3D MODELING OF FRACTURE OF BRITTLE POROUS MATERIALS USING MOVABLE CELLULAR AUTOMATON METHOD*

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Movable cellular automaton method, which is a representative of particle methods in solid mechanics, is used for computation. In an initial structure the automata are positioned in FCC packing. The pores are set up explicitly by removing single automata from the initial structure. The computational results show that the curve of porosity dependence of strength and elastic properties of the modeled specimens has a break at the porosity about 20%, i.e. percolation threshold. The obtained results are in a good agreement with the available experimental data.

Introduction

It is well known that porosity dependence of strength and elastic properties of porous materials is determined by the pore morphology. If porosity is small, each pore is closed and isolated form the others. With porosity increasing the number of pores becomes greater and the distance among pores decreases. When porosity reaches percolation threshold the pores are not closed anymore and consequently form new morphology. Thus, porosity dependence of strength and elastic properties should be changed when percolation threshold is exceeded.

Note, it is very difficult to study the problem experimentally, because of stochastic nature of the pore morphology in real materials. For example, it is impossible to make specimens with various porosity value and the same porous structure. At the same time potentialities of the modern computational mechanics allow to study in detail not only deformation of complex heterogeneous materials but also fracture of such materials.

1. Computational model for porous ceramics

For 3D computer simulation of mechanical behavior of a porous material under uniaxial compression we used the movable cellular automaton method (MCA) [1]. MCA is a method in discrete computational mechanics which allows modeling deformation and fracture of heterogeneous material with taking into account the structure of the material explicitly.

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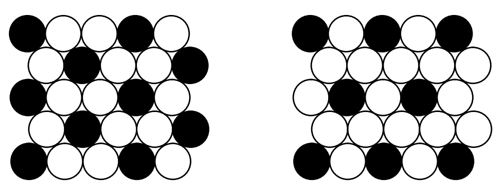
Modeled material is represented as a set of elements of finite size (automata) interacting with each another according to some pre-determined rules. Mechanical interaction among automata are defined by so called response function, which can be interpreted as a local stress-strain diagram. Equation of translation motion and rotation of the automata are written in many-body approach. This means that interacting force between two automata depends not only on position and state of these automata but also on position and state of their neighboring automata. This allows modeling solid and granular material behavior within the framework of one MCA method.

Response function of automata used in this study corresponded to ZrO_2 ceramics with average size of pores commensurable with the grain size of the material. According to the pore distribution diagram of this material [2] the automaton size in the computations was $1\,\mu$m. All the modeled specimens where bricks with a square base. The loading was applied by assignment of vertical velocity for automata of the top layer of a specimen. At the same time the substrate automata were rigidly fixed. At the initial stage of the loading velocity of the upper automata increased by a sinusoidal law from 0 to 1 cm/s and then was constant.

Pores were generated by removing single automata from the basic structure. The porosity values were varied from 0 to 50 %. Note, that the maximal porosity on the assumption of pore disconnection in closed packing for 2D is $1/2 = 50\,\%$ (Fig. 1,a) while for 3D it is $1/4 = 25\,\%$ (Fig. 1,b). In this case the pores are regularly situated.



(a) (b)

Fig. 1. Periodic pores (black) in closed packing

The maximal value of closed porosity for random removing of single automata from FCC packing is 17.6 %. The percolation limit for 3D FCC packing is 19.8 %. Consequently, all the specimens used in this study with porosity greater than 20 % contained clusters of interconnecting pores. For the specimens with porosity greater than 25 % their porosity was interconnected.

In [3] it was shown that porosity structure defined not only elastic, but also strength properties of a material. The clusters of interconnecting pores present a new element of structure in addition to single closed pores. Thus, with porosity increasing the changes of elastic and strength properties of a material are expected after transition of the percolation limit.

2. Determining the representative volume

At the first stage it is required to determine the representative volume of the modeled material. For material without pores the representative volume was determined based on four solid specimens. For this purpose the convergence of effective elastic modulus of the specimen E_{eff} to the automaton elastic modulus E_0 with increasing the specimen size was analyzed.

The convergence was assumed to be satisfied if E_{eff} differed from E_0 not greater then $3\,\%$. The computations showed the representative volume was equal $10\,\mu$m of the brick base size. The fracture pattern (cracks) in this specimen is shown in Fig. 2 The cracks are generated from the stress concentrators and propagate along maximum tangential stress direction.

