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Study of Strength Properties of Ceramic Composites with Soft Filler Based on 3D Computer Simulation

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Abstract. The movable cellular automaton method which is a computational method of particle mechanics is applied to simulating uniaxial compression of 3D specimens of a ceramic composite. Soft inclusions were considered explicitly by changing the sort (properties) of automata selected randomly from the original fcc packing. The distribution of inclusions in space, their size, and the total fraction were varied. For each value of inclusion fraction, there were generated several representative specimens with individual pore position in space. The resulting magnitudes of the elastic modulus and strength of the specimens were scattered and well described by the Weibull distribution. We showed that to reveal the dependence of the elastic and strength properties of the composite on the inclusion fraction it is much better to consider the mathematical expectation of the corresponding Weibull distribution, rather than the average of the values for the specimens of the same inclusion fraction. It is shown that the relation between the mechanical properties of material and its inclusion fraction depends significantly on the material structure. Namely, percolation transition from isolated inclusions to interconnected clusters of inclusions strongly manifests itself in the dependence of strength on the fraction of inclusions. Thus, the curve of strength versus inclusion fraction fits different equations for a different kind of structure.

INTRODUCTION

The problem of predicting the physical and mechanical properties of composite materials depending on the inclusion fraction has a long history. It has been solved by many authors in various statements but is still not completely understood, and is 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 of creating materials with a very complex structure both of the porous/inclusion space and of the matrix itself, which in fact provides the material with high functional properties. For the analytical solution of this problem the most successful approaches are the micromechanics of composites that is based on the method of self-consistent field (definition of the property contribution tensor) as shown, for example, in [1], and the method of random functions [2]. However, these approaches allow predicting only the properties that determine the propagation of disturbances of various types: elastic, thermal and electromagnetic. Regarding the strength, the capability of these approaches is limited mostly to the periodic structure materials. It should be noted that experimental determination of the strength properties of materials produces a large scatter of data, which is caused not only by the heterogeneity and complexity of the material structure but also by technical reasons. 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.

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DESCRIPTION OF THE MODEL

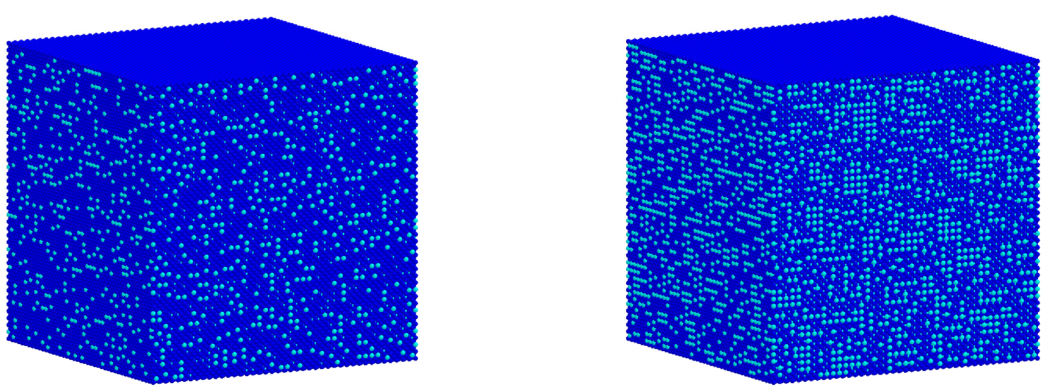
At present, the methods mainly used for simulating the mechanical behavior of materials are numerical methods of continuum mechanics (namely, the finite element method [3, 4]). Recent methods based on a discrete representation of material have been successfully developed and widely used. For example, the method of movable cellular automata (MCA) is an 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 the mechanical behavior of a solid at different scales, including deformation, initiation and propagation of damages, fracture and further interaction of fragments after failure [5–7]. The automaton motion is governed by the Newton–Euler equations. The forces acting on automata are calculated using deformation parameters, i.e. relative overlap, tangential displacement and rotation, and conventional elastic constants, i.e. shear and bulk moduli. A distinguishing feature of the method is the calculation of forces acting on the automata within the framework of multi-particle interaction [7, 8] which among other advantages provides for an isotropic behavior of the simulated medium. Removing of automata from initial dense packing allows an explicit account of voids or pores in the material. Changing the sort (i.e. mechanical properties) of automata in the initial packing allows the account of various kind of inhomogeneity in the material.

A pair of elements might be considered as a virtual bistable automaton having two stable states (bonded and unbound), which permits simulation of fracture and coupling of fragments (or crack healing) by MCA. These capabilities are taken into account by means of the 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 the tensor form [7].

