phase (dark patches) and between 30 and 70% β phase were determined to be 0.189, 0.055 and 0.376, respectively. The length of the transect during the simulations was $L = 40$ length units (the horizontal length of the picture contains 640 length units). The areal fraction of β-phase is $\xi_\beta = 0.42$. The probability of existence of a minimum free path of length $L = 40$ units in the α-phase was determined from Eq. (25)

$$P(40) = \frac{T(40)}{T(0)} = 0.189/0.58 \approx 0.33$$

since $T(0) = \xi_\alpha = 1 - \xi_\beta = 0.58$.

An efficient way of producing the distribution of the total intercept or the largest continuous segment from one of the phases (β or α) is by scanning the microstructure as a bitmap file [24,25] and subsequent sampling of the microstructural image by random segments using the Bresenham algorithm [26,27]. The intercept from β for example is calculated by dividing the number of pixels belonging to β to the total number of pixels composing the transect. For each placement of transect, the maximum length segment intercepted from the phase of interest is also determined. Fig. 7 gives the distribution of the maximum length segments intercepted from β (the dark patches) by a line transect with length 140 units. The algorithm for obtaining the distribution of the largest continuous segment from β can be modified easily to eliminate thin borders of α between two β segments and to count them as a single β segment (Appendix B). In many cases thin borders of α will not make a noticeable difference if large β aggregates exist along the transect length (e.g. for problems related to absorption of a signal or radiation).

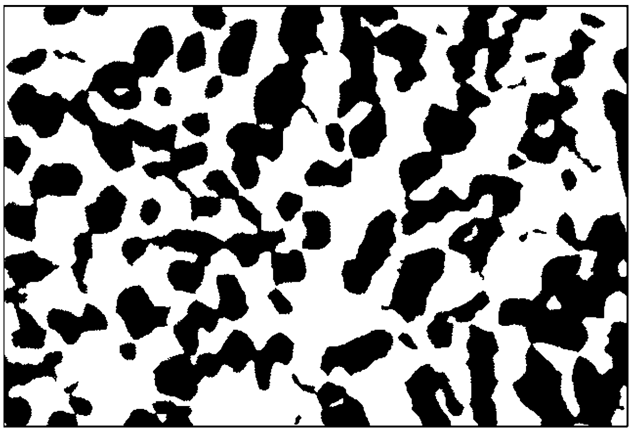

Fig. 6. Scanned image of a duplex stainless steel microstructure. The white zones are austenite ($\xi^\alpha = 0.58$) and the dark zones are ferrite ($\xi^\beta = 0.42$).

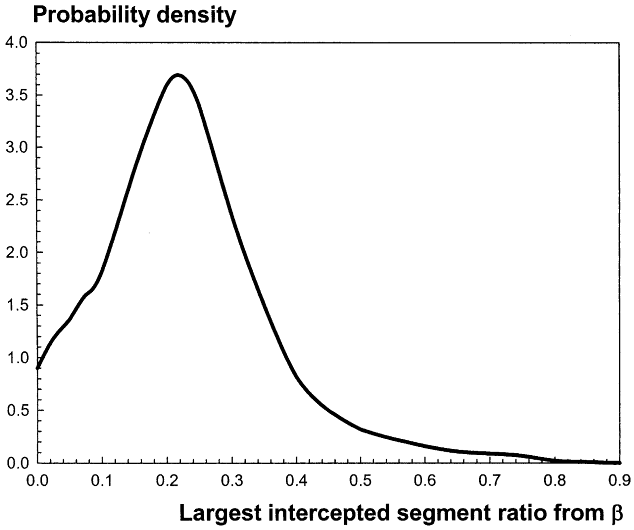

Fig. 7. Probability density distribution of the maximum size segment intercepted from β (the dark zones in Fig. 6) by a line transect with length 140 units (the horizontal length of Fig. 6 contains 640 units).

5. Discussion

The uncertainty (variability) of properties associated with inhomogeneous media formed by nucleation and growth is *intrinsic* and the description of the material properties distribution benefits significantly from using statistical methods. Eq. (3) gives the probability of sampling matrix phase only by a transect of size x in a system of growing Poisson distributed spherical nuclei. The equation is time dependent and of significant importance to the kinetics of phase transformations proceeding with nucleation and growth. If the length of the transect x is zero, the equation gives the exact quantity of untransformed matrix phase at any instant during the phase transformation (Eq. (11)). For nuclei characterised by a small volume ratio and constant nucleation rate ($I(t) = I = \text{const}$), Eq. (11) can be simplified. Since for small ratios $[(4/3)\pi r^3(\tau - \nu)]/V$, $(V = 1)$, $\ln[1 - (4/3)\pi r^3(\tau - \nu)] \approx -(4/3)\pi r^3(\tau - \nu)$, after integrating, Eq. (11) transforms into the Kolmogorov–Johnson–Mehl–Avrami equation [23] (KJMA equation):

$$\xi_\beta(\tau) = 1 - \exp[-(\pi/3)Ir^3\tau^4] \tag{26}$$

As a result, the KJMA equation and the exact equation (11) describing kinetics of phase transformation are both special cases of the derived equation (3).

