FRACTURE PARAMETERS OF FERROELECTRIC CERAMICS CONNECTED WITH THE ROUGHNESS OF THE EDGES OF THE CRACK AND ITS DEFLECTION

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A numerical experiment and a model of the region of contact of the edges of a crack are used as the basis for evaluating different parameters of fracture for two types of ferroelectric ceramics — PbTiO₃ and BaTiO₃ — obtained by hot pressing. Consideration is given to features associated with inhibition of anomalous grain growth, deviation of the crack from a straight line due to structural nonuniformity, and the roughness of the fracture surface. The effect of roughness is independent of the parameter that characterizes inhibition of grain growth and causes the results for both ceramics to be close to one another.

Introduction. In the development and production of new ceramics for service under extreme conditions, special attention is given to their resistance to fracture. Fracture toughness changes (increases or decreases) in response to the character of the fracture and the acting toughening mechanisms. The resolution of this problem is made additionally difficult by the complex physico-mechanical phenomena manifested during production and use of the material and the existence of grains, pores, microcracks, impurity phases, and other microstructural features (such as the domain structure of ferroelectric ceramics), which are related to special properties that the material possesses.

Also, predicting the behavior of ceramics and optimizing their physico-mechanical properties is complicated by the brittle and quasi-brittle behavior of materials of the given type. This behavior makes it difficult to correct defects that form in the material during processing. Thus, no progress can be made on this problem without extensive microstructural investigations and examination of characteristic features of the behavior of ceramics.

Certain characteristic toughening mechanisms and features of the growth of macrocracks have already been established within the framework of the numerical approach described in [1] for jointly studying the production and fracture of ceramics made by hot pressing. In particular, researchers have examined the effects of microcracking, which can either increase or decrease the fracture toughness of the material [2-5]. The branching of a crack and the formation of a bridge behind the crack front have also been investigated [4, 5]. Another subject of inquiry has been the processes that directly influence the toughening of ferroelectric ceramics: the interaction of a crack with 90% domain boundaries [6], twinning [7], and phase transformations near the crack tip due to the coexistence of tetragonal and rhombohedral phases near a morphotropic boundary [8].

The goal of the present investigation is to use a numerical experiment and a model of the region of contact of the edges of a crack to evaluate parameters of the fracture of a ferroelectric ceramic that are due to the roughness of the fracture surface and the deviation of the macrocrack from rectilinearity. We chose hot-pressed ceramics PbTiO₃ and BaTiO₃ as the subjects of the research.

Model representations. Without going into detail on the subject of modelling the processes involved in the formation of the microstructure of the material during sintering and cooling, we will mention that models of the propagation of the thermal front, recrystallization of the molding powder, anomalous controllable grain growth, and the microcracking of grain boundaries were examined in detail in [2, 3, 9]. In our model, the nonporous granular structure is represented in the form of a square two-dimensional grid containing 2000 cells of the size δ. Each cell corresponds to a particle of the molding powder.
Cells with identical numbers form the corresponding grain (Fig. 1a). Microcracks formed during cooling and under the influence of excess stresses near a growing macrocrack are modeled at the grain boundaries. The trajectory of the crack in the microstructure of the ceramic is determined by the grid of grain boundaries and features of the interaction of the crack with microcracks. These determinations are made by modeling on graphs [3, 10]. A computer model such as this makes it possible to find all of the microstructural characteristics necessary to determine the fracture parameters that will be evaluated below.

Roughness of the fracture surface and shielding of the crack. The projecting irregularities on the fracture surface formed due to the structural nonuniformity of the material result in a change in the fracture toughness of the ceramic. It was shown in [1-1] that the locking of the interface that occurs because of this is a much greater obstacle to movement of the edges of a crack than the effects associated with the friction of the contacting surfaces on the straight sections.

Let us evaluate the reduction in stress intensity, i.e., the shielding of the crack, caused by the contact region in which the effects of locking are manifested. Ignoring the effect of friction, we will use the model shown in Fig. 2a [11]. Due to the absence of friction, the opening of the crack \( u \) is determined solely by the stress-intensity factor (SIF) \( K_I \) for fracture mode I. The stress-intensity factor is related to the applied loads. Here, \( K_I' = K_I \) (SIF at the crack tip) [11]:

\[
u(r) = 8(1 - v^2)K_I \sqrt{r} / (\sqrt{2\pi E} \).
\]

In this equation, \( r \) is the distance from the crack tip; \( E \) and \( v \) are the elastic modulus and Poisson's ratio. The length \( L \) of the region over which the irregularities on the edges of the crack are in contact with one another is found from the condition

\[
u(L) = H,
\]

where \( H \) is the height of a projection at the interface (Fig. 2a). We then find from (1) and (2) that

\[
L = (\pi/32) \left\{ EH / [(1 - v^2)K_I] \right\}^2.
\]

Inside the contact regions, the shear stresses \( \tau \) and displacements \( v \) are elastic and are analogous to those connected with the linear mass of the microcracks (Fig. 2b [12]). Thus, to evaluate the shielding efficiency \( \Delta K_{II} = K_{II} - K_{II}' \), we represent the microcrack mass by using the continuous model of elastic springs (Fig. 2c [13]). In this model, the stresses \( \tau \) and the displacements \( v \) are related as follows [12]:

\[
v = \frac{8r(1 - v^2)\ln[1/\sin(\pi D/2D)]}{\pi E},
\]