Multilevel approach to description of deformation and fracture of brittle media with hierarchical porous structure on the basis of movable cellular automaton method

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Abstract. An approach to multilevel description of deformation and fracture of brittle porous media on the basis of movable cellular automaton method was proposed. The media characterized by pore size distribution function having two maxima were considered. The core of the proposed approach consists in finding the automaton effective response function by means of direct numerical simulation of representative volume of the porous medium. A hierarchical two level model of mechanical behavior of ceramics under compression and shear loading was developed. The ceramics on the basis of zirconium oxide with pore size greater than the average grain size was considered. At the first level of model the small pores (corresponding to the first maximum of distribution bar chart of pore size) were taking into account explicitly as well as representative volume and effective elastic characteristics of the porous medium were evaluated. At the second scale level of the model, big pores were taking into account explicitly (by removing automata from the initial structure) and the parameters of matrix corresponded to the ones of the first level. Simulation results showed, that the proposed multilevel model allows performing correct qualitative and quantitative description of deformation and fracture of brittle media with hierarchical porous structure.

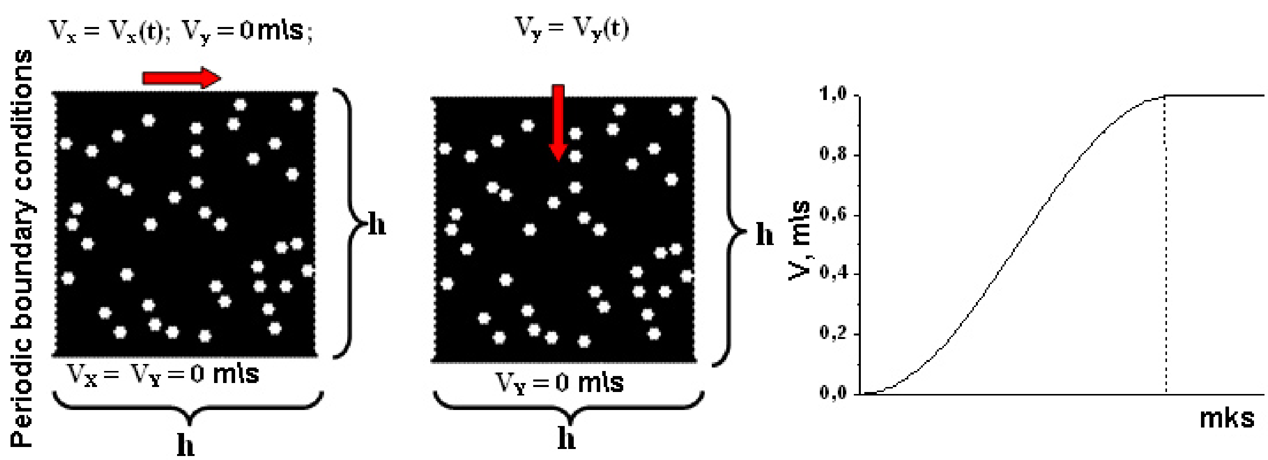
Introduction

Porous materials are characterized by hierarchical pore structure and complex mechanical behavior at fracture [1-3]. To study and describe these materials the information about their structure and mechanical properties on a few scale levels is needed. One way of getting this information is a numerical simulation. In the framework of one-level approach direct accounting for peculiarities of structure and mechanical behavior of material on each scale level seems to be impossible. As a result, the goal of this investigation is the development of multilevel approach, represented at [4] and corresponding hierarchical model for describing deformation and fracture of nanostructure porous ceramics under compression and shear on the basis of movable cellular automaton method (MCA) [5]. The choice of this method caused by the fact that he has successfully proved itself in the study of mechanical behavior of brittle porous media from the initiation of the first damages until massive fracture [6-9]. The calculations were performed for a model material with mechanical properties of nanocrystalline $ZrO_2(Y_2O_3)$ (yttria-stabilized zirconia) with the average pore size greater than the average grain size and two maxima in its pore size distribution function [2, 3].

