# Multiscale numerical study of fracture and strength characteristics of heterogeneous brittle materials using the particle-based MCA method

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**Abstract**

In the present paper the multiscale approach to the construction of multiscale rheological models of brittle materials with heterogeneous internal structure is implemented within the numerical method of movable cellular automata (MCA). Nikolaevsky's plasticity model with non-associated flow law was chosen as a rheological model for zirconium alumina concrete at the different structural scales. An example of application of the implemented approach to determine the mechanical properties(including parameters of the rheological model and strength values) of brittle materials with multiscale internal structure at both macroscopic and mesoscopic scales is described. The effect of strain rate on brittle material behavior in case of uniaxial compression and tension was analyzed.

The majority of natural and technical materials have multiscale heterogeneous internal structure, which can be represented as a hierarchy of three principal structural scales: micro-, meso- and macroscopic scales. To model such materials at different structural/spatial scales the so-called "multiscale approach" [1] can be efficiently used. In the framework of this approach a representative volume of the material is determined for each structural scale from the lowest to macroscopic one. According to the results of theoretical study (analytical description or numerical simulation) of the response of representative volume the integral rheological function and the values of its parameters (including strength) are defined. Constructed in this way rheological models are used as input data for the components of the structure (regions with different structural and phase composition) at the next (higher) structural/spatial scale. Sequential implementation of this procedure from the lowest scale up to macroscopic one provides construction of a macroscopic rheological model of material.

It is known that characteristics of the material are determined not only by the features of the internal structure, but greatly depend on the load type and stress/strain rate as well. Therefore, the determination of adequate methods for obtaining dynamic strength characteristics of materials is an important trend in mechanics and materials science. This is due to the fact that the effect of strain rate on the results of the experiment is observed even at low rates, while under the dynamic impact the influence of strain rate becomes determinative. Numerical simulation is an efficient way to reveal the influence of strain rate and applied boundary conditions on material behavior and mechanical properties under dynamic loading.

In the present work we used an approach to the construction of multiscale rheological models within the numerical method of movable cellular automata (MCA). The MCA

method belongs to the group of computational particle-based methods [2]. The formalism of this method combines mathematical formalisms of discrete element and cellular automaton numerical methods. The non-associated plastic flow law with Drucker-Prager failure criterion (Nikolaevsky's plasticity model) is used as the rheological model in the formalism of MCA [3]. The model parameters (such as compressive and tensile strengths, dilation and internal friction coefficients) are considered as functions of both accumulated inelastic strain and strain rate.

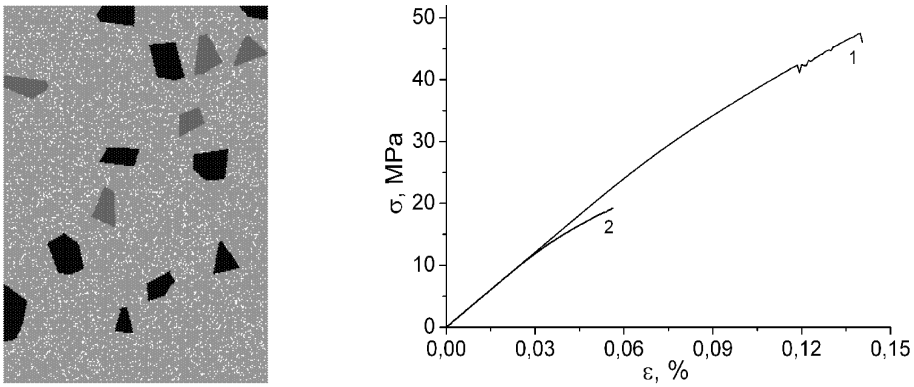
In the study the multiscale approach [1] was applied to construct a multiscale structural model of zirconium alumina concrete (ZAC) with reinforcing particles of electrofusion zirconium dioxide and barium-alumina cement binder. Topicality of the study of mechanical properties of ZAC is associated with the big prospects of its application in nuclear reactor protection systems against the spread of radioactive substances into the environment in case of severe accidents.

