Numerical Study of Mechanical Behavior of Ceramic Composites under Compression Loading in the Framework of Movable Cellular Automaton Method

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Abstract. Movable cellular automaton method was used for investigating the mechanical behavior of ceramic composites under uniaxial compression. A 2D numerical model of ceramic composites based on oxides of zirconium and aluminum with different structural parameters was developed using the SEM images of micro-sections of a real composite. The influence of such structural parameters as the geometrical dimensions of layers, inclusions, and their spatial distribution in the sample, the volume content of the composite components and their mechanical properties (as well as the amount of zirconium dioxide that underwent the phase transformation) on the fracture, strength, deformation and dissipative properties was investigated.

Keywords: Numerical simulation, movable cellular automaton method, ceramics composites, phase transitions, deformation and fracture, mechanical properties

INTRODUCTION

Ceramic composite materials are used in manufacturing critical parts in many industries. Such an important role of the composites imposes strict requirements on the structure, mechanical behavior and properties of these materials. It demonstrates the study of those as topical and important both for the practical applications and for the fundamental science [1, 2]. The composites based on nanocrystalline oxides $ZrO_2(Y_2O_3)$ and Al_2O_3 are some of the most widely used representatives of this class of materials. In contrast to other ceramics composites, they are characterized by ductile fracture which is stipulated, in particular, by the polymorphic transformations of $ZrO_2(Y_2O_3)$ under mechanical loading. Detailed experimental investigation of the $ZrO_2(Y_2O_3)$–Al_2O_3 composite is very difficult because the mechanical response of the latter depends on many parameters [1, 2]. Thus, the goal of this paper was to research the mechanical behavior of the $ZrO_2(Y_2O_3)$–Al_2O_3 composite via a wide set of structural parameters, using a particle-based computational model: the volume content of components, the size of inclusions and interlayers in different crystal modifications and the fraction of $ZrO_2(Y_2O_3)$ that undergoes polymorphic transformations. This model was developed on the basis of the movable cellular automaton (MCA) method; the model was used herein for modeling ceramic composites under uniaxial compression loading.

MODEL CONSTRUCTION AT MESOSCALE

Within the frame of the MCA method [3], a numerical model of the mechanical behavior of a ceramic composite based on nanocrystalline $ZrO_2(Y_2O_3)$ fiber-reinforced by Al_2O_3 under uniaxial compression was developed.

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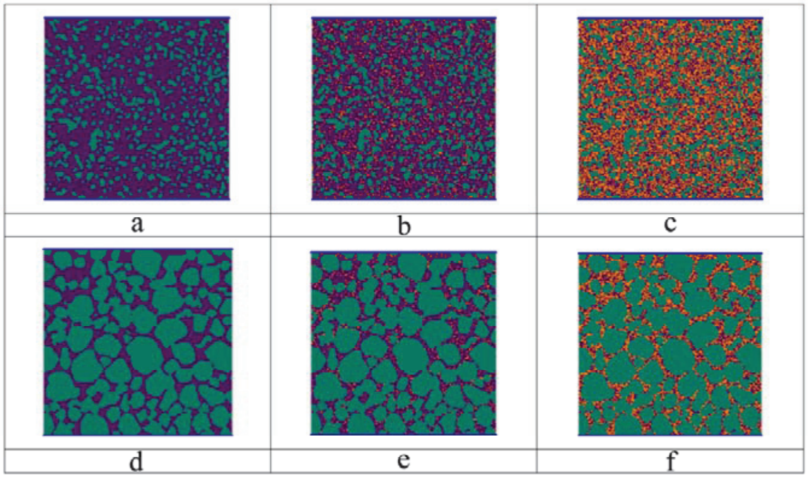

FIGURE 1. Initial structures of the ZrO_2 (Y_2O_3)–Al_2O_3 composite with different structure parameters: (a–c) $\Psi = 0.3$, $L = 2$ μm, $H = 6$ μm; (d–f) $\Psi = 0.7$, $L = 6$ μm, $H = 2$ μm; $\Omega = 0$ (a, d), 0.1 (b, e), 0.5 (c, f)

The possibility of taking into account the tetragonal-monoclinic (T–M) transition in the matrix of a real composite and the slowdown of the development of defects and cracks in the material during mechanical loading associated with this transition were implemented in the model.

Model composites with different setsq and values of structural parameters (such as the volume content of components, the size of inclusions and interlayers (structural elements) and the fraction of the matrix that undergoes phase transformations during mechanical loading (Ω)) were generated. Model specimens with two typical dimensions of inclusions (i. e. filler) L and interlayers (i. e. matrix) H were generated from the analysis of the real composite's structure (namely the images obtained by the electron microscopy of the microsections of the real composite [1]). At the mesoscale of the model, the composite structure was taken into account explicitly (Fig. 1). In case of small inclusions and thick interlayers, their typical dimensions were $L = 2$ μm and $H = 6$ μm, and the volume content of the filler was $\Psi = 0.3$ (Fig. 1(a)). In case of coarse inclusions and thin interlayers, $L = 6$ μm and $H = 2$ μm and $\Psi = 0.7$ (Fig. 1(d)) [1, 2]. The specimens under consideration had the dimensions (i.e. the side of a square sample) of 32 μm. The size of the movable cellular automata was 0.2 μm. The ideal adhesion (bonding) conditions were established at the interfaces of the components.

