Multiscale Modeling of Strength Properties of Dispersion-Reinforced Ceramic Composite Materials

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Abstract. In this work a three-level model of ceramic composites materials based on a reaction bonded silicon carbide is developed. Numerical solution is based on the method of multiscale homogenization along with the finite element method. As a result a series of local problems on the periodical cells of 3 structure levels are solved. The calculations of stress concentration tensors in matrixes and weighing materials are presented. New criteria for matrixes and weighing materials is used to calculate the strength properties in multiaxis stressed condition. This criteria includes essential differences (more than an order of magnitude) of ceramic properties under straining and compression. The model which includes scale effect of strength of ceramic composite materials is proposal. The computational research of sequential micro-destruction processes of ceramic composite until complete destruction is done. The results show that changing of concentration of larger fractions is less significant then content of smaller fractions in the presence of polydisperse structure in ceramics.

Keywords: ceramic composites, reaction bonded SiC, microdestruction, numerical simulation, finite-element method, multiscale homogenization method, strength criterion, stress concentration tensor, scale strength effect

1 Introduction

Composite materials based on reaction bonded silicon carbide matrix (RBSiC) and SiC disperse filler are perspective materials for creation of shockproof protecting systems because of their high strength, stiffness, destruction energy and relatively low cost. However characteristics of this materials significantly depend on manufacturing technological processes and on receipt of composite components. In addition during the hardening details can give strong shrink, giving significant residual stresses. This residual stresses can give deformation and even breakdown in the final product. To select the optimal content of ceramic composite components of SiC system and to calculate strength properties of such materials it is demanded to develop special mathematic model, which can forecast strength properties of composite materials including variation of content, form and disperse filling. This model also should take into account locked-up stresses, appearing in ceramic composite during agglomeration of particles.

Existing analytical and numerical models of composite materials, armed with particles, allow to forecast elastic properties with certain precision, however numerical calculation of strength properties is essentially more complex problem, because it is necessary to build the appropriate model of microcrack emission in heterogeneous structure. Attempts to build such models using simple concentration of finite-element mesh were not successful, because of dramatic increase of non-physical singularity effect of calculation. Widely known commercial software not always allow to get adequate results of microdestruction modeling of composite.

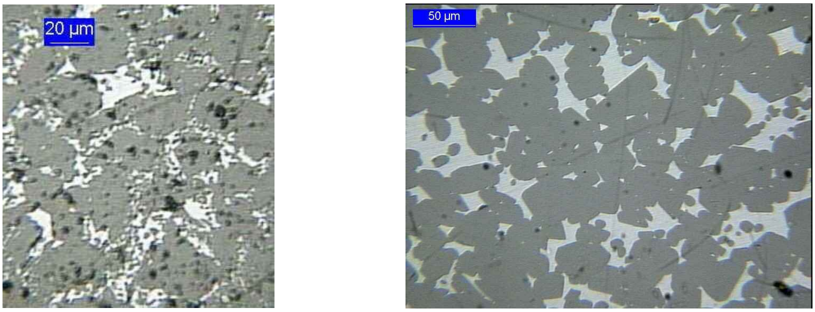
Nowadays the great attention is paid to the development of numerical finite element methods of microstress modeling in composites [4, 18, 21]. One of the most efficient method for calculation of microstress in composites is the method of asymptotic averaging (MAA) (or homogenization method) [2, 3, 5, 23, 25], which ensures the high accuracy of calculation of microdestruction in mathematical terms. Possible errors of calculation by this method can be related only to errors of its numerical application as well as to inaccurate specifications of the component characteristics and the microstructure geometry. In [1, 6–8, 13] algorithms of finite element solution of the so-called local problems in periodicity cells, which appear when MAA is used, were developed.

This work continues the development cycle [14, 16, 17, 20] of creating models and numerical methods for modelling microdestruction processes in composite materials. The new 3-level strength model of ceramic composite is presented. This model is based on RBSiC and allows to describe the effect of strengthening of composite material during the changing particles content of SiC including the production technology of its manufacturing.

