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FRACTURE MODELING IN SPECIMENS WITH I-, V- AND U-SHAPED NOTCHES: A PROBABILISTIC APPROACH IN EXCITABLE CELLULAR AUTOMATA METHOD

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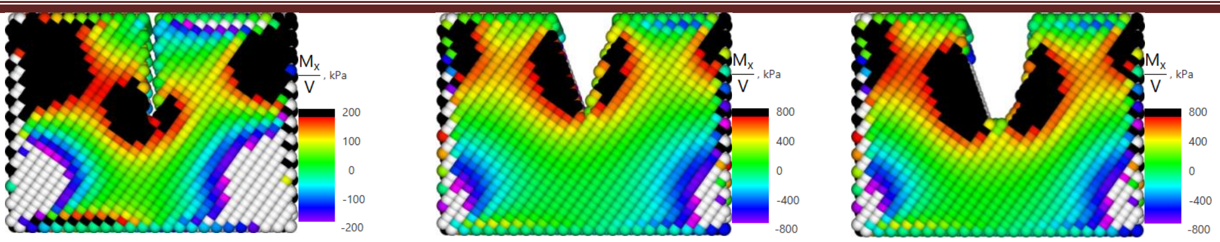
When conducting full-scale tests of loaded structural materials the information obtained is often either incomplete or difficult to be extracted from a real experimental data. Additional information and appropriate interpretation of the results can be obtained using numerical modeling. The application of this approach within a reasonable calculation time allows one to obtain results and formulate preliminary recommendations. To solve this problem, along with determining the optimal set of physical-chemical properties, of particular influence is geometrical shape of the machine part that, among other factors, is taken into account at the design stage. In doing so during the calculation the required thickness, shape, number and size of holes, grooves, fillets and other geometric heterogeneities are to be determined [1].

The previously proposed method of excitable cellular automata allows one to vary the shape and structure of the specimen under simulation. This approach has proven its correctness at solving similar problems [2]. However, the authors previously did not pay attention to aspects of modeling fracture processes, primarily due to the complexity of developed fracture criteria that could be effectively used. In this paper, it is proposed to use a probabilistic approach to model crack nucleation in local regions of the material. This approach is based on the ideas of the physical mesomechanics of materials where particular attention is paid to the aspects of the influence of the effective curvature of the crystalline lattice at the mesoscale [3].

To describe the processes of energy redistribution in a loaded solid an original method of excitable cellular automata (SECAM) was previously developed and described in detail [4]. This approach is aimed at simulation of open system behavior with continuous energy pumping. In doing so, development of self-organization and nucleation of new structures processes can be studied. The main difference of the proposed method from the most of discrete ones is related to the fact that an active element of the cellular automaton describes a fixed region of a space through which energy and matter flow.

The method of excitable cellular automata allows explicitly taking into account the influence of internal interfaces. The mesh of active elements is divided into clusters each of which models a grain that has its own orientation of the crystalline lattice with corresponding Euler angles. The basis of the method is a modified Thornbull relation according to which the velocity of the energy flow through the boundary between neighbours is proportional to the stress at this boundary. In doing so, in a loaded solid there are zones with nonzero force moments. When they reach maximum values at the interfaces the local increase in the material curvature takes place.

Numerical experiments were carried out for aluminum specimens 40×10×30 μm in size with I-, V- and U-shaped notches. For each experiment the application of tensile load was simulated along the horizontal axis X at the velocity of $400 s^{-1}$ during 100 μs. The distribution pattern of the X component of the specific angular momentum at the front faces of the studied specimens (Fig. 1) indicates on the following. The region located at the notch tip accumulates elevated values of this component, and this effect is most pronounced in the case of the sharpest *I*-shaped notch. It should also be noted that the highest values of the *X* component in the vicinity of the notch are achieved in the specimen with *U*-shaped notch. Such an increase in the level of the local moments of forces can lead to further nucleation and propagation of a crack in the notch tip zone.



a b c

Fig. 1. Distribution patterns of the *X* component of the specific angular momentum in the specimen with I-, V- and U-shaped notches at time point of 5 (a, b, c) µs.

In fact, in the framework of solid mechanics fracture should more intensively develop in the material with a sharper notch at least for a reason of higher stress concentration coefficient. In this study, we did not aim at analysis of crack growth itself but the processes of plastic deformation preceding it. From this point of view, a gradual local stress relaxation in the region of the sharper notch tip contributes to their less intense accumulation. This explains the reason why the component *X* of the specific force moment for the I-shaped notch is less than that for the specimens with V- and U-shaped ones.

On the other hand, in a specimen with a blunt notch, the probability of crack nucleation in front of the notch tip is the smallest. This is consistent with the classical ideas of fracture mechanics. This favors the promise of the proposed approach for modeling the processes of crack propagation by the method of excitable cellular automata. This will be the subject of the next research in the development of this study.

The use of the method of excitable cellular automata made it possible to determine the geometrical shape of the notch which is most effective for reducing the likelihood of crack initiation in the specimen under uniaxial tension. Further studies including the implementation of the transition of the active element to a fracture state as well as parametric studies of the influence of the plasticity coefficient to the fracture criteria will provide a more objective pattern of the simulated processes.

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