Studying the influence of numerical simulation parameters on the solutions of boundary value problems on the destruction of bodies with crack-like defects

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Abstract. The work is devoted to the study of damage accumulation processes in solving problems on the fracture of bodies with crack-like defects. Scientific publications in the field of studying the influence of various parameters on the results of numerical simulation are considered. The boundary-value problem of the deformation and fracture process is determined, the degradation algorithm is written taking into account the staging and the dispersion of the strength properties of finite elements over the three-parameter Weibull distribution. The results of numerical simulation are presented in the form of a calculated diagram of deformation in the axes “force - displacement” and patterns of the fracture area, patterns of development of defects. The influence of the stochastic nature of the strength properties of the material on the fracture process is shown.

1. Introduction

For a more accurate simulation of the processes of defect development and the occurrence of fracture processes, a more complete understanding of the processes accompanying postcritical deformation of materials is required, which is associated with obtaining relevant experimental and theoretical data on the behavior of constructions under various types of stress-deformation state. Moreover, mathematical models describing the behavior of materials should accurately indicate the main effects of loading behavior, describe the main stages of damage development in materials and take into account the influence of these damages on the deformation and fracture processes [1, 2].

Initially, structural defects present in the material, such as voids, shells, inclusions of other materials, can become centers of cracking and lead to fracture. In simulation, various approaches are used to simulate crack growth, so in [3, 4] an approach is used according to which each finite element is an element of a material with a certain number of grains. Crack development is simulated by successive fracture of elements according to the law of damage accumulation and the selected fracture criterion. In fractured elements, the stiffness decreases by several orders compared with the stiffness of the surrounding material. In this case, the size of the element is a incremental step of the crack length in the area of construction fracture. However, this approach can only be used to simulate cracks with a
predetermined growth direction. Since fracture is a multilevel and multistage process [5, 6], which includes the stage of nucleation and development of microdefects with their subsequent merging into one or several main cracks, approaches based on the use of ratios of damaged medium mechanics to analyze fracture processes, may be more promising for use, allowing to predict the entire process of development of defects in the material from the moment of their nucleation to the maximum opening of the main crack.

However, when using numerical calculations to simulate physical processes, it is necessary to take into account a large number of factors that directly affect the calculation results. These parameters include the type of finite-element grid, the number of elements in the computational domain, their quality, the dispersion of elastic and strength characteristics, etc. So, in the work [7], the dependence of some calculation results on the parameters of partitioning an unstructured grid was studied. At the same time, while solving the problems of fracture, some researchers noted that the crack can take off in one direction or another, regardless of its “true” direction, corresponding to the physics of the fracture process. To minimize this phenomenon, the authors of the works [8, 9, 10] simulate a two-level finite-element grid, which automatically rebuilds as it increases, while to reduce the sensitivity of the finite-element grid other researchers formulated their own models, in which the result does not depend on the size of the finite-element [11]. Along with the influence of the finite-element grid, it was also noted that the course of the fracture process is affected by the dispersion of strength properties in structural elements [12, 13].

2. Formulation of the problem and discussion of the results

Within this work, we consider the features of the formation of macro-fracture conditions for various characteristics of the distribution law of random strength constants. To solve the numerical problem, a structural-phenomenological model is used [6], in which the stress \( \sigma_{ij}(r) \) and deformation fields \( \varepsilon_{ij}(r) \) are found through a closed system of equations that includes equilibrium equations without taking into account mass forces (1):

\[
\sigma_{ij}(r) = 0
\]

Cauchy geometrical relationship (2)

\[
\varepsilon_{ij}(r) = (u_{i}(r)+u_{j}(r))/2
\]

and determining ratios for an isotropic medium (3):

\[
\sigma_{ij}(r) = (3K(r)(1-k) V_{jmn} + 2G(r) H_{jmn}) \varepsilon_{ij}(r)
\]

in which the elastic properties are described by the volumetric compression moduli \( K(r) \) and shift \( G(r) \). The measures of the damage tensor \( \Omega \), which is calculated as (4)

\[
\Omega_{klmn} = \omega_{1}\delta_{kl}\delta_{mn} + \omega_{2}(\delta_{km}\delta_{ln} + \delta_{km}\delta_{ln})
\]

are independent material functions \( k \) and \( g \), which are included in the defining ratios where \( V_{jmn} = 1/3 \), \( \delta_{kl}\delta_{mn} \) and \( H_{jmn} = I_{jmn} - V_{jmn}k = 3\alpha_{1}+2\alpha_{2}, g = 2\alpha_{2} \), where \( K = E/3(1-2\nu) \), \( G = E/(1+\nu) \). Material functions express the change in deformation properties that determine the behavior of materials under hydrostatic pressure and pure shear. They depend on the invariants of the deformation or stress tensor.

\[
j_{\sigma}^{(1)}(r) = \sigma_{kl}(r) \quad \text{and} \quad j_{\sigma}^{(2)}(r) = \sqrt{\sigma_{ij}^{(1)}\sigma_{ij}^{(1)}}, \quad \text{where} \quad \sigma_{ij}^{(1)} = \sigma_{ij} - \left( \frac{1}{2} \right) \sigma_{kk}\delta_{ij}.
\]

The stress tensor invariants are related to the deformation tensor invariants: \( j_{\sigma}^{(1)} = K(1-k)j_{\varepsilon}^{(1)} \), \( j_{\sigma}^{(2)} = 2G(1-g)j_{\varepsilon}^{(2)} \).