When constructing the MCA-based multiscale model of ZAC the internal structure of investigated material on macroscopic and mesoscopic structural scales was taken into account. Each automaton at the macroscale was characterized by physical and mechanical parameters corresponding to the integral response of mesoscopic representative volume of ZAC. Samples describing mesoscopic representative volumes were designed with explicit consideration of irregularities of internal structure (reinforcing ceramic particles, pores and damages). Properties of cellular automata modeling components of mesostructure were determined using available experimental data in the literature. At the macroscopic scale a concrete is considered as a structural monophase material. Herewith, its complicated multiscale internal structure is implicitly taken into account through the agency of parameters of the mechanical response of movable cellular automata. The presence of macroscale heterogeneities is modeled by specifying the type and parameters of stochastic spatial distribution of properties such as yield stress, strength and others.

To determine the required mechanical properties of cellular automata at the macroscale the constructed mesoscopic samples of concrete (with explicit modeling of the large-size fraction of $ZrO_2$) was subjected to mechanical tests (including uniaxial compression and tension). Figure 1a shows an example of the internal structure of the representative volume sample of concrete with 10% volume fraction of reinforcing $ZrO_2$ aggregates (samples with 30% and 50% volume fraction of aggregates were similarly considered). Black inclusions in the figure show the nonporous ("monolithic") mesoparticles of $ZrO_2$, dark gray inclusions correspond to the weakly bounded conglomerates of $ZrO_2$ microparticles. The matrix (binder) is light gray. The model takes into account the fact that the porosity of concrete is determined primarily by the porosity of the binder. In the carried out two-dimensional simulation it was assumed to be equal to 10% that corresponds to 15-20% volume porosity.

The general properties of mesoscopic concrete components are shown in table 1. The properties of monolithic mesoparticles and microparticles conglomerates of $ZrO_2$ were taken from the experimental data, which are available in literature, for low-porous and high-porous zirconium dioxide respectively. The mechanical properties of movable cellular automata modeling the binder corresponded to properties of the cement with ideal defect-free internal structure.

Using the data shown in table 1, the uniaxial compression and tension tests (in quasi-static approximation, $\dot{\varepsilon} = d\varepsilon/dt$=0.01) of mesoscopic concrete samples were conducted. The basic strength and rheological characteristics of the samples with different volume fractions of reinforcing $ZrO_2$ particles were obtained. For example, Figure 1b shows the diagrams of uniaxial compression and tension of mesoscopic concrete sample with 10 % volume fraction of reinforcing particles. The characteristics obtained by the series of similar




a) b)

Figure 1: An example of the internal structure of the concrete sample at the mesoscale (a) and tipical diagrams of uniaxial compression (plot 1) and tension (plot 2) for mesoscopic concrete samples (b).

tests of the mesoscopic samples with different spatial configurations of aggregates were averaged. The table 2 summarizes the main integral strength and rheological properties of ZAC concrete with different volume fractions of reinforcing aggregates at the mesoscopic scale.

The strength and rheological characteristics of the mesoscopic concrete samples were used to specify the properties of movable cellular automata modeling the concrete at the macroscopic scale for the simulation of the dynamic tests of macroscopic concrete samples. The influence of loading velocity on material response was taken into account by defining the dependences of mechanical parameters of concrete (including yield stress, dilation and internal friction coefficients, compressive and tensile strength and so on) on strain rate (fig. 2). These dependences were obtained by generalization of the large set of experimental data for a wide range of brittle materials including concretes [4]. For example, figure 2 shows the generalized dependence of the compressive strength $\sigma_c/\sigma_c^0$ (fig. 2a) and tensile strength $\sigma_t/\sigma_t^0$ (fig. 2b) on the strain rate. Here, the values of the strengths $\sigma_c$ and $\sigma_t$ are normalized by the values of static compressive strength ($\sigma_c^0$) and tensile strength ($\sigma_t^0$) respectively. Obtained generalized dependences determined dynamic mechanical response of movable cellular automata modeling fragments of concrete samples at the macroscopic scale.

