An improved cellular automaton based on physical energy distribution for microcrack evolution analysis

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An improved cellular automaton based on physical energy distribution for microcrack evolution analysis

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Abstract. Microcracks are important factor in the early stage of structural material failure. The cellular automata method was improved in this paper to simulate microcracks evolution process for material failure analysis. Basic rules based on generalized energy were defined including cells status, failure thresholds and energy input. The Voronoi algorithm was used to construct a random grid to simulate the influence of grain boundaries. Combining overall and local stress status, a sensitivity parameter was introduced to decide the energy distribution, and the new energy distribution rule could accurately reflect the energy competition mechanism between microcracks. Numerical results are in reasonable agreement with experimental results in related literature. The relation between input energy and cracks numerical density could be used in reliability evaluation.

Keywords. Microcrack; Cellular automata; Energy distribution.

1. Introduction

Microcracks play an important role in the early stage of structural material failure process. In general, microcracks are found in larger amounts in mild carbon steel or alloy structural steel, and have length less than 10^{-4} m. The irregular distribution of microcracks is a bottleneck for relevant studies [1], hence numerical calculation methods are widely used to study the evolution of microcracks.

Cellular Automata (CA) is an effective method for analysis of complex systems. It is constructed by clear mathematical rules and random initial conditions, and describes the internal interaction of discrete dynamic systems [2, 3]. When applied to mechanical simulation, there are two ways for cellular automata. CA based on force and deformation regards cells as nodes, and defines rules through equilibrium conditions, geometric relations and constitutive equations. CA based on energy regards cells as continuous domains of material with energy status, and defines rules through energy transfer and storage.

The purpose of this paper is to improve the CA based on energy for microcracks evolution, so that it could be more practical and accurate. More realistic initial conditions and energy distribution rule would be defined.

2. Rules of the improved cellular automata

Major rules of energy-based CA include initial conditions, energy input and failure criteria. In order to make the simulation closer to physical reality, rules of energy-based CA were improved from initial conditions and energy distribution.

2.1. Basic rules

2.1.1. Cell. The cellular automaton is defined on a two-dimensional 100 × 100 grid. An index (i, j) is used to describe the location of a cell.

2.1.2. Failure threshold. At the initial moment, failure thresholds are assigned to each cell as $F(i, j)$. For general cells, the failure threshold is F_g. For defective cells, the failure threshold is F_d. For grain boundaries, the failure threshold is F_b. Initial conditions are discussed in section 2.2.

2.1.3. Generalized energy. Generalized energy $E(i, j)$ is used instead of actual energy. Generalized energy is dimensionless quantity and uses integer metrics. The initial generalized energy is $E_0(i, j)$.

2.1.4. Generalized time and energy input. The cellular automaton is executed in each time step, and generalized time T is used to represents time steps. Generalized time is also dimensionless quantity and uses integer metrics. There is 1 unit of generalized energy been put into the system in each time step, and the energy distribution rule is discussed in section 2.3.

2.1.5. Failure. Any cell will failure when $E(i, j) \geq F(i, j)$, and failure cells will not receive energy.

2.2. Initial conditions based on material microstructure

For common metal and alloy materials, microcrack lengths and material microstructure characteristic lengths are in the same range. During the damage process, grain boundaries have considerable influence on the expansion of microcracks. To simulate grain boundaries structure of materials, the voronoi algorithm was used to construct a mesh with certain randomness. A high grain boundaries failure threshold F_b was set, so that most cracks will be blocked when extending through grain boundaries. The geometry of generated grain boundaries is shown in Figure 1.

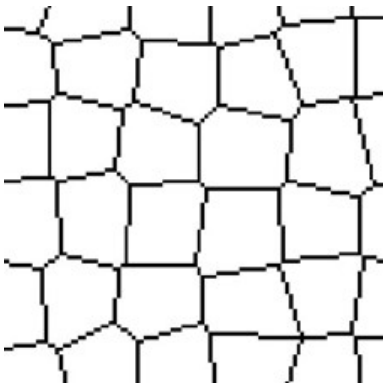

Figure 1. The geometry of generated grain boundaries.

Defective cells represent inclusions, dislocation pluggings, processing defects or other defects. The extension and aggregation of defects will accelerate crack growth dramatically. Based on the actual material microstructure, random defective cells was generated and been assigned a lower failure threshold F_d.