Eq. (24) establishes a simple link between three fundamental statistical characteristics of inhomogeneous microstructures: (i) the probability $T(x)$ that a transect of length x will sample only matrix phase; (ii) the probability $P(x)$ of existence of a free path of minimum length x and (iii) the volume fraction ξ_a of the matrix phase. Thus, the concept 'line transect' is very flexible in terms of characterisation of a spatial arrangement and volume fraction. Indeed, from characterising spatial arrangement in case of non-zero transect length, the transect of zero length measures of volume fraction (Eq. (7)). The probability of sampling only matrix phase by a transect of given length x is much easier to quantify (measure) than the probability of a free path of minimum length x. According to Eq. (25), the latter probability is obtained as a ratio of the probability of sampling only matrix phase by a transect of length x (from Monte Carlo simulations) and the volume fraction of the matrix (these two are derived by Monte Carlo simulations).

From Eq. (23), for example, it follows that microstructures characterised by similar values of the integral $\int_0^\tau I(\tau-\nu)\pi r^2(\tau-\nu)\mathrm{d}\nu$ are characterised by approximately the same distribution of the free paths. For a small size of the growing nuclei compared to the volume of the system where they nucleate, from Eqs. (17)–(21) it follows that microstructures with the same value of the product, $\lambda \times$ *mean projection size of the nucleus*, are characterised by the same mean free path and variance. This can be used for topological optimisation of microstructures in order for example to decrease the mean free path and its variance. This is important for problems from radiation and diffusion transport and scattering in inhomogeneous solids.

In the simple case of convex nuclei of the same type, the mean free path in the α-phase and its variance are $\bar{x} = 1/(\lambda\bar{t})$ and $V = 1/(\lambda\bar{t})^2$, where $\bar{t}$ is the mean projection area of the nucleus on a plane perpendicular to the direction of the transect. Substantial decrease of the mean free path and the free path variance can be expected if the nuclei number density λ or their size $\bar{t}$ are increased.

An important application of the method of random transects is for problems related to absorbing radiation emitted from a particular point of an inhomogeneous media. Suppose that the scanned microstructure in Fig. 6 is a result of combining various random sections from a material composed of constituents α and β with different absorption capability. A source of radiation can be activated anywhere in the material. Suppose that the constituent β absorbs radiation and the decrease y of the initial radiation intensity I_0, is described by $y = (I_0 - I)/I_0 = 1 - \exp(-\lambda_\beta L x)$, where I is the radiation (signal) intensity after the absorption from β, λ_β is the linear absorption coefficient through unit thickness of β, L is the distance from the source (the length of the transect), $x = L_\beta/L$ is the penetrated lineal fraction of β along the distance L (the intercept from β). Thus, the absorbed radiation intensity depends only on the intercept from β and does not depend on the ordering of α and β along the distance from the source (along the transect). Performing Monte Carlo simulations involving numerous random transects of given length placed on Fig. 6 yields the probability that the radiation intensity will be attenuated by a certain critical value.

Similar application is determining the probability of an attenuation by a certain amount of a signal propagating through an inhomogeneous media. Another application is the microstructural microanalyses where a probability is determined that a random scan of specified length will sample more than a certain amount of a chemical component present with different quantity in both microstructural constituents.

Consider a material with brittle matrix α (initiates fracture easily during loading) and tough second microstructural constituent β (second phase). The distribution of the intercept from α is then related to the probability of initiation of brittle fracture. Thus, if the probability of a large intercept from the brittle matrix phase is large, the probabilities of low toughness and brittle fracture are correspondingly large. If, for example a sharp notch or a long zone of stress intensification traverses inhomogeneous structure, during loading, the initiation of brittle fracture is likely to occur in the largest continuous segment of the brittle phase α traversed by the notch. Hence, the distribution of the largest continuous segments intercepted from α is also related to the likelihood of initiating brittle fracture and together with the distribution of the total intercept from α is a useful 'statistical fingerprint' of inhomogeneous structures.

