ACCUMULATION OF FATIGUE MICRODEFECTS – ENTROPY INTERPRETATION

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Abstract

The authors of the paper presented some of the models describing the process of micro-cracks' development. In this study, the process of a selected model of micro-cracking was analyzed. In the model it was assumed that the damage to the material has some "thermodynamic properties" or rather universal properties inherent in most complex systems. In order to calculate the long-term fatigue strength properties of a structure, it is important to have a good understanding of the distribution parameters of the number of defects of different sizes. A model was built using the entropy principle, which is effectively used to test complex systems that are difficult to formalize. As a result of many experimental studies it was found that the development of fatigue damage is closely related to the process of plastic deformation of the material at the contact point of local defects. The results of computer calculations and simulations led to the conclusions presented in the final part of this paper.

Keywords: distribution of microcracks, entropy interpretation of microcracks, fatigue curve formula

1. INTRODUCTION

Currently, there are a lot of models describing the process of microcracks growth. They may be divided into three groups [1]. The first group of models based on building design schemes of loading attempts to take into account the microstructure of the material. The second group is based on the introduction of a formal parameter of damage and postulates for this a certain evolution equation relating the tension and the growth rate of damage. In the third group of models, it

is assumed that the dynamics of damage has some "thermodynamic" properties, or rather, universal properties inherent in most complex systems [2].

The approach used in this part of the research, gravitate more to the third group. Here, as the starting points the variational principle of maximum entropy and the law of conservation of energy were used.

An important parameter in the study of the mechanics of fatigue fracture is the crack size. However, when the multiplicity of fatigue defects of their size can vary greatly in the material at the same time there are cracks that differ by several orders of magnitude. To calculate the characteristics of long-term strength of the structure it is important to have an idea about the distribution parameters of the number of defects of various sizes.

In the literature works can be found devoted to the study of crack size distribution of their size. This is basically the experimental data obtained as a result of painstaking measurement and counting a huge number of microdefects within control area. A good review of the literature on these issues is available in the paper [3]. Here are the details of various studies on the accumulation of microdefects not only from the action of cyclic loads, but also as a result of processes such as creep, static stretching, and pore formation in superplastic alloys. Below there are some of the characteristic curves discussed in the review cited (see Figure 1 - 3). The symbols used in these drawings are as in the original. Their meaning is clear from the caption text. Graphs are shown: in ordinary and universal coordinates (in the Figures they are marked respectively by letters a) and b)).



Figure 1. The distribution of the pore size in polycrystalline iron samples (0.006% C), creep tested [4] at a strain of 9.3 MPa and a temperature of 700 ° C: $1-\varepsilon = 2.1\%$, $\tau = 23$ h; $2-\varepsilon = 6.2\%$, $\tau = 142$ h; $3-\varepsilon = 9.3\%$, $\tau = 262$ h. Here ε – the relative deformation, τ – during load steps



Figure 2. Distribution of microcracks in size in copper single crystals tested for fatigue [5] at different strain amplitudes and the number of cycles: $1 - \Delta \varepsilon = 2 \cdot 10^{-3}$, $K = 40 \cdot 10^{3}$ - cycle; $2 - \Delta \varepsilon = 4 \cdot 10^{-3}$, $K = 20 \cdot 10^{3}$ - cycle; $3 - \Delta \varepsilon = 2 \cdot 10^{-3}$, $K = 80 \cdot 10^{3}$ - cycle; $4 - \Delta \varepsilon = 4 \cdot 10^{-3}$, $K = 40 \cdot 10^{3}$ - cycle



Fig.3. Derivative dn|dl depending on the radius l of the pores in the samples of copper (purity: 99.999%), fatigue tested at 34 MPa at a strain, frequency 17 Hz, temperature 405°C different numbers of cycles and [5]: $1 - N = 2.5 \cdot 10^3$ cycle; $2 - N = 2.5 \cdot 10^4$ cycle; $3 - N = 2.5 \cdot 10^5$ cycle



Fig.4. Distribution share different height levels in plain annealed brass single crystals deformed in tension at temperatures within the step [3]: 1-77K; 2 300K; 3 - 393K

The graphs show that regardless of the nature of the considered failure, distribution curves of the amount of accumulated defects of their size have the same shape. The graph has two branches - ascending and descending. This statement applies not only the curves in Figure 2, where the given empirical distribution characterizes the fatigue cracks on their size. But, as it can be seen below, this is due to a lack of resolution of the method of detection of small defects. A more accurate measurement (Figure 3), carried out by the method of neutron scattering, allowed to evaluate defects in nanometer size [6]. Increasing the resolution of the two orders allowed to observe the same pattern in the form of distribution curves for fatigue cracks resulting from the action of cyclic loads.

