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THE INVARIANTS OF KINETICS OF STRUCTURAL ELEMENTS OF METAL SURFACES

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Abstract: The symmetry of space and time properties allows us to use the principle of least action to determine the invariants in the processes occurring on the interface of metals. The invariants established by the author and the criterion allowing to estimate the state of the interface are proposed.
Keywords: properties of space and time, principle of least action, invariants, interface, invariant criterion.

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1. Introduction.

The complexity of the study of the interface under external influences is determined by the simultaneous course of a variety of processes (heat conduction, diffusion, mass transfer, hardening, amorphization, destruction, etc.) and the correct choice of the scale factor (load-rate parameters, etc.) of the external influence. The latter allows to establish the course of the dominating process in their variety and, as a consequence, to reveal and establish the basic fundamental laws (invariants) describing this process. It is necessary to break down a complex process into its component parts in the form of simpler processes. In each simple process, isolate the main fundamental laws and describe them using invariant relations [1].

At present there are no scientifically grounded fundamental principles applied both in the field of physics, chemistry, mechanics, and in the field of metal physics and materials science [2]. The modern state of the problem of creation, destruction and wear of materials is characterized as a transitional period between the accumulation of experimental data and their interpretation in the categories of mechanics, physics, chemistry and elaboration of basic structural laws (invariants) of contact interaction during contact interaction. May it be necessary to work up other invariant, independent from the schemes and regimes of solid tests, criteria and characteristics, and then – work out the means for measurements? What quantity or criterion may be laid as the foundation for description of complex contact solid phenomena? Understanding of the mechanism of proceeding complex contact phenomena will allow working out intellectual materials with inverted connection, including nana-materials [3, 4].

It should be emphasized that the author of this report fifteen years ago raised the question of finding invariants [5]. The principle of least action (Hamilton's principle) was proposed as a theoretical justification for the search for invariants. Systematic and painstaking research work carried out by the author made it possible to define and formulate these invariants [6–9].

2. Experimental

Polycrystalline nickel of 99.99% purity, armco-iron, bearing steel, bronze, and cast iron were investigated. The nickel samples in the form of thin disks were polished electrolytically and annealed in a vacuum of 0.133 mPa at 973 K. The friction test of Ni – Mo pair was carried out on the machine AE-5 according to the finger-disk scheme with precise setting of the contact area at a specific load of ≈ 84 kPa and linear speed of ≈ 0.5 m/s. Electron microscopic studies of nickel were carried out on a microscope EVM-100AK and Hitachi-H800 by the method of thin foils on "lumen". The resolution of the Hitachi-H-800 is ≈ 0.1 nm. The technique of preparation of nickel samples for transmission electron microscopy is given in work [10]. The dislocation structure in the nickel-molybdenum pair under friction

loading was studied using the ferromagnetic resonance method (FMR) and electronic microscopy. FMR methods appear to be the most appropriate for the study of the dislocation structure in ferromagnetic. At external electromagnetic field frequencies of 9600 MHz (ν = 9600 MHz), the broadening of the FMR absorption lines in a deformed ferromagnetic is caused by elastic stress fields, while small-scale defects (such as impurity atoms or vacancies) and large-scale defects (e.g. cracks or pores) lie outside the absorption spectrum [10]. In the above works, a linear relationship was established between the breadth of the FMR line (Δ H) and dislocation density (ρ). Another advantage of the method is that the depth of penetration in the skin metal layer (δ) is $10^{-7} – 10^{-6}$ m at external electromagnetic field density of 9600 MHz. This makes the method sufficiently selective and sensitive when used for the study of defect microstructures in thin surface layers, particularly under friction loading, when the depth of the surface layers affected by plastic deformation is comparable to the thickness of the skin layer [11]. Samples of bearing steel, bronze, cast iron were investigated by the roller-particle liner scheme, etc. on the SMT friction machine and other facilities [12].

3. **Results and discussion**.

Sub microcrystalline (SMC) and nanocrystalline structural states (NC) are formed in zones with strongly disoriented crystal areas, arising from the convergence of powerful dissimilar clusters of dislocations (dipoles) built during their polygonization into walls. The latter determines the stress state of the metals with the formation of a high gradient of misorientation between the formed structural elements, where the sliding band blocked by the grain boundary can be simplistically represented as a curved segment of fixed length L (Fig. 1, a).

