Computer Modelling Based on the Percolation Theory of the Third Stage of Cracks Formation and Development on the Steel Microstructures Surfaces

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Abstract

The modeling of the process of destruction of structural materials under cyclic loads in the field of high-cycle fatigue was considered. A phenomenological analysis of the main stages of the formation of cracks, mechanisms and schemes of their initiation, formed in the process of destruction of real objects, was carried out. The implementation of these mechanisms using the tools of the percolation theory made it possible to increase the reliability of modeling the processes occurring in real conditions during the destruction of a structure. The parameter of the model of damage accumulation on the images of the microstructure of the surface of metals and alloys was formulated, which makes it possible to detect the moment of completion of the formation of a crack. The fractal dimension of the percolation cluster obtained on the cells belonging to the damage was chosen as a parameter. To calculate the sizes of percolation clusters the Hoshen – Kopelman multiple labeling algorithm was used. The existing algorithm was supplemented with an auxiliary label for open cells belonging to the percolation cluster, which made it possible to get rid of the additional operation of comparing labels and re-marking nodes when combining parts of a single cluster. To confirm the effectiveness of the proposed parameter, simulation the process of damage accumulation on images of the surface microstructure was made. The magnitude of the error did not exceed 6.6% for calculations using the values of the fractal dimension of percolation clusters built on the cells belonging to the crack.

Keywords

Modeling of fatigue fractures, percolation cluster, fractal dimension, simulation.

1. Introduction

The material used in structures and subjected to periodic loading gradually deteriorates. Fatigue failures occur during the accumulation of damage, i.e. initiation and development of cracks [1]. It is customary to distinguish three stages of this process. The first stage is associated with the formation of slip bands in the near-surface layer of the sample. This process is called incubation or preparatory, because it is reversible and cannot be considered as destruction. Stable slip bands are fine lines on the ground surface of the specimen. During the second stage, crack initiation occurs, i.e., damage is formed within individual grains, submicrocracks are formed in slip bands. During the second stage of destruction, microstructures are accumulated uniformly over the entire surface of the sample. The third stage is the stage of stable crack growth. It begins at the moment when a microcrack grows into a macrocrack, i.e. crosses the border of several grains. The development of macrocracks is the fatigue failure of the material [1]. The third stage ends when the macrocrack reaches a critical size.

GraphiCon 2022: 32nd International Conference on Computer Graphics and Vision, September 19-22, 2022, Ryazan State Radio Engineering University named after V.F. Utkin, Ryazan, Russia
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2. Model

The process of forming a sequence of images reflecting the dynamics of changes in the metal microstructure in response to cyclic loading is a long and expensive process under laboratory conditions. As a result, modeling algorithms are relevant, the development, automation and subsequent verification of which will allow obtaining a reliable and sufficiently large sample of images. Simulation provides images of the microstructure at each loading cycle. In work [2], the rules of cellular automata were proposed and designed, which make it possible to simulate the accumulation of damage to the microstructure of the surface of metals and alloys under cyclic loads. An algorithm was also proposed for adding a mechanism for the formation and development of coarse slip bands (CSB) to the developed model of damage accumulation in the microstructure of the surface of metals and alloys. As a result of the functioning of the proposed system, after one loading cycle, a new configuration of the microsection surface is obtained. After performing several cycles, the change in state over time can be observed.

It should be noted the importance of determining the parameters of the model of cellular automata of surface microstructures, which make it possible to characterize images of a defective surface microstructure. For this, it is necessary to consider in more detail the process of crack formation.

The third stage of fatigue failure is the stage of stable crack growth. It begins at the moment of the formation of a macrocrack, that is, a crack that crosses the boundary of several grains, and ends when the macrocrack reaches a critical size. In order to detect the moment of completion of the third stage, let's turn to the theory of percolation.