Below is presented an approach that allows, based on maximum entropy principle, to obtain the theoretical relationship describing both at the same branch of the curve n = f(l). The resulting dependence has the property of self-similarity and explains the exponential nature of the curves in the illustrations (Figure 1 - 4).

2. SET OF FATIGUE DEFECTS AS A THERMODYNAMIC SYSTEM

In this part of the work we will try to identify the physical basis for the formation of such distributions to identify the factors influencing its parameters. In [7, 8] the idea related to many distributed self-organized systems, including microcracks, seen from a single point of view, namely, from the perspective that on the set of some "consumers" distributed a limited set of "resources" (especially, on an absorbing set of microcracks distributed energy) is proposed. Moreover, the allocation is not arbitrary, but in accordance with the principle of entropy.

As used herein, the entropy principle can be effectively applied to the study of complex hard-formalized systems. It is based on the understanding that certain allocated quantity that characterizes the state of the system (in our case, it is the energy of defect formation), is distributed within this system in the most likely way. Therefore, with this distribution the entropy reaches its maximum value. Conditional maximum entropy acts as an integral criterion that the system realizes itself in this particular configuration.

The above experimental curves are well described on the basis of this approach. The actions of the alternating load of the energy consumed in the formation of fatigue defects. Their total number can be divided into classes (Figure 5), each of which n_i is composed of representatives of consuming the same amount of energy equal ε_i .



Figure 5. Distribution n_i - "media" and W_i - "resources" include the phase space M cells

In this notation:

$$\sum_{i=1}^{M} n_i = N, \qquad \qquad 1)$$

$$\sum_{i=1}^{M} W_i = \sum_{i=1}^{M} n_i \varepsilon_i = W.$$
 2)

We assumed that the energy absorbed by a single defect ε_i is related to its linear size l_i by functional relations:

$$\mathcal{E}_i = \mathcal{E}(l_i), \qquad 3)$$

and the expression (2) will have the form:

$$\sum_{i=1}^{M} n_i \cdot \varepsilon(l_i) = W.$$
⁴)

The problem of finding the distribution of the number of defects by their size $n_i = f(l_i)$ is reduced to finding the defect distribution of the value of their creating energy $n_i = \varphi(\varepsilon_i)$. In accordance with the principle of entropy, this dependence is formed such that all selected *M* classes of defects energy distribution realized with the maximum achievable expansion and, therefore, conditional maximum entropy $W_i = n_i \cdot \varepsilon_i$ is reached. To this purpose it is convenient to use Shannon entropy:

$$H = -\sum_{i=1}^{M} p_i \cdot \ln(p_i) .$$
 5)

Here, p_i – the frequency (probability) of occurrence of the *i* – outcome. In the case of energy distribution $W_i = n_i \cdot \varepsilon_i$ by grade it is $p_i = \frac{n_i \cdot \varepsilon_i}{W}$

Thus, we obtain the required distribution $n_i = f(\varepsilon_i)$ as a result of solving the problem with the conditional maximum entropy, recorded as follows:

$$H_{W}(n_{i}) = -\sum_{i=1}^{M} \frac{n_{i} \cdot \varepsilon_{i}}{W} \cdot \ln \frac{n_{i} \cdot \varepsilon_{i}}{W}$$

$$\tag{6}$$

where conditions act as requirements (1) and (2). [9]

If the entropy of the function appears, this approach is known as the formalism of Jaynes-Gibbs. Its essence lies in the fact that to achieve a conditional maximum $H_W(n_i)$, it is sufficient to solve the problem of finding the unconditional extremum of a new feature $\Phi(n_i)$ that includes an additive $H_W(n_i)$, and constraint equations (1) and (2), and weighted Lagrange multipliers α and β :

$$\Phi(n_i) = -\sum_{i=1}^{M} \frac{n_i \cdot \varepsilon_i}{W} \cdot \ln \frac{n_i \cdot \varepsilon_i}{W} + \alpha \cdot (\sum_{i=1}^{M} \frac{n_i}{W} - \frac{N}{W}) + \beta \cdot (\sum_{i=1}^{M} \frac{n_i \cdot \varepsilon_i}{W} - 1)$$
(7)

Equating to zero the partial derivatives:

$$\Phi(n_i) = -\sum_{i=1}^M \frac{n_i \cdot \varepsilon_i}{W} \cdot \ln \frac{n_i \cdot \varepsilon_i}{W} + \alpha \cdot (\sum_{i=1}^M \frac{n_i}{W} - \frac{N}{W}) + \beta \cdot (\sum_{i=1}^M \frac{n_i \cdot \varepsilon_i}{W} - 1)$$