2 Microstructure of the reaction bonded silicon carbide composite

A composite based on reaction bonded silicon carbide consists of a filler and a silicon carbide matrix. The filler is powder of silicon carbide of the different fractions. The silicon carbide matrix is synthesized by chemical reaction of liquid silicon, carbon and solid carbon, which is produced during the pyrolysis of phenol-formaldehyde resin [22, 24]. The filler is, as a rule, fission fragments which have random character and big difference in fractions. Generally it can be identified large fractions of the size of 20-100 microns and small fractions of 1-10 microns. Photographies of real microstructure of RBSiC are shown in Fig. 1.

We consider a model of reaction bonded silicon carbide composite material which has three structure levels [5, 15, 6, 19, 26] (Fig 2). The first level is formed by the periodicity cells 1 (PC1) consisting of a filler of a coarse fraction and a matrix m_1. On the second level the matrix m_1 is formed by the periodicity



a) b)

Fig. 1. The microstructure of the material with the original grains of silicon carbide of 28 microns.

cells 2 (PC2), each of them consists of a filler of a fine-grained fraction and a reaction bonded silicon carbide matrix m_2. The matrix m_2 has defects, for example, high concentration of dissolved, but unreacted component C and Si, microcracks due to technological stresses and mainly pores. So, we introduce the third structural level formed by the periodicity cells 3 (PC3). Each periodicity cell of type 3 is formed by a zero defect silicon carbide matrix m_3 and a defect.

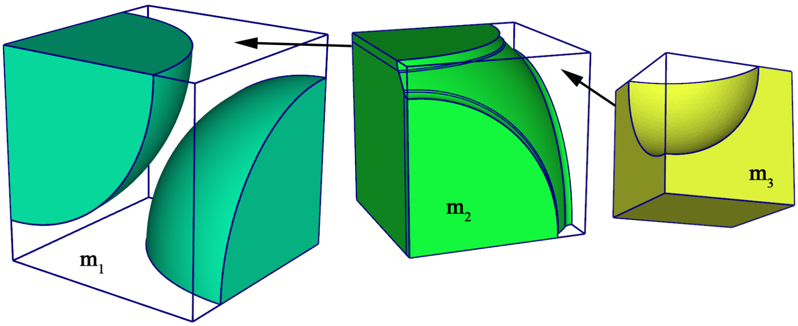


Fig. 2. The three level structure of silicon carbide ceramics.

3 Mathematical formulation of local problems

All structural levels may be considered as independent according to the method of multiscale homogenization [17]. At first we compute the effective elastic and strength properties of the third level, then we calculate the effective characteristics of the second level, considering the composite matrix m_2 as a homogeneous material with effective characteristics of the third level, and then we calculate the characteristics of the first level.

Consider the solution of local problems for the periodicity cell of the second level having the volume V_ξ. It includes the matrix m_2 and fine-disperse filler. We believe that the PC2 has three-axial symmetry, therefore instead of a full volume of PC2 V_ξ we can consider its 1/8th part of volume $\tilde{V}_\xi$. This volume $\tilde{V}_\xi$ consist of the N components: $N-1$ pieces of fine-disperse particulate of filler of the volume $\tilde{V}_{\xi\alpha}$, $\alpha = 1...N-1$, and binding matrix m_2 ($\alpha = N$). For calculating microstresses in PC2 by homogenization method [15, 11, 12] we formulate a series of the so-called local problems L_{pq} of the elasticity theory on the 1/8th part of the periodicity cell