The term percolation itself can be literally translated as flow; within the framework of this theory, the processes of the formation of connected objects in disordered media are studied [3]. In the theory of percolation, it is customary to distinguish a certain set of terms. A chain of connected objects, for example, filled black squares, is called a cluster. The subset of black squares continuously connected to the starting cell (or collection of cells) is a percolation cluster. The percolation threshold is understood as the critical concentration of the filled black squares at which a percolation cluster appears [4, 5].

The first works on the theory of percolation appeared in the forties of the twentieth century [6, 7], in which the dynamics of the formation of gels during polymerization was studied. Currently, the percolation approach is used in many areas, including the study of the behavior of materials under various conditions. For example, in [8, 9], the process of damage accumulation in materials was investigated, and the moment of formation of a percolation cluster representing a microcrack was chosen as a condition for the transition of a sample to a fractured state. It should be noted that in the works [8, 9] there is no analysis of the main mechanisms of crack formation; schemes of their origin, formed in the process of destruction of real objects. Taking these mechanisms into account will increase the reliability of modeling the processes occurring in real conditions.

Let's introduce into the system being developed the parameter D_{M} - the fractal dimension of the percolation cluster obtained on the cells belonging to the damage (CSB and crack that will be marked with the symbols S and C, respectively). Note that this parameter D_{M} can be calculated from both real and model images of the surface microstructure. To determine the value of D_{M}, it is necessary to build a percolation cluster on the cells belonging to the damage.

Consider the process of constructing clusters on a square eight connected lattice, assuming that the diagonal elements are also adjacent. To calculate the size of the clusters, the Hoshen − Kopelman multiple labeling algorithm was chosen [4]. It allows to determine the belonging of a particular cell to a particular cluster in one iteration. In this algorithm, an LxL lattice is considered, the nodes of which are randomly filled with zeros or ones. The Hoshen-Kopelman labeling algorithm uses an array of cluster labels. The main essence of this algorithm is the sequential marking of the occupied nodes bordering the cluster (marked by one), but not belonging to any cluster of nodes, until all neighboring nodes of the current cell become free. Then the perimeter of the marked cluster is determined. At the next iteration, the above procedure (marking) is applied to the boundary nodes of the found perimeter of already occupied nodes [10].

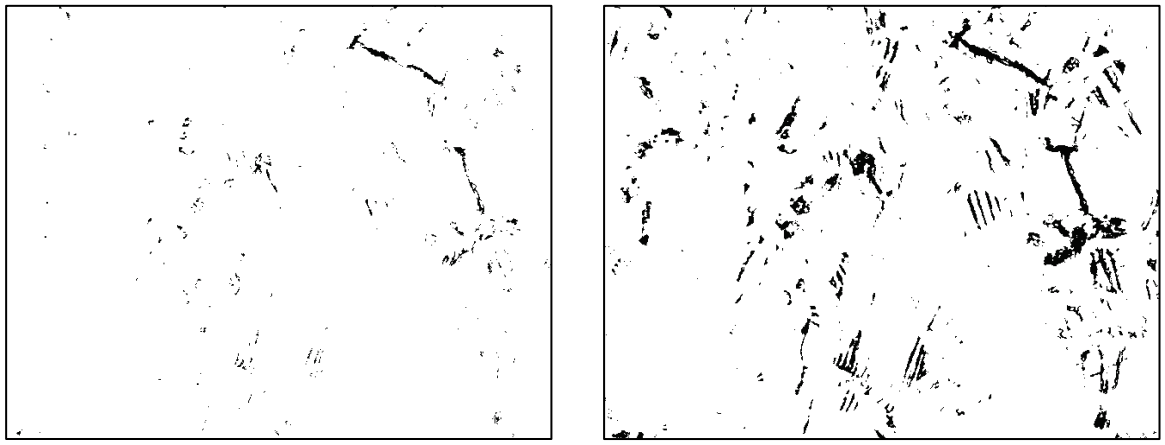
In current case, the size of the lattice will correspond to the size of the calculated field of the cellular automaton. When the algorithm is running, an arbitrary cell of the cellular automaton as the initial cell for constructing a cluster will be chosen. Within the framework of the developed algorithm, it is considered closed all cells that do not belong to damage, i.e. not marked with symbols S and C, but

open - cells marked with S and C. Let's introduce a system of labels by analogy with the method described in [11]:

- "0" - for closed cells that do not belong to the HPS and the crack;
- 1" - for open cells that do not belong to the percolation cluster;
- "2" - for open cells belonging to the percolation cluster.

