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Self-Organization of Structure Formation Processes in Intense Treatment and Operation of Materials

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Abstract

Structural self-organization of metals and alloys has been analyzed and the mode sustainability of technological and operational processes under intense complex heat and deformation exposure has been determined. The ways of structure formation intensification in the material processing and structure stabilization in material operation that combine control pressure and thermal effects parameters have been proposed.

Keywords

Metals and alloys; phase transitions; pressure treatment; structure formation; synergetic conception; thermal operations; thermo-mechanical effect.

Introduction

To ensure operational properties of metals and alloys the latter have to undergo irreversible changes caused by phase transitions as a result of deformation, thermal or other intense effects. If the material, having been intensively affected, is in structurally non-equilibrium state, it also has to be processed, although phase transformations do not occur in it [1].

Changes in the structure and properties of metals and alloys with time are determined by temperature, pressure and other intense factors of their formation [2]. The processes occurring during the materials processing are described in the theory of heat treatment of metals, specifying the kinetics of transformations at different temperatures and factors affecting its course [3]. Up to date uniform pressure has not been actively used to control structure formation in materials [4]. The use of pressure treatment for structure formation in metals and alloys is restrained by technological complexities to control the process and lack of clarity how effectively pressure can be used to obtain special properties of materials [5].

The purpose of the work is to develop theoretical and technological foundations of structure and phase formation in metals and alloys using crystallization modes of a change in pressure on the basis of the integrated approach to phase transitions and structure formation during thermal operations, pressure treatment and thermo-mechanical effects from the synergetic perspective.

The synergetic concept of the state of a thermodynamic system

It is reasonable to determine the dominant processes of structure formation under intense effects in terms of synergetics using the concept of a mode in the distributions of continuous random variable of controlled parameter [6].

By a mode we mean such a value of the parameter at which the density of its distribution is at a maximum. According to the synergetic concept, stable modes adjust to the dominant unstable modes and consequently can be excluded. This leads to a drastic reduction in the number of controlled parameters – degrees of freedom of a thermodynamic system. The remaining unstable modes can serve as the parameters of order that determine the processes of structure formation [7].

The equations of state of the thermodynamic systems, resulting from the reduction of the parameters, are grouped into several universal classes of the form [6, 7]:

$$\frac{\partial}{\partial \tau}U = G(U, \nabla U) + D\nabla^2 U + F(\tau),$$

where U – a controlled parameter; τ – current time; G – a non-linear function of U and may be U gradient; D – the coefficient that describes either the diffusion when its value is real or the propagation of waves when its value is imaginary; F – fluctuating forces due to the interaction with the environment and dissipation inside the system.

Equations of this type are similar to the equations describing phase transitions of the first and second kind. In accordance with the synergetic concept, phase transitions occur as a result of self-organization, a process which is described by three degrees of freedom, corresponding to the order parameter (**O**), its conjugate field (**F**) and control (**C**) parameter [7].

To use a single degree of freedom – the order parameter – is possible only for describing the quasi-static phase transformation. In the systems which are far from being in thermodynamic equilibrium, each of these degrees of freedom acquires an independent significance. The processes of self-organization in them result from the competition of the positive feedback of the order parameter with the control parameter and the negative feedback with the conjugate field. Consequently, except for the process of relaxation, at the equilibrium state over time τ^p with two degrees of freedom a self-oscillating mode can be realized, and with three degrees – a transition into a chaotic state can take place [6, 7].

Thus, the state of thermodynamic systems under intense treatment and operation is characterized by a number of modes [8, 9]:

1) *memorising* – which is determined by a "frozen" disorder in the transition from a disordered state and is implemented when the time of the order parameter relaxation is much smaller than any other time $\left(\tau_{\mathrm{O}}^p << \tau_{\mathrm{C}}^p \text{ and } \tau_{\mathrm{O}}^p << \tau_{\mathrm{F}}^p\right)$;

2) *relaxation* – is realized when the time of relaxation of the order parameter is much greater than the relaxation time of the remaining degrees of freedom $\left(\tau_{\mathrm{O}}^p >> \tau_{\mathrm{C}}^p \text{ or } \tau_{\mathrm{O}}^p >> \tau_{\mathrm{F}}^p\right)$;

3) *self-oscillation* – which requires the commensurability of the characteristic time of a change in the order parameter and the control parameter or the conjugate field $\left(\tau_{\mathrm{O}}^p \gtrless \tau_{\mathrm{C}}^p \text{ or } \tau_{\mathrm{O}}^p \gtrless \tau_{\mathrm{F}}^p\right)$;

4) *stochastic* – is characterized by a strange attractor and is possible if all of the three degrees of freedom are commensurable $\left(\tau_{\mathrm{C}}^p \gtrless \tau_{\mathrm{O}}^p \gtrless \tau_{\mathrm{F}}^p\right)$.

