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PROBABILISTIC DESCRIPTION OF STOCHASTIC PROCESSES OF STRUCTURAL FAILURE IN ADVANCED POLYDISPERSE COMPOSITES

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Abstract. The aim of this research is to develop new theoretical models and simulation tools for analysis of microstructural stress fields in components of composites with complex stochastic geometry and for prediction of multiscale failure of considered materials during deformation. Non-periodic randomly reinforced composites were studied. Deformation process is characterized with multipoint statistical moments of stochastic stress fields in components of composites. These moments are determined analytically from solution of stochastic boundary-value problems taking into account statistical properties of the microstructure and loading conditions. Geometry of microscopic structure of materials is characterized with high-order multipoint correlation functions.

1 INTRODUCTION

Composites application in high-tech industry is rapidly increasing due to combination of their mechanical properties, for instance, low strength-to-weight ratio, high corrosion and fatigue resistance, good formability at the manufacturing stage. New materials, most suitable for prescribed purposes, loading and conditions of use, can be designed for each specific application [1]. The key parameters, which determine homogenized properties of the material and can be varied during manufacturing and design processes are mechanical and physical properties of the phases and geometrical characteristics of microstructure [1, 4, 9].

The effective homogenized mechanical properties of composites are differ from properties of the distinct phases. Such multiscale hierarchy of composites is typically investigated using the representative volume element (RVE) concept when parameters of larger scale models are measured and calculated on a smaller scale [2, 3].

The urgent question in new composite materials design is developing precise mathematical models that would allow predicting their behavior and could be used for developing recommendations for the optimal combination of microstructure parameters and properties of the phases. Composite materials usually have stochastic microstructure which specifics' description is quite challenging task. Such structural parameters as volume fraction of constituents, shapes, sizes and distribution of inclusions affect significantly effective (homogenized) characteristics of composites [1, 7, 9]. One of the ways to consider these features in mathematical modelling is stochastic approach based on random functions theory [1, 8, 13]. According to such methods, all the equations and relations of the mechanics of composites at the RVE scale have the radius-vector as a variable, so that they can discriminate different constituents of the material. For instance, in order to consider the internal microstructure of the two-component composites, the following indicator function is used [13]:

$$\lambda(\vec{r}) = \begin{cases} 1, \text{if radius-vector } \vec{r} \text{ indicates inclusion} \\ 0, \text{if radius-vector } \vec{r} \text{ indicates matrix} \end{cases} \quad (1)$$

Statistical method are used for estimation of failure inside the RVE, calculation of characteristics of deformation process in phases of materials as well as effective characteristics with due regard for the possible effects brought by microstructure geometry stochastic features.

2 MULTISCALE FAILURE PROBABILITY OF COMPOSITES

Let's consider the RVE of composite as a system of micro-volumes dV. Each of such micro-volumes can be either in fractured or initial state. By analogy with the indicator function (1), the function of microscopic damageability can be introduced to characterize the failure inside the RVE during deformation process [8]:

$$w(\vec{r},t) = \begin{cases} 1, \text{if radius-vector indicates that micro-volume } dV \text{ is fractured} \\ 0, \text{if radius-vector indicates that micro-volume } dV \text{ is not fractured} \end{cases} \quad (2)$$

Assuming that $w(\vec{r},t)$ is ergodic by the radius-vector $\vec{r}$, the failure probability $p(\vec{r},t)$ of micro-volumes dV is equal to mathematical expectation of the function $w(\vec{r},t)$:

$$\left\langle w(\vec{r},t) \right\rangle_{\vec{r}} = p(\vec{r},t) \quad (3)$$

In designing new materials it is important to know which of the phases will subject to fracture mostly under specified loading conditions. The failure probability $p(t)_C$ (where C defines phase of composite) can be calculated for each of the phases:

$$p_C(t) = \int_{\sigma_{\text{limiting}}^{(u)}}^{\infty} f(\sigma_u) d\sigma_u, \quad (4)$$

where σ_u is a failure criterion of the phase, $f(\sigma_u)$ is probability density function of σ_u in RVE, $\sigma_{\text{limiting}}^{(u)}$ is limiting value of the criterion after which the phase constituent will rupture. The geometric sense for the phase failure probability is the area under the $f(\sigma_u)$ function plot limited by the $\sigma_{\text{limiting}}^{(u)}$ value from one side and infinity from another (see Fig. 1).