$$\begin{cases} \sigma_{ij(pq)/j} = 0, \quad \tilde{V}_\xi \\ \sigma_{ij(pq)} = C_{ijkl}(\xi_s, z)(\varepsilon_{kl(pq)} - \alpha_{kl}(\theta - \theta^*)), \quad \tilde{V}_\xi \cup \Sigma'_s \cup \Sigma_s \\ \varepsilon_{ij(pq)} = \frac{1}{2}\left(U_{i(pq)/j} + U_{j(pq)/i}\right), \quad \tilde{V}_\xi, \\ [U_{i(pq)}] = 0, \ [\sigma_{ij(pq)}]n_j = 0, \quad \tilde{\Sigma}_{\xi\alpha N}, \end{cases} \tag{1}$$

where p and q are the indexes of the local problems changing from 1 to 3 (there are a total of nine different problems L_{pq}); $U_{i(pq)}\,(\xi_s)$ are the components of the displacement vectors (the unknown functions) in the problem L_{pq}; $\sigma_{ij(pq)}$, $\varepsilon_{ij(pq)}$ are the components of the stress and deformation tensors in $\tilde{V}_\xi$; ξ_s are the local Cartesian coordinates in the 1/8th PC; $_{/i} = \partial/\partial\xi_i$ are the derivatives of the local coordinates; $\left[U_{i(pq)}\right]$ are the jumps of functions at the interface $\tilde{\Sigma}_{\xi\alpha N}$ of the cell components; $C_{ijkl}(\xi_s, z)$ are the components of the tensors of the elasticity moduli of the composite structural components of PC2 (they are described by the dependencies of the coordinates ξ_s); z is the parameter of the component damageability; $\alpha_{kl}\,(\theta)$ are the components of the tensor of thermal expansion, which depend on the temperature; θ is the current temperature; $\theta^*(\xi_s)$ is the sintering temperature of the ceramic particles, depending on the local coordinates.

System (1) is supplemented by the special boundary conditions at the surfaces $\Sigma'_s = \{\xi_s = 0.5\}$ of the 1/8th part of PC

$$\begin{array}{llll} at\ \Sigma_i^{'}: & U_{i(pp)} = 1/2\bar{\varepsilon}_{pp}\delta_{ip}, \quad S_{j(pp)} = 0, \quad S_{k(pp)} = 0, & i \neq j \neq k \neq i, \\ at\ \Sigma_j^{'}: & U_{i(pq)} = (1/4)\bar{\varepsilon}_{ip}\delta_{ip}, \quad S_{j(pq)} = 0, \quad U_{k(pq)} = 0, & i, j = \{p, q\}, \\ at\ \Sigma_k^{'}: & S_{i(pq)} = 0, \quad S_{j(pq)} = 0, \quad U_{k(pq)} = 0, & i \neq j \neq k \neq i, \end{array} \tag{2}$$

where $\bar{\varepsilon}_{pq}$ are the components of the averaged deformation tensor for PC, $S_{i(pq)} \equiv \sigma_{il(pq)}n_l$ are the vectors of forces.

The boundary conditions at the symmetry planes $\Sigma_s = \{\xi_s = 0\}$ are similar to relations (2), where we assume $\bar{\varepsilon}_{pq} = 0$.

4 Effective elastic characteristics of the periodicity cells of the second level structure

Using the numerical solution of problems L_{pq} (1), (2) we find the fields of displacements $U_{i(pq)}$ and stresses $\bar{\sigma}_{ij(pq)}(\xi_s)$ in the PC2 at given values of average deformations $\bar{\varepsilon}_{kl}$.

