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# MACHINE BUILDING AND MACHINE SCIENCE
# МАШИНОСТРОЕНИЕ И МАШИНОВЕДЕНИЕ

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## Analysis of the initial stage of fatigue wear in heterostructure materials under contact cyclic loading [***]

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## Анализ начальной стадии усталостного износа гетероструктурных материалов в условиях контактных циклических нагрузок[*]

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*Introduction.* The process of formation of fatigue defects in metal alloys with different structural morphology is considered. The work objective is to develop a computational tool for determining the moment of the defect nucleation under cyclic loading.

*Materials and Methods.* A physical model is built, calculation expressions are presented. The physical model is based on the theory of dislocations. It is shown that a structure factor is particularly important in the process of fracture nucleus origination under dynamic cyclic loading. Depending on the structure and properties of the material, as well as on the nature of the loads, the critical fatigue defect develops in the form of cracks, pores or micro-crater wear.

*Research Results.* A numerical experiment was performed to determine the moment of nucleation of the critical-size defect in iron-base alloys under the drop hypervelocity impacts. Comparative data of calculations and bench tests for droplet impingement erosion of steels and alloys with the structure of ferrite, austenite, sorbitol and martensite are presented. The efficiency of the nucleation stage during the incubation period of erosive wear of the materials studied was evaluated.

*Discussion and Conclusions.* There are no strict instrumental methods for determining the duration of the nucleation stage; therefore, it is recommended to use the proposed analytical model. In addition, the work performed gave a significant application result, i.e. it showed that the focused design of the material structure can significantly increase the wear resistance.

**Keywords**: iron-base alloys, alloy substructure, cyclic loadings, fracture nucleus origination, physical model, numerical experiment, droplet impingement erosion.

*Введение*. Рассмотрен процесс формирования усталостных дефектов в металлических сплавах с различной структурной морфологией. Цель работы — создание расчетного аппарата для определения момента зарождения указанных дефектов в условиях циклического нагружения.

*Материалы и методы.* Построена физическая модель, представлены расчетные выражения. В основу физической модели положена теория дислокаций. Показано, что при динамических циклических нагружениях определяющее значение в процессе зарождения очагов разрушения имеет структурный фактор. В зависимости от структуры и свойств материала, а также от характера нагрузок, критический усталостный дефект развивается в форме трещины, поры или микрократера износа.

*Результаты исследования.* Выполнен численный эксперимент по определению момента зарождения дефекта критического размера в сплавах на основе железа при высокоскоростных капельных соударениях. Представлены сравнительные данные расчетов и стендовых испытаний по каплеударной эрозии сталей и сплавов со структурой феррита, аустенита, сорбита и мартенсита. Оценен вклад стадии зарождения в инкубационный период эрозионного износа исследованных материалов.

*Обсуждение и заключение.* Строгие инструментальные методы для определения продолжительности стадии зарождения отсутствуют, поэтому рекомендовано использовать предложенную расчетно-аналитическую модель. Кроме того, выполненная работа дала важный прикладной результат — продемонстрировала, что целенаправленное конструирование структуры материала может существенно увеличить износостойкость.

**Ключевые слова**: сплавы на основе железа, субструктура сплавов, циклические нагрузки, зарождение очагов разрушения, физическая модель, численный эксперимент, каплеударная эрозия.



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**Introduction.** Modeling specific unpredictable phenomena is a pressing challenge in terms of preventing their undesirable consequences. For example, in aeronautics, heat power engineering, gas turbine production and agriculture, the problem of droplet impingement erosion remains unsolved. The issue is discussed on the world level [1–4]. The first success in modeling this phenomenon concerned single0020 droplet collisions [5–10]. Some papers [11–13] attempted to quantify the ability of materials and coatings to resist the action of dynamic cyclic loads. In particular, it was possible to create an analytical model tested under the conditions of liquid droplet shock [14–18]. Many authors [19–21] do not differentiate the behaviour of a material or coating at the stages of nucleation and development of fracture. Nucleation is problematically identified in the experiment. In the model mentioned above, it was estimated using empirical coefficients that did not have a universal theoretical foundation, and this is a clear drawback of the solution. This work objective is a deeper theoretical study of the stage of the defect nucleation in the coating causing its wear and destruction, as well as the creation on this basis of a calculating apparatus for determining the moment of nucleation of cracks or pores in various materials and coatings under cyclic loading.

