Multiscale numerical study of mechanical response of zirconia alumina concrete with particle-based MCA method

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Abstract

In the present work the "multiscale" model is developed for numerical study of materials with multiscale heterogeneous internal structure at different structural/spatial scales. This model is implemented within the numerical method of movable cellular automata (MCA). Implemented multiscale model is applied to zirconia alumina concrete (ZAC) with reinforcing particles of electrofusion zirconia and barium-alumina cement binder. The numerical simulations allowed to obtain a set of strength and rheological properties of concrete ZAC at the macroscopic and mesoscopic scales. The detail analysis of the effect of parameters of the internal structure of ZAC (volume fraction of aggregates, porosity, etc.) on the mechanical properties of concrete was conducted.

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) of a 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.

In the present work the proposed approach to the construction of multiscale rheological models is implemented within the numerical method of movable cellular automata (MCA) belonging to the group of computational particle-based methods [2, 3]. The formalism of this method combines mathematical formalisms of discrete element method (P.A. Cundall) and the approach of cellular automata.

Implemented multiscale approach is applied to construct a multiscale structural model of zirconia alumina concrete (ZAC) with reinforcing particles of electrofusion zirconia and barium-alumina cement binder. It should be noted that the topicality of the study of mechanical properties of ZAC is connected 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.

Nikolaevsky's plasticity model with non-associated flow law was chosen as a rheological model for ZAC at the different structural scales. The main feature of Nikolaevsky's model is the postulated linear relationship between the bulk and the shear components of plastic strain rate [4]. Coefficient of this relationship is a function of both accumulated inelastic strain and strain rate.

When constructing the MCA-based multiscale model of ZAC the internal structure of the 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 of mesoscopic representative volume were designed with explicit consideration of irregularities of internal structure. 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 the mobile cellular automata. As noted above, these parameters correspond to Nikolaevsky's plasticity model. 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 mesoscopic structural model of concrete (with explicit modeling of the large-size fraction of ZrO_2) was constructed and the required mechanical tests of mesoscale samples was conducted.

At the mesoscopic scale a concrete can be represented as a dispersion reinforced composite material with reinforcing zirconia particles and cement as a binder. The volume fraction of reinforcing particles in concrete is specifying parameter of model. In the carrying out calculations the various values of the volume concentration of reinforcing particles in the range of 10% to 50% was considered. It should be noted that the content of the smallest ("microscale") fraction of ZrO_2 particles can vary significantly for different batches of supplied ceramics. It was assumed that the volume concentration of this fraction in the binder is small and has no significant effect on mechanical properties of concrete. Therefore, the parameters of response function of cellular automata modeling mesoscopic binder were close to the corresponding properties of the cement. It is well known that when mixing concrete the degree of uniformity of distribution of the particles in volume is the important factor. In reality, to ensure the uniform spatial distribution in the binder is not always possible. The smallest smallest ("microscale") fraction of the particles tends to form aggregates of a mesoscopic scale (the size of hundreds of micrometers). Microparticles in the conglomerates are bonded by microscopic cement layers. In addition, these conglomerates may have quite high porosity (tens of percent) with characteristic pore sizes of the order of the size of microparticles ZrO_2 and less. Described mesoscopic conglomerates of fine-dispersed particles were explicitly simulated, along with consolidated particles of ZrO_2. However, their internal structure was modeled implicitly by specifying the parameters of the mechanical response of cellular automata. The porosity of mesoscopic conglomerates was assumed to be high and equal 40% in the carried out calculations. Note that in the developed model the compressive and tensile strength of conglomerates were assumed to be equal to strength characteristics of a binder (cement). This assumption is implying high adhesion of microparticles to interlayers of cement in the conglomerates volume and low porosity of these interlayers. The volume fraction of mesoscopic aggregates in the ZrO_2 mesoscale aggregates can vary significantly for different batches of concrete and is one of the input parameters of the model mezostrukturnoy concrete. In the carried out calculations, it was assumed to be 30%.

At the microscopic scale each component of mesostructure concrete can be represented as a material with a complicated heterogeneous structure. In particular, in the consolidated mesoparticles of ZrO_2 the grain structure can be identified. Conglomerated mesoparticles at the microscale can be represented as a group of nonporous microparticles of ZrO_2, separated by cement interlayers.

But at this stage of present work the development of microscale model hasn't been carried out yet, and the corresponding properties of cellular automata at the mesoscale were determined from the available experimental data. In particular, the parameters of elasticity and plasticity model and strength characteristics of ZrO_2 aggregates were taken from the experimental data for nonporous samples of zirconium dioxide stabilized with yttrium oxide Y_2O_3. The same parameters for automata simulating conglomerates of microparticles of ZrO_2 corresponded to parameters of the zirconia ceramics with appropriate porosity.

