Numerical simulation of mesomechanical behavior of porous brittle materials

I.Yu. Smolin\textsuperscript{a,b}\textsuperscript{*}, P.V. Makarov\textsuperscript{a,b}, M.O. Eremin\textsuperscript{a,b}, K.S. Matyko\textsuperscript{a}

\textsuperscript{a}Tomsk State University, Lenin Prospekt, 36, Tomsk 634050, Russia
\textsuperscript{b}Institute of Strength Physics and Materials Science SB RAS, Pr. Akademicheskii, 2/4, Tomsk 634055, Russia

Abstract

The influence of the types of porous structure on the features of deformation, damage accumulation and fracture of mesovolumes of brittle materials is studied. At the mesoscale, the pores of different shape are taken into account explicitly. The digital models were made using random values of coordinates and radii of spherical voids or solid spheres. For numerical modeling of the mechanical behavior up to failure, the evolutionary approach is applied with considering the nonlinear constitutive equations to describe damage accumulation and its influence on the degradation of the strength properties of the frame of porous ceramics. The calculated averaged stress-strain diagrams were shown to be sensitive not only to the value of porosity but also to the shape of pores. The simulation results are validated with experimental data for zirconia and alumina ceramics. Good qualitative and quantitative agreement of modeling results with experimental data suggests that taking into account of two-scale porosity in the form of explicit consideration of large pores at the mesoscale and implicit integrated consideration of tiny pores and cracks from the microscale in the form of accumulated damage is quite sufficient in the framework of the hierarchical modeling.

Keywords: Ceramics; Porous structure; Modeling; Structure – property relationship; Damage.

1. Introduction

Because of the manufacturing process, all ceramics acquire a certain degree of porosity. Of special interest are the highly porous ceramics that are widely used as filters, thermal insulator, catalyst, prosthetics, etc. The problems of
modeling of porous materials can refer to three areas: (i) modeling the porous structure per se; (ii) determining the effective properties of porous materials; (iii) direct numerical simulation of deformation and fracture of porous materials at different scales. While there is a vast literature devoted to all of the three, quite a number of problematic issues still exist (e.g., Bruno and Kachanov 2013a; Kalatur et al. 2014; Manoylov et al. 2013).

Concerning the first of mentioned area of problems, it should be mentioned that in analytical approaches due to mathematical restrictions some simplified hypotheses about porous structure are usually introduced. For example, it is suggested that all pores are isolated and periodically located in space, have spherical or ellipsoidal shape and the same size. The computational approach is free of these limitations and makes it possible to take into consideration an extensive variety of periodical or stochastic structures (Michel et al. 1999; Kanit et al. 2011; Xu et al. 2015). Besides, now it is possible to get the features of the porous morphology of real materials using tomography as shown by Chen et al. (2014) and Saxena and Keller (2000).

Initially, to predict the effective physical mechanical properties of heterogeneous and composite materials the analytical approaches were used. The use of numerical modeling for that purposes started from the two-dimensional approximation that still have been used in some cases (e.g., Konovalenko et al. 2013; Karakulov et al. 2014). However, with the rise of different numerical methods and computer power it became possible to solve three-dimensional problems as shown, e.g., by Smolin et al. (2014a, b). There are a lot of articles devoted to estimation of elastic properties of porous ceramics but not too much discussing the strength-porosity relations. To describe the effective properties and even peculiarities of the mechanical behavior at the stages of non-elastic deformation, cracking and fracture, the corresponding comprehensive nonlinear constitutive equations are needed. Examples of such models for heterogeneous solids have been reported by Ursenbach (2001), Makarov (2008), Makarov and Eremin (2013), Bruno and Kachanov (2013b). As usual, highly porous materials are hierarchically organized multiscale systems. Under external forces applied the evolution of such a multiscale system leads to accumulation of damage of different scales and to the formation of new structures, i.e. complexification of the system. A basic problem of the simulation of such materials is the construction of constitutive equations describing all aspects of the mechanical behavior of these materials, including the deformation response and, especially, the failure.