These fields are used to find the average values of stress:

$$\bar{\sigma}_{ij} =< \sigma_{ij} >= \sum_{p,q}^{3} \bar{\sigma}_{ij(pq)},$$

where

$$\bar{\sigma}_{ij(pq)} = \left\langle \sigma_{ij(pq)} \right\rangle = \int\limits_{\tilde{V}_\xi} \sigma_{ij(pq)}(\xi_s) dV_\xi. \tag{3}$$

Then the components of the tensor of effective elasticity moduli of the composite are calculated by the formulas

$$\bar{C}_{ijpq} = \frac{\bar{\sigma}_{ij(pq)}}{\bar{\varepsilon}_{pq}}, \tag{4}$$

where there is no summation over p and q. After that we calculate the effective tensor of elastic compliances $\bar{\Pi}_{ijpq}$, that is inverse to $\bar{C}_{ijpq}$, and technical elastic constants of the composite, such as effective Young moduli $E_\alpha = 1/\bar{\Pi}_{\alpha\alpha\alpha\alpha}$, effective Poisson constants $v_{\alpha\beta} = -\bar{\Pi}_{\alpha\alpha\beta\beta} E_\alpha$, and effective shear moduli $G_{\alpha\beta} = \bar{C}_{\alpha\beta\alpha\beta}$.

The components of the tensor of stress concentrations $B^{(\alpha)}_{ijkl}$ connect microstresses $\sigma^{(\alpha)}_{ij}(\xi_s) = \sum\limits_{p,q}^{3} \sigma_{ij(pq)}(\xi_s)$ in the matrix and the filler (the fine disperse particles SiC) with average stresses $\bar{\sigma}_{kl}$ in the PC2 by the formulas

$$\sigma^{(\alpha)}_{ij}(\xi_s) = B^{(\alpha)}_{ijkl}(\xi_s)\bar{\sigma}_{kl}, \quad \xi_s \in \tilde{V}_{\xi\alpha}, \quad \alpha = 1...N. \tag{5}$$

The components $B^{(\alpha)}_{ijkl}$ in the matrix and the filler are calculated by the formulas

$$B^{(\alpha)}_{ijkl}(\xi_s) = \sigma_{ij(pq)}(\xi_s)\bar{\Pi}_{pqkl}, \quad \xi_s \in \tilde{V}_{\xi\alpha}, \quad \alpha = 1...N. \tag{6}$$

5 Model of the strength properties of the components

The strength criterion of ceramic materials should take into account the significant differences in their properties in tension and compression. Therefore, we introduce a failure criterion of isotropic matrix m_2 and filler particles [19] based on Pisarenko-Lebedev criterion:

$$z = \frac{\sigma_u^{(\alpha)2}}{3\sigma_S^{(\alpha)2}(1 + B^{(\alpha)} V(\sigma_-^{(\alpha)}))}, \tag{7}$$

where $\sigma_-^{(\alpha)} = \frac{1}{2}\left(\left|\sigma^{(\alpha)}\right| - \sigma^{(\alpha)}\right)$, $\sigma^{(\alpha)} = \sigma^{(\alpha)}_{11} + \sigma^{(\alpha)}_{22} + \sigma^{(\alpha)}_{33}$ are the invariants of the stress tensor in the matrix and fillers, $\sigma_u^{(\alpha)}$ are stress intensity [10], $B^{(\alpha)} = \left(\frac{\sigma_C^{(\alpha)2}}{3\sigma_S^{(\alpha)2}} - 1\right)\frac{1}{\sigma_C^{(\alpha)}}$ is the constant, $\sigma_C^{(\alpha)}, \sigma_T^{(\alpha)}, \sigma_S^{(\alpha)}$ are the ultimate compression strength, ultimate tensile strength and ultimate shear strength. For ultimate strengths the following relationships should be taken into account: $\sigma_C > \sqrt{3}\sigma_S$, $\sigma_C > 0, \sigma_S > 0$. In (7) a continuous positive function of the 1st invariant $V(\sigma_-^{(\alpha)})$ is introduced

$$V(\sigma_-^{(\alpha)}) = \begin{cases} 0, & \sigma^{(\alpha)} > 0, \\ -\sigma^{(\alpha)}, & -\sigma_C^{(\alpha)} < \sigma^{(\alpha)} < 0, \\ \sigma_C^{(\alpha)}, & \sigma^{(\alpha)} < -\sigma_C^{(\alpha)}. \end{cases} \quad (8)$$