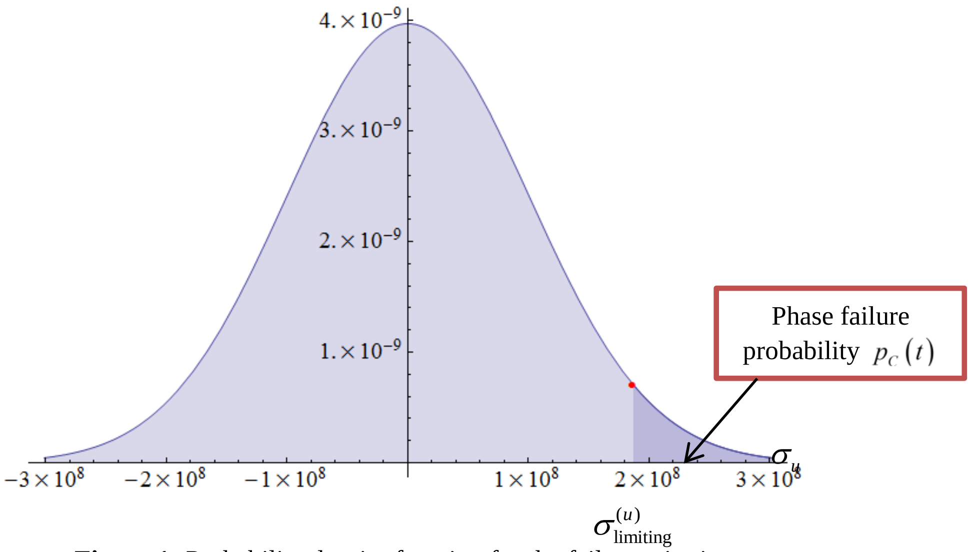

Figure 1: Probability density function for the failure criterion

Hence, to compute the failure probability for the phase on a micro-scale under defined loading of RVE it is essential to set the failure criterion and obtain its probability density function. This function can be reconstructed with first k statistical moments of the failure criterion σ_u [6].

3 STATISTICAL MOMENTS OF MICROSCOPIC STRESS FIELDS

Many conventional failure criteria σ_u depends on the first and second order invariants $j_\sigma^{(1,2)}$ of microscopic stress tensor σ_{ij}. The criterion, for instance, could be the following [8]:

$$\sigma_u^2 + 3(\sigma_c - \sigma_t)\sigma \leq \sigma_t \sigma_c, \tag{5}$$

where σ_t is tensile strength of the phase, σ_c is compressive strength of the phase, $\sigma_u^2 = \sigma_{11}^2 + \sigma_{22}^2 + \sigma_{33}^2 - \sigma_{11}\sigma_{22} - \sigma_{11}\sigma_{22} - \sigma_{22}\sigma_{33} + 3(\sigma_{12}^2 + \sigma_{13}^2 + \sigma_{23}^2)$, $\sigma = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33})$, σ_{ij} are components of micro-stress tensor.

Thus, in order to calculate statistical moments of σ_u we will need statistical moments of the same order for the components of the microscopic stress tensor σ_{ij}:

$$\langle \sigma_{ij} \rangle_C, \ \langle \sigma'_{ij}(\vec{r})\sigma'_{\alpha\beta}(\vec{r}_1) \rangle_C, \ \ldots, \ \langle \sigma'_{ij}(\vec{r})\sigma'_{\alpha\beta}(\vec{r}_1) \ldots \sigma'_{\xi\psi}(\vec{r}_{n-1}) \rangle_C \tag{6}$$

where $\langle \sigma_{ij} \rangle_C$ is mean stress in phase C (first order moment), $\langle \sigma'_{ij}(\vec{r})\sigma'_{\alpha\beta}(\vec{r}_1) \rangle_C$ is dispersion of stress in phase C (second order moment), $\langle \sigma'_{ij}(\vec{r})\sigma'_{\alpha\beta}(\vec{r}_1) \ldots \sigma'_{\xi\psi}(\vec{r}_{n-1}) \rangle_C$ is n-order moment. Values of these moments can be numerically calculated with finite element methods or with boundary-value problem solution for the RVE. The second approach is used in this work. The RVE concept allows to apply the traditional mechanics methods and relations on a micro-scale, where different constituents of the material can be discriminated. Hence, the stochastic boundary-value problem on the RVE scale consists of the following equations [13]:

$$\sigma_{ij,j}(\vec{r})=0, \qquad \varepsilon_{ij}(\vec{r})=\tfrac{1}{2}\left(u_{i,j}(\vec{r})+u_{j,i}(\vec{r})\right),$$
$$\sigma_{ij}(\vec{r})=C_{ijkl}(\vec{r})\varepsilon_{kl}(\vec{r}), \qquad u_i(\vec{r})\big|_{\vec{r}\in\Gamma_V}=\varepsilon^*_{ij}r_j, \tag{7}$$

where $\sigma_{ij}(\vec{r})$ and $\varepsilon_{kl}(\vec{r})$ are microscopic stress and strain fields, $C_{ijkl}(\vec{r})$ is field of structural elasticity modulus, $u_i(\vec{r})$ is field of displacements. The boundary conditions on a surface of the RVE are set in displacements with the constant symmetric tensor of strain ε^*_{ij} and presume uniformity of the macroscopic deformation.

One of the simplified ways for obtaining the probability density function $f(\sigma_u)$ is to assume the normal distribution of σ_u criterion:

$$f(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \tag{8}$$

where μ is mean of distribution, σ^2 is dispersion. With such assumption the failure probability can be calculated with only two first moments (mean value and dispersion) of σ_u and, consequently, of two first moments of stress fields in the phases. Analytically, these moments (6) depend on solution of the boundary-value problem as well as on high order correlation functions $K^{(n)}_{\lambda}(\vec{r},\vec{r}_1,...,\vec{r}_n)=\langle\lambda'(\vec{r})\lambda'(\vec{r}_1)...\lambda'(\vec{r}_{n-1})\rangle$ for the RVE of the considered material [11, 12]:

$$\left\langle\sigma_{ij}\right\rangle_C=F\left(\left\langle\varepsilon_{ij}\right\rangle_C,\left\langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r}_1)\right\rangle_C,\left\langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\right\rangle_{RVE},K^{(n)}_{\lambda'}(\vec{r},\vec{r}_1,...,\vec{r}_{n-1}),u'^{(\chi)}_{i,j}(\vec{r})\right) \tag{9}$$

$$\left\langle\sigma'_{ij}(\vec{r})\sigma'_{\alpha\beta}(\vec{r}_1)\right\rangle_C=F\left(\left\langle\varepsilon_{ij}\right\rangle_C,\left\langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\right\rangle_C,\left\langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\right\rangle_{RVE},K^{(n)}_{\lambda'}(\vec{r},\vec{r}_1,...,\vec{r}_{n-1}),u'^{(\chi)}_{i,j}(\vec{r})\right) \tag{10}$$

where stroke ' denotes fluctuation of a field towards its mean value: $\varepsilon'_{ij}(\vec{r})=\varepsilon_{ij}(\vec{r})-\langle\varepsilon_{ij}(\vec{r})\rangle$, $\sigma'_{ij}(\vec{r})=\sigma_{ij}(\vec{r})-\langle\sigma_{ij}(\vec{r})\rangle$, $u'_m(\vec{r})=u_m(\vec{r})-\langle u_m(\vec{r})\rangle$, $\lambda'(\vec{r})=\lambda(\vec{r})-\langle\lambda(\vec{r})\rangle$, angle brackets $\langle\ \rangle$ denote volume averaging.

The values of correlation functions were obtained for each model of RVE geometry. These functions are used in analytical expressions if the appropriate approximating expression for them is found. This question was studied in [11].

In elastic case, the boundary-value problem (7) has the following solution in displacements [10, 12]:

$$u'_{i,a}(\vec{r})=e_{kl}C^{(M)}_{jnkl}\int_{V_1}G_{ij,\alpha}(\vec{r},\vec{r}_1)\left(\lambda'(\vec{r}_1)\right)_{,1n}dV_1, \tag{11}$$

where $,\alpha$ stands for d/dx_{α}, $G_{ij,\alpha}\left(\vec{r},\vec{r}_1\right)$ is the Green's function [1, 10], $C^{(M)}_{jnkl}$ is tensor of structural elasticity modulus of matrix, e_{kl} is macroscopic strain tensor equal to ε^{*}_{ij}.

The solution (11) substituted in the strain-displacement equations $\varepsilon'_{i\alpha}\left(\vec{r}\right)=1/2\left(u'_{i,a}(\vec{r})+u'_{\alpha,\mathrm{i}}(\vec{r})\right)$ allows to obtain the analytical expressions for the statistical moments (9) and (10).