We may set them to the extreme (7) distribution:

$$\frac{\partial \Phi(n_i)}{\partial n_i} = -\frac{\varepsilon_i}{W} \cdot \ln \frac{n_i \cdot \varepsilon_i}{W} - \frac{\varepsilon_i}{W} + \alpha \cdot \frac{1}{W} + \beta \cdot \frac{\varepsilon_i}{W} = 0, \qquad 8$$

where $C_l = W \cdot exp(\beta - l)$.

The physical meaning of the multiplier α becomes clear after determining extremes of a function $n_i = f(\varepsilon_i)$ defined by the formula (8). This is the easiest way to find the extremum of the corresponding continuous distribution $n = \varphi(\varepsilon)$, which is obtained when $M \to \infty$. The condition $\frac{dn}{d\varepsilon} = 0$ follows $\alpha = -\varepsilon_*$ a constant $C_1 = n_* \cdot \varepsilon_* \cdot e$. Here $e \approx 2.718$, ε_* and n_* – the coordinates and the point at which the distribution (8) reaches the maximum.

As a result, the distribution $n_i = \varphi(\varepsilon_i)$ can be written as:

$$\frac{n_i}{n_*} = \frac{\varepsilon_*}{\varepsilon_i} \cdot \exp\left(1 - \frac{\varepsilon_*}{\varepsilon_i}\right)$$
9)

As with the growth of the influence of the argument ε_i of the exponential factor in the expression (9) is almost eliminated, it asymptotically approaches the exponential (hyperbolic) relationship:

$$n_i = \frac{n_* \cdot \varepsilon_* \cdot e}{\varepsilon_i} = \frac{C_1}{\varepsilon_i}$$
 10)

Therefore, in Fig. 6 is shown the hyperbolic limit law of distribution.



Fig. 6. Limit the hyperbolic distribution law

3. DISTRIBUTION OF DEFECTS OF VARIOUS KINDS OF DESTRUCTION - THE CALCULATION AND COMPARISON WITH EMPIRICAL DATA ACCUMULATED

The distribution of the number of defects n_i of size l_i can be obtained by substituting the formula (11), the expression (3) between the size of the defect to the magnitude of the absorbed energy $\varepsilon_i = \varepsilon(l_i)$ to them:

$$\frac{n_i}{n_*} = \frac{\varepsilon(l_*)}{\varepsilon(l_i)} \exp\left(1 - \frac{\varepsilon(l_*)}{\varepsilon(l_i)}\right),$$
11)

Where l_* and n_* - the coordinates of the point of extremum of the curve. To assess the type postulated dependence linking microcrack energy $\varepsilon_i = \varepsilon(l_i)$ absorbed with its size, we will resort to some phenomenological considerations, and we will update the findings in the empirical example of the above curves. Obviously, the energy consumed in the fracture during cyclic loading is expended in two aims. One part $\varepsilon_{i(break)}$ of it is the destruction of inter crystalline bonds, that is, to increase the area of the crack itself; second $\varepsilon_{i(diss)}$ - is transformed into heat in its zone of plasticity.

Given that the micro-cracks per unit area accounted for approximately the same number of broken inter crystalline bonds, it can be assumed that the energy of fracture is proportional to its area, which means:

$$\mathcal{E}_{i(break)} \propto l_i^2$$
 12)

Somewhat, more complicated to evaluate is the second dissipative component $\varepsilon_{i(diss)}$.

As a result, in many experimental studies [10, 11], there was an understanding that the development of fatigue damage is closely linked to the process of plastic deformation of the material, localized at the interface of these defects. On the one hand, this area of localized plasticity "sets the stage" for the growth of microcracks size, on the other hand, it is also a major consumer of that part of the energy coming from the outside, which is defined as the energy dissipation. Measurements made by using infrared thermography method [9, 10] have shown that the most intense heat occurs on cracks border.

As a result, microcracks energy dissipation can be estimated as:

$$\varepsilon_{i(diss)} \propto P \cdot \Delta h \propto l_i^2 \cdot (l_i^2)^{\delta} = l_i^{\gamma}$$
 (13)

Thus, the exponent, which connects γ it with the size of microcracks energy dissipation can be represented as the sum of:

$$\gamma \approx 2 + 2 \cdot \delta$$
, where $\delta > 1$.