**Materials and Methods.** Difficulties in evaluating the stage of fracture and wear nucleation under the repeated exposure (for example, at high-speed liquid-droplet collisions that provoke droplet impingement erosion of metal products) are associated not only with instrumental determination of nuclei of cracks or pores. At this stage, the presence of structural elements in the material does not allow us to present the process as a continuum and to use linear fracture mechanics (for example, the Paris-Erdogan fatigue theory) for calculations. Therefore, in the fracture mechanics, the initial stage of the fatigue defect nucleation is singled out in a special stage. It is called “microstructural fracture mechanics” and proceeds until the defect reaches the size of $l_k = (4…10)\cdot d$, where $d$ is the size of a structural element of the material [22]. An analytical estimation of the stage of fatigue defect nucleation requires, first of all, a metal physical approach. The task is to find a calculated expression for the number of cyclic loads $N_3$ necessary for the formation of a critical size fatigue defect in the material. As an empirical foundation for the computational model, the experimental data of bench tests for droplet impingement erosion, where the number of drop collisions plays the role of $N_3$, can be used.

In the general case, the equation for the number of dynamic cyclic loads $N_3$ should include three components: mechanical, kinetic, and structural.

The metal physical concept of a mechanical component is related to the number (density) of mobile dislocations $\rho_m$ arising from a single shock loading (collision).

. In the process of multiple collisions, the number of mobile dislocations increases, they move in the metal matrix along slip planes under the action of tangential stresses $\sigma_s$ until they form flat clusters with critical density $\rho_{kr}$ at the nearest impassable barriers. Exceeding $\rho_{kr}$ causes spontaneous breaking of interatomic bonds in the metal and the origination of a crack nucleus. The $\rho_{kr}$ values for various materials and coatings are known [23]. A mechanical component of the number of collisions is expressed in the form of the dependence $N_3 = f(\rho_{kr}/\rho_m)$.

A kinetic component of the number of collisions $N_3$ takes into account the dependence of the dislocation energy on its velocity $V_d$. From the theory of dislocations, it is known that with an increase in speed of dislocation, its energy increases according to the expression of Einstein for bodies moving at speeds close to the light speed. The only limit for the dislocation velocity is the sound speed in a $C_0$ crystal, at which the dislocation energy becomes infinite. Therefore, considering the specifics of the drop impact, a kinetic component of the number of collisions is expressed as $N_3 = f(V_d / C_0)$.

A structural component of the number of collisions $N_3$ has two aspects. The first is that the dislocation motion under impact is limited by the size of the structural element of the $D$ matrix, within which a free path of dislocations is possible. In the general case, a grain size is considered as such an element, and its thickness – for thin coatings. The second aspect considers that within the grain or coating, there can be obstacles to the dislocation motion: second-phase particles, small-angle boundaries, immobile dislocations fixed by atmospheres, stacking faults, lattice resistance (Peierls

stress). As noted above, these both aspects are reflected in the structural component of the number of collisions, and it is a function of two variables $N_3 = f(D, \Delta G)$, where $\Delta G$ is the Gibbs free energy to activate the process of obstacle negotiation within the structural element $D$. The negotiation mechanism depends on the nature of the obstacle, which determines the value of $\Delta G$ for each specific case of the material structure (their classification is given in [23]).

Thus, all the components of the desired number of collisions $N_3$ affect the process of fatigue defect nucleation at the same time — with each collision. This fact determines the commutative nature of the interaction of the mechanical, kinetic, and structural components. Then, in the most general form, $N_3$ is determined from the expression

$$N_3 = \frac{\rho_{kr}}{\rho_m} \cdot \sqrt{1 - \left(\frac{V_d}{C_0}\right)^2} \cdot \frac{D}{l_0} \cdot e^{-\frac{\Delta G}{kT}}, \quad (1)$$

where $k$ is the Boltzmann constant; $T$ is thermodynamic temperature, K; $l_0$ is the path covered by mobile dislocations in one loading cycle (collision).