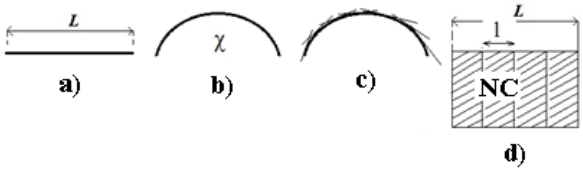


Figure 1. Scheme of formation of SMC and NC states: a) initial structure in the form of a segment; b) evolution of the structure in the form of a segment bending under the action of external influences; c) beginning of formation of SMC- and NC- states; d) formed SMC- and NC- states

The more curved the segment, the greater the local gradient of orientation of the structural elements in the crystal lattice or the curvature of the crystal lattice of the metal and, accordingly, the amount of stored energy in it (Fig. 1, b). Since the middle of the segment bends more and its ends bend less, the components of the curvature gradient will be different from zero. It is natural to assume that the structure of the crystal represented by the segment will tend to a state with minimal free energy, which is possible by its relaxation in accordance with energy profitability or the principle of least action (Fig. 2, where H is enthalpy) [6, 13].

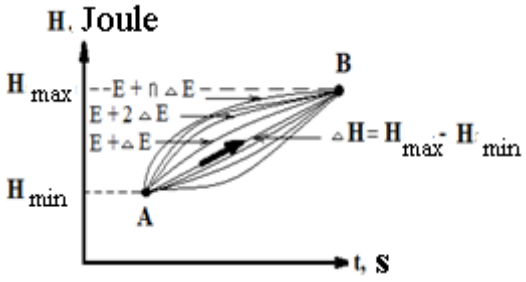


Figure 2. Kinetics of system transition from one structural state (A) to another (B) according to the principle of least action (Hamilton's principle)

Energy relaxation is carried out by shifting and rotating the corresponding segments, which make up the segment (Fig. 1, c), that is, it is energetically advantageous for the material to break into segments (straight sections) with zero or minimal possible (tending to zero) local curvature. The kinetics of the

realization mechanism proceeds in accordance with the principle of least action with the simultaneous triggering of all possible channels of energy relaxation: absorption or release of heat depending on the energy advantage, changing the direction of point defects flows in a high gradient of elastic fields, which determines the energy flow change through the local space zone and, respectively, the launch of phase transformations and chemical reactions. The complexity of material research under external influences is determined by the simultaneous course of several processes (heat conduction, diffusion, mass transfer, hardening, amorphization, fracture, etc.) and the correct choice of scale factor (load-rate parameters, etc.) of external influence, which allows to establish the course of the dominant process in their variety and, consequently, to reveal and establish the basic fundamental laws describing this process [10–13]. The latter is confirmed experimentally by the existence of NC states characterized by a high dislocation density $\rho \approx 10^{18}$ m^{-2} due to the boundaries of the block structure and the dislocation density $\rho \approx 10^{12}$ m^{-2} inside the block, characteristic of annealed unstrained nickel [11]. Inside the NC block of states, the dislocation density is very low and is similar to the cellular structure shown in Fig. 1, c. The segments or blocks that make up the segment are mutually disoriented, which is described by the local curvature or the ratio of the angle of disorientation between the segments to the distance between them. One of the main mechanisms of crystal structure fragmentation is the formation of inter-nodal bifurcation states [14]. A nanocrystalline material consists of a number of structures that are formed by intense plastic deformation in regions of high crystal lattice curvature in a certain volume, and the formation of one NC structure leads to a decrease in the local curvature of the crystal lattice directly in the local zone of formation. Relaxation of the stored free energy of plastic deformation in local zones will form a set of disoriented local zones, the union of which forms the volume of the nanomaterial.

The main laws of formation and kinetics of deformation defects at the nano, micro, meso, and macroscale levels of plastic deformation of the nickel surface layer were revealed, which determines the main deformation mechanisms in hardening and fracture of metal surfaces under external influences (rolling, triboloading, etc.), namely:

– the invariant associated with the asymmetric kinetic dependence between dislocation density and fracture or wear [15] intensity can be related to the time homogeneity property and the related energy conservation law, namely, an increase in the dislocation density to a certain critical value causes hardening of the surface layer, which in turn determines a decrease in the fracture intensity and vice versa [1, 3, 7]:

$$\rho \cdot I = const \quad , \tag{1}$$

where ρ is dislocation density and I is wear intensity, const ≥0;

