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Probabilistic Approach for Analysis of Strength of Ceramics With Different Porous Structure Based on Movable Cellular Automaton Modeling

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Abstract

Movable cellular automaton method which is a computational method of particle mechanics is applied to simulating uniaxial compression of 3D porous ceramic specimens. Pores were considered explicitly by removing automata selected randomly from the original fcc packing. Distribution of pores in space, their size and the total fraction were varied. For each values of porosity there were generated several represented specimens with individual pore position in space. The resulting values of elastic modulus and strength of the specimens were scattered and well described by the Weibull distribution. We showed that to reveal dependence of the elastic and strength properties on porosity it is much better to consider not average of the values for the specimens of the same porosity, but the mathematical expectation of the corresponding Weibull distribution. It is shown that relation between mechanical properties of the material and its porosity depends significantly on pore structure. Namely, percolation transition from closed porosity to interconnected pores strongly manifests itself on strength dependence on porosity. Thus, the curve of strength versus porosity fits different equations for different kind of pore structure. Composite ceramics which pores are filled by plastic filler shows the similar behavior.

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Keywords: Ceramics; pore structure; elastic modulus; strength; simulation; Weibull analysis

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1. Introduction

The problem of predicting the physical and mechanical properties of ceramic materials as depending on their porosity have a long history. It has been solved by many authors in various statements, but is still not completely understood and therefore relevant. The complexity of this problem consists, first of all, in the fact that the properties of real materials are mainly determined by their multiscale structure. Modern production technology of ceramics is capable to create materials with a very complex structure both of the porous space and the matrix itself, which in fact provides the material with high functional properties. For analytical solution of this problem the most successful approaches are the micromechanics of composites, which is based on the method of self-consistent field (definition of the property contribution tensor) as shown by Kachanov and Sevostianov (2013), and the method of random functions (Vildeman et al., 1997). However, these approaches allow predicting only the properties that determine propagation of disturbances of various types: elastic, thermal and electromagnetic. Regarding the strength, the capability of these approaches is limited essentially to the periodic structure materials. It has to be noted, that experimental determination of strength properties of the materials produces a large scatter of data, which is caused not only by the heterogeneity and complexity of the material structure, but technical reasons also. Taking into account all the aspects mentioned above, one may conclude that to solve this problem it is promising to use computer simulation and statistical analysis.

2. Description of the Model

At present, the methods mainly used for simulating the mechanical behavior of materials are numerical methods of continuum mechanics (namely, the finite element method). However, recently the methods based on discrete representation of material have been successfully being developed and widely used. For example, the method of movable cellular automata (MCA) is a new and effective method in discrete computational mechanics, which assumes that the material consists of a set of elementary objects (automata), interacting with the forces determined in accordance with the rules of many-particle approach. MCA allows one to simulate mechanical behavior of a solid at different scales, including deformation, initiation and propagation of damages, fracture and further interaction of fragments after failure as shown by Shilko et al (2015) and Smolin et al. (2015). In MCA, the automaton motion is governed by the Newton-Euler equations:

$$\begin{cases} m_i \frac{d^2 \mathbf{R}_i}{dt^2} = \sum_{j=1}^{N_i} \mathbf{F}_{ij}^{\text{pair}} + \mathbf{F}_i^{\Omega}, \\ \hat{J}_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{N_i} \mathbf{M}_{ij}, \end{cases} \quad (1)$$

where \mathbf{R}_i , $\boldsymbol{\omega}_i$, m_i and \hat{J}_i are the location vector, rotation velocity, mass and moment of inertia of i th automaton, respectively; $\mathbf{F}_{ij}^{\text{pair}}$ is the interaction force of the pair of i th and j th automata; and \mathbf{F}_i^{Ω} is the volume-dependent force acting on i th automaton and depending on the interaction of its neighbors with the remaining automata. In the latter equation, $\mathbf{M}_{ij} = q_{ij}(\mathbf{n}_{ij} \times \mathbf{F}_{ij}^{\text{pair}}) + \mathbf{K}_{ij}$, where q_{ij} is the distance from the center of i th automaton to the point of its interaction (“contact”) with j th automaton, $\mathbf{n}_{ij} = (\mathbf{R}_j - \mathbf{R}_i)/r_{ij}$ is the unit vector directed from the center of i th automaton to the j th one and r_{ij} is the distance between automata centers (Fig. 1), \mathbf{K}_{ij} is the torque caused by relative rotation of automata in the pair as shown below.