In simulating the elastic-brittle fracture, the functions \( g \) and \( k \) change from 0 to 1 steplike when the fracture criterion (5) is satisfied:
The system of equations is supplemented by kinematic boundary conditions on the surface of the body: \( U_i(r) \mid s = U_i^0 \).

The simulation of the deformation and fracture process is implemented in the Ansys software engineering package using program code written in the built-in programming language APDL and includes at the initial step the developing of a geometric model, its division into finite elements and the application of boundary conditions in displacements. In this case, the value of the applied displacements \( U_0 \) is chosen so that no element is destroyed by its action. The boundary-value problem of the theory of elasticity is solved under given boundary conditions. The fulfillment of the fracture criterion in all finite elements is checked. If the fracture criterion is fulfilled in any of the elements, such an element is considered to be fractured, its stiffness characteristics are reduced to a small value. If there are several similar elements, then the element with the highest ratio of the current equivalent stress to the critical one is selected. Further, in the iterative mode, the stress and deformation fields are recalculated in the computational domain without changing the boundary conditions. If the fracture criterion is not satisfied in all elements, then the applied displacement is automatically scaled so that only one final element is fractured at the next iteration. In such a case, the sequence of actions is repeated from the verification step of the fulfillment of the fracture criterion in all finite elements. A similar technique allows most accurate capturing the start of the fracture process. The procedure is repeated until there are no elements satisfying the fracture criterion. At the same time, the process of properties degradation in the elements subjected to fracture is performed once, and new properties are used at the next iteration. The condition for the end of the algorithm is the achievement of a certain minimum value of the total force acting on the upper edge of the plate. As a result of solving the problem, deformation diagrams of the computational domain in the force-displacement axes and fracture area patterns are constructed.

This work considers the influence of such a parameter of numerical simulation on the calculation results as a dispersion of the strength properties of finite elements. The random strength constants of the elements correspond to the three-parameter Weibull distribution, the probability-distribution function of which is given as (6):

\[
F(\sigma) = 1 - \exp \left[- \left(\frac{\sigma_{cr} - \sigma_0}{\sigma_{cr} - \sigma_0}\right)^b \right] \tag{6}
\]

where \( \sigma_0 > 0 \) – minimal strength parameter, \( \sigma_{cr} \) – characteristic strength parameter, \( b > 0 \) – shape parameter. Distribution parameters associate with variation coefficient \( \kappa \), and mathematical mean value \( \langle \sigma_{cr} \rangle \) of random value by equation (7):

\[
\sigma_0^{cr} = \langle \sigma_{cr} \rangle \left[1 - \frac{k_1}{\sqrt{c_2-c_1^2}}\right], \quad \sigma_0^{cr} = \kappa_1 \langle \sigma_{cr} \rangle + \sigma_0^{cr} \tag{7}
\]

where \( c_1 = \Gamma(1 + 1/b), c_2 = \Gamma(1 + 2/b), \Gamma(z) \) – Gamma- function.

The stochasticity of the fracture process is considered by the example of uniaxial tension of a homogeneous square plate with a side length \( L = 0.2 \) m, the lower face of which was fixed along the longitudinal axis \( y \), the left side was fixed along the \( x \) axis. Moreover, tensile forces in the form of displacement along the \( y \) axis were applied to the upper face (Figure 2, a). The computational domain was decreed for 2772 finite elements. The fracture process was carried out with a dispersion of the strength properties of the elements over the three-parameter Weibull distribution with the mathematical expectation \( \langle \sigma_{cr} \rangle = 150 \) MPa, the coefficient of variation \( \kappa = 0.52 \) and the shape parameter \( b = 2 \).

As a result of the solution, a deformation diagram, which is shown in Figure 1, and patterns of the fracture areas (Figure 2), corresponding to the points marked in Figure 1, are built. The stage of diffuse damage accumulation is observed (Figure 2, a) when the defects are distributed throughout the plate volume and do not actually interact with each other; the localization of the fracture process (Figure 2, b, c) in...
which the field of the stresses of the defects, which appeared at a certain close distance, begins to interact and a large concentration of stresses arises in the space between two close defects, which leads to fracture in this region. As a result, the defects are combined to form a larger crack, which creates even a greater concentration of stresses. Subsequently, larger cracks also begin to interact and merge, forming one or more main cracks (Figure 2, d, e), which lead to fracture of the sample (Figure 2, f).

![Deformation diagram in axes «Force-displacement»](image)

**Figure 1.** Deformation diagram in axes «Force-displacement»

![Fracture areas pictures constructed for the deformation diagram points (a-f), shown in Figure 1.](image)

**Figure 2.** Fracture areas pictures constructed for the deformation diagram points (a-f), shown in Figure 1.
From the development patterns of defects shown in Figure 2, it can be seen that the stochastic nature of the strength properties of the finite elements significantly affects the course of the fracture process, and at the postcritical stage of deformation, a “phased” fracture pattern is realized, in which an avalanche-like fracture of several finite elements occurs and then, the softening process is stopped. At point $f$, the deformation process stops due to the fracture of the model region during through crack propagation.

3. Summary

As a result of the work, a methodology for mathematical simulation of the deformation and fracture process was developed taking into account a random dispersion of the strength constants of finite elements corresponding to the three-parameter Weibull distribution, demonstrating the possibility of a multi-step process of body damage based on the use of a two-level structural and phenomenological model. A review of the scientific literature in the field of studying the influence of numerical simulation parameters on the solution of boundary-value problems on the fracture of bodies with crack-like defects is presented. The results of numerical simulation are presented in the form of a calculated diagram of deformation in the axes “force - displacement” and patterns of the fracture area.

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