Multiscale Simulation of Porous Ceramics Based on Movable Cellular Automaton Method

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Abstract. The paper presents a model for simulating mechanical behaviour of multiscale porous ceramics based on movable cellular automaton method, which is a novel particle method in computational mechanics of solid. The initial scale of the proposed approach corresponds to the characteristic size of the smallest pores in the ceramics. At this scale, we model uniaxial compression of several representative samples with an explicit account of pores of the same size but with the random unique position in space. As a result, we get the average values of Young’s modulus and strength, as well as the parameters of the Weibull distribution of these properties at the current scale level. These data allow us to describe the material behaviour at the next scale level were only the larger pores are considered explicitly, while the influence of small pores is included via the effective properties determined at the previous scale level. If the pore size distribution function of the material has \( N \) maxima we need to perform computations for \( N - 1 \) levels in order to get the properties from the lowest scale up to the macroscale step by step. The proposed approach was applied to modelling zirconia ceramics with bimodal pore size distribution. The obtained results show correct behaviour of the model sample at the macroscale.

1. Introduction

Nowadays, ceramic materials are being widely used in medicine, electrical, electronics industries, body armor, etc. Advanced technologies of ceramics production are capable of creating 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 example, in the medical application, the porous structure of ceramics has to be interconnected in order to allow the bone tissue to fill the porous space [1]. Mainly, this leads to bimodal pore size distribution in the material. As a result, mechanical behaviour of the material can be nonlinear and even unpredictable.

The problem of predicting the physical and mechanical properties of porous materials has been being solved by many authors in various statements. The complexity of this problem consists, first of all, in the fact that the properties of advanced materials are mainly determined by their complex multiscale structure [2]. For the analytical solution of this problem, the most successful approaches are (i) the micromechanics of composites, which is based on the method of self-consistent field (definition of the property contribution tensor) as shown, for example, in [3]; and (ii) the method of random functions [4]. However, these approaches allow predicting only elastic, thermal, and electromagnetic properties of the material. Regarding the strength, the
capability of these approaches is limited essentially to the periodic structure materials. At the same time, novel computational techniques allow correct simulation of the material behaviour from atomic scale up to the macroscale. Taking into account all the aspects mentioned above, we may conclude that for predicting the mechanical properties of the advanced ceramics it is promising to use multiscale computer simulation [5, 6].

2. Description of the model

At present, numerical methods of continuum mechanics are mainly used for simulating the mechanical behaviour of materials at meso and macroscale [7, 8]. However, recently methods based on the discrete representation of materials have been successfully developed and widely used [6, 9, 10]. One of them is the method of movable cellular automata (MCA), which assumes that the material consists of a set of elementary objects (automata), interacting with each other by the forces determined in accordance with the rules of many-particle approach. MCA allows one to simulate mechanical behaviour of a solid at different scales, including deformation, initiation, and development of damages, fracture and further interaction of fragments after failure [6, 11, 12, 13].

An automaton motion is governed by the Newton-Euler equations:

\[
\begin{align*}
\frac{d^2 \vec{R}_i}{dt^2} &= \sum_{j=1}^{N_i} F_{\text{pair}}^{ij} + F_i^{\Omega}, \\
\frac{d\vec{\omega}_i}{dt} &= \sum_{j=1}^{N_i} M_{ij},
\end{align*}
\]

where \(\vec{R}_i\), \(\vec{\omega}_i\), \(m_i\) and \(\vec{J}_i\) are the location vector, rotation velocity vector, mass and moment of inertia of \(i\)th automaton, respectively, \(F_{\text{pair}}^{ij}\) is the interaction force of the pair of \(i\)th and \(j\)th automata, \(F_i^{\Omega}\) is the volume-dependent force acting on \(i\)th automaton and depending on the interaction of its neighbours with the remaining automata. In the latter equation, \(M_{ij} = q_{ij}(\vec{n}_{ij} \times F_{\text{pair}}^{ij}) + \vec{K}_{\text{rot}}^{ij}\), here \(q_{ij}\) is the distance from the center of \(i\)th automaton to the point of its interaction with \(j\)th automaton, \(\vec{n}_{ij} = (\vec{R}_j - \vec{R}_i)/r_{ij}\) is the unit vector directed from the centre of \(i\)th automaton to the \(j\)th one and \(r_{ij}\) is the distance between automata centres, \(\vec{K}_{\text{rot}}^{ij}\) is the torque caused by relative rotation of automata in the pair.

The forces acting on automata are calculated using deformation parameters, i.e. relative overlap, tangential displacement and rotation, and conventional elastic properties of the material, i.e. shear and bulk moduli. A distinguishing feature of the method is calculating of forces acting on the automata within the framework of multi-particle interaction [13, 14] using volume-dependent force \(F_i^{\Omega}\), which among other advantages provides for an isotropic behaviour of the simulated medium.

A pair of the elements may 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 realized by means of the corresponding change of the state of the pair of automata. A fracture criterion used in simulation essentially depends on the physical mechanisms of material deformation and failure. An important advantage of the MCA formalism is that it makes possible direct application of conventional fracture criteria (Huber-Mises, Drucker-Prager, Mohr-Coulomb, etc.), which are written in the tensor form [14]. In this work a fracture criterion based on critical value of the equivalent stress was used. Switching of a pair of automata to an unbound state would result in a changeover in the forces acting on the elements; in particular, they would not resist moving away from one another.