The uniaxial compression and tension tests of the ZAC concrete samples at the macroscopic scale were simulated at various impact velocities. Strain rate ranged from $\dot{\varepsilon}= 0.1$ to $\dot{\varepsilon}= 1000$. Note that at the initial stage of dynamic loading the value of applied loading velocity increased gradually to the final value and then was held constant. At high strain

| Parameter | Binder | $ZrO_2$ | Conglomerates of $ZrO_2$ microparticles |
|---|---|---|---|
| Young's modulus E (GPa) | 55 | 172 | 27 |
| Yield stress $\sigma_y$(MPa) | 35 | 1000 | 175 |
| Dilation cefficient $\Lambda$ | 0,16 | 0,25 | 0,25 |
| Internal friction coefficient $\omega$ | 0,16 | 0,25 | 0,3 |
| $\sigma_c/\sigma_t$ (MPa)/(MPa) | 170/75 | 2100/831 | 170/75 |

Table 13: Physical and mechanical properties of the concrete components at the mesoscale.

| Parameter | Aggregate concentration 10% | Aggregate concentration 30% | Aggregate concentration 50% |
|---|---|---|---|
| E (GPa) | 38,6 | 44,4 | 53,1 |
| $\sigma_y$ (MPa) | 21,8 | 27,4 | 24 |
| $\Lambda$ | 0 | 0 | 0 |
| $\omega$ | 0,21 | 0,27 | 0,272 |
| $\sigma_c/\sigma_t$ (MPa)/(MPa) | 45,8/21 | 50,5/18,3 | 51,5/18,5 |

Table 14: Physical and mechanical properties of concrete samples at the macroscale.

rates the time of increase in loading velocity is comparable with the total time of loading and this definitely influences the characteristics of the mechanical response of material. Figures 3 and 4 show examples of loading diagrams of the concrete sample in the cases of uniaxial compression and tension respectively (here mechanical properties of movable automata corresponds to the properties of mesoscopic concrete samples with 10% aggregate concentration).

Analysis of the simulation results has shown that the dependence of the strength characteristics of concrete on strain rate is strongly non-linear. This generally corresponds to the experimental data [4]. However, quantitative comparison of the values of concrete strength has shown a significant difference between the results of the numerical simulation and the experimental data [4, 5, 6]. Figure 5 shows numerically obtained dependences of the compressive and tensile strength on strain rate for uniaxial compression and tension tests of ZAC concrete samples. At high strain rates values of dynamic concrete strength are order of magnitude higher than experimental magnitudes presented in figure 2.

Huge increase in the concrete strength in numerical experiments is accompanied by the change of the type of sample fracture. In the case of compression test at strain rates not exceeding $\dot{\varepsilon} \approx 1$ fragmentation of samples is typical for quasistatic regime of loading (fig. 6a), while at high strain rates (up to $\dot{\varepsilon}$=1000) fracture develops in frontal regime (fig. 6c). In the last case the region of extremely intensive fracturing (crushing) extends behind the front of incident elastic wave. At rates of the order $\dot{\varepsilon}$=10 (fig. 6b) first damages are localized near the loading surface, and then, after the elastic wave reflection from the bottom surface of the sample, the remaining (lower) part of the sample is being destroyed.