The invariant associated with the rate of increase and decrease of dislocation density under triboloading can be correlated with the homogeneity property of space and the momentum conservation law associated with it. The rate of increase and decrease of dislocation density is determined by the size of the preformed during hardening, rolling, triboloading structure and the misorientation of the internal interfaces. The rate of increase in dislocation density (K_1) during hardening of the nickel surface layer determines both the rate of decrease in dislocation density (K_2) and strain stress relaxation, respectively, for one, and each cycle of change in strength properties, which determines the major role of the size of structural elements on the rate of change in strength properties at each of the structural-scale strain levels [7, 8]:

$$\frac{K_1}{K_2} = const, \tag{2}$$

where $K = \Delta H/\Delta t$, ΔH is the ferromagnetic resonance line broadening, Δt is time, $0 \leq const \leq 1$;

Isotropy of space and the associated law of momentum conservation can be correlated with the invariant associated with the mechanisms of deformation and destruction of the tribosystem surface or material at all mesoscopic structural and scale levels in accordance with the scale invariance. A possible implementation mechanism would be through inter-granular shear, relative rotation and slippage. According to the law of momentum conservation, the macro rotation should be compensated by the sum of all rotations in the hierarchy of mesoscale levels [16]:

$$\sum_{i=1}^{N} rot\ I_i = 0, \quad (3)$$

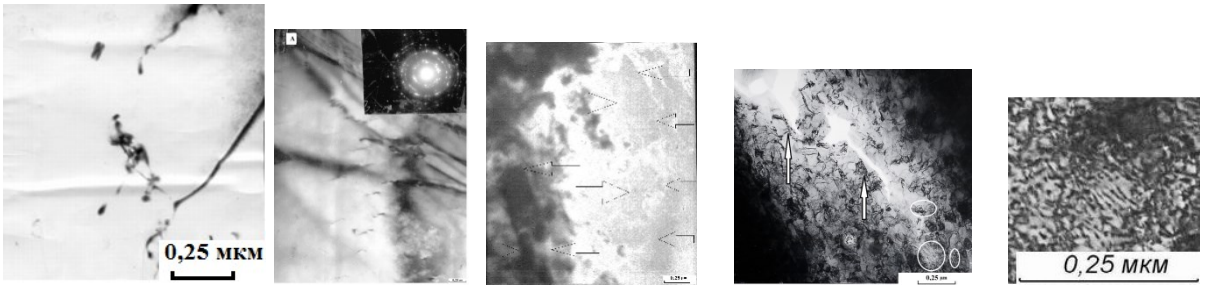
where I_i is the fluxes of defects at the i-th mesoscopic level.

The formation of defect fluxes Ii is a kinetic process that requires periodic crack stopping to bring the material state before the crack apex to the critical level of nanostructural states.
Are there still other invariants [17]? The laws of physics do not forbid this, even if they cannot be related to the properties of space and time due to our current understanding of physical processes. Increasing the degree of porosity of a metal determines grain sliding and intercristalline cracking [18].
– analysis of experimental data on evaluation of wear (I-volumetric wear intensity, [I] = m^2) of nickel samples, subjected to preliminary deformation by rolling and prolonged triboloading) and comparison of data on evaluation of pore area (S-pore area at all structural-scale levels of deformation covering the volume of the metal, [S] = m^2) of the same samples by transmission electron microscopy shows that there is a directly proportional relationship between these parameters, that is, the expression is executed [7]:

$$\frac{I}{S} = const, \quad (4)$$

where const ≥ 0.

Determination of the const values depending on the triboloading and wear regime requires further elaboration.
Thus, the kinetics of formation, evolution and destruction of the boundaries of structural elements under the action of external influences (rolling, triboloading, etc.) proceeds in the space-time continuum in accordance with the energy benefit or in a broader sense in accordance with the principle of least action, which determines the search and establishment of invariants, including the creation and evolution of nanomaterials [3, 9].
As a result of a long triboloading of the nickel surface (≈ $150 \cdot 10^3$ s) in the presence of surface-active substances contained in the plastic lubricant CYATIM-201 the formation of a defective structure whose size varies from 30 μm to 3 nm (Fig. 3).



a) **b)** **c)** **d)** **e)**

Figure 3. Kinetics of the nickel surface structure under triboloading: a) – initial structure of annealed nickel; b) – structure corresponding to the minimum oscillation dependence of the ferromagnetic resonance line broadening; c) – forming the curvature of the sliding bands; d) – subgranular microstructure; e) – nanocrystalline structure

The grain size of the nickel annealed before triboloading was ≈ 30 μm. Submicrocrystalline (SMC) and nanocrystalline structural states (NC) have a closed form and are formed in areas with strongly disoriented crystal sections [19]. There is a cyclic strain hardening of the nanocryslline nickel surface [20]. The kinetics of defect structure formation can be simplified as a circle of decreasing diameter size (Figure 3).