The simulation methods discussed here can be used to determine which nuclei distribution produces the smallest variance of the intercepted fraction from the weaker component and yields the smallest scatter of the corresponding material property (e.g. fracture toughness). Assume for simplicity that circular nuclei of the same radii are present. Then, for a line transect of specified length, the variation of the intercepted fraction from β-phase nuclei will be small if for any direction of the transect similar number of nuclei centres is likely to be found inside the exclusion zone Z (Fig. 4(a)). This is approximately fulfilled by nuclei whose centres form a Poisson field. For this type of distribution, the variation of the number of nuclei inside the exclusion zone Z is not particularly sensitive to the orientation of a curvilinear transect of any shape and therefore the variation of the intercept from β-phase nuclei will not be unduly large. Furthermore, a distribution of nuclei may be sought which minimises the probability that a random transect will sample more than a specified fraction from the weaker phase, which is an useful type of topological optimisation leading to materials with improved toughness.

Eq. (11) which is a special case of Eq. (3) can be used for determining the volume fraction of transformed phase during phase transformations proceeding with nucleation and growth. Eq. (11) is exact and more precise than the analogous KJMA equation (26). Thus, for a small number of nuclei in a system with finite volume, Eq. (26) shows large deviations from the true values [23]. For any number of growing nuclei, however, Eq. (11) gives correct predictions regarding the quantity of the transformed phase. Unlike the KJMA equation (26) valid for constant nucleation and growth rate, Eq. (11) also handles the case where the nucleation and growth rate are arbitrary functions of time.

The methods developed in the paper also have important application to determining the reliability of stressed inhomogeneous materials. Since the lower tail of the strength distribution is a function of the lower tail of the material properties distribution, the distribution of the intercept from one of the constituents can be used for determining the strength distribution and finally the reliability of the material. Reliability can be improved by reducing the variation of material properties due to inhomogeneity and its propagation into variation (uncertainty) associated with strength.

Another important application is limiting the risk from premature fracture of an inhomogeneous material with a sharp crack or a long zone of stress intensification. Suppose a minimum failure-free operating period is specified, during which an inhomogeneous material containing a sharp notch or a long stress intensification zone experiences sequential random shocks.

The risk R from premature fracture for the specified minimum failure free operating period MFFOP is related to the cost C of the consequences from fracture by the simple relationship $R = p_f C$ where p_f is the probability of fracture (i.e. the probability that fracture will occur before the end of the specified operating period. For a specified maximum acceptable risk R_{max} of fracture, the maximum acceptable probability of fracture p_{fmax} can be determined from $p_{fmax} = R_{max}/C$.

The critical load level that triggers brittle fracture depends on the amount of intercepted quantity from the brittle constituent: a larger intercept corresponds to a smaller critical load and vice versa. Suppose the maximum load is normally distributed during the specified minimum failure-free operating period with particular mean value and variance. Suppose also that the mean value of the load (but not its variance) can be controlled.

The calculated maximum acceptable probability of premature fracture p_{fmax} (together with the specified minimum failure free period) can then be used for setting reliability requirements. These are related to the maximum acceptable mean load during the specified period so that the R_{max} of premature fracture remains below the maximum acceptable level. For a particular mean load, the actual probability of fracture can be calculated on the basis of a load-strength interference model involving the load distribution and the strength distribution [1–3] giving the distribution of the critical stress triggering brittle fracture. The strength distribution is determined from the distribution of the intercept from the brittle constituent, which is in turn determined by random sampling of an image of the inhomogeneous structure.

Early-life failures of components and systems can significantly be reduced due to (i) better understanding of the effect of material inhomogeneity on the strength distribution; (ii) identifying and controlling design variables dependent on inhomogeneity, with significant contributions to the variability of strength; (iii) implementing new designs characterised by reduced sensitivity to material inhomogeneity and properties variation due to inhomogeneity. These will deliver new solutions for increasing the reliability of mechanical components and systems.

6. Conclusions

1. A fundamental time-dependent equation has been derived for the probability of sampling only matrix phase by a random line transect in a system containing growing Poisson distributed spherical nuclei. The KJMA equation and the exact equation dealing with phase transformation kinetics are special cases of the derived equation.
2. The probability of sampling matrix phase only by a line transect measures simultaneously the product of two fundamental characteristics of duplex media: (i) the volume fraction of the matrix phase and (ii) the probability of existence of a free path of specified minimum length.
3. For a small ratio of the size of the nuclei and the volume of the system, the distribution of the free paths in the matrix phase is exponential.
4. Increasing the number density of the nuclei and decreasing the size of the mean projection of the nuclei (on a plane perpendicular to the line transect) by the same factor does not affect the mean and the variance of the free paths in the matrix phase.
5. A statistical derivation has been proposed of an exact time-dependent equation describing the evolutionary change in the quantity of the transformed phase with time for structures formed by nucleation and growth.
6. Using a maximum acceptable level of the risk of faliure and a minimum failure free operating period, reliability requirements can be set regarding the acceptable loading of inhomogeneous materials containing zones of stress intensification of known size. The maximum acceptable level of the probability of fracture can be obtained from the ratio of the maximum acceptable risk of fracture and the cost of the consequences from fracture.
7. The probability distribution of the intercept from the weaker microstructural constituent gives an important indication regarding the probability of brittle fracture. A simulation method and software routine have been developed for identifying the largest continuous segment intercepted from the weaker microstructural constituent and the continuous sub-segment containing the smallest property value.