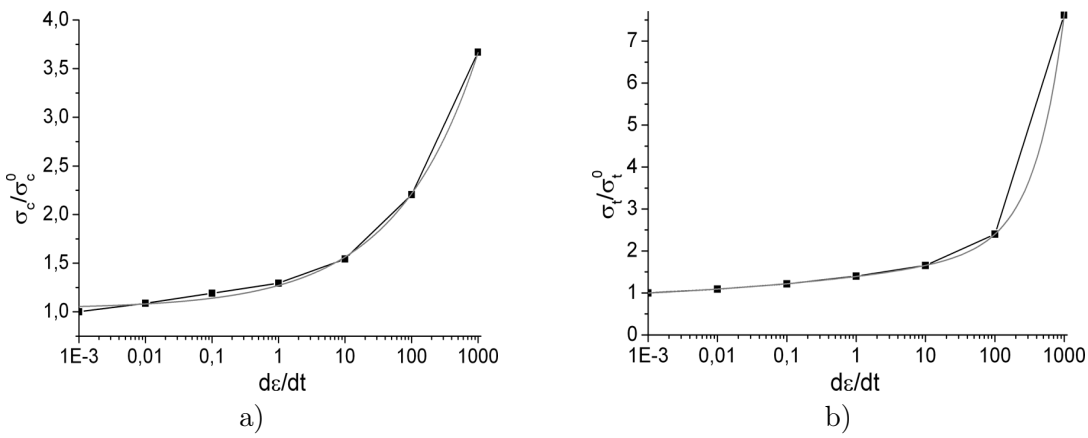
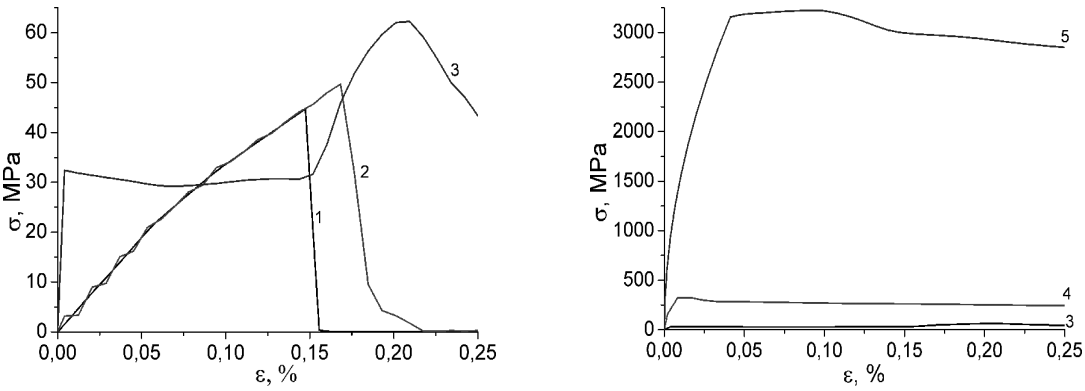
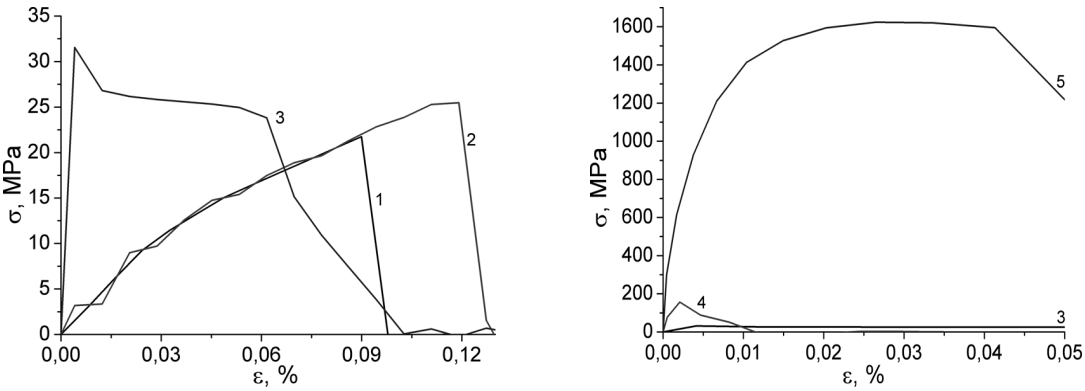



Figure 2: Generalized experimental dependencies of the compressive (a) and tensile (b) strengths on the strain rate.




a) b)

Figure 3: Loading diagram of uniaxial compression of the concrete sample with strain rate: 1 - $\dot{\varepsilon}$=0.1; 2 - $\dot{\varepsilon}$=1; 3 - $\dot{\varepsilon}$=10; 4 - $\dot{\varepsilon}$=100; 5 - $\dot{\varepsilon}$=1000.




a) b)

Figure 4: Loading diagram of uniaxial tension of the concrete sample with strain rate:1 - $\dot{\varepsilon}$=0.1; 2 - $\dot{\varepsilon}$=1; 3 - $\dot{\varepsilon}$=10; 4 - $\dot{\varepsilon}$=100; 5 - $\dot{\varepsilon}$=1000.