Building up a hierarchical model was performed by several stages. At the first stage to find automaton effective response function on macroscopic scale level the calculation were performed with explicit taking into account the structure of material on micro level (this is the scale level where pores structure of model specimens with the size of 20÷250 μm was defined explicitly). The representative volume of porous medium on this scale level was found. At the second stage the calculations performed on the macro-level. At this scale level the porous structure of specimens was taking into account in the same way (explicit manner) as at the previous scale-level. The third stage was a verification of the developed model

1. Finding the representative volume of porous medium and corresponding effective response functions on the macroscopic scale level

On "micro-scale" level the representative volume was determined by means of convergence analysis of elastic and strength properties of the model porous specimens with their size increase. Mechanical behavior of six groups of porous ceramics specimens under uniaxial compression and simple shear was performed. All specimens in each group had the same geometrical size, but different pore space distribution. Each group consisted of six specimens. Square specimens under consideration had dimension (square side) of 20, 60, 100, 150, 200 and 250 μm according to the groups. It was supposed that all pores in ceramics under investigation, as well as the model material, had spherical shape. The pore size of the model material, according to maximum in ceramics pore size distribution function [1], was 3 μm [2, 3]. Diameter of movable cellular automata, according to the average grain size [1], was 1 μm. Pore structure of model specimens was made by moving away an automaton randomly and its six nearest neighbors. The total porosity in all the samples was 7% [2, 3]. The initial structure of a model specimen is shown in Fig. 1,a,b.



a) b) c)

Fig. 1. The initial structure of the model specimen with a side h = 60 μm and scheme of application of mechanical stress during shear loading (a) and uniaxial compression (b); the law of variation of velocity of the upper automata layer of the specimen (c)

The simple-shear loading was simulated by setting equal velocities in horizontal direction to all automata in the upper layer (fig. 1,a,c). The value of this velocity gradually increased from 0 to 1 m/s in sinusoidal manner and then remained constant. The automata in the bottom layer were fixed. This regime ensured a quasi-static character of loading and allowed dynamic effects to be avoided until the first damage appears. All samples had periodic boundary conditions in the direction of loading. The uniaxial compression loading was simulated by setting equal velocities in vertical direction (up to 1 m/s) to all automata in the upper layer (fig. 1,b,c). The velocities of automata in the bottom layer were set to zero. Displacement in horizontal direction were allowed to automata in the bottom and upper layers. The lateral surfaces of specimen were free. The problem was solved under plane strain conditions. The response function of automata corresponded to the diagram of loading for nanocrystalline $ZrO_2(Y_2O_3)$ with total porosity of 2% and an average pore size comparable with the grain size [2, 3]. Shear modulus of movable cellular automaton G = 59.2 GPa, Poisson ratio ν = 0.3. Inter-automaton bond fracture criterion used for intensity of shear stresses [10].