Eqs. (9) and (10) contain also moments of strain fields:

$$\left\langle \varepsilon_{ij}\right\rangle_C = F\left(\left\langle \varepsilon'_{ij}\left(\vec{r}\right)\varepsilon'_{\alpha\beta}\left(\vec{r}\right)\right\rangle_{RVE}, K^{(\mathrm{n})}_{\lambda'}(\vec{r},\vec{r}_1,...,\vec{r}_{n-1}), u'^{(\chi)}_{i,j}(\vec{r})\right) \tag{12}$$

$$\left\langle \varepsilon'_{ij}\left(\vec{r}\right)\varepsilon'_{\alpha\beta}\left(\vec{r}\right)\right\rangle_C = F\left(\left\langle \varepsilon'_{ij}\left(\vec{r}\right)\varepsilon'_{\alpha\beta}\left(\vec{r}\right)\right\rangle_{RVE}, K^{(\mathrm{n})}_{\lambda'}(\vec{r},\vec{r}_1,...,\vec{r}_{n-1}), u'^{(\chi)}_{i,j}(\vec{r})\right) \tag{13}$$

where $\left\langle \varepsilon'_{ij}\left(\vec{r}\right)\varepsilon'_{\alpha\beta}\left(\vec{r}\right)\right\rangle_{RVE}$ is moment of micro-strain field in the whole RVE.

Eqs. (9) and (10) are directly used in averaging of Eq. (5). The details of boundary-value problem solution method as well as procedures of statistical moments (6) values calculation in elastic and elastoplastic cases are described in [10, 11].

4 POROUS MATERIALS FAILURE ESTIMATION

The implementation of such methodology can be demonstrated on the example case of porous matrix composites, in which inclusions are considered vacuum. In application to such type of materials, this methodic can be used for calculation of matrix failure probability on a micro-scale. In this work some specific porous material were considered, which matrix mechanical properties matches the ceramics (alumina porcelain) properties:

$$\nu_M = 0.3,\ E_M = 3.5\times10^2\,\mathrm{GPa},\ \sigma_c = 0.205\,\mathrm{GPa},\ \sigma_t = 0.170\,\mathrm{GPa}, \tag{14}$$

where ν_M is Poisson ratio, E_M is modulus of elasticity, σ_t is tensile strength of the matrix, σ_c is compressive strength of the matrix.

The RVE microstructure geometry model has been defined as a cube with polydesperse spherical inclusions (pores), as shown on Fig. 2:

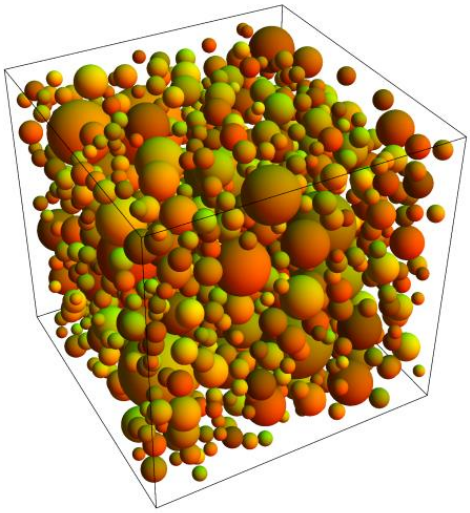

Figure 2: Model of a stochastic structure with spherical inclusions

The synthesis of such structures was performed using the Hard-Core Model [5]. The characteristics of some of the studied structures are presented in Table 1.

Table 1: Geometrical parameters of the synthesized structure models

Volume fraction, p	Number of inclusions	Minimal radius of inclusion	Maximal radius of inclusion
0.30	976	4.0	27.0
0.40	1456	5.0	9.0
0.50	2000	4.0	14.0

The simple shear boundary conditions for the RVE were considered. The components of the tensor ε_{ij}^{*} in (7) had the following values:

$$\varepsilon_{12}^{*} = \begin{pmatrix} 0 & 5\times10^{-8} & 0 \\ 5\times10^{-8} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{15}$$

With these loading conditions, microstructure parameters and matrix properties, the values of statistical moments (9) and (10) can be calculated using boundary-value problem solution (11). The results are presented in Table 2, only for components with index combination $i=1,\ j=2$. The others components are considered negligible.

