Wear nucleation in vacuum ion-plasma coatings and methods of its assessment

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Abstract. The paper discusses coatings of different composition and structure. The object of the study was the stage of nucleation wear of the coatings. Coatings up to 10–12 µm thick were obtained by ion-plasma deposition in a vacuum. The analytical part of the work is based on the theory of dislocations. This made it possible to create a computational model of the stage of nucleation of wear under conditions of cyclical impacts, which is problematically identified by instrumental methods. The comparison of calculated data with experimental data are given.

1. Introduction
In our previous works [1, 2], attempts were made to quantify the ability of materials and coatings to resist the action of external shock cyclic loads. In particular, it was possible to create a calculation and analytical model that was tested under the conditions of the liquid droplet shock [3, 4]. However, the model we developed did not differentiate the behavior of a material or coating at the stages of nucleation and development of destruction. The moment of nucleation is being identified in the experiment very problematically. In our model, it was estimated using empirical coefficients that did not have a universal theoretical justification, which can be considered an obvious drawback of the model. Therefore, this work aims to provide a more in-depth theoretical consideration of the stage of the formation of defects in the coating, leading to its deterioration and destruction, as well as the creation on this basis of a calculating method for determining the moment of nucleation of cracks or pores in various materials and coatings under cyclic loading.

Difficulties in estimating the nucleation stage of fracture and wear during cyclic impacts (for example, during a high-speed liquid-droplet impacts, which provoke droplet impingement erosion of metal products) are associated not only with the instrumental determination of the nuclei of cracks or pores. At this stage, the presence of structural elements in the material does not allow to represent it as a continuous continuum and to use linear fracture mechanics for calculations, for example, the Paris-Erdogan fatigue theory. Therefore, in the fracture mechanics, the initial stage of fatigue defect nucleation stands out as a special stage of “microstructural fracture mechanics”, which runs until the defect reaches the size $l_i = (4 \ldots 10) \cdot d$, where $d$ is the size of the structural element of the material [5]. In this regard, the analytical evaluation of the nucleation stage of fatigue defects requires, above all, a metal physical approach. The task is to find the calculated expression for the number of cyclic
loadings (droplet impacts) \( N_i \), necessary for the formation of a fatigue defect of a critical size in material.

2. Physical model

In the general case, the equation for the number of collisions \( N_i \) should include three components: mechanical, kinetic, and structural.

The mechanical component is associated with the number (density) of mobile dislocations \( \rho_m \) arising from a single shock loading (droplet impact). In the process of a repeated impacts, the number of moving dislocations increases, they move in a metal matrix along slip planes under the action of tangential stresses \( \sigma \), until they form flat pile-ups with critical density \( \rho_{kr} \) on the nearest insurmountable barriers. The excess of \( \rho_{kr} \) leads to the spontaneous breaking of interatomic bonds in the metal and the formation of a nucleating crack. The values of \( \rho_{kr} \) for various materials and coatings are known [6]. Then the mechanical component of the number of a droplet impacts is expressed as \( N_i = f(\rho_{kr}/\rho_{m}) \).

The kinetic component of the number of droplet impacts \( N_i \) takes into account the dependence of the dislocation energy on its velocity \( V_d \). It is known from the theory of dislocations that as the speed of the dislocation increases, its energy increases in accordance with Einstein’s expression for bodies moving at speeds close to the speed of light. The only limit for the dislocation velocity is the speed of sound in a \( C_0 \) crystal, at which the dislocation energy becomes infinite. Therefore, taking into account the specifics of a droplet impact, the kinetic component of the number of collisions will be expressed as \( N_i = f(V_d/C_0) \).

The structural component for the number of droplet impacts \( N_i \) has two aspects. The first is that the motion of dislocations upon impact is limited by the size of the structural element of the matrix \( D \), within which a free path of dislocations is possible. In general case, the grain size is considered as such an element, and for thin coatings its thickness is considered. Another aspect involves the fact that within the grain or coating there may be various obstacles to the movement of dislocations: particles of secondary phases, low-angle boundaries, dislocations fixed by atmospheres, packing defects, lattice resistance (Peierls stress). Therefore, the structural component of the number of collisions must take into account both of these aspects. This component will be represented as a function of two variables \( N_i = f(D, \Delta G) \), where \( \Delta G \) is the Gibbs free energy to activate the process of overcoming obstacles that are within the structural element \( D \). Mechanism of obstacles overcoming depends on the nature of the obstacle, that determines the value of \( \Delta G \) for each specific case of the structure of the material (their classification is given in [6]).