The selected system of labels differs from the one presented in the Hoshen – Kopelman algorithm by the presence of an auxiliary label - "2" for open cells belonging to the percalation cluster, which makes it possible to get rid of the additional operation of comparing labels and re-labeling nodes when combining parts of a single cluster [11].

Supply to the input of the algorithm for constructing a percolation cluster a two-dimensional matrix of a given size (the calculated field of a cellular automaton) obtained at the stage of forming the principles of crack formation. This matrix contains information about cells labeled C and S. The output is a two-dimensional array containing information about the resulting clusters. In figure 1 shows examples of constructing percolation clusters for a fixed size of the computational field and various values of the concentration of diffusing particles γ, added at the stage of forming the rules for the development of CSB [2], for the number of loading cycles N = 55 thousand cycles.



a b

Figure 1: Percolation clusters at the concentration of diffusing particles, a: γ = 0.31; b: γ = 0.50 for the number of loading cycles N = 55103 cycles

Note that the topological dimension of the set is distinguished, i.e. for a line it is equal to 1, for a square – 2, for a cube – 3 [12, 13] and fractal (fractional) dimension characterizing the coefficient of change of a set with a change in scale [14, 15].

Let's calculate the fractal dimension D_{M} of the obtained percolation clusters on the cells belonging to the HPS and cracks (marked with the symbols S and C) using the relation presented in [16]:

$$N = p \cdot (R/R_0)^{D_M}, \qquad N \to \infty ,$$

where R is the radius of the cluster, R_0 is the radius of the structural units that make up the cluster, N is the number of structural units that make up the cluster, p is the density of structural units in the cluster.

The density p depends on how the structural units are packed in the cluster. The fractal dimension of the D_{M} cluster is a quantitative characteristic of how the cluster fills the space it occupies [16, 17].

It should be noted that diffusion-limited aggregation processes generate clusters with fractal dimension D_{M} (2) = 1.71 [16]. However, in our case, the fractal dimension is calculated for clusters built on the cells belonging to the crack (marked as C), the marking of which occurs in accordance with the rules for the formation of a crack on real objects, which means that their fractal dimension may differ from that obtained in [16] values.

In the process of calculating, the values of the fractal dimension of the image (model and real), containing the damage accumulated over a certain number of loading cycles, are sequentially covered with grids with square cells with different sizes of the side of the square. The number of cells is counted and the percentage of the areas occupied by the damaged and undamaged slip bands of the surface microstructure is determined. Comparison of the number of damaged and undamaged cells with the size

of the side of the mesh cell, at which these numbers were obtained, allows us to obtain dependences of the same type, which will be used for the analysis.

To calculate the fractal dimension of percolation clusters built on cells belonging to damage (CSB and cracks), the clusters were covered with a mesh, after which the number of cells Qi covering the surface microstructure defects (CSB and cracks) was calculated. Subsequently, the mesh size was changed and the number of cells occupied by the cluster (microstructure defect) at the current mesh size was calculated. Eleven meshes of various sizes were used, followed by plotting the dependence of the number of cells occupied by clusters corresponding to damage to the surface microstructure on the mesh cell size ri.

As an example, the first five results of calculating the number of cells superimposed on damaged elements of the surface microstructure of one image from the test set presented (the number of loading cycles N = 5·104 cycles) (Table 1).

