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Effect of the Features of Functionalized Structure on Elastic Properties and Strength of Partially-Filled Brittle Porous Materials

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Abstract. A two-scale mechanical model of brittle porous material partially filled with plastic filler (inclusions) was developed within the framework of the formalism of movable cellular automaton method. The model was applied to study the mechanical properties of mesoscopic samples with a linear distribution of the local porosity in the depth of the material. Calculation results showed essentially nonlinear dependence of their elastic and strength properties on the degree of pore space filling. It is found that depending on the sign of the gradient of porosity the value of shear strength of partially filled samples can significantly increase or remain constant with increase in the value of the degree of filling.

INTRODUCTION

A significant number of implants and bone endoprosthesis are produced from ceramic metal oxide [1, 2]. Due to the good biomechanical and biochemical compatibility with human bone tissue, this material is widely used in medical practice. Despite the widespread use of ceramic materials, a number of important questions, concerning the influence of characteristics of internal structure on the mechanical properties, are still not fully understood. For example, to achieve a strong integration of ceramic endoprosthesis with a bone the following two conditions should be fulfilled: the bone should ingrow into the implant pores and the resulting porous composite “ceramic-bone” should have the specified values of strength and elastic moduli. One way to fulfill these conditions is to provide materials with functionalized internal structure, such as porosity gradient along a certain direction. Experimental study on the effect of the porosity gradient on the mechanical properties of material is complex and expensive. In addition, the experimental approach does not allow a detailed study of the dynamics of damage accumulation and fracture. Therefore, in this paper, the mechanical properties of porous ceramic materials with different values of porosity gradients and varying degree of filling of the pore space with inclusions imitating bone, was studied on the basis of numerical simulation. Movable cellular automaton method [3] was used as a numerical method.

MODEL DESCRIPTION

The calculations were carried out for a model material with mechanical properties close to nanocrystalline $ZrO_2(Y_2O_3)$ (yttria-stabilized zirconia) with the average pore size greater than the average grain size. Pore size distribution of considered ZrO_2 has two maxima [2, 4]. The values of partial porosity, corresponding to the first and the second maximum, are 26 and 14%. The value of total porosity is about 40%. The characteristic pore sizes corresponding to these maxima are 1 μm (microscale pores) and 18 μm (so-called mesoscale pores), respectively. A two-scale model developed in [5, 6] was applied to describe the structure and mechanical properties of the ceramic

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material. Mesoscale pores were set explicitly in the model. Microscopic pores in mesoscale pore walls were taken into account implicitly by means of specifying the mechanical properties (elastic constants and strength) of the walls [2, 4].

The model elastic-plastic material was used as a filler of mesoscopic pores. The mechanical parameters of the filler are close to those of human cortical bone: Young modulus E = 20 GPa, Poisson ratio ν = 0.31, yield stress σ_{el} = 120 MPa, compressive strength σ_c = 150 MPa and corresponding ultimate strain ε_c = 3%. Ceramic matrix was assumed elastic-brittle. Its mechanical properties are close to those of ceramics $ZrO_2(Y_2O_3)$ with porosity 30%: E = 40 GPa, ν = 0.34, σ_c = 150 MPa, ε_c = 0.375%. The perfect adhesion (ideal bonding) condition was imposed at the interface between the matrix and inclusions of the model composite. The problem was solved under plane strain condition.

Functionalized structure of model ceramics was set by creating a constant value of porosity gradient along the vertical axis (Fig. 1). Three groups of square specimens (with a side length H = 1.4 mm) were generated. Each group was consisted of seven specimens with individual arrangement of pores. Samples of each group were characterized by the same value of the local porosity gradient grad$C = \partial C/\partial y$. In the first group of specimens pores were homogenously distributed in the volume of the specimen ($|\text{grad}C| = 0$). In the second and third groups of specimens absolute gradient values were the same, and directions were opposite. Thus, in the second group the local porosity value decreases from the top (C_{top} = 19.43%) to the bottom surface of specimen (C_{bottom} = 8.57%), while in the third group it increases from C_{top} = 8.57% to C_{bottom} = 19.43%. All the specimens have the same value of total porosity (14%) that corresponds to the second peak of pore size distribution in $ZrO_2(Y_2O_3)$. All the pores in the model specimens are equiaxed and have the same size 18 µm.

Filling voids by elastic-plastic filler was carried out from the top to bottom surface of the specimen at the same depth h over the entire length of the sample (Fig. 1). The degree of pore space filling in the specimen was characterized by a dimensionless geometrical parameter $\chi = h/H$. We considered partially filled specimens with $\chi \in [0;\ 1]$. The effect of the value of the parameter χ on the mechanical response of composite with different gradients of porosity under the condition of simple shear (Fig. 1) was studied. Periodic boundary conditions were applied on the vertical sides of the specimens.