The calculations were performed for the composites both having ordinary matrix (which was characterized by brittle fracturing) and damping matrix (capable of undergoing the T–M phase transition). The volume ratio of the matrix undergoing the structural transformation during mechanical loading Ω was specified explicitly and was equal to 0.1 (Fig. 1(b, e)) and 0.5 (Fig. 1(c, f)) [1, 2]. Phase transition in the MCA method was implemented on the basis of the phenomenological approach, the main point of which was the formulation of the principle of irreversible mechanical behavior of the material.

The automaton response functions were constructed in such a way as to qualitatively and quantitatively correspond to the deformation diagrams of the appropriate materials. The automaton response functions of ceramic Al_2O_3 and ZrO_2 (Y_2O_3) in the (T)-phase conform to the elastic behavior of the material. Their parameters were: for Al_2O_3—the compression strength of $\sigma = 600$ MPa, the modulus of elasticity of $E= 400$ GPa; for (T)–$ZrO_2(Y_2O_3)$—$\sigma = 1300$ MPa, $E = 220$ GPa. The automaton response function of $ZrO_2(Y_2O_3)$ in the (M)-phase contained a section corresponding to the irreversible behavior of the material. Inside this section its parameters were as follows: the effective modulus of $E_1 = 197$ GPa and $\sigma = 315$ MPa [1, 2]. Thus, up to some value of stress intensity (namely, 125 MPa) in a pair of $ZrO_2(Y_2O_3)$ automata in the (T)- and (M)-state, their behavior defined by the automata response function is identical. Above this value, it is different. In reality, this corresponds to an initiation (T–M) transition at a certain value of shear stress. In reality, this corresponds to the initiation of the (T–M) transition at a certain value of shear stress.

An increase in the fracture toughness of ceramics after a (T–M) transition was implemented in the model by introducing the kinetics of the transition of the automata pair from "bound" to "unbound" state (which permits the simulation of a fracture by the MCA method). For this purpose, a crack propagation rate parameter was explicitly introduced into the MCA model; this parameter could slow down the transition of the automata pair into "unbound" state by several time steps. Normally, for the MCA method this transition occurs within a single time step, which corresponds to the crack propagation with the longitudinal sound speed. In the simulation of (T–M) transition, the magnitude of crack propagation velocity in corresponding (T–M) automata pairs was lower than the velocity of sound in the material and was equal to 0.735 m/s. The velocity of compression loading of model specimens was equal to 0.5 m/s. Thus, to describe the fracture of the material undergoing the (T–M) transition, controlled crack growth mode was implemented in the model. For the rest of the materials, the uncontrolled growth mode was implemented.

INVESTIGATION OF MECHANICAL BEHAVIOR OF THE COMPOSITE UNDER UNIAXIAL COMPRESSION

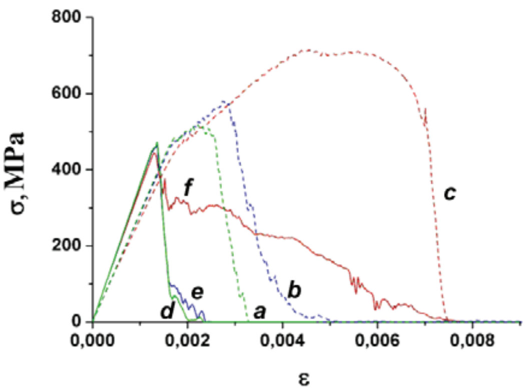

FIGURE 2. Loading diagrams of model composites with different structural parameters (curves in Fig. 3 correspond to specimens in Fig. 1 with the appropriate lettering)

The analysis of composite loading diagrams (Fig. 2) has shown that an increase in Ω (from 0 to 0.5) leads to increases in the fracture energy E_{fr}, tensile strength σ_b and ultimate strain ε_c of the material. Thus, in case of composites with the volume content of filler $\Psi = 0.3$ (Fig. 1(*a–c*)) the increase was 287% for E_{fr}, 38% for σ_b and 117% for ε_c (curves *a–c* in Fig. 2). For composites with $\Psi = 0.7$ (Fig. 1(d–f)) the corresponding increase is observed only for E_{fr} (234%) and for ε_c (218%) (curves *d–f* in Fig. 2). No growth of strength properties of composites with $\Psi = 0.7$ (with increasing Ω) is observed due to the small volume content of matrix in them and the peculiarities of the material structure (thin interlayers of matrix, coarse inclusions of filler). The comparison of loading diagrams of specimens having different values of Ψ and identical Ω has shown that the dissipation, strength and deformation properties of the specimens with $\Psi = 0.3$ were higher than those of the samples with $\Psi = 0.7$ (Fig. 2). Thus, in case of composites with $\Omega = 0$ the difference in their E_{fr}, σ_b and ε_c is 134%, 10% and 64%, respectively. With the increasing Ω, this difference becomes more distinct and is 171%, 62%, 106% (for E_{fr}, σ_b and ε_c, respectively). Thus, one can assume that in the range of variation of these parameters, the integral strength, deformation and dissipation properties of the composite increase with the growth of the volume content of matrix ($1–\Psi$) and that of its portion undergoing the T–M transformation (Ω).