The failure criterion z, which is calculated by the formula (7), has the value 0 if the stress is absent in the composite. It is ranged within $0 < z(\sigma_{ij}^{(\alpha)}) \leq 1$ in the loaded condition if there is not damage. And it takes the values $z(\sigma_{ij}^{(\alpha)}(\xi_s)) \geq 1$, if the fracture initiation occurs at some point ξ_s. If the failure criterion reaches the value $z = 1$, then we obtain strength surface of a component

$$\sigma_u^{(\alpha)2} = 3\sigma_S^{(\alpha)2}(1 + B^{(\alpha)}V(\sigma_-^{(\alpha)})). \quad (9)$$

In the tensile area $\sigma^{(\alpha)} > 0$ the strength surface is the von Mises ellipsoid $\sigma_u^{(\alpha)2} = 3\sigma_S^{(\alpha)2}$. In the compression area $-\sigma_C^{(\alpha)} < \sigma^{(\alpha)} < 0$ the tensile strength is increased. And in the "supercompression" area $\sigma^{(\alpha)} < -\sigma_C^{(\alpha)}$ the strength surface again is the von Mises ellipsoid, but with the modified tensile strength: $\sigma_u^{(\alpha)2} = \sigma_C^{(\alpha)2}$.

If the condition $z(\sigma_{ij}^{(\alpha)}(\xi_s)) \geq 1$ is satisfied at the point ξ_s or in a certain area PC2, there is no complete destruction. This is partial destruction of PC2, hereinafter called microdestruction. Introduce the dependence of the components of the elastic modulus of the failure criterion for accounting microdestruction of components in the model:

$$C_{ijkl}(\xi_s, z) = (1 - h(z(\sigma_{ij}^{(\alpha)}(\xi_s) - 1))C_{ijkl}^{(\alpha)}, \quad \xi_s \in \tilde{V}_{\xi\alpha},\ \alpha = 1...N, \quad (10)$$

where $C_{ijkl}^{(\alpha)}$ are the components of the tensor of elasticity moduli of the composite components (they are constants). According to the formula (10) if microdestruction occurs at the point ξ_s, elasticity modulus is equal to zero at this point.

To calculate the strength of the composite as a whole, we need to calculate the limit values of average stresses $\bar{\sigma}_{kl}$. At this stresses an initial microdestruction occurs at least in one of its components (fillers or matrix) in a point $\xi_s^* \in \tilde{V}_\xi$ at a time t^*, and then complete destruction occurs. For the calculation of limit values of stresses in experimental research usually implement a process of linear load, in which the average stresses are proportional the time: $\bar{\sigma}_{kl}(t) = \tilde{\sigma}_{kl}t$, where $\tilde{\sigma}_{kl}$ are the components of the stress gradient tensor. Substituting (5) in the strength criterion of the matrix or fillers (7) we obtain the initial failure condition of composite

$$\max_{\xi_s \in \tilde{V}_\xi} \{z(B_{lnkm}^{(\alpha)}(\xi_s)\bar{\sigma}_{km}(t^*))\} = 1, \quad (11)$$

where $\xi_s = \xi_s^*$ are coordinates of the point in the PC2, t^* is the time point at which the condition (11) is executed first, $\bar{\sigma}_{km}(t^*)$ are limit stresses.

After appearance of the initial failure elastic moduli are changed in the destroyed areas of the matrix and/or fillers in accordance with the model described above. With further increase in average stress values $\bar{\sigma}_{km}(t)$ failure condition (11) is satisfied in a large number of points of PC2, that is, there is the process of propagation of microdestruction. Some area $V_{\xi}^{*}(t)$ of the partial destruction of the composite is formed in the periodicity cell 2.

For modeling of effective elastic and strength properties of PC3 and PC1 is used a similar method. The stresses occur due to the thermal strain $\varepsilon_{kl}^{0} = \alpha_{kl}\,(\theta - \theta^{*})$ of the ceramic composite during cooling after the laser sintering.