Table 1

Results of calculating the number of cells for different mesh sizes

№	Sample	Number of loading cycles	Cell size, pixel	Qdamaged	Qintact
1	1	5·104	1.00	895383	912655
2			2.00	222434	228646
3			4.00	55841	57057
4			8.00	14003	14248
5			16.00	3506	3536

3. Testing and results analysis

To confirm the effectiveness of the proposed criterion, let's simulate the process of damage accumulation on test images of the surface microstructure. Test images were obtained from fatigue tests. Fatigue tests were carried out on flat rectangular specimens manufactured in accordance with GOST 25.502-79. The samples were subjected to elastoplastic cyclic deformation according to the cantilever bending scheme with a frequency of 9 Hz until a macrocrack with a length of about 1 mm appeared [18]. The images obtained after fatigue tests of specimens made from three different alloys were combined into three test sets. The test parameters are presented in Table 2.

Table 2

Test parameters when forming test samples

№ test set	Steel grade	Number of loading cycles before crack formation	Number of images in each sample
1	08Х18Н10Т	6·106	45
2	15ЮТА	2,2 ·105	28
3	07ГБЮ	6,95·105	21

For test set № 1 of steel microsection images, the modeling of the process of accumulation of damage to the surface microstructure was carried out. The simulation was carried out in two ways. In the first, according to the algorithm described in [2], without taking into account the formation and development of the CSB, using incomplete threshold for the initial initialization of the computational field. In the second case, an algorithm was used for modeling, taking into account the formation and development of CSB and the formation of a crack [2].

To adjust the parameters of the model, the values of the fractal dimension D_M of percolation clusters built on the cells belonging to the crack for each image from the test set has been calculated. The model parameters were adjusted so that the D_M value for the model images coincided with the real ones.

In Tables 3 and 4, the values of the number of loading cycles for the model images correspond to the number of iterations of the cellular automaton during the simulation. The value of the error ε for N* was calculated by the formula:

$$\varepsilon = \frac{|N_{actual} - N^{**}|}{N_{actual}} 100\%,$$

where N^{**} - is the number of loading cycles obtained by a material scientist or an automated classifier when analyzing the current state of the surface microstructure.

Table 3

Values of fractal dimension (D_M) and the number of loading cycles (N) for test set № 1 of images

Sample number	Number of loading cycles when fixing real images, ·103	Dm for real images	Dm for model images	The number of loading cycles when fixing model images, ·103	The error in estimating the number of loading cycles ε (based on model images),%
1	0	-	-	-	-
2	80	1,58	1,58	78	2,5
3	160	1,58	1,57	148	7,5
4	250	1,57	1,58	252	0,6
5	1250	1,58	1,58	1250	0,0
6	3250	1,59	1,57	3209	1,3
7	4250	1,58	1,58	4250	0,0
8	5750	1,57	1,57	5750	0,0
9	6050	1,58	1,58	6050	7,1
				mean ε	2,37

Table 4

The values of the fractal dimension (D_M) and the number of loading cycles (N) for the test set № 1 (taking into account the CSB)

Sample number	Number of loading cycles when fixing real images, ·103	Dm for real images	Dm for model images	The number of loading cycles when fixing model images, ·103 (incomplete thresholding, taking into account the formation of CSB and cracks)	The error in estimating the number of loading cycles ε (based on model images), %
1	0	-	-	-	-
2	80	1,58	1,57	79	0,6
3	160	1,58	1,57	159	0,8
4	250	1,57	1,58	252	-0,6
5	1250	1,58	1,58	1250	0,7
6	3250	1,59	1,57	3209	1,3
7	4250	1,58	1,58	4250	0,8
8	5750	1,57	1,57	5750	0,0
9	6050	1,58	1,58	6050	0
				mean ε	0,44

Similar values were obtained when simulating the process of cyclic loading for test sets № 2 and № 3. The calculated values of D_{M} for real images indicate that the value of fractal dimensions is characteristic for each set of experiments, and, consequently, for each set of factors acting on sample under fatigue testing. The magnitude of the error did not exceed 6.6% for calculations using the values of the fractal dimension D_{M} of percolation clusters built on cells belonging to the crack.

Thus, the fractal dimension D_{M} of the percolation cluster obtained on cells belonging to lesions can be a parameter of the cellular automaton model of surface microstructures, which makes it possible to characterize images of a defective surface microstructure.

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