Note that the automata of the pair may represent the parts of different bodies or one consolidated body. Therefore its interaction is not always really contact one. That is why we put the word “contact” in quotation marks. More of that, as it shown in Fig. 1, the size of the automaton is characterized by one parameter d_i , but it does not mean that the shape of the automaton is spherical. Real shape of the automaton is determined by area of its “contacts” with neighbors. For example, if we use initial fcc packing, then the automata are shaped like a rhombic dodecahedron; but if we use cubic packing then the automata are cube-shaped.

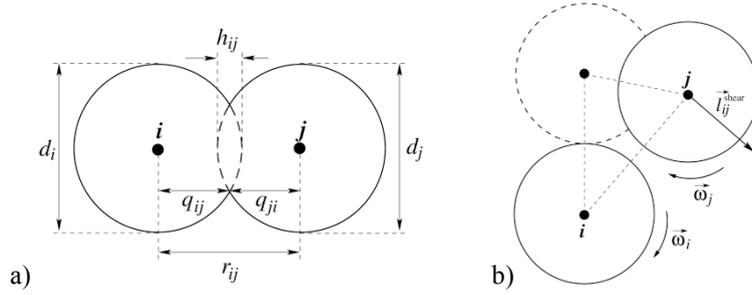


Fig. 1. Schematic of determining the spatial parameters for central (a) and tangential (b) interaction of a pair of the movable cellular automata.

For locally isotropic media, the volume-dependent component of the force can be expressed in terms of the pressure P_j in the volume of the neighboring automaton j as follows:

$$\mathbf{F}_i^\Omega = -A \sum_{j=1}^{N_i} P_j S_{ij} \mathbf{n}_{ij} \tag{2}$$

where S_{ij} is the area of interaction surface of automata i and j ; and A is a material parameter depending on elastic properties.

The total force acting on the automaton i can be represented as a sum of explicitly defined normal component \mathbf{F}_{ij}^n and tangential (shear) component \mathbf{F}_{ij}^τ :

$$\mathbf{F}_i = \sum_{j=1}^{N_i} (\mathbf{F}_{ij}^{\text{pair}} - AP_i S_{ij} \mathbf{n}_{ij}) = \sum_{j=1}^{N_i} [(F_{ij}^{\text{pair},n}(h_{ij}) - AP_j S_{ij}) \mathbf{n}_{ij} + F_{ij}^{\text{pair},\tau}(\mathbf{l}_{ij}^{\text{shear}}) \mathbf{t}_{ij}] = \sum_{j=1}^{N_i} (\mathbf{F}_{ij}^n + \mathbf{F}_{ij}^\tau) \tag{3}$$

where $\mathbf{F}_{ij}^{\text{pair},n}$ and $\mathbf{F}_{ij}^{\text{pair},\tau}$ are the normal and tangential pair interaction forces depending respectively on the automata overlap h_{ij} (Fig. 1(a)) and their relative tangential displacement $\mathbf{l}_{ij}^{\text{shear}}$ (Fig. 1(b)) calculated with taking into account the rotation of both automata. Note that, although the last expression of Eq. (3) formally corresponds to the form of element interaction in conventional discrete element models, it differs from them fundamentally in many-particle central interaction of the automata.

Using homogenization procedure for computing stress tensor in a particle described by Potyondy and Cundall (2004), the expression for the components of the average stress tensor in the automaton i takes the form:

$$\bar{\sigma}_{\alpha\beta}^i = \frac{1}{V_i} \sum_{j=1}^{N_i} q_{ij} \mathbf{n}_{ij,\alpha} F_{ij,\beta} \tag{4}$$

where α and β denote the axes X, Y, Z of the global coordinate system; V_i is the current volume of the automaton i ; $\mathbf{n}_{ij,\alpha}$ is the α -component of the unit vector \mathbf{n}_{ij} ; and $F_{ij,\beta}$ is β -component of the total force acting at the point of “contact” between the automata i and j .