The evolutionary methodology developed by Makarov (2008), Makarov and Eremin (2013), Kostandov et al. (2013) seems to be an effective approach to solving this problem. Mathematically, the complete set of differential equations of continuum mechanics together with the constitutive equations is a set of nonlinear dynamic equations. Makarov (2008) and Makarov and Eremin (2013) have shown that the solutions of these solid mechanics equations demonstrate all the main features of the evolution of non-linear dynamic systems, including the slow dynamics, bifurcation and change in the scenarios of evolution. It has been also shown that material failure at the final unstable stage develops as a catastrophe in the blow-up regime. From a physical standpoint, a material under loading is considered as a nonlinear dynamic multiscale system. The nonlinear positive and negative feedbacks are explicitly specified in the set of equations, which regulate the interaction between the state of stress and the strain emerging in the material, as well as its response to the loading (accumulation of damage at different scales, degradation of strength properties). Such an approach can effectively describe the mechanical evolution of porous materials at different scales, including the localized accumulations of damage and inelastic deformation at micro- and meso-scales, strength degradation, the formation of cracks of different scales and the macroscopic failure.

The purpose of this paper is to demonstrate the possibilities of combination of a known approach to modeling porous structure of materials (a geometrical problem) and a new approach to simulation of mechanical behavior (deformation, damage accumulation, and fracture) of porous material mesovolumes.

2. Geometric models of the porous medium

Following the pioneering work by Roberts and Garboczi (2000) and subsequent contributions by Bruno et al. (2011) or Smolin et al. (2014c), we will consider two statistical models of porous structures with different morphologies: overlapping spherical pores (OSP) and overlapping solid spheres (OSS). In the first case, a model of porous medium represents a sample of solid comprising spherical voids of different radii at random uncorrelated points in space. This model mimics the morphology of isolated pores in realistic materials at low porosity caused by the processes of coalescence and spheroidization of pores, e.g., in ceramics at the last stage of sintering. In the second case, the geometric model is constructed by filling an empty space by solid spherical particles of different
radii, which are placed at randomly selected points in space and may overlap. This model correlates with the process of sintering of ideal spherical particles, e.g., ceramic powder.

We have generated a series of geometric structures consisting of voxels, which represent the two types of pore morphology considered above. Two of them are shown in Fig. 1a, b. These voxel structures were used as an input for the following computer simulation of their deformation and fracture. To estimate how these model structures mimic reality, one can compare them with the photo of the surface of porous zirconia ceramics shown in Fig. 1c. The ceramics were obtained by sintering of nanostructured zirconia powders (Buyakova and Kulkov, 2007). It is seen that in realistic ceramics there are pores of different morphologies in one and the same material. This is due to various factors, such as changing the process conditions, different forms of individual powder particles, etc. The greater interest then arises in the numerical investigation of ideal porous structures when one can separately study the contribution of each pore morphology to the features of their mechanical characteristic and behavior.

![Fig. 1. 3D model structures having different pore morphology: (a) OSP structure; (b) OSS structure; and (c) SEM image of the porous structure in the zirconia ceramics by Buyakova and Kulkov (2007).](image)

### 3. The mathematical framework of the evolutionary approach to modeling deformation and failure

In accordance with the concept of the evolutionary description of deformation and subsequent fracture of materials developed by Makarov (2008), the complete set of equations includes the fundamental laws of conservation of mass, momentum and energy, as well as two groups of constitutive equations. The first group of constitutive equations defines the elastic response of the media, and in the concept represents the well-known linear hypoelastic relation between the Jaumann rate of Cauchy stress and rate of deformation. The concern of the evolutionary constitutive equations of the second group is to determine the rate of inelastic strains in the first group of constitutive equations. Here, strain rate is determined by the plastic flow theory:

\[
\dot{\varepsilon}_{ij} = \lambda \frac{\partial g(\sigma_{ij})}{\partial \sigma_{ij}} \quad \text{if} \quad f(\sigma_{ij}) \geq 0
\]