SIMULATION RESULTS AND DISCUSSION

Simulation results showed that in partially filled specimens with homogeneously distributed pores damage accumulation and formation of the main crack take place near the fixed bottom specimen boundary (Figs. 2a and 3a). In the specimens with $|\text{grad}C| \neq 0$ the spatial arrangement of the region of localized fracture is defined by the value of χ as well as by the gradient of porosity. In particular, in specimens with porosity decreasing into the bulk of material (from the top to the bottom) at $\chi \leq 0.4 \div 0.5$, fracture is typically localized at the border between filled and unfilled parts of the specimen (Fig. 2b). In case of the opposite direction of the porosity gradient a main crack path passes through the region near the fixed bottom boundary of the specimen (Fig. 2c). At $\chi > 0.5$ crack develops in close proximity to the bottom boundary and partially propagates along the border between filled and unfilled parts of the specimen (Figs. 3b and 3c)

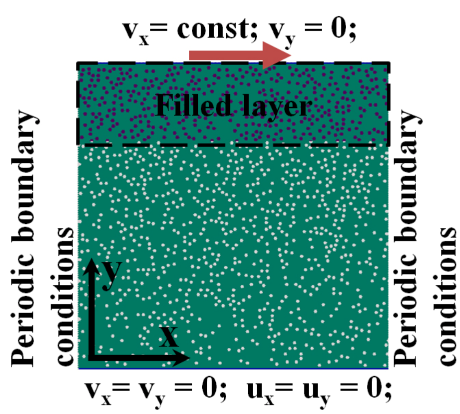

FIGURE 1. Example of pore structure and loading scheme of model specimen

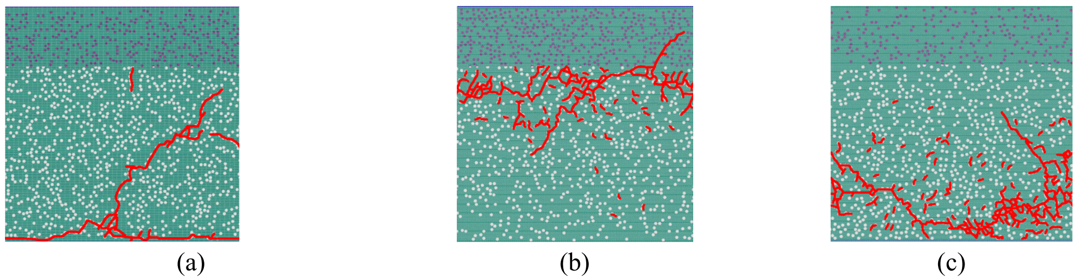

FIGURE 2. Pore structure and fracture pattern of partially filled ($\chi = 0.25$) model specimens: $\partial C/\partial y = 0$ (a), 78 (b), $-78\ \mathrm{m}^{-1}$ (c)

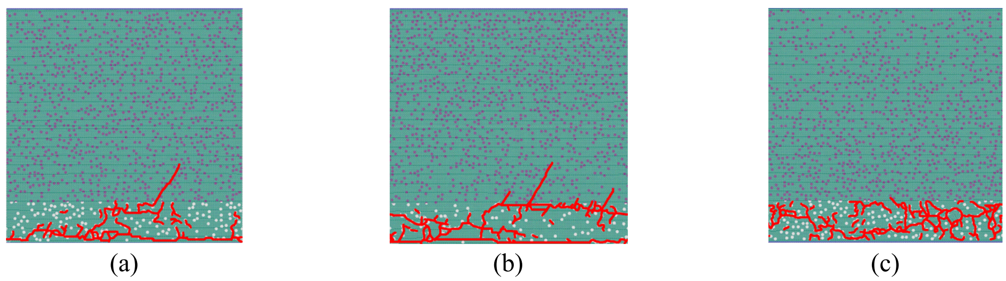

FIGURE 3. Pore structure and fracture pattern of partially filled ($\chi = 0.83$) model specimens: $\partial C/\partial y = 0$ (a), 78 (b), $-78\ \mathrm{m}^{-1}$ (c)

Influence of functionalized porous structure of the composite on effective shear modulus (G) and shear strength (τ) was studied on the basis of analysis of the dependences $G(\chi)$ and $\tau(\chi)$. Corresponding curves are shown in Fig. 4.

The calculation results showed that the value of G increases nonlinearly with the growth of χ (Fig. 4a). One can see that even in samples with $|\mathrm{grad}C| = 0$ (curve *1* in Fig. 4a) the rate of increase in composite shear modulus ($\partial G/\partial \chi$) gradually increases with χ and reaching a maximum at $\chi \to 1$. In specimens with $|\mathrm{grad}C| \neq 0$ the value of ($\partial G/\partial \chi$) increases/decreases in case of increasing/decreasing porosity with depth (curves *2* and *3* respectively). Note that in the specimens with porosity decreasing with depth ($\partial C/\partial y > 0$) a character of the nonlinearity is replaced by the opposite ($\partial G/\partial \chi$ gradually decreases with increasing χ and reaches a minimum at $\chi \to 1$, curve *2* in Fig. 4a). The difference in the value of G for samples with $\chi = 0$ and $\chi = 1$ is determined by volume content of the pores and the elastic properties of the filler. In the considered case this difference is about 50%. Note that in both limiting cases the elastic constants of material do not depend on the magnitude and sign of the porosity gradient. At the same time, the maximum difference between G values of specimens with the same porosity, but characterized by opposite direction of the porosity gradient is achieved at $\chi = 0.5$ and amounts 12% in the considered specimens. These results show that the functionalized structure of composite with a partially filled pore space can have a significant effect on its elastic properties.