For further convenience, the interaction parameters of movable cellular automata are considered in relative (specific) units. Thus, the central and tangential interactions of the automata i and j are characterized by the corresponding stresses η_{ij} and τ_{ij} :

$$\begin{cases} F_{ij}^n = \eta_{ij} S_{ij} \\ F_{ij}^\tau = \tau_{ij} S_{ij} \end{cases} \tag{5}$$

To characterize the deformation of the automaton i in its normal interaction with the automaton j , we can use the following dimensionless parameter (normal strain)

$$\xi_{ij} = \frac{q_{ij} - d_i / 2}{d_i / 2} \tag{6}$$

In general case, each automaton of a pair represents different material, and the overlap of the pair is distributed between i th and j th automata :

$$\Delta h_{ij} = \Delta q_{ij} + \Delta q_{ji} = \Delta \xi_{ij} d_i / 2 + \Delta \xi_{ji} d_j / 2 \tag{7}$$

where symbol Δ denotes the increment of a parameter per time step Δt of numerical integration of the motion equation (1). The distribution rule of strain in the pair is intimately associated with the expression for computing the interaction forces of the automata. This expression for central interaction is similar to Hooke's relations for diagonal stress tensor components:

$$\Delta \eta_{ij} = 2G (\Delta \xi_{ij}) + (1 - 2G/K) P_i \tag{8}$$

where K is the bulk modulus; G is the shear modulus of the material of i th automaton; and P_i is the pressure of the automaton i , which may be computed using Eqs. (3) and (4) at previous time step or by predictor-corrector scheme.

To determine a parameter characterizing shear deformation in the pair of automata $i-j$, we start with kinematics formula for free motion of the pair as a rigid body

$$\mathbf{v}_j - \mathbf{v}_i = \boldsymbol{\omega}_{ij} \times \mathbf{r}_{ij} \tag{9}$$

where $\mathbf{r}_{ij} = (\mathbf{R}_j - \mathbf{R}_i)$, \mathbf{v}_i is the translation velocity of the i th automaton centroid; and $\boldsymbol{\omega}_{ij}$ is the rotational velocity of the pair as a whole (rigid body). If we multiply both sides of Eq. (9) on the left by \mathbf{r}_{ij} and neglect rotation about the axis connecting centers of the automata of the pair (i.e. let $\boldsymbol{\omega}_{ij} \cdot \mathbf{r}_{ij} = 0$ because the rotation about the axis of the pair does not produce a shear deformation), then we get the following formula

$$\boldsymbol{\omega}_{ij} = \frac{\mathbf{n}_{ij} \times (\mathbf{v}_j - \mathbf{v}_i)}{r_{ij}} \tag{10}$$

Besides such rotation of the pair as a whole (defined by the difference in translational velocities of the automata), each automaton rotates with its own rotational velocity $\boldsymbol{\omega}_i$. The difference between these rotational velocities produces a shear deformation. Thus, the increment of shear deformations of the automata i and j per time step Δt is defined by the relative tangential displacement at the contact point \mathbf{l}_{ij}^{shear} divided by the distance between the automata :

$$\Delta \gamma_{ij} + \Delta \gamma_{ji} = \frac{\Delta \mathbf{l}_{ij}^{shear}}{r_{ij}} = \frac{(q_{ij} (\boldsymbol{\omega}_{ij} - \boldsymbol{\omega}_i) \times \mathbf{n}_{ij} + q_{ji} (\boldsymbol{\omega}_{ij} - \boldsymbol{\omega}_j) \times \mathbf{n}_{ji}) \Delta t}{r_{ij}} \tag{11}$$

The expression for tangential interaction of movable cellular automata is similar to Hooke's relations for non-diagonal stress tensor components and is pure pairwise:

$$\Delta \boldsymbol{\tau}_{ij} = 2G (\Delta \boldsymbol{\gamma}_{ij}) \tag{12}$$

The difference in automaton rotation leads also to the deformation of relative “bending” and “torsion” (the last only in 3D) of the pair. It is obvious that the resistance to relative rotation in the pair cause the torque, which value is proportional to the difference between the automaton rotations:

$$\Delta \mathbf{K}_{ij} = -(G_i + G_j)(\boldsymbol{\omega}_j - \boldsymbol{\omega}_i)\Delta t. \quad (13)$$

Eqs. (1)–(8), (11)–(13) describe the mechanical behavior of a linearly elastic body in the framework of MCA method. Note that Eqs. (7), (8), (11)–(13) are written in increments, i.e., in the hypoelastic form. Psakhie et al. (2011) showed that this model gives the same results as the numerical solving usual equation of continuum mechanics for isotropic linearly elastic medium by finite-difference method. That makes it possible to couple MCA method with the numerical methods of continuum mechanics. Smolin et al. (2009) showed that involving the rotation allows the movable cellular automata to describe the isotropic response of material correctly.