MODELING RESULTS

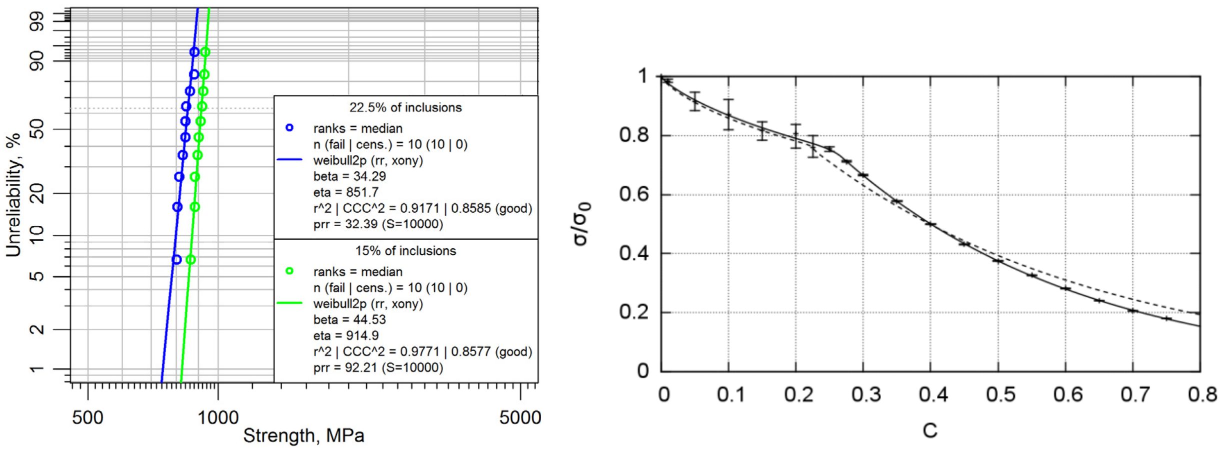
In this paper, MCA method is applied to study three-dimensional ceramic composite specimens of cubic shape under uniaxial compression. The inclusions are taken into account explicitly by changing the sort (i.e. properties of human bone) for randomly selected automata from the original fcc packing. The inclusion distribution in space and their size are varied. The automaton size is equal to one micron.

As previously done in [9], for each value of inclusion fraction a few representative specimens with individual inclusion 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 inclusion arrangement. It should be noted that the scatter of strength values is sufficiently larger, especially for the inclusion fraction in the range from 5 up to 30%, which is of particular interest since in this range there is percolation transition from the system of isolated inclusions to the permeable inclusion structure.



(a) (b)

FIGURE 1. The modeled specimens with different fraction of inclusions: 10 (a) and 30% (b)



(a) (b)

FIGURE 2. Weibull plot (a) and normalized strength versus inclusion fraction (b) for the modeled ceramic composites

To determine the functional dependence of the mechanical properties of specimens on the porosity, the authors [9] used a few well-known functions for the approximation of 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, in [10] the time to occurrence of the "weakest link" of many competing failure processes is governed by the Weibull distribution model that assumes the following cumulative distribution function

$$F(t) = 1 - \exp(-(t/\eta)^{\beta}), \tag{1}$$

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 on the inclusion fraction based on the use of mathematical expectations for the corresponding Weibull distribution, rather than the arithmetic mean of simulation data. Note that for large values of β, the expectation of the Weibull distribution $\langle t \rangle = \eta\Gamma(1 + 1/\beta)$ 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 the transformation of Eq. (1) to a 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/.

Figure 2a shows the Weibull plot for strength analysis of a ceramic specimens for two values of the fraction of small inclusions (equal to automaton size) for which there were maximum scatters 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%.

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

As noted in [9], this dependence is substantially determined by the structure of inclusions/pores. 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 this function is

$$\sigma = \sigma_0 (C_0 - C/C_{\max})^m \tag{2}$$

and if the inclusions form permeable structure the function changes to

$$\sigma = \sigma_0 \frac{1-(C/C_{\max})^m}{1+(C/C_n)^n}, \tag{3}$$

where $C_{\max}$, C_n, n and m are adjustable parameters, σ_0 is the strength of pure ceramics (matrix). The solid curve in Fig. 2b approximates the simulation data by Eqs. (2) and (3). It is seen that both parts are perfectly joined at the percolation limit.

The dotted line in Fig. 2b shows the fitted result for the simulation of ceramics with large inclusions. These inclusions are generated by changing the sort for one of the randomly selected automata and its twelve nearest neighbors. As one can see from Fig. 2b, the strength of ceramics with small inclusions is larger than that of the ceramics with large inclusions at the inclusion fraction range from 0 to 40%, and the strength of the ceramics with small inclusions is conversely less at the fraction larger than 40%.

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 the fraction of inclusions 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 inclusions is determined by the structure of the material. In particular, this relationship changes its "nature" when passing over the percolation limit: the functions that best fit the simulation results on both sides of the limit are different. Moreover, the strength of the specimens with large inclusions is less than the strength of the specimens with small inclusions if their fraction is less than 40%, and when the fraction is greater than this limit the strength of the specimens with large inclusions becomes higher.

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