Quantitative difference between the experimental results (fig. 2) and results of numerical simulation (fig. 5) is due to the differences in the methods of obtaining the strength characteristics of material under dynamic impact. In most experimental studies considered in the paper [4] the compressive and tensile strengths are determined by indirect methods, which analyze the wave processes, the fracture energy intensity value, etc. In the present study the value of compressive or tensile strength was assumed to be equal to the maximum compressive or tensile stress at the uniaxial compression or tension test of the sample. So, numerical simulation has shown that in a direct uniaxial compression (or tension) test the sample inertia and finite dimensions hinder to obtain real (correct) strength properties of the material.

This fact indicates that at strain rates corresponding to the dynamic regime of loading ($\dot{\varepsilon} \gg 1$) the method of experimental realization of the specified kind of stress state (uniaxial compression or tension, nonequiaxial compression and so on) plays the determining role in the studying the strength properties of material. So, numerical modeling is a perspective and economically efficient way for the development of adequate experimental methods of determining the strain rate dependences of mechanical (including strength) characteristics of heterogeneous solids.

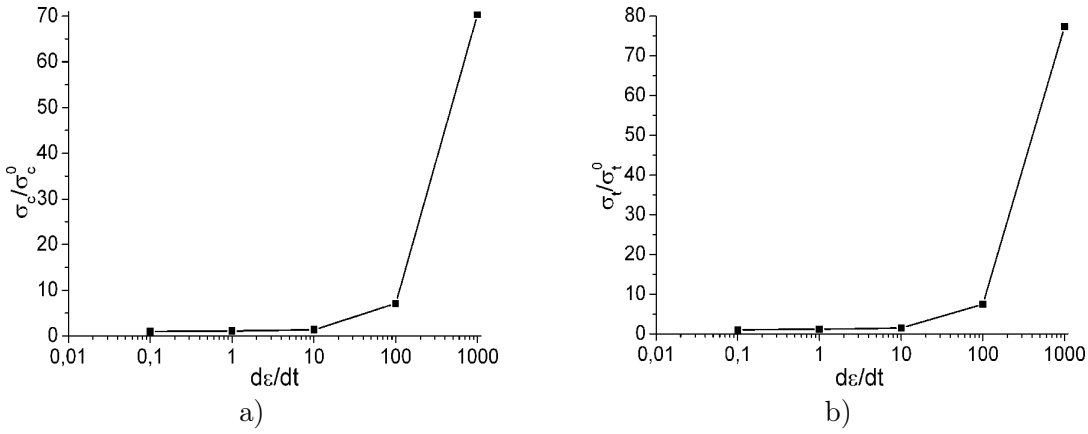



Figure 5: Dependences of normalized compressive (a) and tensile (b) strengths on the strain rate. Numerical simulation results.

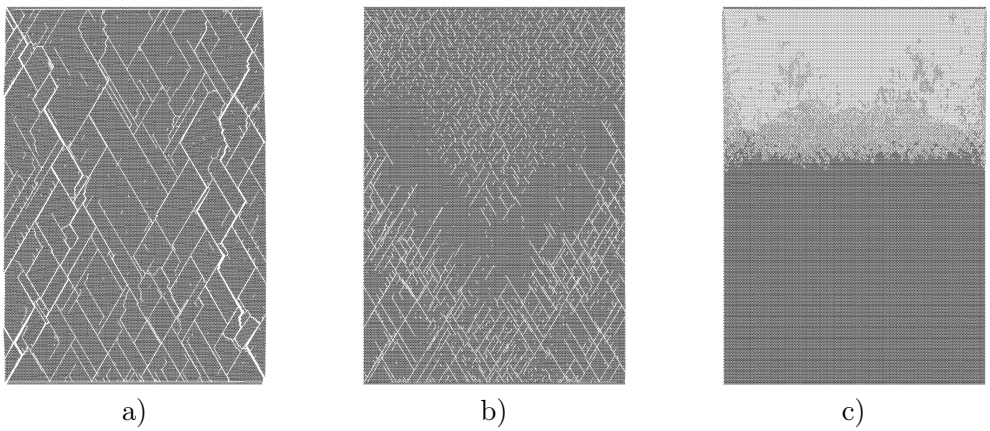



Figure 6: Examples of sample fracture at the uniaxial compression at the strain rates $\dot{\varepsilon}$=0.1 (a), $\dot{\varepsilon}$=10 (b), $\dot{\varepsilon}$=100 (c).

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