3D probabilistic cellular automation modeling of transition to fracture in rocks under loading

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Abstract. The three-dimensional model of the probabilistic cellular automaton, which has previously been constructed on the basis of the kinetic theory of strength, is studied in this paper. It describes the process of rock damage accumulation and formation of a damage cluster structure. Comparing the kinetic curves of damage accumulation and correlation functions of the model experiments, it is found that, depending on the sprouting probability of the damage cluster perimeter, which simulates the rate of material fracture under the action of local overstresses near the existing damage clusters, two qualitatively different modes of damage accumulation are observed in the 3D model. For the sprouting probabilities of the cluster perimeter higher than 0.2, the process of transition to irreversible fracture is significantly accelerated and becomes strongly correlated. Along with this, the best agreement of correlation functions in the model and in the physical experiments is observed for the sprouting perimeter probability values smaller than 0.2.

1. Introduction
Advance in the stress–strain monitoring and fracture prediction in rock mass using the pulsed electromagnetic and acoustic emission data [1, 2] calls for new techniques of the experimental evidence interpretation. Pulsed emission means liberation of energy every time when a new defect appears, thus, emission records identify initiation of new defects or propagation of existing defects, which informs on the kinetics of damage accumulation. Characteristics of pulsed emission only indirectly inform on spatial pattern of damages and on their clustering dynamics, which is of the prime concern in fracture prediction. The current technological level has no capabilities to allow simultaneous monitoring of accumulation of damages and their dynamic cluster structure. Such analysis is possible with computer-aided modeling. Advantages of this approach are proved by the general regularities present at the pre-fracture stage [3] when the multi-level structural hierarchy of defects reaches the self-organized criticality [2], characterized by fractal spatial and temporal similarity of at all hierarchical levels. From the acoustic tests, microcracks form in rocks on a mesoscopic scale (tens fraction of micrometer) [4]; for this reason, the process of transition from the mesoscopic scale to the macroscopic scale can be described without delving into detailed dynamics of initiation of separate elementary damages but only using the geometrical characteristics of the structure under analysis from the model of percolation with regard to the stochastic nature of the process. Based on the kinetic theory of strength, the cellular automata and isotropic model of brittle fracture proposed in [5–7] considers kinetics of accumulation of damages as a single space–time process with regard to internal dynamics. The model enables analyzing separately although synchronously and consistently the kinetics of accumulation of new damages (analogues of emission
pulses in physical experiments) and the space–time dynamics of the resultant cluster structure formation, with obtaining of static characteristics of these processes, such as correlation functions, Hurst exponent, size distribution of clusters, etc. This enables a reasoned comparison of the statistical characteristics of flows represented by elementary damages of the model with the characteristics of experimental flows represented by emission pulses. As a result, it is possible to reveal such statistical characteristics which are reflective if transition of the system to the pre-fracture stage (minimum crossing of the autocorrelation function of time in the domain of negative values, or bend of the Hurst exponent).

The probabilistic cellular automata of modeling is defined by a set of probabilities which characterize formation of elementary damages by a few complementary mechanisms and which generate time series of the numbers of elementary damages and clusters of elementary damages as a result of evolution of the spatial cluster structure. A probability of a new elementary damage to appear at a free point of lattice (occupation probability) \( p_{occ} \) is reflective of damage rate under the influence of mechanical stresses averaged on a spatial scale, which are much higher than a characteristic size of an elementary damage, and is governed by the external loading conditions of a material. The sprouting probability of the damage cluster perimeter, \( p_{spr} \), describes an increased damage rate under the action of local over-stresses nearby the existing elementary damage (or cluster of damages). The merging probability of clusters when approach at a critical distance, \( p_{mer} \), takes into account mutual effect of a couple of damage clusters on their counter growth. The cellular automata allows implementation of various modeling scenarios of damage accumulation.

As soon as the modeling scenario is selected and the input parameters are put in, each iteration within the generation algorithm for random process of accumulation of damages runs as follows: damages accumulate at undamaged points of lattice, perimeters of the existing clusters sprout, the clusters which approach at a critical distance merge, and a cluster structure of elementary damages forms. Each iteration ends with termination of the cluster structure of the previous step and with generation of a new cluster structure with automatic updating of all characteristics of the clusters. The final stage of the evolution is a cluster connecting the opposite faces of a cube. Formation of the connection cluster is interpreted as fracture of the whole system, and the number of implemented iteration is identified as the time to fracture. Configuration of a cluster structure in the lattice at a specific time is assigned by the number of clusters as well as by such characteristics as mass (number of elements in cluster), root-mean-square radius, and spans per strings, columns and layers. As a result, each iteration yields a point in each sampling of time series “number of elementary damages” and “number of clusters of elementary damages”, which are used to calculate characteristics of these time series.

2. Mathematical modeling and results

This study focused on the internal dynamic scenario on the sprouting probability of a cluster versus its size—root-mean-square radius \( R^2 \) in terms if stress concentration at the cluster boundary:

\[
p_{spr} = p_{spr}(T) \exp \left( \frac{\gamma \sigma \sqrt{R^2}}{kT\sqrt{l}} \right),
\]

where \( T^{1/2} \sigma \sqrt{R^2} \), \( R^2 \) is the model estimate of stress concentration; \( l \) is the characteristic size of an elementary damage; \( k \) is the Boltzmann constant; \( T \) is the temperature; \( \gamma \) is the structural parameter; \( \sigma \) is the tensile stress far from a crack.