Removing automata from initial dense packing allows the explicit taking into consideration voids or pores in the material.
Herein we present a multiscale approach based on MCA method for 3D modelling zirconia ceramics with bimodal pore size distribution [15]. In general, the approach is similar to 2D one described in [16], the main difference and advantage consists in employing Weibull distribution of the elastic and strength properties of a heterogeneous material at higher scales. The initial lowest scale of the proposed approach corresponds to the characteristic size of the small pores. At this scale, we model uniaxial compression of several representative samples with an explicit account of pores of the same size but with the unique position in space. As a result, we get the average values of Young’s modulus and strength, as well as the parameters of the Weibull distribution of these properties at the current scale level. These data allow us to describe the material behaviour at the next scale level were only the large pores are considered explicitly. Simulations of the samples compression at this level provide us with the material properties used for final simulation at the macroscale.

3. Simulation results and discussion
Let us consider the simulation results of the samples compression at the lowest scale of the model corresponding to small pores of the ceramics which size is equal to 1 µm and comparable to the grain size of the material [15]. Here it is natural to use the size of automata to be equal to 1 µm too. The response function of automata was taken to be corresponding to the loading diagram for nanocrystalline ZrO$_2$(Y$_2$O$_3$) with total porosity of 2% and an average pore size being equal to about the grain size [15]. Inter-automaton bond rupture criterion used in calculations was formulated as a threshold value for equivalent shear stress. A typical model sample with an explicit account of pores is shown in Figure 1a. The pores were obtained by removing the randomly selected automata from the original close fcc packing.

There were considered five representative samples with pores of the same size but with the unique position in space. Typical loading curves for these samples are shown in Figure 1b. Using these curves the elastic modulus in compression (the slope of the linear part of the curve) and the compression strength (its maximum value) were determined for each sample. These values are random variables due to random pore arrangement in the samples. As shown, for example, in [17] the time to occurrence of the “weakest link” of many competing failure processes is governed

![Figure 1](image)

**Figure 1.** (a) a typical model sample with 15 % of porosity and (b) the loading curves for five samples of the lowest scale level with different spatial distribution of pores.
by Weibull distribution model, which assumes the following cumulative distribution function

\[ F(t) = 1 - \exp\left(-\left(\frac{t}{\eta}\right)^\beta\right) \]  

(2)

where \( \eta \) is the scale parameter (also called as the characteristic life), and \( \beta \) is the shape parameter.

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 \( \eta \) and \( \beta \) these programs use several methods, the most important of which is the method of maximum likelihood estimation. But if the random sample size is small (five in our case), it is recommended to use the median rank regression, which is reduced to the transformation of Eq. 2 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 plot of the normalized probability density function (solid line) for the strength of the samples with porosity of 15% obtained from the Weibull analysis of the presented modelling results. The same analysis was performed for the elastic modulus in compression of the model samples.

![Figure 2](image.png)

**Figure 2.** Distribution of the material strength at mesolevel: \((a)\) normalized probability density function, \((b)\) the spatial distribution in a model sample.

To verify the proposed approach against the behaviour of the real ceramics with hierarchical porous structure, let us consider the final results of simulation at the macroscale depicted in Figure 3. Figure 3a shows the loading curves for compression of two samples with the same Weibull distributions for elastic modulus and strength, but different scatter of these properties in space. One can see that this difference reveals itself only at the stage of macrocrack propagation (descending part of the curves). The main reason for such a difference is that the relative scatter of the elastic modulus is rather small compared to the strength scatter. That is why the elastic behaviour of different samples is very similar. Nevertheless, the strains when the macrocracks are generated in different samples differ, as well as the macrocrack paths. The failure pattern of
the macrosamples shown in Figure 3b is typical for heterogeneous material and consists of a large number of small fragments. This is a result of a large number of local stress concentrators in the macrosample due to scatter of strength properties. In contrast to the samples with an explicit account of the pores, where crack paths are curved [16], in our macrosamples cracks propagate along a plane direction and just deviate at new stress concentrators. However, the obtained results allow us to conclude that the proposed approach is capable for correct simulating the ceramics with hierarchical porosity.

The obtained data provide us the ability to pass from one scale level to the next scale level (herein and after referred to as mesolevel) of the model where these data describe the effective properties of the material of large pore walls. This is a heterogeneous material with stochastically distributed elastic and strength properties. To model mechanical behaviour of samples at this scale, we scatter elastic and strength properties for each automaton according to the Weibull distribution obtained from the previous scale level. The automaton size at mesolevel corresponds to the representative sample of the previous scale and is equal to 60 µm. A typical model sample for this level is shown in Figure 2b, where the automaton colour corresponds to the strength of the automaton. The crosses in Figure 2a correspond to the distribution of automata strength over the sample in Figure 2b, so one can see that these random values are really described by the specified distribution law.

4. Conclusions
A 3D multiscale model for porous ceramics based on movable cellular automaton method is proposed in the paper. The important issue of the model is a determination of the Weibull distribution parameters for elastic and strength properties at the current scale from modelling uniaxial compression of the model samples with an explicit account of pores. These parameters allow correct transfer of the effective ceramics properties to the upper scale level of the model. The proposed approach was applied to modelling zirconia ceramics with bimodal pore size distribution. The obtained results show the correct behaviour of the model sample at the macroscale.
Acknowledgments

The investigation has been carried out at financial support of the Project No. III.23.2.3 of the Basic Research Program of State Academies of Sciences for 2017–2020.

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