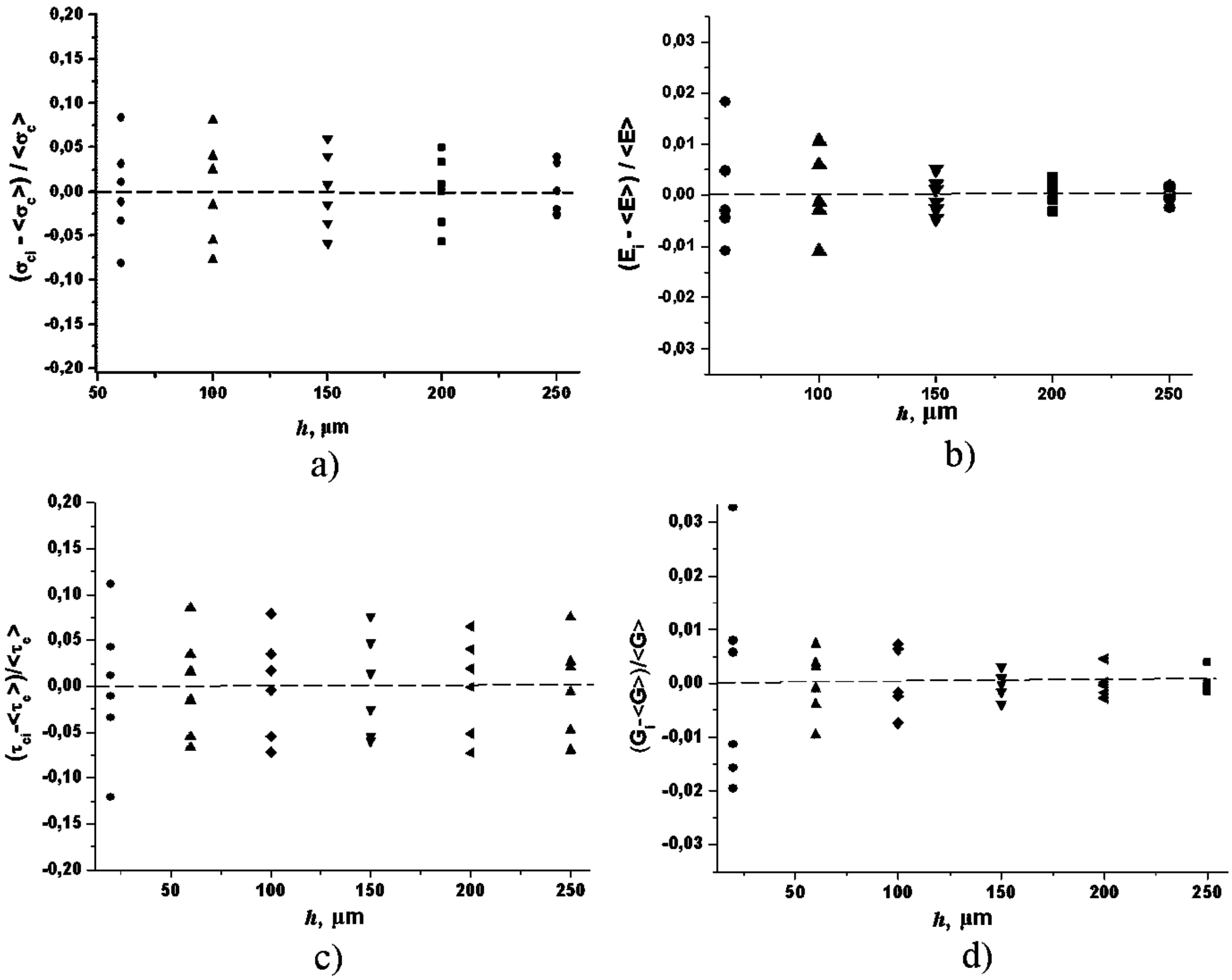


Fig. 2. Relative deviation of elastic modulus E_{eff}, shear modulus G_{eff}, compression strength σ_c, shear strength τ_c of model specimens from corresponding mean values $<E_{eff}>$, $<G_{eff}>$, $<\sigma_c>$, $<\tau_c>$ under uniaxial compression (a, b) and shear loading (c, d).

Convergence analysis of mechanical properties for porous model specimens with increase of their size was performed in terms of estimated deviation of effective elastic and strength properties of specimens (modulus of compression-elongation E_{eff}, shear modulus G_{eff}, compression strength σ_c and shear strength τ_c - parameters of diagram of loading) from corresponding mean values in the groups $<E_{eff}>$, $<G_{eff}>$, $<\sigma_c>$ and $<\tau_c>$. The specimen size, for which deviation didn't exceed 3% for E_{eff}, G_{eff} and 15% for σ_c, τ_c was accepted as the size of representative volume. Simulation results (fig.2.) showed nonlinear convergence of strength and elastic properties of model specimens. Relative deviation of E_{eff} , G_{eff}, σ_c and τ_c of model specimens with 150 μm sides from corresponding group average was 0.51, 0.38, 6 and 7.6%. These values did not exceed of the desired limits. Thus, it was shown, that porous specimens with 150 μm sides is the representative volume of the model media under consideration. The values of $<E_{eff}>$ and $<\sigma_c>$ were taken as characteristics of response function of automata on macroscopic level. Slight deviations of these values (- 9.5% и 36%) from ones evaluated by experimental way are related with two-dimensional formulation of problem, kind of stress state and incomplete correspondence the pore morphology in the model and in the ceramics. They were corrected (by means of) introducing a correction ratio. The transition from the elastic modulus determined by the calculated diagram of loading under plane strain conditions EPSS to the Young's modulus was based on the ratio $E = E_{PSS}(1-\nu^2)$ [11].