The expression (1) is obtained on the basis of the theory of dislocations and represents a theoretical concept. To use (1) in assessing the wear resistance of materials and coatings under the conditions of cyclic liquid-droplet collisions, it is necessary to specify its constituent quantities (such as $\rho_m$, $V_d$, $l_0$, $\Delta G$) through measured impact parameters (e.g., impact velocity $V_0$ and droplet size $R_0$). The authors have already completed the corresponding refining of the model (1) and are preparing material for publication.

**Research Results.** The computational model has been tested for iron-based alloys of various compositions and structures. This selection is due, first of all, to the difference in the behaviour of dislocations in these alloys and makes it possible to identify the capabilities of the computational model. So, in ferrite and austenite, the factor hindering dislocations is the lattice resistance (Peierls stress). In a sorbitol structure, the glide of dislocations is determined by the morphology and distribution of obstacles — by carbides Fe and Cr. In martensite, the dislocation motion is hindered as given. Thus, the subject of research in this part of the work is actually a structure factor.

Since all the materials studied are alloys based on iron, their basic stress-strain properties differ insignificantly. The following values were used in the calculations: elastic modulus $E$ = 186 ... 218 GPa; Poisson ratio $\nu$ = 0.20 ... 0.31; shear modulus $\mu$ = 64 ... 80 GPa; Burgers vector $b = 2.5 \cdot 10^{-10}$ m. The data of numerical experiments on the implementation of the presented model and bench tests of Fe-based alloys with different structural morphology, including heterogeneous ones, are given in Table 1 and in Fig. 1.

Table 1

Experimental $m_0$ and calculated $N_3$ values of the number of collisions* for Fe-based alloys

| Material (structure) | Structure parameters | | | | Collision parameters | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | $V_0$ = 250 m/s; $R_0$ = 0.55 mm | | | $V_0$ = 340 m/s; $R_0$ = 0.32 mm | | |
| | Lattice ($M_p$) | $\alpha_1$ | $D$ [m$^{-6}$] | $l$ [m$^{-6}$] | Calculation | | Exp. | Calculation | | Exp. |
| | | | | | $N_3$ | $\alpha_0$ | $m_0$ | $N_3$ | $\alpha_0$ | $m_0$ |
| ARMKO Fe (ferrite) | BCC (2.9) | 0.5 | 100 | 3.0 | 2197 | — | — | 1187 | — | — |
| 08X18H10T (austenite) | FCC (3.06) | 0.5 | 100 | 3.0 | 2446 | 0.253 | 9680 | 1322 | 0.154 | 8597 |
| 20X13 (sorbitol) | BCC (2.9) | 2.0 | 100 | 0.35–0.50 | 4655 | 0.280 | 16630 | 3742 | 0.254 | 14768 |
| 20X13 (martensite) | Tetrag. (2.95) | 0.02 | 0.01 | 0.01 | 9844 | 0.550 | 17861 | 5705 | 0.470 | 12140 |

* Number values of droplet collisions falling at one point are presented (determined in the software of the test bench).