The strength characteristics of automata that simulate the binder at the mesoscopic scale is determined by modeling mechanical tests of mesoscale cement samples and comparing the results with experimental data for cement samples of mark M500 with appropriate porosity. Note that the cement of mark M500 has similar mechanical (including strength) characteristics with barium-calcium aluminate cement used in creating the ZAC. The resulting rheological and strength characteristics of the binder and reinforcing particles are shown in Table 1 (Notation: E - Young's modulus; ω and Λ - coefficients of internal friction and dilation; σ_c and σ_t - strength values during uniaxial compression and tension and compression; σ_y - the yield stress at the uniaxial compression; σ_y, (σ_{h1}, ε_{h1}) and (σ_{h2}, ε_{h2}) parameters - anchor points in the polygonal approximation of the diagram of uniaxial compression. Linearized diagram of uniaxial compression is used to calculate the dependence of the yield surface on the equivalent strain $Y(\varepsilon_{ms})$). The Table 1 shown that the elastic and strength properties of the components of concrete are significantly different. The difference of the elastic moduli promotes stress concentration at the interfaces. Therefore, the adhesion of the binder to the reinforcing mesoparticles is the significant factor determining the strength of concrete at the mesoscale. Also, the high strength of cement on the microscale can be seen. This is due to the fact that in the model the cement at the microscale is assumed to have uniform nonporous structure.

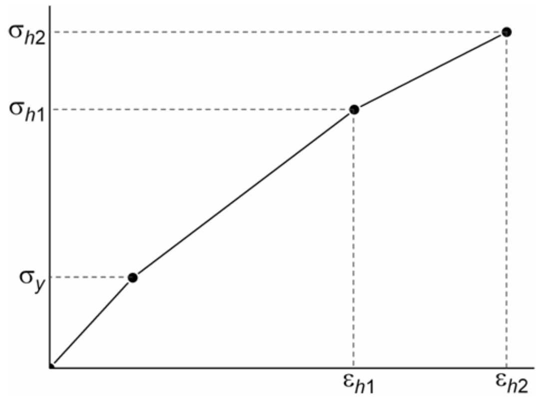


Figure 1: Schematic representation of the diagram of uniaxial compression

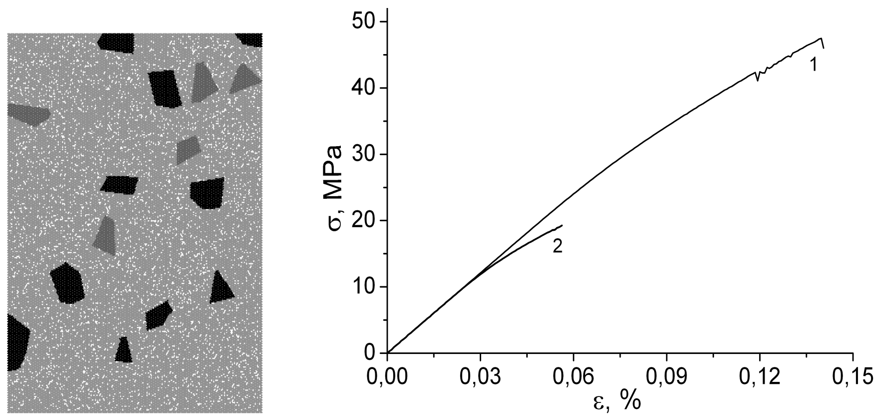
The porosity of concrete samples is primarily determined by porosity of binder. According to the literature the general part of the total porosity is the mesoscale pores (the size of tens to hundreds of micrometers). So, the porosity is explicitly taken into account by random removal of automata simulating the binder (cement paste with a low content of microparticles of ZrO_2) to achieve the desired value of the integral porosity of binder. Typical values of porosity for this type of concrete can be 10-20% or more. In the two-

Parameter	Binder	ZrO_2	Conglomerates of ZrO_2
E (GPa)	55	172	27
σ_y(MPa)	35	1000	175
σ_{h1}(MPa)	111	1200	178
ε_{h1}	0,0027	0,00698	0,00659
σ_{h2}(MPa)	130	2100	180
ε_{h2}	0,0033	0,0122	0,00667
Λ	0,16	0,25	0,25
ω	0,16	0,25	0,3
σ_c/σ_t (MPa)/(MPa)	170/75	2100/831	170/75

Table 11: Physical and mechanical properties of the concrete components at the mesoscale.

dimensional calculations the specified value of 2D porosity of binder was assumed to be 10%, which corresponds to 15-20% of the 3D porosity.

