

# The Numerical Study of Fracture and Strength Characteristics of Heterogeneous Brittle Materials under Dynamic Loading

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**Abstract.** In the present paper the multiscale approach to the construction of rheological models of brittle materials with heterogeneous internal structure is implemented within the numerical method of movable cellular automata. An example of application of the implemented approach to determine the mechanical properties (including parameters of the rheological model and strength) of brittle materials with complicated internal structure at both macroscopic and mesoscopic scales is described. The effect of strain rate on brittle materials behavior under uniaxial compression and tension is analyzed.

**Keywords:** multiscale numerical simulation, zirconium alumina concrete, movable cellular automaton method, fracture

## INTRODUCTION

The majority of materials have complicated 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 material properties are determined not only by the features of the internal structure, but greatly depend on the load type and 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 rheological models within the numerical method of movable cellular automata (MCA). The movable cellular automata method belongs to the group of computational particle-based methods [2]. The formalism of this method combines features of discrete elements 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 movable cellular automata method [3].

## MODEL DESCRIPTION

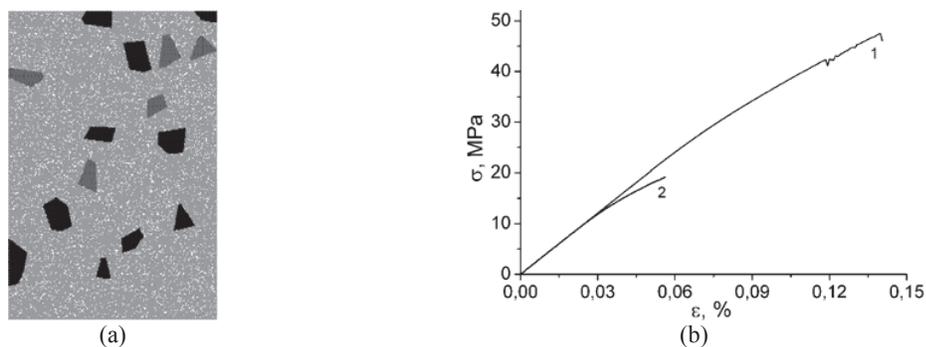
In the study the multiscale approach [1] was applied to construct a structural model of zirconium alumina concrete with reinforcing particles of electrofusion zirconium dioxide and barium-alumina cement binder. Topicality of the study of mechanical properties of zirconium alumina concrete is associated 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 structural model of zirconium alumina concrete the internal structure of investigated material at 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 zirconium alumina concrete. 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 experimental data. Experimental investigation of the mechanical properties of zirconium alumina concrete was conducted using the modified Kolsky method (split Hopkinson bar method). The features of the mechanical response of concrete under dynamic splitting and dynamic compression of concrete samples constrained by the rigid girdle were analyzed. At the macroscopic scale a concrete is considered as a structural monophasic material. Herewith, its complicated multiscale internal structure is implicitly taken into account by means 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.

## RESULTS AND DISCUSSION

To determine the mechanical properties of cellular automata at the macroscale the mesoscopic samples of concrete (with explicit modeling of the large-size fraction of  $ZrO_2$ ) were subjected to uniaxial compression and tension tests. Figure 1(a) 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 conglomerates of  $ZrO_2$  microparticles 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.



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

TABLE 1. Physical and mechanical properties of the concrete components at the mesoscale

Parameter	Binder	ZrO <sub>2</sub>	Conglomerate of ZrO <sub>2</sub> Microparticles
Young's modulus $E$ , GPa	55	172	27
Yield stress $\sigma_y$ , MPa	35	1000	175
Dilation coefficient $\Lambda$	0.16	0.25	0.25
Internal friction coefficient $\omega$	0.16	0.25	0.30
$\sigma_c / \sigma_t$ , MPa	170 / 75	2100 / 831	170 / 75

TABLE 2. Physical and mechanical properties of concrete samples at the macroscale

Parameter	Aggregate Concentration		
	10%	30%	50%
$E$ , GPa	38.6	44.4	53.1
$\sigma_y$ , MPa	21.8	27.4	24.0
$\Lambda$	0	0	0
$\omega$	0.210	0.270	0.272
$\sigma_c / \sigma_t$ , MPa	45.8 / 21	50.5 / 18.3	51.5 / 18.5

Using the data shown in Table 1, the uniaxial compression and tension tests (quasi-static approximation,  $\dot{\varepsilon} = d\varepsilon/dt = 10^{-2}$ ) of mesoscopic concrete samples were conducted. The basic strength and rheological characteristics of the samples with different volume fractions of reinforcing ZrO<sub>2</sub> particles were calculated. For example, Fig. 1b shows the diagrams of uniaxial compression and tension of mesoscopic concrete sample with 10 % volume fraction of reinforcing particles. The characteristics calculated by the series of similar tests of the mesoscopic samples with different spatial configurations of aggregates were averaged. The Table 2 summarizes the main integral properties of zirconium alumina concrete concrete with different volume fractions of aggregates at the mesoscopic scale.