(1)

where

\[
g(\sigma_{ij}) = J_2 - \lambda P(2Y + \alpha P) + \text{const}
\]

(2)

\[
f(\sigma_{ij}) = -\alpha P + \sqrt{J_2} - Y_0(1-D)
\]

(3)

\[
D = \int_{\varepsilon_0}^{\varepsilon_{\text{eff}}} \left[ H(\mu_\sigma)(\varepsilon_{\text{eff}} - \varepsilon_0^C)^2 + (1 - H(\mu_\sigma))(\varepsilon_{\text{eff}} - \varepsilon_0^T)^2 \right] dt
\]

(4)


$$\mu_\sigma = 2 \frac{S_2 - S_1}{S_1 - S_3} - 1$$

Here $\dot{e}_{ij}^p$ are the components of the inelastic strain rate tensor, $\sigma_{ij}$ are the stress tensor components, $J_2 = 0.5 \sigma_{ij} \sigma_{ij}$ is the second invariant of deviatoric stress tensor, $P$ is the mean hydrostatic stress (pressure), $\alpha$ is the internal friction coefficient, $\Lambda$ is the coefficient of dilatancy, $Y_0$ is the reference cohesion (shear strength when pressure equals zero), $D$ is the damage. The plastic multiplier $\lambda$ in Eq. (1) is determined by the requirement that the stress must meet the yield condition $f(\sigma_{ij})$.

Limiting stress surface $f(\sigma_{ij})$ is written in the von Mises–Schleicher form with taking into account the dependence of the shear strength on the pressure, which in turn results in different tensile and compressive strength of the material. A non-associated flow rule is used in Eq. (1), which means $\Lambda$ is independent of $\alpha$. In this case, the plastic potential $g(\sigma_{ij})$ given by Eq. (2) is different from the yield function $f(\sigma_{ij})$ given by Eq. (3).

The failure of a material in this approach is described as the process of downfall degradation of the material strength to zero when damage accumulation takes place. The function of medium degradation (damage) $D = D(t) \leq 1$ is represented by Eq. (4) as a function of the current effective accumulated inelastic strain $\varepsilon_{eq} = \varepsilon_{eq} + \alpha \theta \varepsilon_{cur}$ in the medium and of the stress state type (Lode–Nadai parameter $\mu \sigma$). Here $H(x)$ is the Heaviside function, $\varepsilon_{eq}$ is the equivalent inelastic strain, $\theta$ is the inelastic bulk strain, $\varepsilon_0^C$, $\varepsilon_0^T$ are the strains on the elastic stage at which the material begins to accumulate damage under conditions of compression and tension, respectively, $\varepsilon_0$ is a parameter of the model, $t_0^C$ and $t_0^T$ have the meaning of the characteristic time of the process in compression and tension, respectively. $S_1$, $S_2$, $S_3$ are the principal deviatoric stresses. Note that $\varepsilon_0^T < \varepsilon_0^C$, so damage accumulation begins at substantially lower stress in the zones of tension plus shear ($\mu_\sigma < 0$) than in the zones of compression plus shear where $\mu_\sigma > 0$. The rate of damage accumulation $1/t_0^T$ in the local zones where $\mu_\sigma < 0$ is also significantly higher than the rate $1/t_0^C$ in the zones where $\mu_\sigma > 0$. Consequently, the strength parameters will degrade much faster in the regions of the medium where the Lode–Nadai parameter is negative. Thus, the medium response to the type of stress state is yielded in the medium during its loading.

4. Calculation results and their discussion

The simulation of deformation and fracture of porous ceramics were performed by solving the total set of equations in a three-dimensional formulation using the finite difference scheme described in detail by Wilkins (1999).

The size of the computational domain was always $9 \times 9 \times 9 \ \mu m^3$. The uniform computational grid consisted of $150 \times 150 \times 150$ nodes. The media in pores were modeled by an effective elastic material with mass and elastic properties of several orders of magnitude smaller than the corresponding characteristics of ceramics.