The dominating processes of structure formation are determined by the intensity of energy and matter transfer in non-equilibrium thermodynamic systems. The stability of structure formation is provided by the control of the stability of the processes of intensive processing and operation through the use of positive and negative feedbacks [9, 10].

Thermal treatment of metals and surface exposure to energy flows

The purpose of any thermal treatment process is to provide a desired material structure by heating (or cooling) it up to a certain temperature and subsequently changing it [1]. The mode of thermal treatment is typically characterized by the following basic parameters: the temperature of heating and holding time, the speed of heating and cooling of the material [4].

All the types of thermal treatment, according to A. A. Bochvar [2], are divided into four main groups of operations, which in terms of the synergetic concept of structure formation, can be associated with the modes of the thermodynamic system behavior.

The modes are defined by relaxation time τ^p: of the order parameter while cooling, structure formation parameter conjugate with it, and the control thermal treatment parameter – heating. The presence of two degrees of freedom generates a thermal cycle and that of three degrees provides the cycle with phase transitions.

As a result, groups of operations of thermal treatment are implemented [2, 4]:

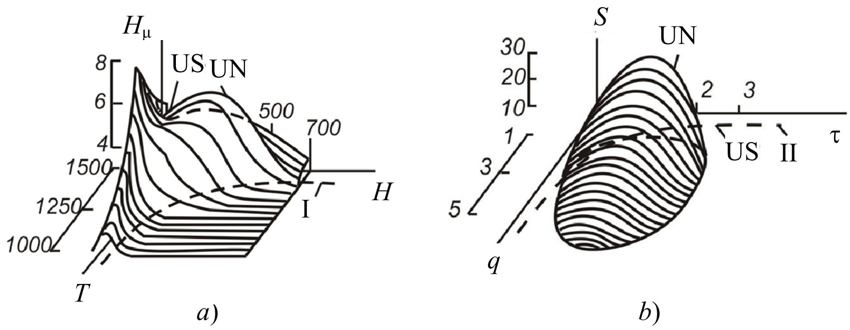
1) *hardening* – heating above the transformation temperature, followed by rapid cooling to obtain a structurally unstable state;

2) *tempering* – heating of the hardened material below the transformation temperature followed by cooling to obtain a more stable structural state;

3) *annealing* of the first kind – heating the material in an unstable state after the pre-treatment, followed by slow cooling, resulting in a more stable structural state;

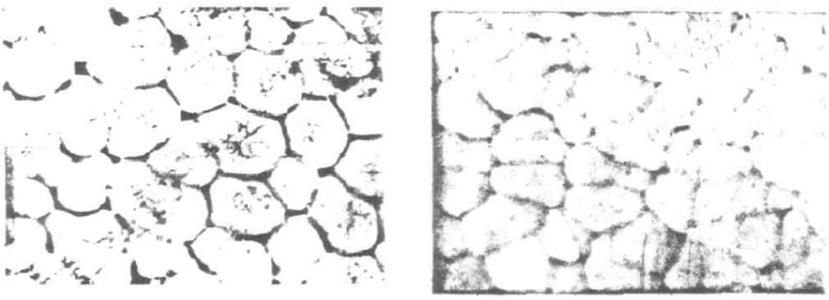
4) *annealing* of the second kind – heating above the transformation temperature followed by slow cooling to obtain a structurally stable state.