The properties of the mesoscopic concrete samples were used to specify the properties of movable cellular automata modeling the concrete at the macroscale 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 on strain rate. These dependences were obtained by generalization of the large set of experimental data for a wide range of brittle materials including concretes [4]. Fig. 2 shows the generalized dependence of the compressive ( $\sigma_c/\sigma_c^0$ , Fig. 2(a)) and tensile strength ( $\sigma_t/\sigma_t^0$ , Fig. 2(b)) 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.

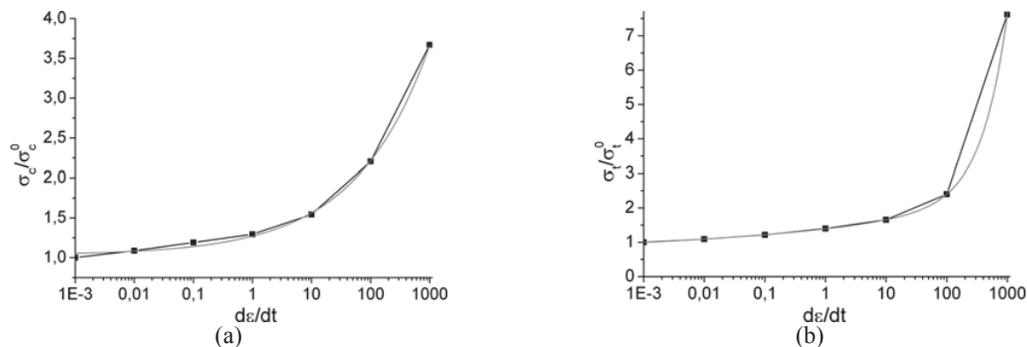


FIGURE 2. Generalized experimental dependencies of normalized compressive (a) and tensile (b) strengths on the strain rate

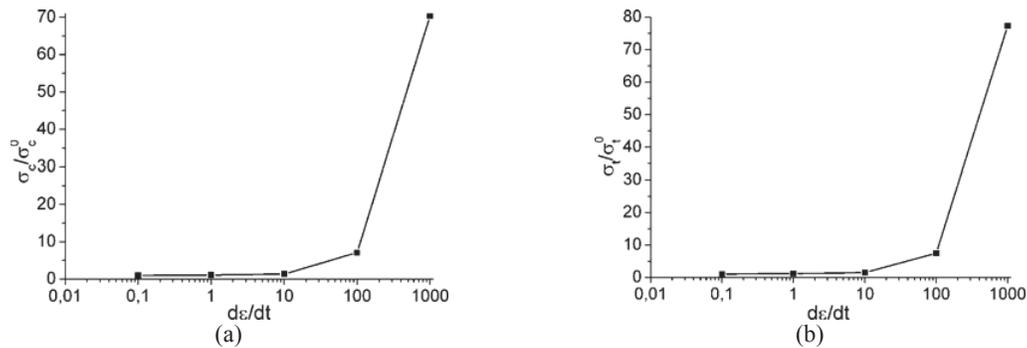


FIGURE 3. Dependences of normalized compressive (a) and tensile (b) strengths on the strain rate. Numerical simulation results

The uniaxial compression and tension tests of zirconium alumina concrete samples at the macroscopic scale were simulated at various impact velocities. Strain rate ranged from  $\dot{\varepsilon} = 10^{-1}$  to  $\dot{\varepsilon} = 10^3$ . Analysis of the simulation results has shown that the dependence of the strength characteristics of concrete on strain rate is strongly non-linear. It is 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 [4–6]. Figure 3 shows numerically obtained dependences of the compressive and tensile strength on strain rate for uniaxial compression and tension tests of zirconium alumina concrete samples. At high strain rates values of dynamic concrete strength are order of magnitude higher than experimental magnitudes presented in Fig. 2.

Quantitative difference between the experimental data (Fig. 2) and results of numerical simulation (Fig. 3) is due to the differences in the methods of obtaining the strength characteristics of material under dynamic impact. In most experimental studies considered in [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 strength value was assumed to be equal to the maximum stress at the uniaxial compression/tension test of the sample. So, numerical simulation has shown that in a direct uniaxial compression/tension test the sample inertia and finite dimensions hinder to obtain real (correct) strength properties of the material.

## CONCLUSION

The properties of zirconium alumina concrete at the macroscopic and mesoscopic scales were calculated. The dependences of concrete properties on strain rate were analyzed. The results of the study indicate that at strain rates corresponding to the dynamic regime of loading ( $\dot{\varepsilon} \gg 1$ ) the strength properties of material are significantly determined by the method of experimental realization of the specified kind of stress state.

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