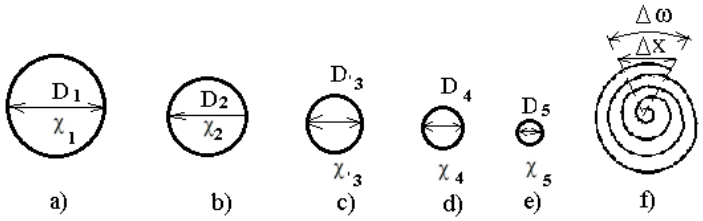


Figure 4. Scheme of the formation of structural defects at different structural-scale levels of deformation: a) initial structure; b)-e) evolution of the structure under the action of external influences (triboloading), namely: b) formation of microstructure; c) submicro-; d) nanoscale structural states; e) nanocrystalline structural states; f) evolution of kinetics of increase of local disorientation ($\Delta\omega/\Delta x$) of structural elements

Table 1. The summarizes parameters describing the structural states shown in Figure 3 and Figure 4.

Size of structural elements (diameter (D)), 10^{-6} m	Angle ($\Delta\omega$), degree	Local curvature of the nickel crystal lattice (χ), degrees/10^{-6} m
30	360^0	12
3	360^0	120
0.3	360^0	1200
0.03	360^0	12000
0.003	360^0	120000

The local curvature of the nickel crystal lattice increases by an order of magnitude when the size of the structural element decreases by an order of magnitude (table 1). The expression is executed:

$$\chi_{ij}(10^{-n}\cdot x_1;\ 10^{-n}\cdot x_2;\ 10^{-n}\cdot x_3) = 10^n\ \chi_{ij}^{o}(x_1, x_2, x_3), \qquad (5)$$

where x_1, x_2 and x_3 are space coordinates, and χ_{ij} is the tensor of local curvature of the nickel crystal lattice, n = 0, 1, 2, 3, 4, χ_{ij}^{o} is the tensor of local curvature of the nickel crystal lattice corresponding to the initial structure.

Thus, the existence of another invariant, namely, the scale invariance of the local curvature of the nickel crystal lattice, has been proved [3, 7]. The latter once again confirms that the kinetics of formation and evolution of structures at all structural-scale levels of deformation, as well as the relaxation of energy stored in the material, including its destruction, proceeds in accordance with the principle of least action (Hamilton's Principle) [6, 13].

Analysis of the dependence of the tunnel resistance (R_t) calculation on the thickness of boundary lubricating layers (BLL) and the actual contact area in rolling bearings shows that when the load increases by two orders of magnitude, the actual contact area changes by an order of magnitude, and the contribution from the BLL thickness to the calculated value of R_t increases by ten orders of magnitude, i.e., 10^{10} Ohm [12]. The main contribution to the calculated value of the tunnel resistance is made by the thickness of BLL. Therefore, the BLL thickness can be estimated not only in statics, but also in dynamics, when the actual contact area changes under the action of the load [21, 22]. The boundary conditions are defined and an invariant criterion (Dirichlet condition) for evaluating the state of metal surfaces under triboloading is developed. The ratio of the measured value of contact resistance under the action of load-rate parameters to the value characterizing the initial state of the surface determines the processes occurring on it [23]. The invariant criterion establishes the relationship between the load-rate modes of triboloading and the kinetics of structure formation with the nature of its response, namely the change in nanometer thickness of the boundary lubricating layer or coating and its state. The latter determines the mechanism and character of fracture of the mating surfaces from low-amplitude and multi-cycle to scoring and seizure, accompanied by catastrophic fracture [24, 25].

4. Conclusions.

The degree of my understanding allowed me to propose to apply the principle of least action to describe the processes occurring on the metal interface and to define the invariants of the kinetics of structural elements of metal surfaces under external influences. The fundamental role of the crystalline lattice curvature of the nickel surface layer in the formation of defect structure elements at different scale levels of deformation under triboloading has been shown. The existence of scale invariance of the local

curvature of the crystal lattice of the nickel surface layer once again confirms the universality of the scientifically valid use of the fundamental principle of the least action for the creation, evolution, and destruction of materials, including nanomaterials of various functional purposes. It is proved that the application of this principle, which describes various kinetic processes at the junction of different sciences: physics, chemistry, mesomechanics, nonequilibrium thermodynamics, etc. determines not only the kinetics of evolution, but also the search and establishment of fundamental, invariant regularities for processes occurring in the space-time continuum.

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The author is seeking the sponsor to publish the monograph on the topic of this report.

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