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A Study of the Influence of Soft Particle Size and Concentration on Strength and Strain Properties of Ceramic Composites

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Abstract. In the paper a theoretical study of the influence of particle distribution of soft inclusions-agglomerates in a ceramic composite sample on its strength and deformation characteristics was carried out. A movable cellular automaton method was used to simulate a uniaxial compression test of two-dimensional rectangle composite samples. It was found that the average size of inclusions agglomerate-while maintaining the volume fraction of the particles of the soft phase has little effect on the strength and deformation properties of the simulated samples. The simulation results can help to understand the mechanical properties of such objects within any generalized model.

INTRODUCTION

The development of ceramic materials that retain dimensional stability during temperature changes, with a zero coefficient of thermal expansion ZTE [1, 2], would solve many technical problems associated with the dimensional variance not only in the oil and gas sector, but also in many other industries, including rocket, electronic, high-temperature, and high-precision measuring technologies.

One approach of creating ceramics with zero thermal expansion coefficients is to create a composite, in which the dimension of the invariance under heating is achieved due to the gradient between the thermal expansion and compression. In such a material linear expansion of the material of one component is compensated by linear compression of another component with a negative coefficient of linear expansion. As a material with a negative thermal-expansion (NTE) coefficient [3, 4] the zirconium tungstate ZrW_2O_8 is a particular interesting to the researchers [2, 3]. The uniqueness of this compound is that unlike many other NTE materials a compression of ZrW_2O_8 under heating occurs isotropically in a wide temperature range. The limitations of this approach lie in the fact that the increase in the volume fraction of zirconium tungstate, as well as other known materials with a negative coefficient of linear expansion is accompanied by a decrease in mechanical properties. Thus, the task of creating a ceramic material with a ZTE coefficient is supplemented by the problem of finding the optimal structure of the composite particle size and concentration of inclusions.

In the paper, a computational method of the discrete approach—the method of movable cellular automata—is used to solve this problem. The aim of the study is to find a relationship between the characteristics of the structure and strength characteristics of the composite material as a whole. For this a simulation of uniaxial compression of samples in which the concentration of inclusion particles was fixed while their size was varied was carried out. The results can be used to optimize the structure of ceramic materials with a zero coefficient of linear expansion.

Advanced Materials with Hierarchical Structure for New Technologies and Reliable Structures
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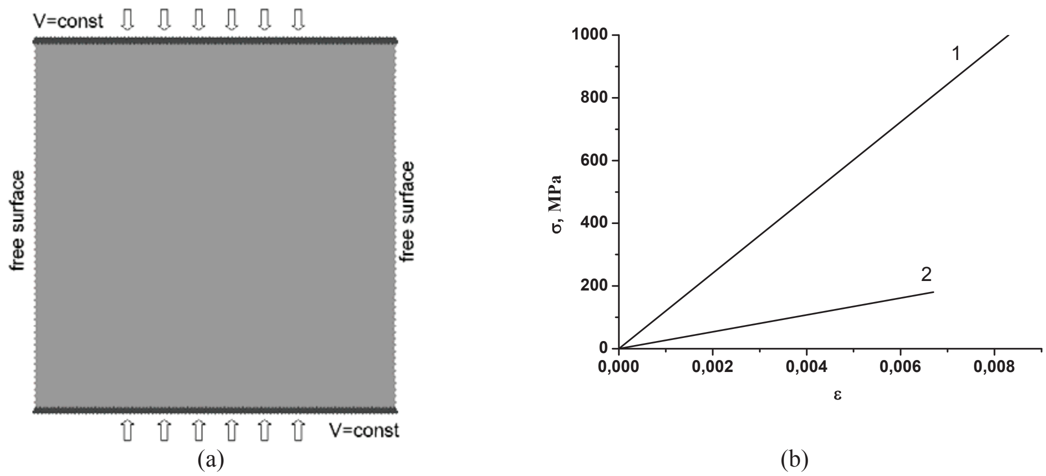

FIGURE 1. A loading scheme for the uniaxial compression test (a), loading diagrams used to set the response functions of the model materials: *1*—matrix, *2*—inclusions (b)