A pair of elements might be considered as a virtual bistable automaton having two stable states (bonded and unbonded), which permits simulation of fracture and coupling of fragments (or crack healing) by MCA. These capabilities are taken into account by means of corresponding change of the state of the pair of automata. A fracture criterion depends on the physical mechanisms of material deformation. An important advantage of the formalism described above is that it makes possible direct application of conventional fracture criteria (Huber-Mises-Hencky, Drucker-Prager, Mohr-Coulomb, Podgorski, etc.), which are written in tensor form.

3. Simulation Results

In this paper, MCA method is applied to study three-dimensional porous ceramic specimens of cubic shape under uniaxial compression. The pores are taken into account explicitly by removing the randomly selected automata from the original fcc packing. The pore distribution in space and their size are varied. In addition, the variant of pore filling with plastic filler is also considered (i.e., the composite of ceramic matrix with inclusions of the bone particles). The automaton size was equal to one micron.

As previously done by Smolin et al. (2014), for each porosity value a few representative specimens with individual pore arrangement were generated. A quasi-static uniaxial compression of each specimen was simulated, which resulted in the calculated loading diagram (σ - ε). Using this diagram the elastic modulus in compression (the slope of its linear part) and the tensile strength (its maximum value) were determined for each individual specimen. The values of the elastic modulus and tensile strength obtained from the simulation are random variables due to random pore arrangement. It has to be noted, that the scatter of strength values is sufficiently larger, especially for the porosity in the range from 5 up to 30 %, which is of particular interest since in this range there is a percolation transition from the system of isolated pores to the permeable pore structure. To determine the functional dependence of the mechanical properties of the specimens on the porosity, Smolin et al. (2014) used a few well-known functions for approximation of the calculation points, in which the properties for each porosity value were determined as the arithmetic mean of all specimens with the same porosity. However, as shown, for example, by Rinne (2009) the time to occurrence of the “weakest link” of many competing failure processes is governed by Weibull distribution model, which assumes the following cumulative distribution function

$$F(t) = 1 - \exp\left(-\left(t/\eta\right)^\beta\right), \quad (14)$$

where η is the scale parameter (also called as the characteristic life), and β is the shape parameter. Invented by Swedish scientist Waloddi Weibull in 1937, Weibull analysis is widely used for life data (also called failure or survival) analysis today. The Weibull distribution can be used to predict failure times of products, even based on extremely small sample sizes. Because the Weibull is a natural extension of the constant failure rate exponential model, the mean value (mathematical expectation) of the corresponding random variable can vary significantly from the arithmetic mean of the sample, meaning the assumption of its uniform distribution.

In this paper, we propose to determine the functional dependence of the strength properties on porosity based on the use of mathematical expectations for the corresponding Weibull distribution, but not arithmetic mean of simulation data. Note, that for large values of β , the expectation of the Weibull distribution $\langle t \rangle = \eta \cdot \Gamma(1 + 1/\beta)$ is almost equal to the scale parameter η .

Currently, there are many commercial software products performing reliability or survival analysis based on the Weibull model, such as Weibull++, Visual-XSel, Statgraphics, Statistica, and others. In order to determine the parameters η and β these programs use several methods, the most important of which is the method of maximum likelihood estimation. But in the case of a small sample size it is recommended to use the median rank regression, which is reduced to transformation of Eq. (14) to linear equation, and to the linear approximation of this equation by means of simple least-square regression. There is also free software for the analysis of large data based on the R statistical programming language, available at <https://www.R-project.org/>. In our work, we used a special package designed for the R, providing basic functionality needed to perform Weibull analysis available at <http://r-forge.r-project.org/projects/abernethy/>.

3.1. Simulation of Porous Ceramics

Fig. 2,a shows the Weibull plot for strength analysis of the ceramic specimens for two values of the fraction of small pores (equal to automaton size), for which there were maximum scatter of strength. One can see that the simulation data are well described by the Weibull distribution. Note, that the values of the arithmetic mean for all porosity values are higher than the mathematical expectation of no more than 0.5 %.