Table 2: Statistical characteristics of stress field in matrix

Pores volume fraction	Mean stress in matrix, Pa $\left\langle \sigma_{12} \right\rangle_M$	Dispersion of stress in matrix, Pa $\left\langle \sigma'_{12}\sigma'_{12} \right\rangle_M$
0.30	9686.76	1.80×10^7
0.40	8381.21	3.33×10^7
0.50	7051.20	5.27×10^7

The transition to the failure criteria (5) gives the results for the mean value and dispersion of σ_u, matrix failure probability according to the normal distribution (see Table 3).

Table 3: Failure criterion statistical characteristics and failure probability

Pores volume fraction	Mean of distribution, Pa $M\left[\sigma_u\right]$	Dispersion of distribution, Pa $D^{(2)}\left[\sigma_u\right]$	Matrix failure probability, p_M
0.30	16778	5.41×10^7	0.001
0.40	14516.7	1.00×10^8	0.029
0.50	12213	1.58×10^8	0.117

The results showed that for the considered materials the matrix failure probability significantly increases with growth of pores volume fraction, while mean stress in matrix decrease.

In general case, the described mathematical model allows to calculate the failure probability of phases of the two-component materials in dependence of stress-strain state of the RVE, mechanical properties of the matrix and internal stochastic geometry of microstructure.

5 CONCLUSIONS

- Described stochastic methods allow to perform the probability analysis of failure of randomly reinforced composites. Using the RVE concept, deformation process can be studied at a microscopic level, in each of the phases. The microstructure details were taken into account by means of high order correlation functions.
- To determine the characteristics of microscopic stress fields, the stochastic boundary-value problem solution was obtained. Deformation is defined by setting the loading conditions at the boundaries of the RVE.
- The failure probability estimation for the distinct phases and whole RVE depend on failure criteria, probability density function of which is expressed through the statistical moments of micro-stress fields.
- This approach was applied to porous ceramics composites. The case of simple shear state of strain was studied for which the numerical results for statistical characteristics of stress and failure probability were obtained.

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REFERENCES

[1] V. Buryachenko, *Micromechanics of heterogeneous materials*, 1st ed., Springer, New York (2007).

[2] Hill, R., Elastic properties of reinforced solids: some theoretical principles. *Journal of the Mechanics and Physics of Solids*, 11 (1963): 357–372.

[3] Kanit, T., Forest, S., Galliet, I., Mounoury, V., Jeulin, D., *Determination of the size of the representative volume element for random composites: statistical and numerical approach*, International Journal of Solids and Structures, 40 (2003): 3647–3679.

[4] M.M. Kaminski, *Computational Mechanics of Composite Materials,* Springer, 2005.

[5] P. Kanouté, D.P. Boso, J.L. Chaboche, B.A. Schrefler, *Multiscale Methods for Composites: A Review*, Arch. Comput. Methods. Eng. 16 (2009): 31–75.

[6] M.G. Kendall, A. Stuart, *The Advanced Theory of Statistics*, Griffin, Vol. 1 (1967).

[7] V.V. Silberschmidt, *Account for random microstructure in multiscale models*. In: *Multiscale Modeling and Simulation of Composite Materials and Structures*. Eds. Y.W. Kwon, D.H. Allen and R. Talreja. Springer, New York (2008): 1-35.

[8] Y. Sokolkin, A. Tashkinov, *Mechanics Of Deformation And Fracture Of Structurally Heterogeneous Media*, Nauka, Moscow (1984) (in Russian).

[9] S. Torquato, *Random Heterogenous Materials, Microstructure And Macroscopic Properties*, Springer-Verlag (2001).

[10] M. A. Tashkinov, V. E. Vildeman, N. V. Mikhailova, *Method Of Successive Approximations In A Stochastic Boundary-Value Problem In The Elasticity Theory Of Structurally Heterogeneous Media*, Composites: Mechanics, Computations, Applications, An International Journal 2(1), (2011): 21–37.

[11] Mikhail Tashkinov, *Statistical characteristics of structural stochastic stress and strain fields in polydisperse heterogeneous solid media*, Computational Materials Science (2014). DOI: 10.1016/j.commatsci.2014.01.050.

[12] M. Tashkinov, *Multipoint approximations of stochastic elastic boundary value problem for polydisperse composites,* Proceedings of 6th European Congress on Computational Methods in Applied Sciences and Engineering, Vienna (2012).

[13] V.E. Wildemann, Y.V. Sokolkin, A.A. Tashkinov, *Nonelastic Deformation and Fracture Mechanics of Composition Materials*, Nauka, Moscow (1997) (in Russian).