The investigation of the influence of the Ψ, Ω, L and H structural parameters on fracturing of the composites was performed on the basis of the analysis of inter-automaton bond nets of model specimens, some of which are shown in (Fig. 3). The study of inter-automaton bond nets corresponding to different values of the compression strain of the specimens revealed that the T–M transition in the structure of ceramics $ZrO_2(Y_2O_3)$ resulted in the slowdown of defects and crack growth in the composite. This trend becomes stronger with increasing Ω. In the inter-automaton bond nets of the specimens, it manifests itself as the growth of the compression strain value, corresponding to specimen destruction (ultimate strain).

To study fracturing of the composite in more detail, the number of broken inter-automaton bonds in its components (in the volume of the T–$ZrO_2(Y_2O_3)$ matrix and the Al_2O_3 filler) under different values of compression strain of the specimens was calculated. The analysis of the results obtained has shown that the matrix of the composite with $\Psi = 0.3$ and $\Psi = 0.7$ contains up to 13% and 5% of broken inter- automaton bonds, respectively. Increasing Ω from 0 to 0.5 results in the growth of the fraction of broken inter-automaton bonds by more than 3 times. The analysis of the number of broken inter-automaton bonds in the filler of the composite has shown that increasing Ω resulted in the growth of the fraction of defects in filler by up to 300%. These results indicate that the matrix of the composites with higher values of Ω is more effective in transmitting the mechanical load on the filler particles and receives a greater relative number of defects (in T–$ZrO_2(Y_2O_3)$) during the deformation of the material than the samples with lower Ω values. It results in increasing the mechanical energy required for specimen failure (dissipation properties).

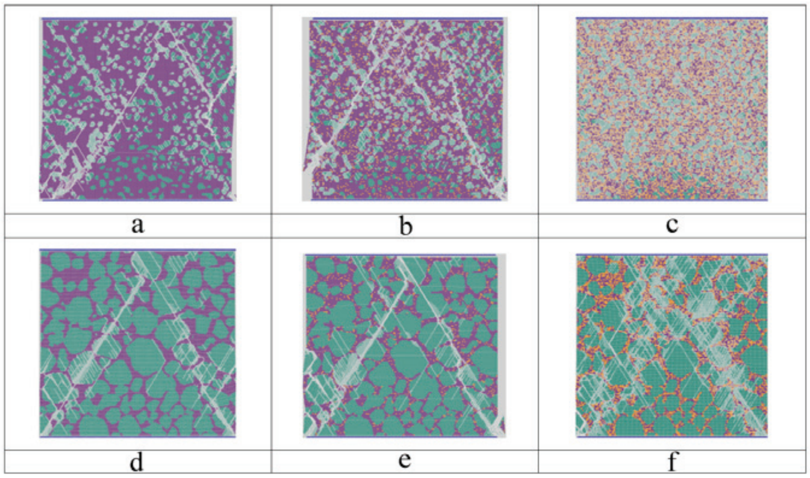

FIGURE 3. Fracture pattern of the $ZrO_2(Y_2O_3)$–Al_2O_3 model composites with different values of structural parameters at the moment of macrocrack propagation under uniaxial compression: (a–c) $\Psi = 0.3$, $L = 2$ µm, $H = 6$ µm; (d–f) $\Psi = 0.3$, $L = 6$ µm, $H = 2$ µm; $\Omega = 0$ (a, d), 0.1 (b, e), 0.5 (c, f)

The analysis of the fracture patterns of model specimens (Fig. 3) revealed two peculiar deceleration mechanisms of local cracking of matrix (T–$ZrO_2(Y_2O_3)$) and filler (Al_2O_3) of the composite associated with structural parameters *L* and *H*. Thus, in case of a composite with small inclusions and thick interlayers, macrocrack propagation is slowed down to a certain point at brittle inclusions (Al_2O_3) and continues after their partial or complete failure (Fig. 3(a–c)). In case of a composite with coarse inclusions and thin interlayers, the defects are localized in the filler particles to a certain point thus slowing the development of macrocracks in the specimens (Fig. 3(d–f)). In all the cases, the fracture of the filler and the matrix is an additional way of mechanical loading energy dissipation.

SUMMARY

As a result of the simulation, one can conclude that the mechanical behavior of ceramical composites is determined by a combination of interrelated factors. In particular it is shown that the fracture, strength, deformation and dissipation characteristics of the composites are determined by the heterogeneity of their structure (the geometrical dimensions of interlayers and inclusions and their spatial distribution in the material), the volume content of the components as well as their mechanical properties. The phase transitions in the structure of zirconium dioxide play a special role in the mechanical behavior of the composite under consideration.

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