Groups of operations of thermal treatment can be associated with thermodynamic system equilibrium modes [8, 9]. Among the six possible equilibrium states of a controlled two-parameter system there is not the most stable state – a stable node (**SN**) [9]. The mode which corresponds to hardening is an unstable node (**UN**). From this most unstable state, through the mode – an unstable focus (**UF**) – the system transforms in the course of tempering or annealing of the first kind into the states characterized by modes of a stable focus (**SF**) or a limit cycle (**LC**). Phase transformations during annealing of the second kind after hardening convert a thermodynamic system from



a) *b*)

Fig. 1. Distribution of microhardness H_μ, GPa along the depth *H*, μm of the surface layer of a titanium alloy with a chrome-nickel coating with a change in temperature *T*, K (*a*) and the relative surface area *S*, % with a modified structure depending on the specific power *q*, kW/cm^2 and duration τ, s of the electron-beam heating (*b*); the visible boundary of the modified layer (I) and the melting boundary (II) are marked with dashed lines



a) *b*)

Fig. 2. Cellular structures (×3000) on titanium alloys VT 20 (*a*) and VT6 (*b*) after electron- beam heating with a specific power of 3 kW/ cm^2 for 1 s

a state with UN mode into a state characterized by unstable saddle (**US**) mode.

The above mentioned UN and US modes of equilibrium states of a thermodynamic system are clearly observed under intense treatment (Fig. 1). It is reasonable to compare the values of physico-mechanical parameters of quality treatment (see Fig. 1, *a*) with the amount of the formed structures, characterized by a relative area of the modified surface (see Fig. 1, *b*) [10, 11].

The formation of a cellular structure on the modified surface of a titanium single-phase pseudo-α-alloy (Fig. 2) occurs through the formation of vortex dissipative structures in a liquid state.

The change in the state modes of a thermodynamic system is determined by the prevailing convection mechanisms. At the beginning of fusion the narrow cells formed by a thermocapillary force, described by Marangoni criterion, originate and then move to the periphery. With increasing intensity of electron-beam exposure in the center of the heating zone the natural convection, characterized by Grashof criterion, blurs vortex dissipative structures. Wide toroidal vortices generated by the buoyancy force, described by Rayleigh criterion, under electron-beam exposure are observed only when deep melting of the surface occurs [11, 12].

The study of the relationship between the area S_0 of the surface with a cellular structure and the total area of the fritted section depending on the specific power *q* and heating duration τ showed (see Fig. 1, *b*) that the largest area with a regular structure $S_0 = 40$ % is formed in the narrow heating intensity range [10, 12].

The formation of a cellular structure on the maximum area is characterized by UN mode which is transformed into a limit cycle. The cycle is limited by transition processes of the material transformed from a solid to a liquid state. The formation of the interface – the melting border – is described by US mode. The movements from the interface in the opposite directions, by thermal conduction and convection of heat flows, stabilize the state of the system [8, 9].

The dependences of a change in the structure micro-hardness (see Fig. 1, *a*) characterized by physical and chemical transformations in the surface layer of titanium alloys with coatings look similar to the dependences of cellular structures formation (see Fig. 1, *b*). Chemical reactions, dissolution of coating elements in a solid state, formation of phases having eutectic composition, melting of the coating surface to form a regular structure, submelting of a base to form a transition zone, the formation of diffusion zones under electron-beam exposure [9, 10] lead to a change in the micro-hardness along the depth of the surface layer of a titanium alloy with a chrome-nickel coating (see Fig. 1, *a*). Consequently, to control the strength of coating-base adhesion and improve physical-chemical parameters of the processed surfaces, the intensity range of electron-beam exposure must be strictly controlled in accordance with the chemical composition of the base and the coating as well as its thickness.

Plastic deformation and metal forming

Phase transformations used in thermal treatment are primarily caused by a change in temperature, but varying the other thermodynamic factor – the pressure – it is possible to obtain structural changes that do not occur at constant pressure [1, 4].

According to the synergetic concept of structure formation, types of materials forming, like the types of thermal treatment, can be divided into four main groups of operations related to the modes of behavior of a thermodynamic system [9, 11].

Forming modes are also determined by time τ^p: of the order parameter during relaxation (stress relieving), structure formation parameter conjugate with it, and the parameter of mechanical processing control – pressure. Two degrees of freedom determine cyclic hardening, and three – stochastic cold hardening and destruction.