NUMERICAL MODEL

As noted above, a Movable Cellular Automata (MCA) method was used [5–9]. The main formalism, the equations of motion for a system of movable cellular automata, and the interaction between them are given in [6, 10]. In the paper a fragment of composite ceramic-based sample with dimensions of 100×100 mm shown in Fig. 1a was subjected to uniaxial compression within the plane-strain approximation. To this end, the particles belonging to two upper and two lower layers of the sample, were loaded by constant velocities of 1 m/c, directed towards each other. The size of an individual automaton d was equal to 1 mm. The matrix material was modeled by particles with mechanical properties similar to the properties of zirconia, wherein the volume fraction of porosity reaches 5%. To set the model parameters of inclusion response function the particles with mechanical properties similar to the properties of zirconia, wherein the volume fraction of porosity reaches 40%, were used. This choice is motivated by certain difficulties in identifying the mechanical properties of zirconium tungstate while selected model material provides softening as well. The response functions of both model materials used are shown in Fig. 1b. Selection of model materials and particle size determined the step of integration schemes Δt, which amounted to 2.5×10^{-10} s. Along the direction perpendicular to the applied uniaxial compression, free boundary conditions were simulated.

We consider the structure of the resulting composite sample in which the volume fraction of inclusions γ was nearly constant and equal to 25%. The average size of inclusions-agglomerates Σ_{av} was varied in different tasks and was equal to $6.7\times d$, $11.3\times d$, $11.5\times d$ and $38.5\times d$. In order to get statistical values for each of the considered structures free different specimens with identical parameters γ and Σ_{av}, but with a different arrangement of inclusion, particles in a ceramic matrix were generated.

RESULTS OF SIMULATION

The resulting modeled structure of the initial composite samples in which the average size of inclusion-agglomerate were varied while keeping the volume fraction of inclusions γ at about 25% are shown in Fig. 2.

The simulation results showed that when the strain ε is close to 0.006, in the simulated fragment the process of cracking starts to develop. The place of cracks origination and direction of their propagation are determined by the presence and nature of the location of inclusions. Figure 3 shows the structures of the modeled samples for the three considered configurations during forming of the main cracks. It is seen that cracks primarily occur along the boundaries of the matrix material with inclusions, which explains the difference in their mechanical properties. In the future, initial cracking joined together and formed the main crack, which also passes through on-agglomerates. This result is particularly noticeable in the case of large inclusions when $\Sigma_{av} = 38.5\times d$.

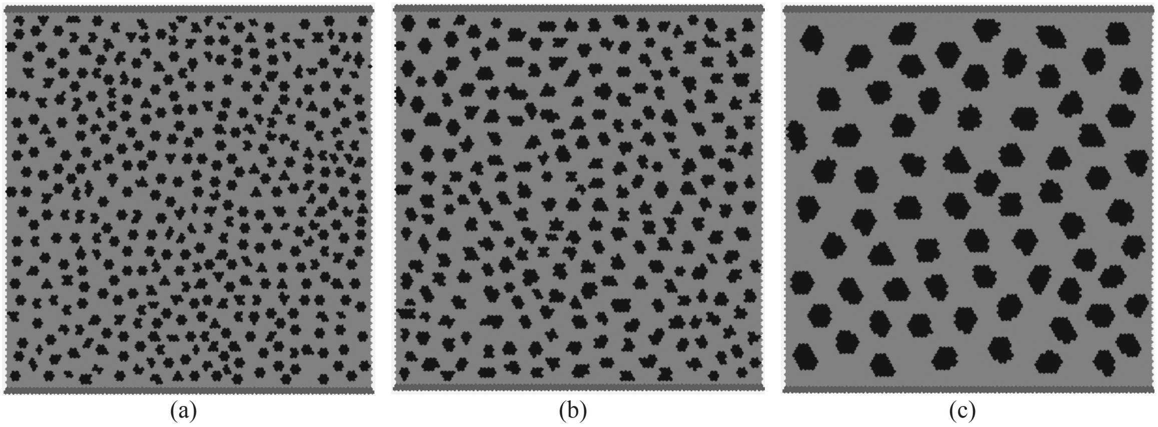

FIGURE 2. Initial configuration of composite samples in which the average sizes of inclusion-agglomerate Σ_{av} were varied: (a) 6.7×*d*, (b) 11.3×*d* and (c) 38.5×*d* while keep the volume fraction of inclusions γ about 25%. Hereafter black circles denote automata with properties of inclusion material; grey indicates the automata of matrix. Dark grey automata at the top and bottom denote loading layers

Figure 4 shows the loading diagrams for the considered composite samples. It is clearly seen that the strength values for all considered samples are close to the level of σ = 450 MPa. For the sample based on pure zirconia dioxide this parameter is above 1 GPa (see curve *1* in Fig. 1b). Thus, despite the variation in the average size of inclusions-agglomerates Σ_{av} in the range 6.6×*d*–38.5×*d*, the resulting mechanical properties of such composites vary within 10% only (420 MPa for Σ_{av} = 11.5×*d* and 450 MPa for Σ_{av} = 6.7×*d*). The resulting deformation properties of generated samples are also very close (ultimate strain varies from 0.006 for Σ_{av} = 38.5×*d* to 0.007 for Σ_{av} = 6.6×*d*).