In view of the changes (12) and (13) we can postulate a kind of dependence linking the entire microcrack energy absorbed with its size:

$$\varepsilon_{i} = \varepsilon_{i(break)} + \varepsilon_{i(diss)} = g(l_{i}) \approx a \cdot l_{i}^{\beta} + b \cdot l_{i}^{\gamma}, \qquad 14$$

where in the case of fatigue cracks $\beta = 2$. This expression reflects the presence of the two components of energy absorbed by the microcrack - fracture energy and energy dissipation. In this case, formula (11) for calculating the distribution of the number of microcracks of the size can be written as follows:

$$\frac{n_{i}}{n_{*}} = \frac{l_{*}^{\beta} + c \cdot l_{*}^{\gamma}}{l_{i}^{\beta} + c \cdot l_{i}^{\gamma}} \cdot \exp\left(1 - \frac{l_{*}^{\beta} + c \cdot l_{*}^{\gamma}}{l_{i}^{\beta} + c \cdot l_{i}^{\gamma}}\right),$$
¹⁵⁾

where l_* and n_* - the coordinates of the extremum distribution (Fig.1 and Fig.4 they correspond to the notation l_{SC} and N_{SC}). From the above the empirical curves

can also be prepared for and evaluation c and γ . Their proper selection will allow to describe these distributions using the dependence (15). The shape of the curves $c \bowtie \gamma$ can be seen in Fig. (7). For these imputations made $\beta = l$ (and the subsequent calculations performed in Mathcad-15).



Figure 7. Calculations using formula (15): - a) in normal and b) in the logarithmic coordinate systems

Expression (15), originally derived from the entropy principle reflects more general rules, which are inherent in complex systems such as the balance sheet, in which a limited amount of "resources" is allocated on a finite set of "carrier" At the heart of this expression is very hyperbolic distribution (9).

Distributions satisfying these rules have precisely the properties which were observed experimentally in the analysis of accumulated defects of different nature destruction (Figure 1 - 2.). They are due to properties such as self-similarity and the nature of the individual branches of power curves (straight sections of the graph represented in logarithmic coordinates).

By the method of adjusting the parameters *c* and γ according to formula (15) the values were determined (Figure 8) at which coincidence calculations and empirical data become sufficiently good. To do this, we have been imposed graphs the calculated values n/n_* and the empirical curve $(dn/dl)/(dn/dl)_{SC}$ shown in Figure 3 (b) for fatigue defects. For the following two graphs the distribution of fatigue cracks, the exponent of the first term is adopted $\beta = 2$, as it was previously argued.



Fig. 8. Results of calculation of the distribution amount of fatigue cracks by the formula (15) and to compare them with experimental data [5] for the copper sample

Fig. 9 shows the same comparison and held for another empirical distribution curve of fatigue cracks on their size, with enough high-resolution detection of small defects. For this reason, in Figure 2 (b) is a right branch of the graph.



Fig. 9. Comparison of inclination calculated in (15) obtained empirically and [5] quantity distribution graph for a sample of fatigue cracks

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4. CONCLUSIONS

- A review of various empirical data [3], the distribution of accumulated defects regardless of the destruction of nature have a similarity. They are inherently self-similarity, and descending parts of the power curves have the form (on a logarithmic scale straight lines);
- A good theoretical basis for the analysis of the distribution of the number of micro-defects on the size of a variational entropy principle and the theory of complex systems [12] (which in the final set of "carrier" is allocated a limited amount of "life." On this basis, maximum hyperbolic distribution rule was obtained (9), subsequently used for calculation of dependences (14) and (15);
- The schedule of the marginal distribution of the hyperbolic law (in the form of (9) or (15)) have the property of self-similarity and asymptotically tend to a power form (straight sections in logarithmic scale (Figure 7)). These two properties correspond to the detected features of empirical empiric distribution of micro-defects [13];
- The calculations (formula (15)), the distribution of the number of accumulated defects on their size showed good agreement with the experimental data. The basic law has the same value in all graphs slope descending lines in logarithmic coordinates. It corresponds to the exponent of the second term in (14) equal. Those are quite remarkable results. From this it follows that the dissipation of energy, as suggested above (see relation (13), (14)), is proportional to the size of the micro-cracks around the 7th degree.
- The difference between the distribution curves of fatigue cracks from the distribution curves of accumulated defects of a different nature (cp. The left branch of the graph in Figure 8, 9) is expressed in the difference between the values of the degree of the first term of expression (14). In the first case it is in the second. Thus, the energy gap relationships with fatigue failure are proportional to the square of the size of the crack, and for the destruction of other species this dependence is close to linear.

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