Modeling was implemented on a cubic lattice 100×100×100. The involved probabilities were: \( p_{occ} = 0.0001 \), \( p_{spr} = 0.18 \) and \( p_{mer} = 0.2 \). The obtained characteristics of random processes were averaged over 10 implementations.

The behavior of the time series “number of elementary damages” essentially depends on the choice of the modeling parameters. In the dynamic internal scenario, the accumulation kinetics of elementary damages in 3D model versus the sprouting probability of the damage cluster perimeter,
$p_{spr}$, shows two qualitatively different evolution regimes of the cluster structure. For instance, in case when $p_{spr}$ is not higher than 0.2, the time series “number of elementary damages”, though growing from the first steps of evolution, fluctuates at the trend-unaffected average value. The number of clusters of damages greatly exceeds the number of new elementary damages (Figure 1a). In the time series “number of elementary damages”, the long-term correlations are observed (Figure 1b), with outcome of the correlation function in the domain of negative values. At $p_{spr} = 0.2$ the number of new elementary damages and the number of clusters of damages exceed by the order of magnitude. The processes in the time series “number of elementary damages” coincide increasingly more.

For the sprouting probabilities of the cluster perimeter higher than 0.2, the process of merging of elementary damages and origination of a connection cluster accelerates so that the number of new elementary damages is a few times higher than the number of clusters of elementary damages (Figure 1c) and, accordingly, the number of iterations until the origination of the connection cluster greatly reduces. The processes in the time series “number of elementary damages” and “number of clusters of damages” totally coincide. The correlation functions also coincide, which means inception of strong and long-term correlations (Figure 1d).

**Figure 1.** (a) Kinetic dependences and (b) autocorrelation functions of time series “number of elementary damages” and “number of clusters of damages” at $p_{spr} = 0.18$; (c) kinetic dependences and (d) autocorrelation functions of the same times series at $p_{spr} = 0.22$: 1—cumulative curve of elementary damages; 2—clusters; 3—single elementary damages; 4—elementary damages of perimeters of clusters.

The time series “number of elementary damages” corresponds to the flow of emission pulses which inform on inception of new microcracks and propagation of the existing microcracks. Therefore, in this study, we compare the behavior of the time series “number of elementary damages” from computer modeling with the characteristics of the flow of electromagnetic emission pulses from the physical experiment. From the earlier research [6, 7], the features of reconstruction of a cluster structure of damages before fracture conform with the minimum crossing of the correlation function of random process “number of elementary damages” in the domain of negative values. At the same time, the correlation function of the random process of elementary damage accumulation can be determined from the physical experiment data, and it is possible to compare the behavior of this function with the computer modeling function as the system approaches the fracture stage. This, the correlation function is a reliable statistical characteristic of a random process and can be used as a pre-sign of the system transition to the irreversible pre-fracture stage.
Figure 2 depicts the comparison of the autocorrelation functions of the time series “number of elementary damages” from the computer modeling with the time autocorrelation function of flows composed of pulses of electromagnetic and light emission from the loading tests of quartz diorite [8]. The autocorrelation functions were calculated from the standard formula [9]:

\[
K(\tau) = \frac{\sum_{i=0}^{N} (x(i + \tau) - \bar{x})(x(i) - \bar{x})}{\sum_{i=0}^{N} (x(i) - \bar{x})^2},
\]

where \(x(i)\) is the value of the random value of interest in an \(i\)-th cycle; \(\bar{x}\) is the current average of the random value.

![Autocorrelation functions of time series “number of elementary damages”](image)

**Figure 2.** Autocorrelation functions of time series “number of elementary damages”: 1—quartz diorite, electromagnetic emission; 2—quartz diorite, photon emission; 3—internal dynamic scenario at \(p_{spr} = 0.18\); 4—internal dynamic scenario at \(p_{spr} = 0.22\).

It is seen in Figure 2 that the autocorrelation functions of the number of emission pulses (both electromagnetic and photon emission) behaves qualitatively similarly as the autocorrelation function of the time series “number of elementary damages” in the regime of the cluster structure evolution in the scenario of the perimeter sprouting probability less than 0.2.

### 3. Conclusions

It has been found that depending on the sprouting probability of the perimeter of a damage cluster, in the 3D model of accumulation of damages, two qualitatively different regimes of evolution of the damage accumulation process are observed. When the sprouting probabilities of perimeter of a damage cluster exceed 0.2, the process of transition to irreversible fracture accelerates and becomes strongly correlated. The best agreement between the modeling and physical experiments is observed in the regime of the cluster structure evolution conformable with the sprouting probability less than 0.2. The accomplished research findings enable the more reliable comparison of the modeling data and the physical experiment results with a view to developing procedures of continuous monitoring and prediction of fracture by the transition of autocorrelation functions of flows of emission pulses in the domain of negative value correlation.

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