Figure 1 shows an example of the internal structure of the ZAC sample with a volume fraction of aggregates equal to 10% . Black shows the nonporous ("monolithic") mesoparticles of ZrO_2, dark gray - the weakly bounded conglomerates of ZrO_2 microparticles, light gray - the binder.



(a) (b)

Figure 2: An example of the internal structure of the sample ZAC concrete at the mesoscale (a) and diagram of uniaxial compression (plot 1) and tension (plot 2) of this sample (b).

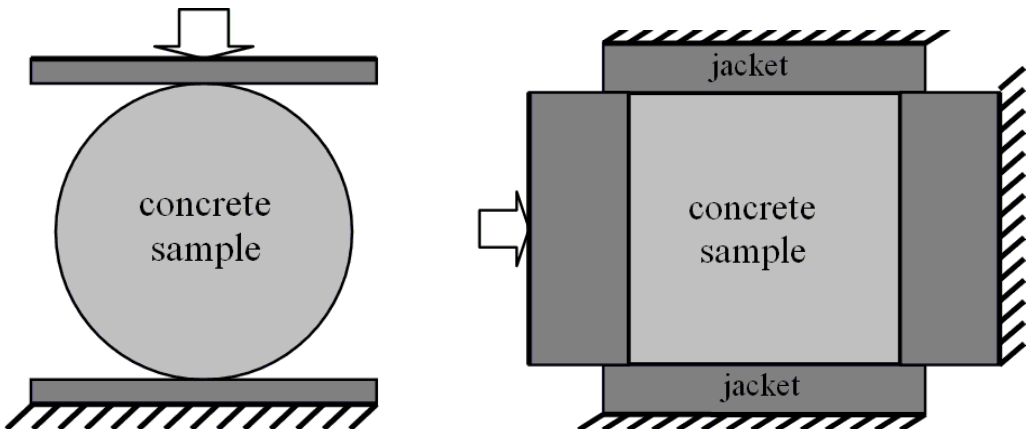
It is well known that an important determinant of the integral strength characteristics of composite materials is the adhesion of binder to reinforcing particles. Due to the lack of reliable information on the bond strength of ceramic aggregates with cement in the ZAC the influence of this parameter on the integral characteristics of mesoscopic concrete was analyzed. As the results of the calculations, the effect of adhesion value to the "mesoscopic" concrete strength is significant under the conditions of the tensile stress. Under the compressive load the influence of the adhesive bond strength on the mechanical response of the sample is much weaker. The influence of adhesion on concrete strength increases along with the volume concentration of binder. Table 2 summarizes the main "mesoscopic" rheological properties of concrete with 10% concentration of ZrO_2 aggregates and low-strength adhesive bond between binder and aggregates.

As a result of series of tension and compression tests the strength and rheological

Parameter	ZAC concrete
E (GPa)	39,8
σ_y (MPa)	24,6
σ_{h1} (MPa)	35
ε_{h1}	0,000911
σ_{h2} (MPa)	48,1
σ_{h2}	0,00142
Λ	0,2
ω	0,2
σ_c/σ_t (MPa)/(MPa)	48,1/21,2

Table 12: Physical and mechanical properties of ZAC concrete at the macroscale.

characteristics of a representative volume of the concrete at the mesoscale were obtained (Fig. 1b). Tests were conducted with different values of the volume fraction of aggregates (Table 2 shows the average values). These characteristics were used as input parameters for modeling concrete ZAC at the macroscopic scale. Two types of mechanical tests were simulated at the macroscale: split ("Brazilian test") and compression in a rigid girdle (to simulate modified Kolsky's test). Schemes of these tests are shown in Fig. 2.



(a) (b)

Figure 3: An example of the internal structure of the sample ZAC concrete at the mesoscale (a) and diagram of uniaxial compression (plot 1) and tension (plot 2) of this sample (b).

The numerical simulations allowed to obtain a set of strength and rheological properties of concrete ZAC at the macroscopic and mesoscopic scales. The detail analysis of the effect of parameters of the internal structure of ZAC (volume fraction of aggregates, porosity, etc.) on the mechanical properties of concrete was conducted. In the carried out investigation the special attention was paid to the analysis of the influence of adhesive strength of interfaces. In particular, the results of the calculations have shown that the influence of adhesion on the strength of "mesoscopic" concrete is the most pronounced under tensile stress condition. At the same time the influence of the adhesive strength on the mechanical response of the sample under compressive stress condition is much weaker. The influence of adhesion value on the concrete strength increases along with the volume concentration of reinforcing aggregates.

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