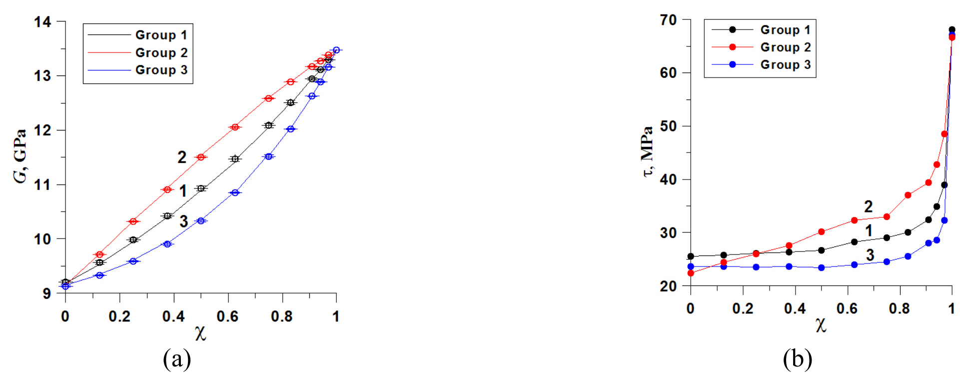

FIGURE 4. The dependence of the effective shear modulus G (a) and shear strength τ (b) of model specimens on the degree of pore space filling χ. Curves *1–3* correspond to different porosity gradients: $\partial C/\partial y = 0$ (*1*), 78 (*2*), $-78\ \mathrm{m}^{-1}$ (*3*)

The nonlinear effect of the functionalized structure on the mechanical properties of brittle porous composites manifests itself in the character of the shear strength (τ) change with χ (Fig. 4b). In all three cases the dependence $\tau(\chi)$ is increasing. Shear strength reaches a maximum value at $\chi = 1$. At the same time, the dynamics of shear strength change in the interval $\chi \in [0; 1]$ substantially differs between the specimens with different porosity gradients.

The maximum difference in the behavior of the specimens is revealed in $\chi \in [0; 0.6]$. Shear strength of specimens with porosity increasing into the bulk material (from top to bottom) is constant in this interval of χ (curve *3* in Fig. 4b). At the same time the strength of the samples with porosity decreasing in the depth of the material increases linearly up to 50% (curve *2* in Fig. 4b). The strength of specimens with $|\text{grad}C| = 0$ also increases in $\chi \in [0; 0.6]$, though much slower than previous one (up to 10%, curve *1* in Fig. 4b).

Such a significant difference is associated with different magnitude and direction of the porosity gradient. The specimens of the second group (Fig. 2b) are characterized by the maximum porosity near the surface (top boundary) of the specimen, while the specimens of the third group (Fig. 2c) have a minimum porosity in this region. Since the region of the sample with the highest local value of porosity is the weakest one, filling of the pores in this region provides a significant hardening and strengthening (Fig. 2b). In accordance with this, the formation of damages in such specimens occurs in the adjacent regions with a lower local porosity and a higher strength. This results in significant increase in shear strength of specimens of the second group with increase in the degree of filling (curve *2* in Fig. 4b). At the same time, the bone filling of pore space of the specimens of the third group begins in the region with minimum local porosity (Fig. 2c) and maximum local strength. Accordingly, hardening of this region does not result in shift of fracture localization area and therefore does not change shear strength of the specimen at small and intermediate values of the degree of filling $\chi \in [0; 0.6]$.

At $\chi \in [0.6; 1]$ all specimens showed the same type of non-linear increase in shear strength τ with χ (Fig. 4b). At $\chi = 1$, the samples are characterized by nearly the same values of τ, which means reducing the role of heterogeneity in spatial distribution of pores in completely filled porous composite.

SUMMARY

The results of numerical simulation of deformation and fracture of brittle materials with a porous structure partially filled with plastic filler, revealed a significant effect of the magnitude and a sign of porosity gradient on the integral mechanical properties of the composite, including strength. Particularly, it is shown that minimum changes in the elastic and strength properties of the porous material with surface layers filled with less rigid and more plastic filler (e.g., bone tissue) can be achieved by formation of the gradient porous structure, characterized by increasing the porosity with the depth of material.

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