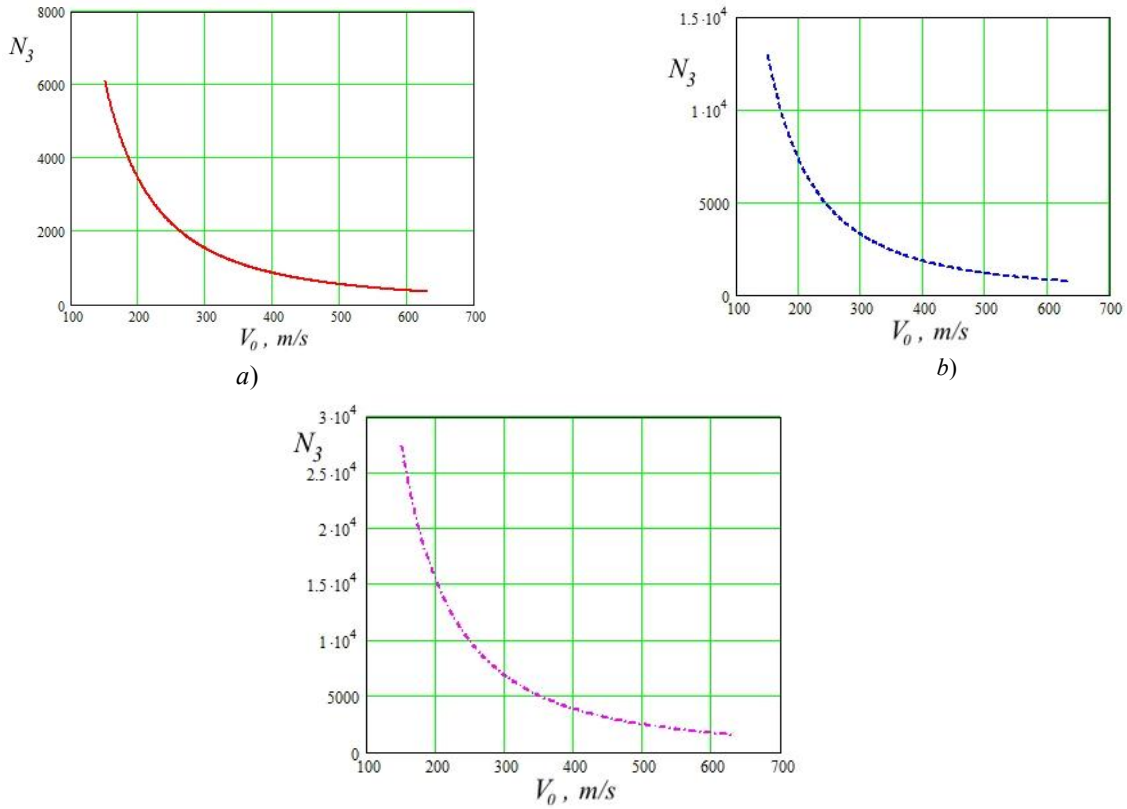


Fig. 1. Dependences of the number of droplet impacts $N_3$ necessary for crack nucleation as a function of impact rate $V_0$ at $R_0 = 0.55$ mm for Fe-based alloys with different structures: *a*) ARMKO Fe (ferrite); *b*) steel sorbitol 20X13; *c*) steel martensite 20X13

Values of some parameters given in Table 1 need explanation. The distance between obstacles $l$ on the path of mobile dislocations in ferrite and austenite is the distance between dislocations, i.e. $l = 1/\sqrt{\rho_d}$ . Given high plasticity of these solid solutions, the density of their dislocations is relatively low $\rho_d = 10^{11}$ m$^{-2}$, which gives $l \approx$ 3 μm. In hardened steel, the dislocation density is close to critical $\rho_{kr}$ = 1016 m$^{-2}$, which not only gives the structural parameter value $l \approx 0.01$ μm in Table 1, but also changes the design procedure for the number of collisions in the source model (1).

For hardened metal materials (for example, for strongly deformed or hardened alloys including 20X13 with a martensitic structure), in the expression (1), the first three factors become a unit. In such materials, the critical dislocation density $\rho_{kr}$ has already been reached; therefore, the concept of mobile dislocations $\rho_m$ loses its meaning. In terms of numbers, this is expressed as follows: $\rho_{kr}/\rho_m$=1; $V_d = 0$; $D = l_0 = 1/\sqrt{\rho_{kr}}$ .

As for the exponent in the expression (1), it retains its meaning with the values of the parameters $\alpha_1$ and $l$ given in Table 1. A crack nucleates in such a structure, an external cyclic action should overcome the existing stresses in a saturated dislocation medium and form a shear defect. Given the above, the designed expression (1) for hardened steel takes the form [23–26]:

$$N_3 = \left(\frac{\mu}{\sigma_s}\right)^2 \cdot e^{\left(-\frac{\Delta F}{kT}\right)\cdot\left(1-\frac{\sigma_s}{\sigma_\tau}\right)}. \qquad (2)$$

Here, $\Delta F$ is the activation energy of the process of overcoming obstacles without applying external voltage, the value $\Delta F$ actually determines the strength of the obstacles from the point of view of their dislocation; $\sigma_\tau$ is the internal stress existing in the material and allowing dislocations to pass through the obstacle at minimum $\Delta G$ values. The yield stress of a solid at $T = 0$K is taken as $\sigma_\tau$. The values $\sigma_\tau$ and $\Delta F$ are the material properties and, in the general case, are expressed through its basic physical characteristics μ and $b$:

$$\sigma_\tau = \mu \cdot b / l; \Delta F = \alpha_1 \cdot \mu \cdot b^3. \qquad (3)$$

In the expressions (3), the coefficient $\alpha_1$ classifies obstacles according to their strength [23].