Hence, the following metal forming processes corresponding to different sections of the generalized curve "strain – stress" are [11]:

1) *impact* – local or uniform pressure to form a state of stress and deformation structures or destruction;

2) *stress relaxation* – no pressure after preloading accompanied by the removal of internal stresses and formation of more equilibrium structures;

3) *cyclic cold hardening* – the creation of hardening deformation structures by cyclic formation of the stress state as a result of the application and removal of the load;

4) *stochastic cold hardening* – the creation of hardening deformation structures by aperiodic formation of stress state as a result of stochastic loading.

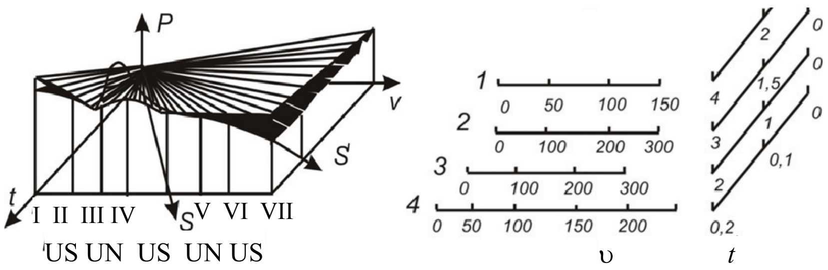
Forming processes as well as thermal ones are associated with equilibrium modes of a thermodynamic system [9]. The results of the research of mechanical materials processing show that there are two possible modes of equilibrium states: unstable node and unstable saddle [8, 9]. During UN mode the dynamic parameters of the working area of the technological system move away from the equilibrium position. The system performs self-excited aperiodic movements which transform into stable self-oscillations of the limit cycle. During US mode at small deviations the dynamic parameters of the system move away from the equilibrium position and approach the stable state in given directions (Fig. 3).

The analysis of the formation of the surface layer structures in the process of mechanical treatment (Fig. 4 and 5) in the study of the effect of the stability of dynamic characteristics on the formation of quality parameters showed the possibility of using UN modes in roughing and allowed to recommend US modes for surface finishing [8, 9].

During processing at a low speed in the formation of advanced fragile glide cracks (see Fig. 4, I; Fig. 5, I) the state of formation zone is defined by the pressure of the technological environment in the direction of the main movement υ by compressive stress σ_z proportional to bulk viscosity ς. If σ_z exceeds a critical value, then the destruction of the crack edges occurs and the resulting particles are split into smaller ones [13].

In case destruction particles are not able to rotate (see Fig. 4, II; Fig. 5, II), they increase the frictional sliding component τ_{yz} between the crack edges and compact by clusters or elements of forming jointed chips during cutting. Such a structure is described by the relation τ_{yz} / σ_z in which τ_{yz} is determined in the direction of the geometric sum of the vectors of the main movement and displacement of compacting clusters [13].

In the process of outgrowth formation (see Fig. 4, III; Fig. 5, III) the forming of the vortex dissipative structures [14] is characterized by relation σ_{yz} / σ_z, in which $\sigma_{yz\ is}$ is a rotary component and σ_z is a translational component of the stress state of the thermo-deformation process. Herewith this rotary



a) *b*)

Fig. 3. Dependencies of deformation and cutting force *P* at various stages (I – VI) of structure formation in the surface layers on the speed υ, m/min, and the depth *t*, mm of exposure for:
1 – titanium alloys; *2* – structural steels; *3* – chromium-nickel steels; *4* – chromium-nickel coatings