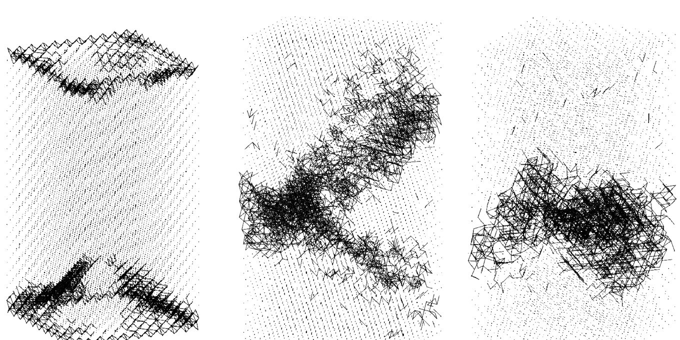
(a) (b)

Fig. 2. Fracture pattern of solid ceramic specimen under compression: a) lines connect linked automata, b) lines connect unlinked automata

If a material contain pores the cracks may initiate not in the corners but in the region of the highest local porosity. The direction of cracks propagation in such material is defined by the porous topology. Fig. 3 shows the first cracks in porous specimens with various values of porosity. One can see that failure behavior of porous material with large porosity and failure of solid material differs dramatically. In particular, the path of the crack propagation in porous material is rather crinkly.

The fracture pattern of the modeled brittle porous 3D specimens qualitative corresponds to 2D simulation results [3]. The quantitative difference is defined by the fact that porosity in 2D specimen is "interconnected" in the normal direction to the computational plane.

To analyze the dependence of elastic and strength properties of the modeled material on its porosity it is necessary to determine the size of representative specimen (volume). It is



C=0% C=20% C=40%

Fig. 3. First cracks in specimens with various values of porosity C under compression

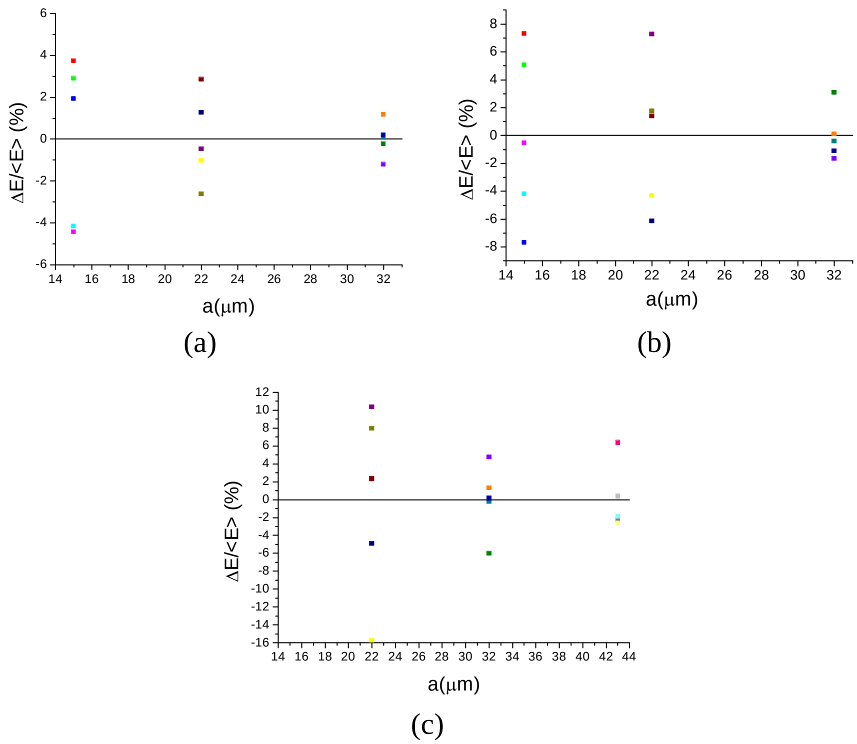


Fig. 4. Convergency of effective elastic moduli of the modeled specimens on their basis size for various porosity: a) 10 %, b) 25 %, c) 50 %

obvious that the representative volume for a porous material will be different for different values of porosity. The simulation showed that for porosity value less then 15 % the representative volume was equal 20 μm (Fig. 4). For porosity value from 15 up to 35 % the size of representative volume was found to be 30 μm (Fig. 4,b). For porosity from 35 up to 50 % — 40 μm (Fig. 4,c).

3. Studying elastic and strength properties of porous ceramics

The loading diagrams of 3D modeled specimens are shown in Fig. 5. They are in good qualitative agreement with 2D simulation results [3, 4]. A quantitative differences is explained by the different influence of porosity on effective porous characteristics in 2D and 3D tasks.

First, it has to be noted that 3D specimens with porosity stochastically distributed in space can demonstrate quasi-viscous regime of fracture like 2D models [4]. To be able to failure in this regime the porosity of 3D specimens has to be greater than 40 % (Fig. 5).