6 Details of numerical simulation

The local tasks (1), (2) are solved by a finite element method which is described in [16, 17, 20]. We use 4-node tetrahedral finite elements, generated by open-source grid generators. The meshes contain different numbers of nodes (from 10^4 to 10^6). Meshes with a large number of finite elements are used in the calculation of effective elastic moduli, when micro destruction is not happened. After microdestruction is beginning, the local tasks become nonlinear, because the elastic modulus of the matrix or fillers is changed, so we use iterative method to solve it. The number of iterations to achieve complete destruction is about 10^3, so for these tasks we use meshes with a smaller number of elements to reduce the time of the numerical experiments. A numerical solution of large systems of linear algebraic equations, preprocessing and postprocessing, including 3D visualization and animation, was implemented in the software package, developed by the scientific and educational center "Supercomputer Engineering Simulation and Development of Software Packages" of the Bauman Moscow State Technical University.

7 Results

7.1 Numerical simulation of microdestruction of ceramics for periodicity cell of the third level

Consider the numerical simulation of microdestruction of ceramics for periodicity cell of the third level with the following properties of SiC matrix m_3: elastic modulus $E_m = 320$ GPa, Poisson's ratio $\nu_m = 0.35$, ultimate strength $\sigma_{Tm}^{0} = 0,07$ GPa; $\sigma_{Cm}^{0} = 4$ GPa; $\sigma_{Sm}^{0} = 0,06$ GPa. We suppose that the pores have a spherical shape. Fig. 3 shows some of the results of microstresses calculations in the PC3. Fig. 3a) shows the distribution of component $B_{1111}^{(\alpha)}$ of the stress concentration tensor in the PC3, where concentration of pore before the start failure is equal to 20%. Fig. 3b) shows the distribution of parameter of damage z in the PC3 under tension in the direction of Ox_1.

Fig. 4 shows the process of microdestruction in the PC3 (matrix with defect) under compression. The failure of the periodicity cell starts on the surface of the pore (defect) and at first is spread in a direction perpendicular to load direction,

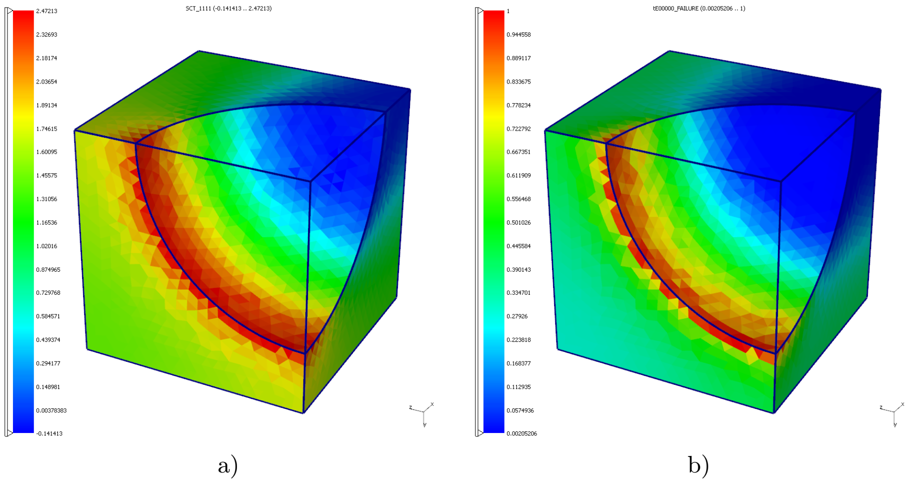


Fig. 3. a) Distribution of the components $B^{(\alpha)}_{1111}$ of the stress concentration tensor in the PC3 (before the start of failure); b) distribution of the parameter of damage z in the PC3 under tension in the direction of Ox_1.

and then the failure zone is turned round and spread in the direction of load action to complete destruction of PC3.