Acknowledgements

The author thanks the reviewers of this paper for the useful comments. The financial support from BP (UK) is gratefully acknowledged.

Appendix A

Consider a coverage of space where m groups of objects with volume ratios $\psi_i = v_i/V$ and numbers n_i, $i = 1,m$ in each group, cover a space with volume V (v_i is the volume of the objects from the ith group). It is clear, that the covered volume fraction is equal to the probability that a randomly selected point in the volume V will be covered. If the point is fixed in V and the objects are introduced one by one, the acts of placing objects can be regarded as random trials, with probabilities ψ_i of success in each trial equal to the probabilities of covering the selected point.

The probability of the event 'no coverage of the selected point at the end of the trials' is $[1-\psi_1]^{n_1}[1-\psi_2]^{n_2}\cdots[1-\psi_m]^{n_m}$, hence the probability of at least a single success (coverage) at the end of the trials is

$$\xi = 1 - (1-\psi_1)^{n_1}(1-\psi_2)^{n_2}\cdots(1-\psi_m)^{n_m} \tag{A1}$$

After taking logarithms Eq. (A1) becomes

$$\ln(1-\xi) = n_1\ln(1-\psi_1) + n_2\ln(1-\psi_2) + \cdots + n_m \ln(1-\psi_m) \tag{A2}$$

which transforms into

$$\xi = 1 - \exp\left(\sum_{i=1}^{m} n_i \ln[1-\psi_i]\right) \tag{A3}$$

If the numbers of the trials and their probabilities of success are functions of time, Eq. (A3) becomes

$$\xi(\tau) = 1 - \exp\left(\int_0^{\tau} n(\upsilon)\ln[1-\psi(\upsilon)]\mathrm{d}\upsilon\right) \tag{A4}$$

where $\xi(\tau)$ is the probability of at least a single success (coverage of the selected point) at the end of the time interval $(0,\tau)$ and $n(\upsilon)$ is the number of trials per unit time at the instant υ (υ is a dummy integration variable). Eq. (A4) describes random coverage by overlapping objects with arbitrary shape, whose volume ratio $\psi(\tau)$ is a function of time. It must be pointed out that the covered fraction depends only on the volume ratios of the covering objects and not on their shape. Indeed, the probability that an object will cover the selected point is the same if the covering object was fixed and the point was randomly cast into the volume. The probabilities of "hitting" two covering objects of different shape are the same if the objects have equal volumes.

Appendix B

Assume for the sake of simplicity that each unit length of α-phase contributes a certain amount p to the average property value under consideration and each unit length of β-phase subtracts a certain amount n from the property. This is the case for example where a signal propagating in duplex media is attenuated by the constituent β more than the average level for the duplex media and less than the average level for the diplex media by the constituent α.

The problem is to determine the continuous sub-segment along the line transect which contains the smallest property value (the sub-segment characterised by the largest absorption). Since each random transect can be decomposed into small elements of unit lengths, each of which either belongs to α and contributes p units to the property or belongs to β and subtracts $|n|$ units from the property, the problem reduces to the following: given an array (vector) of negative (n) and positive (p) real increments, find the length of the continuous sub-array (sub-vector) characterised by the minimum sum of increments (the smallest property value). If for instance, the input vector is $[n,p,n,n,n,p,p,n,n,n,p,n,p,p]$ and $|n|,=p$ the procedure returns the length 8 corresponding to a sub-array that starts at the element with index 3 (the indexes count from 1) and ends at the element with index 10. The sub-array has a minimum sum of $4n$. The problem is very similar to a problem discussed in Ref. [28]. Interestingly, there exists a solution with complexity O(N), or in other words the sub-vector of interest can be found with a single scan of the input vector (line transect). An algorithm of complexity O(N) is given below, which yields the sum, the length and the location of the minimum-value sub-vector.