CONCLUSIONS

The paper examined the strength and strain properties during uniaxial compression of the ceramic composite samples based on zirconia dioxide with soft inclusions whose average size was varied while concentration was kept constant. It was shown that the strength of such composite samples in which the volume fraction of inclusions γ was about 25% changes slightly. Thus, when changing the characteristic average size by more than 5 times the strength properties of the resulting composite do not vary by more than 10%. The corresponding ultimate strain parameter varied within 15%.

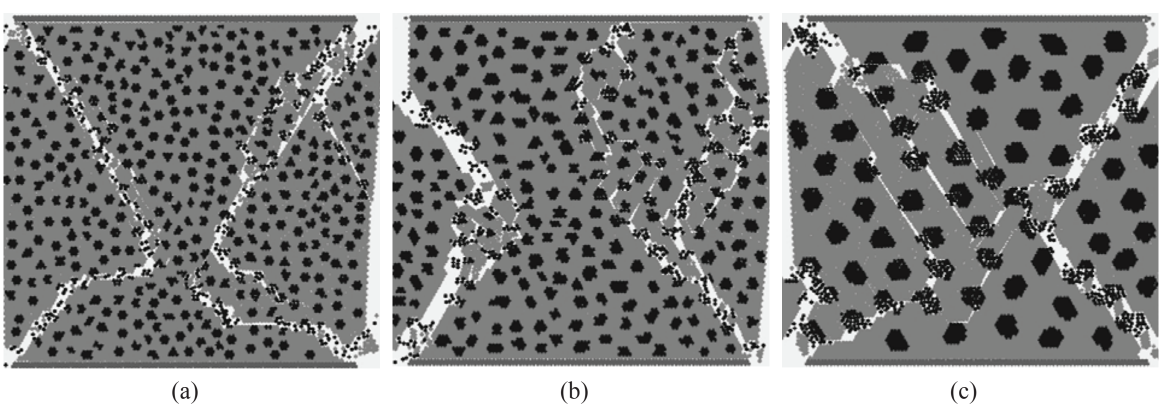

FIGURE 3. Resulting configuration of composite samples at ε = 0.006 in which the average sizes of inclusion-agglomerate Σ_{av} were varied: (a) 6.7×*d*, (b) 11.3×*d* and (c) 38.5×*d* while keep the volume fraction of inclusions γ about 25%

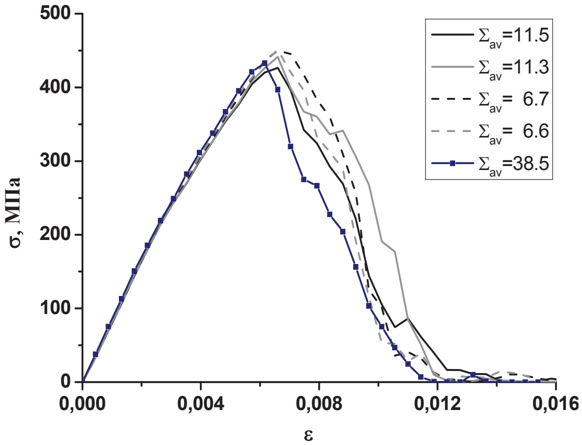

FIGURE 4. Loading diagrams for the modeled samples with different average sizes of inclusions-agglomerates

It is obvious that the description of the behavior of a real structure implies taking into account the availability of many different defects associated with the peculiarities of sintering the powder material, the state of the interfacial grain boundaries of the ceramic matrix and the interface zone matrix including the three-dimensional distribution of the various inclusions, including particles with a negative coefficient of linear expansion, such as zirconium tungstate. Nevertheless, the results obtained in theoretical investigations may be useful in the development of new ceramic-based composite materials, because they provide information about the mechanical properties of objects within the generalized approach. Note that since the main purpose of the selected composite materials is the tribological pair, studies on the impact of these modifications on frictional properties are required. Such investigations are planned for the future.

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