4.1. Uniaxial compression

First of all, the modeling of mechanical behavior of the generated model structures of porous materials was carried out for the conditions of uniaxial compression. Calculations were performed using the isotropic material properties which correspond to the partially stabilized zirconia in the tetragonal phase: the shear modulus $G = 83 \ \mathrm{GPa}$, Young's modulus $E = 220 \ \mathrm{GPa}$, the density $\rho = 6 \ \mathrm{g/cm^3}$, $Y_0 = 2200 \ \mathrm{MPa}$, $\alpha = 0.4$, $\Lambda = 0.1$. The values for the parameters of the kinetics of damage accumulation were taken from the test calculation to produce the features of fracture observed in experiments (Smolin et al. 2014c).

Figure 2a shows the average stress-strain curves for four different samples. One can see that the lower is porosity the higher is the corresponding curve that agrees with experimental observations. For the same porosity, the curve
for OSS morphology lies below. Similar information was reported by Roberts and Garboczi (2000) and Bruno et al. (2011) for the purely elastic behavior.

According to Bruno et al. (2011), the dependence of Young's modulus $E$ on the average porosity $p$ for different morphologies has the form

$$ E = E_d (1 - p)^m $$

where $E_d$ is the Young's modulus of the dense material (or solid domain), and the index of power $m = 2$ for the OSP structures and $m = 4$ for OSS structures. This exponent $m$ is called the pore morphology factor by Bruno et al. (2011). The results obtained in our calculations give the values for this exponent $m = 2.15$ for OSP samples and $m = 3.34$ for OSS samples. The variation may be caused by the fact that the pores have different sizes and are distributed quasi-uniformly which does not comply with the theoretical model assumption. Other authors for the same porous structures bring forward alternative relationships, for example, Roberts and Garboczi (2000) give the formulas

$$ \frac{E}{E_d} = \left(1 - \frac{p}{0.652}\right)^{2.23} $$

$$ \frac{E}{E_d} = \left(1 - \frac{p}{0.818}\right)^{1.65} $$

for OSS and OSP structures, respectively. Smolin et al. (2014a) give the values of maximum porosity 0.7213 and power $m = 1.9026$ for this kind of approximation that are in between the numbers in Eqs (7) and (8), but the pore morphology in their case is also something average due to the features of the numerical movable cellular automaton method applied.

Experimental studies of porous zirconia with the porosity varying in the range from 10% to 75% and different ratio of pore size and ceramics grain size reported by Kulkov et al. (2003) and Savchenko et al. (2014) indicate that the porosity dependence of the Young's modulus is better approximated by the exponential function $E = E_d \exp(-b \cdot p)$. Comparison of the analytical power and experimental exponential dependences, as well as our own calculations point data, are shown in Fig. 2b. It is seen that the exponential and power dependences are very
close for OSS morphology in the selected range of porosity. The difference between them for small and especially for large porosity can be explained by the fact that the pore morphology of the experimental samples does not correspond strictly to the overlapping spherical solids, and in reality, there is a pronounced clusterization (Fig. 1c). The results data obtained in our calculations are also in a good agreement with the power law for the OSS morphology.

Of special interest is also the porosity dependence of strength characteristics. The experimental data for zirconia ceramics was also approximated by the exponential function with different parameters depending on the commensurability of sizes of pores and grains by Kulkov et al. (2003). Figure 2c shows these approximating curves and points obtained in our calculations. The calculated data for the OSS morphology again are in better agreement with the experimental curves.

Figure 3 presents the distributions of damage in different samples at the time corresponding to the last point on the stress-strain curve, i.e. immediately before macrofailure. From the analysis of the nature of the damage accumulation in the frame at the mesolevel, it is worth noting that definitive impact of the total porosity and pore morphology on the shape and the number of cracks could not be stated. Cracks begin to form mainly at the places of high stress concentration near the pores. It may be noted that a thinner frame and a greater curvature of OSS pore structure result in the higher stress concentration. Therefore cracks begin to form and grow through the entire sample of the OSS samples earlier than in the OSP structures.