2. Numerical simulations on macrolevel with explicit taking into porous structure of material

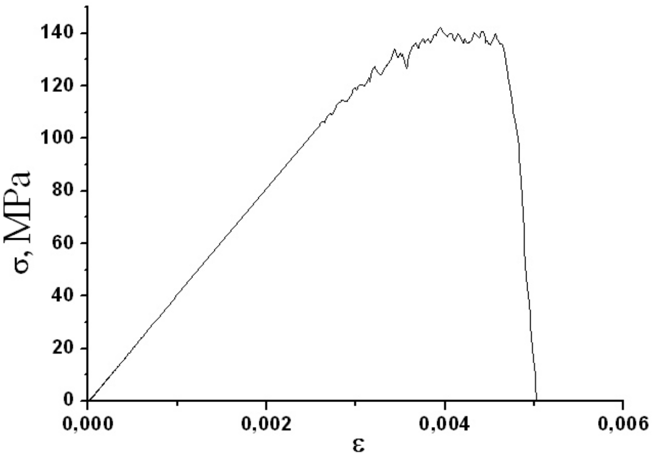
On macrolevel the calculations were performed for nine porous square plane specimens with 22.5 mm side. In according to the size of representative volume the diameter of movable cellular automata was 150 μm. Information about structure and strength properties of material from micro– to macrolevel was transferred by means of response functions with corresponding characteristics of loading diagrams for representative volumes of material on microlevel. The response function of automata corresponded to linear function. Its parameters (the maximal value of specific/unit resistance force to loading and elastic parameter corresponded to Young's modulus) were 846 MPa and 112 GPa. The accounting of porous structure of material on macro-scale level (explicit manner), loading conditions and assumption about stress state were similar with that at the first stage. In according to pore size distribution function the porosity of specimens was 28%, and the size of pore - 450 μkm [2, 3].

3 Model verification

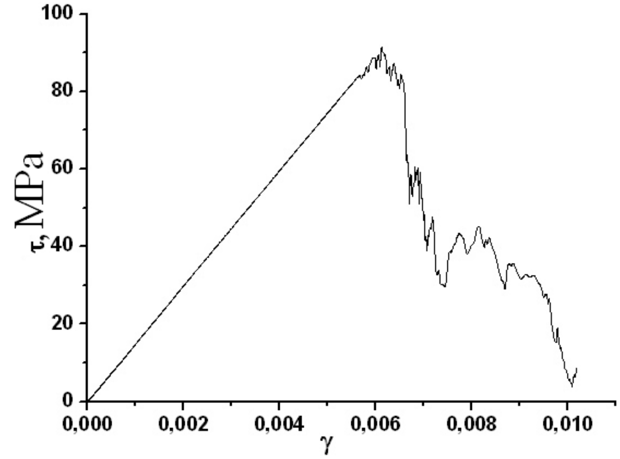
We considered the model as successfully verified (i.e. the model is valid for ceramics under investigation) if the simulation results satisfied the following criteria: 1) Linear loading diagram of model specimens, containing the horizontal section, corresponding to quasi-ductile fracture of porous brittle materials with porosity more than 20%. 2) Qualitative compatibility of the fracture patterns of model specimens and real ceramics. 3) Fall of strength properties of specimens into a certain interval whose limits was found on the basis of processing experimental results.

Loading diagrams typical for all model specimens in case of different types of mechanical loading are presented at figure 3. At these diagrams, you can select several sections. The first linear section, corresponding to elastic deformation of specimen, is typical for brittle materials with any value of porosity. The next section is ascending and not insignificant in extent part of the diagram with multiple stress "oscillations" (just under uniaxial compression – fig. 3, a). These sections correspond to the repetitive processes of damage generation over the entire specimen, the local cracking and then - the elastic deformation of the material, etc. The last section of the diagram is descending. It corresponds to the macrocracks propagation as well as generating separate multiple damages. Under shear loading (fig. 3, b) at the represented diagram after mentioned sections one can see the ascending section of the curve with breakdowns and then - another drop-down area. As a results of the straitened deformation conditions the development of macrocracks in the sample corresponds to precisely this part of the diagram, and the first drop-down section of diagram corresponds to a one-time generation of damages over the entire sample and their development without the formation of macrocracks system.

It should be noted that the horizontal plateau on the compression-test diagram of brittle specimens (fig. 3 a) shows their quasi-ductile fracture, which occurs only when the porosity of the specimen more than 20% [9]. The degree of manifestation of these properties is proportional to the length of this section (plateau) and is different for each model specimens. The reduction of the length of this part of the diagram – tell us that fracture is approximate to brittle failure type. It is natural to assume that as the appearance of quasi-ductile character of the sample destruction and the degree of its manifestation is determined by some critical value of the local porosity. The last one is related, in particular, with the value of total porosity, as well as with the form and size of pores. It should be noted that in this case the quasi-ductile fracture is completely due to structural factor, because the model does not take into account any phase transitions, no rearrangement of the lattice of material.