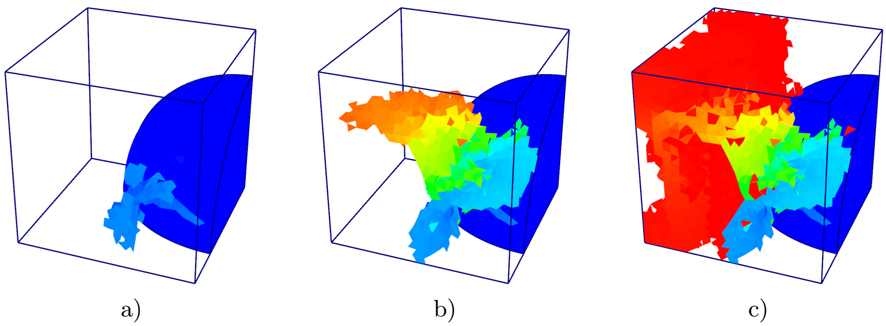


Fig. 4. The process of microdestruction of PC3 (matrix with defect) depending on compressive stress.

7.2 Numerical simulation of microdestruction of ceramics for periodicity cell of the second level

Fig. 5 shows the results of numerical solution of the process of microdestruction in the periodicity cell of the second level under compression. These results are calculated taking into account initial technological stresses, which occurs from the application of laser sintering.

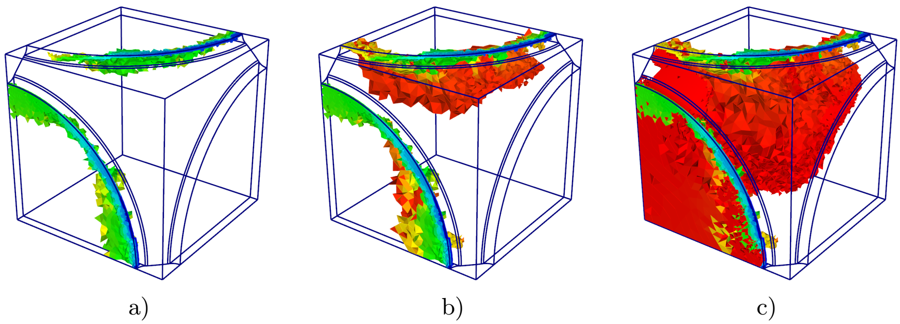


Fig. 5. The process of microdestruction of PC2 under compression taking into account initial technological stresses.

Figure 6 shows the tensile strength of ceramic material depending on concentration of coarse-grained fractions of SiC particle taking into account initial technological stresses.

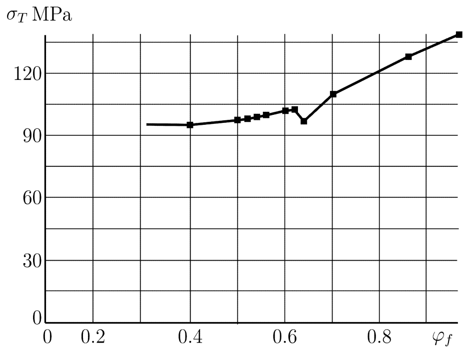


Fig. 6. The tensile strength of ceramic material depending on concentration coarse-grained fractions of SiC particle taking into account initial technological stresses.

8 Conclusions

A mathematical model of microdestruction of reaction bonded silicon carbide has been developed. This model is based on the homogenization method and the finite element method for solution of local problems on periodicity cells. The new strength criterion of ceramic materials has been applied. The comparison with experimental data has shown that this criterion is applicable to solve the problem of microdestruction of the reaction-bonded silicon carbide. It is demonstrated that the developed model allows to simulate the processes of microdestruction of the ceramic composite and can be used as a tool for research and design of new materials with specified properties.

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