The initial generalized energy is a reflection of strain energy status. In this study, the initial generalized energy was set as 0 which means there is no initial stress in the system.

2.3. Energy distribution rule

From the point of view of energy distribution, energy which input to the system is distributed to certain cells for existing crack extension or new crack generation. Since the total amount of input generalized energy is constant during a certain time period, the competition of energy will decide crack evolution results.

There is no doubt that priorities of cells are different, so a parameter S was introduced to describe energy sensibility and define energy distribution rule. The definition of S was combining local stress status and overall stress status. For local stress status, the curvature of defeat was used to reflect the influence of stress concentration. For overall stress status, the amount of effective cells in a certain direction decides the failure tendency of cells. The definition of S is shown in Equation 1.

$$S(i,j)=\left(\left|\frac{1}{2}-\frac{\sum_{round} c_f}{8}\right|\right)^a \times \max\left\{\frac{n}{n-\sum_{x=i} c_f}, \frac{n}{n-\sum_{y=j} c_f}\right\} \tag{1}$$

Where c_f is the quantity of failure cell, a is a constant factor, n = 100 is the grid size.

Then, the probability of each cell obtaining energy could be defined as Equation 2.

$$P(i,j)=\frac{S(i,j)}{\sum_{i=1}^{n}\sum_{j=1}^{n} S(i,j)} \tag{2}$$

3. Results and discussion

The program according to rules in section 2 was implemented in Matlab. Main parameter settings were F_g=2, F_d=1, F_b=5, and the amount of initial defeats was 20. An image in evolution process is shown in Figure 2.

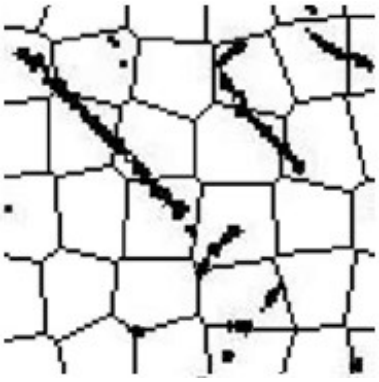

Figure 2. The image of CA in evolution process.

In order to quantitatively study the distribution pattern of cracks, length of cracks must be recorded. The length variable L was defined for each crack as Equation 3.

$$L(k,t)=\sqrt{(x_{\max}-x_{\min})^2+(y_{\max}-y_{\min})^2} \tag{3}$$

Furthermore, a numerical density d was defined to count the amount of cracks in each length range as Equation 4.

$$d(l,t) = \frac{\text{Card}\left\{L \middle| l - \Delta l \le L(k,t) < l + \Delta l\right\}}{2\Delta l} \tag{4}$$

Results are shown in Figure 3 and Figure 4 in the form of crack numerical density. It can be seen that evolution of microcracks divide into three cases. Some microcracks do not expand after nucleation, so lengths of these microcracks are close to 0. Some microcracks expand in a certain extent, and then these cracks were blocked by grain boundaries. Some microcracks break through grain boundaries and continue expanding. The last type of microcrack is the main cause of material failure and should be received significant attention.

Many experiments have been conducted on the fatigue test of mild carbon steel and alloy structural steel [4, 5]. It was found that large amounts of crack length were in the range of 10 μm ~ 17 μm, which were slightly smaller than the average diameter of ferrite. These results indicate that microcracks are considerably hindered when they extend to the grain boundaries, and only a few microcracks could break through the barrier. As the length of microcrack increases, the obstruction will weaken gradually. Simulation results in this paper are in agreement with experiments.