Let us consider dependence of the effective elastic modulus of 3D specimens on its porosity. In Fig. 6,a each square represents the value averaged on five representative specimens with various pore distribution in space. This dependence obviously can be divided into two characteristic parts connected with porous structure: the first corresponds to closed pores (5. . . 20 %), the second corresponds to clusters of interconnected pores (20. . . 50 %). The experimental data taken from [2] are presented in Fig. 6,b for comparison. One can see the computational results are in good qualitative agreement with the experimental data. However, the inclinations of approximating lines showing degree of the influence of porosity on

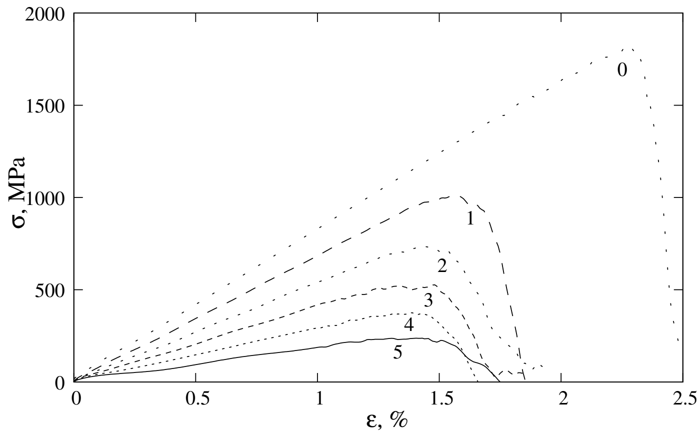


Fig. 5. Loading diagrams for ceramics with various porosity $C = n{\cdot}10\,\%$

elastic characteristics of a material within the intervals are little bit different for the experimental and computational data. It can be explained by stochastic choice of elements for pore generation in the modeled specimens, and hence by the orientations of clusters of interconnected pores, which leads to reduction of porous structure influence on mechanical properties of a material. Besides, according to [2] percolation transitions in ceramics ZrO_2 cause microstructure change. In particular, internal stresses in ceramics with continuous porous structure restrain grain growth. Thus, simulation of uniaxial compression of brittle porous 3D specimens by the movable cellular automaton method showed that percolation transition from the closed pores to interconnected pores in a porous material leads to change in the dependence of its elastic properties on porosity.

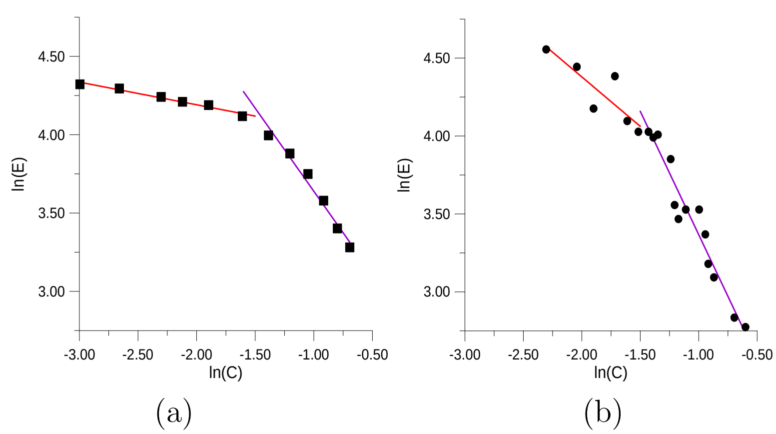
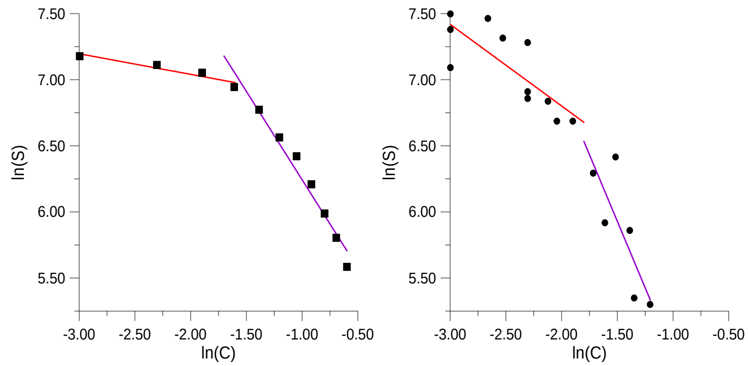


Fig. 6. Dependences of elastic modulus of ceramics on its porosity in logarithmic coordinates: a) simulation; b) experimental data

It is necessary to notice that this result could be obtained only in three-dimensional simulation because two-dimensional specimens with interconnected porosity are not topologically connected and do not resist to the mechanical loading. Besides, the porosity value at which formation of interconnected clusters occur in a two-dimensional case (22.4 %) is considerably less than the corresponding percolation limit (69.62 %).

Fig. 7 shows simulated and experimental dependencies of ceramics strength on its porosity. Again it can be divided into two characteristic parts connected with porous structure.



(a) (b)

Fig. 7. Dependences of ceramics strength on porosity in logarithmic coordinates: a) simulation, b) experimental data

In summary it is necessary to notice that for the purpose of the further application of the proposed 3D MCA model of porous ceramics it is necessary to extend the model with possibility of describing nonlinear properties of materials (degradation of elastic properties, relaxation at high-speed loading, etc.)

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