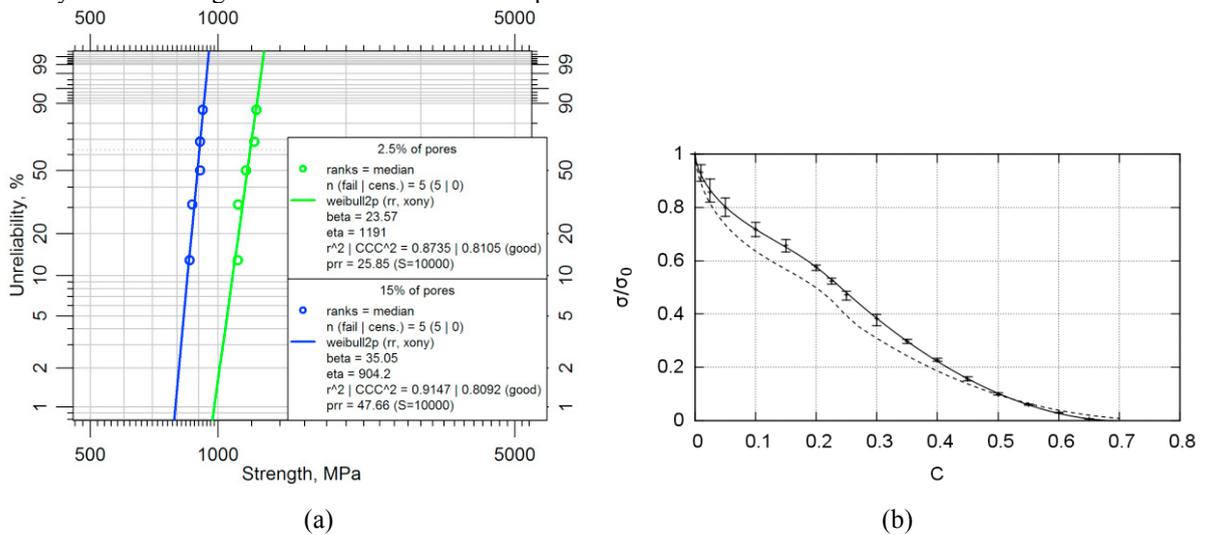


Fig. 2. Weibull plot (a) and normalized strength versus porosity (b) for the modeled porous ceramics.

Let us consider the dependence of the compression strength σ of the model material on porosity C . Points in Fig. 2,b represent values of the mathematical expectation of the Weibull distribution for strength, defined for five model specimens with individual pore positions in space, the deviation intervals are also shown for each porosity value. One can see that the maximum scatter of strength values is observed for small porosity up to 20 %.

As noted by Smolin et al. (2014), this dependence is substantially determined by the structure of the pore space. In particular, it changes at the transition percolation limit. Functions that best fit the simulation data on both sides of the limit are different: for isolated inclusions (pores) this function is

$$\sigma = \sigma_0 (C_0 - C/C_{\max})^m, \tag{15}$$

and if the porosity is permeable the function changes to

$$\sigma = \sigma_0 \frac{1 - (C/C_{max})^m}{1 + (C/C_n)^n}, \tag{16}$$

where C_{max} , C_n , n and m are adjustable parameters, σ_0 is the strength of the intact material. The solid curve in Fig. 2,b approximates the simulation data by the Eqs. (15) and (16). It is seen that both parts are perfectly joined at the percolation limit.

The dotted line in Fig. 2,b shows the fitted result for the simulation of ceramics with large pores. These pores are generated by removing one of the randomly selected automaton and its twelve nearest neighbors. As one can see from Fig. 2,b, the strength of ceramics with small pores is larger than one of ceramics with large pores at the porosity range from 0 to 50%, and the strength of ceramics with small pores is conversely less at porosity larger than 50%.

3.2. Simulation of Ceramic Composites

Next we consider the modeling results for ceramic composites. When generating such specimens, instead of removing the selected automaton it is being replaced by the other automaton with mechanical properties corresponding to the cortical bone, i.e. of material which is much softer and can undergo plastic deformation. Fig. 3.a shows the Weibull plots for strength analysis of the modeled ceramic composite specimens for two values of the fraction of inclusions, which demonstrate the maximum scatter of data. It is evident that these simulation results are also well described by the Weibull distribution for even ten different variants of the spatial arrangement of the inclusions.