4.2. Simple shear

The next problem to study was the behavior of the porous structures under different loading, namely shear. The experimental results for the shear modulus of brittle porous materials are presented by Savchenko et al. (2014) for alumina and zirconia ceramics. In our calculations of the shear loading the following parameters for alumina were used: shear modulus \( G = 152 \text{ GPa} \), Young's modulus \( E = 380 \text{ GPa} \), density \( \rho = 3.9 \text{ g/cm}^3 \), \( Y_0 = 30 \text{ MPa} \), \( \alpha = 0.4 \), \( \Lambda = 0.1 \). Since the OSS structure showed the better results in the case of compression, only this kind of pore morphology was used for shear loading simulations.
The averaged stress-strain curves are shown in Fig. 4(a) for two samples with the total porosity of 20% and 40%. The curves have a shorter elastic part compared with the curve for compressive loading. The descending branch of the $\tau - \gamma$ diagram for shear, on the contrary, is more extensive. Both simulated and experimental dependences of shear modulus versus porosity are depicted in Fig. 4(b). Here again, $G_d$ denote the shear modulus of the dense host material. The comparison of the calculated and experimental data for shear loading shows that the values calculated fit well the experimental curve, especially for porosity varying from 20% to 50%. It is interesting to note that in experiments the porosity was in the range from 20% to 70%.

![Graph](image)

Fig. 4. (a) The averaged shear stress-strain curves calculated for porous alumina OSS samples; (b) The porosity dependence of the reduced shear modulus: experimental curve by Savchenko et al. (2014) and the calculated points.

5. Concluding remarks

Our calculations confirmed that the model structures created by combining overlapping spherical solids mimic well the porous ceramic materials produced by sintering of oxide powders. These geometric models meet better the pore morphology of real samples of porous zirconia ceramics, and they give better agreement for the porosity dependences of the effective Young's modulus and strength when used in modeling of the mechanical behavior of zirconia ceramics under uniaxial compression. A good fit with experimental results for alumina ceramics was also obtained for this kind of morphology in the case of modeling simple shear loading. Some disagreement of calculations results with experimental data should be explained by the fact that the pores were distributed quasuniformly in the model porous structures while in the reality the pore clustering is observed. Besides, in real sintered porous ceramics the pores of different morphology can be found.

The application of the evolutionary approach has provided a suitable description of the formation of areas of high localized damage at the mesoscale and the influence of strength degradation in these local regions of the material on the general nature of the average macroscopic stress-strain diagram including its descending branch. It makes it possible to analyze the influence of pore morphology not only on the elastic moduli but on the strength properties as well. Moreover, it allows for investigating the peculiarities of the material to retain its capacity to fulfill mechanical and functional properties at the stage of damage accumulation.

The medium strength degradation is represented here as a function of accumulated inelastic strain and of the stress state type described by the Lode–Nadai parameter, so that damage accumulation begins at substantially lower stress in the zones of tension plus shear than in the zones of compression plus shear. The rate of damage accumulation in the local areas with the negative Lode–Nadai parameter is also significantly higher. As a result, the strength parameters will degrade much faster in those regions of the medium where the Lode–Nadai parameter is negative. It is very important for heterogeneous materials, such as porous ceramics, because even under simple loading conditions there are regions of various states of stress, and tension is one of them.
Acknowledgements

The research was supported by “The Tomsk State University Academic D.I. Mendeleev Fund Program”, grant 8.2.19.2015 (section 2), and the Program of basic scientific research of the Russian Academy of Sciences in 2013–2020, project 23.2.3 (section 4). Calculations were performed using supercomputer resources of Tomsk State University. The authors thank their colleagues S.N. Kulkov, S.P. Buyakova, N.L. Savchenko and T.Yu. Sablina (ISPMS SB RAS) for providing SEM picture of zirconia and the approximation data of their experimental results.

References