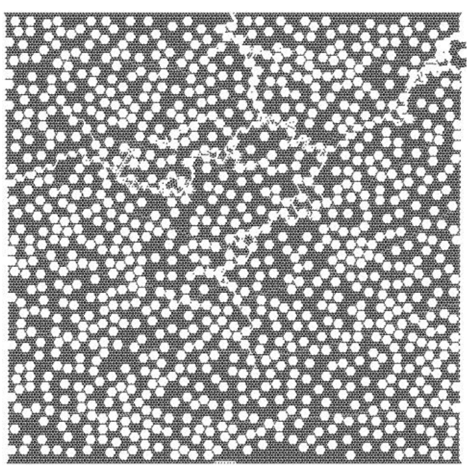
a)



b)

Fig. 3. Diagram of loading of the model specimens with the side h = 22.5 мм under uniaxial compression (a) and shear loading (b).

Performed calculations and comparison of simulated diagrams of loading of model specimens with corresponding diagrams of brittle porous bodies under shear and compression loading [2, 9, 12] revealed their good qualitative compatibility. Thus, the first goodness of fit of the model is satisfied. Typical fracture pattern of model specimens, represented as inter-automaton bond net at the time of first macrocrack propagation, are presented at fig. 4. Under uniaxial compression the specimens were broken-down because of generating therein the asymmetrical system of macrocracks with complex path of crack propagation. In addition, the generation of multiple separated fractures near macrocracks takes place.


a)

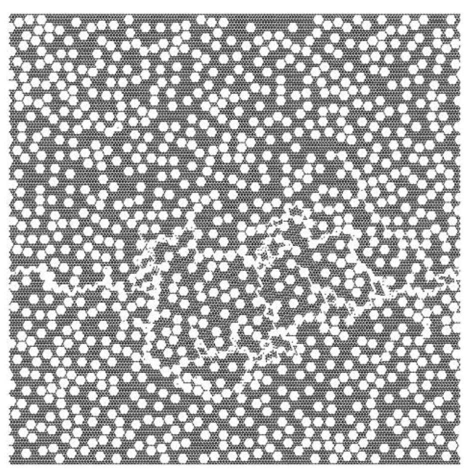

b)

Fig. 4. Fracture pattern of model specimens with the porosity 28% at the moment of first macrocrack propagation under uniaxial compression (a) and shear loading (b)

In the case of quasi-ductile fracture of specimen (Fig. 3, a) the generation of damages and crack growth occur locally, in several places of the sample, characterized by the most-high values of local

porosity (and the least web thickness between isolated pores). Until a certain moment some cracks are not merged into main crack - the stage of its growth, as it were "stretched". It leads to extensive local cracking of the material without losing the integrity of the sample and, consequently, to a substantial dissipation of elastic energy and reduce the effective elastic properties of the material (of the whole sample). Thus, satisfied the second goodness of fit of the constructed model.
To verify the third goodness of fit of the model the average value of the effective elastic modulus ($<E_{\mathrm{eff}}>$) and maximum specific resistance force to loading under uniaxial comression were calculated. Then, they were compared with the corresponding values found in natural experiments. It was shown that the deviation of $<\sigma_{\mathrm{s\_eff}}>$ and $<E_{\mathrm{eff}}>$ model samples from the experimental data does not exceed 30% and 12%, respectively. It is a rather good accuracy in the simulation of highly porous media in plane approximation. This indicates a good quantitative agreement of calculations and experiment and executing the third criterion of the adequacy of the model.
Thus, in this study, the two-level model of porous ceramics with bimodal pore size distribution function, based on a multilevel approach to numerical simulation, was constructed.

Summary

Thus, in this study, the multilevel approach to numerical simulation, developed on the basis of movable cellular automaton method, and constructed corresponding hierarchical model can adequately describe the deformation and fracture of porous materials under mechanical loading. Since the proposed approach is sufficiently general, then, if it is necessary, the heterogeneous media containing more than two scale structural level could be simulated on the basis of mentioned approach.

Acknowledgements

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