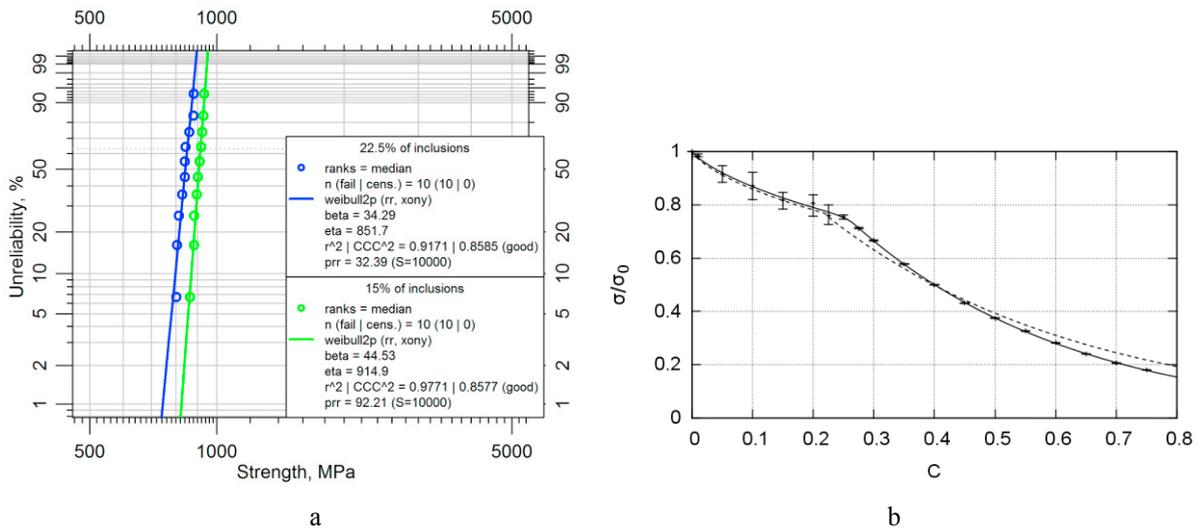


Fig. 3. Weibull plot (a) and normalized strength versus inclusion fraction (b) for the modeled ceramic composites.

Let us consider the dependence of the strength σ of the model composite on the fraction of inclusions C . In Fig. 3,b the points represent values of the mathematical expectation of the Weibull distribution for strength, obtained from ten model specimens with various spatial positions of inclusions; deviation intervals are also shown for each fraction of inclusions. It is seen that the maximum scatter in the composite strength is observed for the range of the inclusion fraction from 5 to 22.5%. At the transition from one function to another there is a brake of the curve.

The dashed line in Fig. 3.b shows a fitted curve for composites with large inclusions (they contain one of the selected automaton and its twelve nearest neighbors). It is significant that for large inclusions the boundary of

transition from one curve to another is a little bit shifted to lower fraction of inclusions, which means that the percolation limit for this size of the inclusions takes place “earlier”. In the plots for porous specimens (Fig. 2), this effect is not so noticeable due to a smooth transition from one curve to another. Similarly to the porous ceramics, the strength of the composite specimens with small inclusions is higher than for ceramics with larger inclusions for low inclusion fraction. The transition when the strength of composite with larger inclusions becomes higher, takes place earlier, namely at the fraction of 40%.

4. Conclusions

The following conclusions can be drawn from the research.

Firstly, it is shown that to determine the dependence of the strength properties of a composite material on fraction of inclusions (pores) it is better to use the magnitudes of mathematical expectation for the corresponding Weibull distribution, not just average values of the measured data.

Secondly, it is shown that the dependence of strength properties of the ceramic composite on the fraction of pores/inclusions is determined by the structure of porous space. In particular, this relationship changes its “nature” when passing over the percolation limit: the functions that best fit the calculation results on both side of the limit are different. Moreover, the strength of the specimens with large inclusions is less than the strength of the specimens with small pores/inclusions if their fraction is less than 40-50%, and when the fraction is greater than this limit the strength of the specimens with large inclusions becomes higher.

Acknowledgements

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