Given a line transect d[N] which contains N pixels each characterised by a value n or p, the algorithm finds the length, the beginning and the end of the sub-segment characterised by the minimum sum (stored in the variable 'min') of pixels' values. After executing the procedure, the length of the sub-segment remains in the variable 'length', the indexes of the pixels corresponding to the ends of the sub-segment remain in the variables 'left_index' and 'right_index'.

```
cur_min := 0; min := 0;
cur_left_index: = 1; cur_right_index := 1;
left_index := 0; right_index := 0; length := 0;
 For i = 1 to n do
  {
    tmp := cur_min + d[i];
    if    (tmp < 0)     then     {cur_min := tmp;
    cur_right_index := i;}
       else {cur_min := 0; cur_left_index := i + 1;
       cur_right_index := i + 1;}
    if (min > cur_min) then {min = cur_min;

left_index := cur_left_index;
right_index := cur_right_index;
length := right_index-left_index + 1;
       }
  }
```

References

[1] Carter ADS. Mechanical reliability and design. New York: Macmillan; 1997.

[2] Haugen EB. Probabilistic mechanical design. New York: Wiley; 1980.

[3] Christensen P, Baker M. Structural reliability theory and its applications. Berlin: Springer; 1982.

[4] Jeulin D. Morphological models for fracture statistics. Mater Sci Forum 1993;123–125:505–14.

[5] Debye P, Bueche AM. Scattering by an inhomogeneous solid. J Appl Phys 1949;20.

[6] Torquato S. Microstructure characterisation and bulk properties of disordered two-phase media. J Stat Phys 1986;45(5/6).

[7] Hilliard JE. Measurement of volume in volume. In: DeHoff RT, Rhines FN, editors. Quantitative microscopy. New York: McGraw-Hill; 1968. p. 45–76.

[8] Saltykov A. Stereometric metallography, 2nd ed. Moscow: Metallurgizdat; 1958.

[9] Hilliard JE, Cahn JW. An evaluation of procedures in quantitative metallography for volume-fraction analysis. Trans Metall Soc AIME 1961;221:344–52.

[10] Fullman RL. Measurement of particle sizes in opaque bodies. Trans AIME, J Metals 1953;(March):447–52.

[11] Weibel ER, Stereological methods: theoretical foundations, vol. 2. London: Academic Press; 1980.

[12] Underwood EE. Quantitative stereology. Reading, MA: Addison-Wesley; 1969.

[13] Todinov MT. On some applications of the random transects. Modell Simul Mater Sci Engng 1999;7:525–39.

[14] Todinov MT. Statistical modelling the scatter of properties from sampling of inhomogeneous materials. Comput Mater Sci 2001;21: 436–51.

[15] Todinov MT. Distribution of properties from sampling inhomogeneous materials by line transects. Probab Engng Mech 2002;17: 131–41.

[16] Todinov MT. Distribution mixtures from sampling of inhomogeneous microstructures: variance and probability bounds of the properties. Nucl Engng Des 2002;214:195–204.

[17] Lu B, Torquato S. Lineal-path function for random heterogeneous materials. Phys Rev A 1992;45(2):922–9.

[18] Lu B, Torquato S. Lineal-path function for random heterogeneous materials. 2. Effect of polydispersity. Phys Rev A 1992;45(10): 7292–301.

[19] Lu B, Torquato S. Nearest-surface distribution functions for polydispersed particle systems. Phys Rev A 1992;45(8):5530–44.

[20] Lu B, Torquato S. Chord-length and free-path distribution functions for many-body systems. J Chem Phys 1993;98(8):6473–82.

[21] Torquato S, Lu B. Chord-length distribution function for two-phase random media. Phys Rev A 1993;45(4):2950–3.

[22] Todinov MT. A new approach to the kinetics of a phase transformation with constant radial growth rate. Acta Materialia 1996;44(12):4697–703.

[23] Todinov MT. On some limitations of the Johnson–Mehl–Avrami–Kolmogorov equation. Acta Materialia 2000;48:4217–24.

[24] Kay DC. Graphics file formats, 2nd ed. New York: Windcrest/ McGraw-Hill; 1995.

[25] Rimmer S. Bit-mapped graphics, 2nd ed. New York: Windcrest/ McGraw-Hill; 1993.

[26] Hearn D, Pauline Baker M. Computer graphics: C version. Englewood Cliffs, NJ: Prentice-Hall; 1997.

[27] Foley JD, van Dam A, Feiner SK, Hughes JF. Computer graphics: principles and practice. Reading, MA: Addison-Wesley; 1996.

[28] Bentley J. Programming pearls. Reading, MA: Addison-Wesley; 1986.