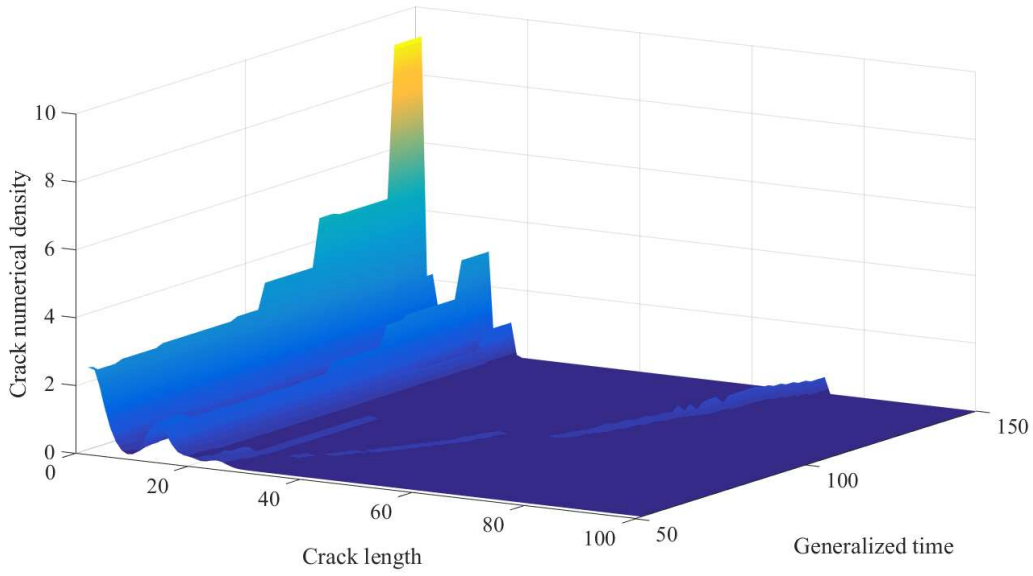

Figure 3. The three-dimensional distribution of crack numerical density.

In early and mid-stages of microcracks evolution, there is no significant difference in the length of microcracks, so the input energy is diluted into lots of microcracks. The energy obtained by ultrashort cracks and blocked cracks are less harmful in the system. However, in the later stage, a small number of microcracks have a length significantly more than others, causing the distribution of energy become imbalance. After getting most energy, these microcracks expand at a faster rate, and lead to final failure. Determining and tracking dangerous microcracks are key issues in damage evolution study.

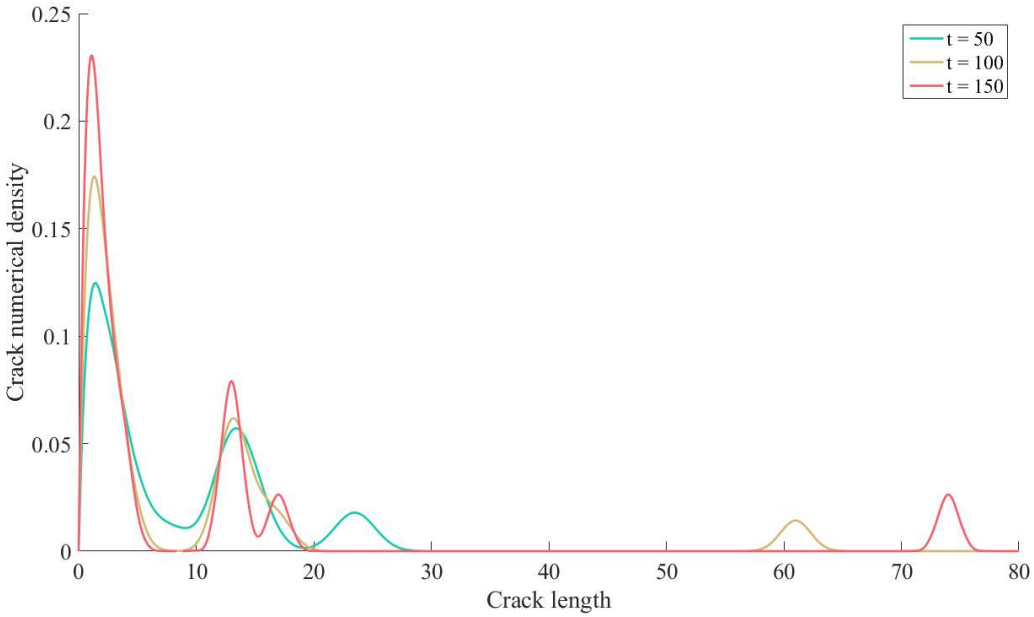

Figure 4. The two-dimensional distribution of crack numerical density.

4. Conclusion

An improved energy-based cellular automaton was proposed to study microcracks evolution. More realistic initial conditions and energy distribution rule make numerical results agree well with experimental results. The relation between input energy and cracks numerical density could be used in reliability evaluation and further coupling analysis.

Acknowledgments

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