It follows from the above that all components of the desired number of impacts \( N_i \) affect the process of formation of a fatigue defect at the same time – with each droplet impact. This fact determines the commutative nature of the interaction of mechanical, kinetic and structural components. Then in the most general form, \( N_i \) will be defined by the following expression:

\[
N_i = \frac{D^{\eta_s}}{\rho_m} \left[ 1 - \left( \frac{V_d}{C_0} \right)^2 \right] \frac{D}{l_0} \cdot e^{-\frac{\Delta G}{kT}}
\]  

(1)

where \( k \) – is the Boltzmann constant; \( T \) – thermodynamic temperature, K; \( l_0 \) – is the path traveled by mobile dislocations in one loading cycle (droplet impact).

3. Results and discussion

Expression (1) is derived from the theory of dislocations and represents a theoretical concept. To use expression (1) when assessing the durability of materials and coatings under cyclic liquid-droplets impacts, it is necessary to disclose the values included in it (such as \( \rho_m, V_d, l_0, \Delta G \)) through parameters of a droplet impact, for example, the impact velocity \( V_0 \) and the droplet size \( R_0 \). Without dwelling on this detailing of model (1), which has already been performed by us and is in preparation for
publication, we will present some results. The data of numerical experiments on the implementation of the presented model and the data of bench tests of ion-plasma coatings are given in tables 1 and 2.

The experimental values shown in Table 2 characterize the incubation period for the erosive wear of the coatings $m_0$. This value includes both the stage of the nucleation of a defect (crack, pore, microcrater), and the stage of its development before the start of mass loss by the sample. It is impossible to instrumentally identify the number of droplet impacts occurring separately at the nucleation stage in experimental values $m_0$. Therefore, the $N_3$ values can only be calculated. The contribution of the nucleation stage to the total value is characterized by the coefficient $\alpha_0 = N_3 / m_0$.

**Table 1.** The main physics and mechanical characteristics of the coatings used in the calculations.

| Coating composition | Characteristics of the coating material |
|---------------------|----------------------------------------|
|                     | Density $\rho$, kg/m$^3$ | Young's modulus $E$, GPa | Poisson's ratio $\nu$ | Shear modulus $\mu$, GPa | Burgers vector $b$, $10^{-10}$ m | Lattice Type (Taylor’s factor $M_p$) |
| Pure Ti             | 4505                      | 110                       | 0.33                  | 41.5                        | 2.92                          | hcp (6.5) |
| Monolayer TiN       | 5430                      | 429                       | 0.23                  | 174                         | 2.995                         | fcc (3.06) |
| 3D-composite of TiAlSi-system | 3840              | 148                       | 0.24                  | 60                          | 3.9                           | fcc (3.06) |

**Table 2.** Experimental $m_0$ and calculated $N_3$ values of droplet impacts for various types of vacuum ion-plasma coatings.

| Coating composition | Structure parameters$^b$ | Impact parameters for initial data $V_0=250$ m/s; $R_0=0.55$ mm |
|---------------------|--------------------------|---------------------------------------------------------------|
|                     | $\alpha_2$, l, m$^{-6}$ | $D$, m$^{-6}$ | Calculations | Experiment |
| Pure Ti             | 0.5                      | 3.0           | 6.1          | 4051       | 0.283       | 14310 |
| Monolayer TiN       | 0.025                    | 1.05          | 4.9          | 6952       | 0.242       | 28760 |
| 3D-composite of TiAlSi-system | 2.0                | 0.05          | 9.3          | 16730      | 0.445       | 37650 |

$^a$ The table shows the values of the numbers of droplet impacts that fall into one point (defined in the software of the test bench).

$^b$ $l$ is the distance between obstacles in the way of mobile dislocations $\rho_m$; $\alpha_2$ - coefficient which is classifying the obstacles by strength [6].

4. Conclusions

The results show that in the absence of instrumental methods for accurately determining the duration of the stage of the nucleation of foci of destruction of coatings for this purpose the proposed analytical model can be used. The model has a versatility of application with respect to various materials and coatings, in which the mechanisms for the nucleation of defects (cracks, pores, microcraters) have a dislocation nature.

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