In the expression (2), the shear stress in the slip plane under the action of which the mobile dislocations move, is considered as the stress $\sigma_s$. Stress $\sigma_s$ is the projection of the external stress vector onto the slip plane and is related to

the lattice slip system through the Taylor factor $M_p$ according to the Schmidt - Boas law for polycrystal [27]. It can be expressed in terms of impact parameters $V_0$ and $R_0$ [28].

The experimental values shown in Table 1 characterize the incubation period of erosive wear of the material $m_0$. This value includes both the stage of the defect (cracks, pores, microcraters) nucleation, and the stage of its development before the sample loss-of-mass start. It does not seem possible to instrumentally identify the number of collisions occurring only at the nucleation stage in the experimental values of $m_0$; therefore, the values of $N_3$ are exclusively theoretical. The contribution of the nucleation stage to the total value is characterized by the coefficient $\alpha_0 = N_3 / m_0$.

In addition to the numerical values presented in Table 1, the model considers the number of collisions $N_3$ necessary for the fracture nucleus origination (cracks, pores, microcraters) and the impact rate $V_0$ at the specified droplet size $R_0$. In addition, using this solution, we can determine the dependence of $N_3$ on $V_0$. Some options of such dependences are presented in Fig. 1.

The results show that the designed data $N_3$ agree with the experiment (the bench test data $m_0$). They also demonstrate compliance with the basic canons of fracture mechanics. In particular, the coefficient $\alpha_0$ characterizes the nucleation energy with respect to the fracture energy. In plastic metallic materials (ARMCO, austenite, sorbitol), the nucleation energy of fatigue cracks is significantly less than the energy of their growth. In hardened alloys (martensite), the nucleation energy is almost always higher than the growth energy. As a rule, this ratio is much larger in favour of the nucleation stage. Table 1 data show that in steel 20X13 with a martensitic structure, the stage of nucleation of fatigue defect $N_3$ is about half of the entire incubation period of the wear formation $m_0$: $\alpha_0 = 0.47$ and 0.55 for collision velocities $V_0 = 340$ m/s and 250 m/s, respectively. Whereas for the same steel with a sorbitol structure, the coefficient $\alpha_0$ is half as much. The values of $\alpha_0$ obtained by us correspond to the data of other authors for similar conditions of cyclic loading (for example, for steel 30ХГСН2А in [29].

The computational dependences in Fig. 1 also correspond to the experimental data. They are located asymptotically with respect to the values $V_0 \approx 100$ ... 150 m/s (the numerical experiment did not study this region in detail). The computational dependences mentioned above correspond to the results of bench tests, which showed that at $V_0 < 135$ m/s, wear is generally not observed in the iron-based alloys [30–34]. That is, the asymptotic property of the graphs in Fig. 1 confirms this empirical fact: at the indicated low collision velocities, fatigue defects of a critical size do not nucleate.

**Discussion and Conclusions.** There are no instrumental methods for accurate determination of the stage duration of fracture nucleus origination of materials, therefore, if necessary, the proposed analytical model is used. It is applicable to materials of various morphologies, in which the mechanisms of defect nucleation (cracks, pores, microcraters) have a dislocation nature. Therefore, under normal conditions, the model is not applicable to ceramic materials with a high proportion of covalent bonds. Another use restriction for the model is, perhaps, too high sensitivity of the exponential factor in the expressions (1) and (2). A small error in determining the numerical values of $\alpha_1$, $\sigma_s$ or $l$ in these formulas prevents from obtaining the results adequate to the experimental data.

The performed work yielded an important applied result, it showed that the focused design of the material structure can significantly increase wear resistance.

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