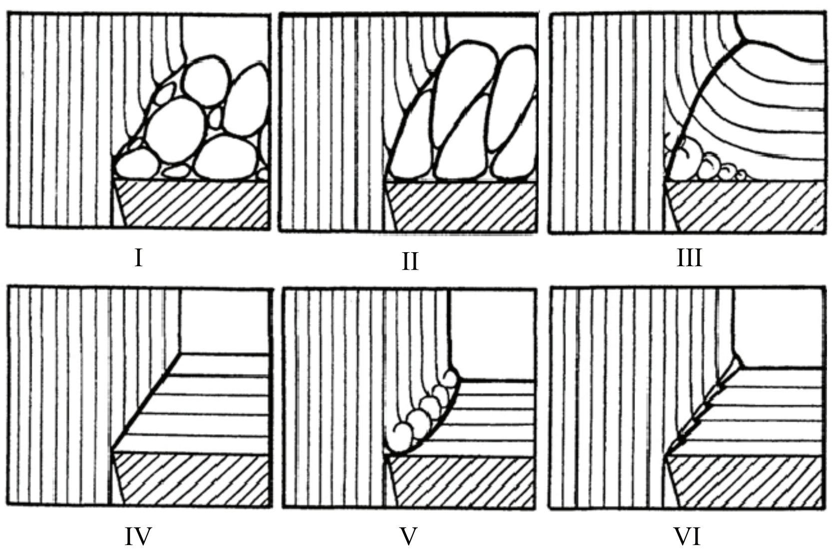


Fig. 4. Schemes of structure formation stages in the processes of surface formation:
I – brittle fracture of the material by advanced crack; II – compacting of destruction particles; III – vortex formation of stagnant structures; IV – plastic flow of the material; V – wave folding; VI – layering of the material by adiabatic shifts

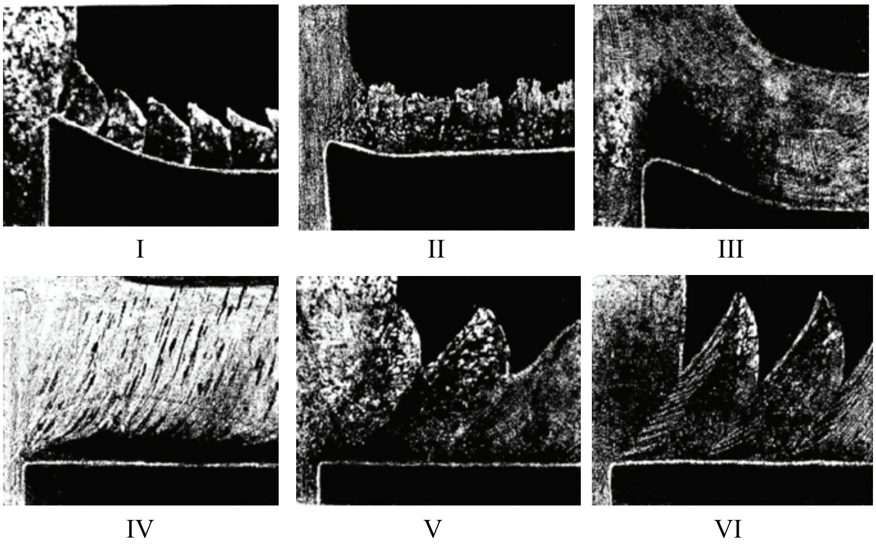


Fig. 5. Chip formation in edge cutting machining:
I – discontinuous chips; II – jointed chips; III – in outgrowth formation; IV – continuous chips; V and VI – stepped chips

component $\sigma_{yz} = \sigma_y\sigma_z$ is determined in the direction of the momentum vector of surface formation [11].

Plastic flow of the surface layers of the processed material or the formation of continuous chips in the cutting process (see Fig. 4, IV; Fig. 5, IV) is described by the shear component τ_{yz} which characterizes the stress state near the reference shear plane [15].

The formation of vortex-like densified structures following the refernce shear plane (see Fig. 4, V; Fig. 5, V) is determined again by the relation σ_{yz} / σ_z of rotational and translational components of the thermal-deformation process [11].

During cyclic adiabatic shears or forming the stepped chips in the cutting process (see Fig. 4, VI; Fig. 5, VI) the stress state is described similarly to jointed chips formation τ_{yz} / σ_z by thermoplastic components of shear τ_{yz} and compression σ_z [16].

The formation of liquid phase between the contacting surfaces is characterized by the molten material flow with dynamic viscosity η proportional to stress tangents τ_{yz} between reference liquid layers [17].

Thus, the kinetics of the formation processes of operational product properties is characterized by the cyclicity of structure states of the surface layer. Herewith, the structure formation in technological environment is described by the transformation of bulk viscosity ς into the dynamic one η through the rotational one μ. Taking into account cyclic characteristics and properties of the environment in the processes of chip formation and structure formation of the surface layer enables to choose the tools for designed processing methods in a rational way.

Wear and fracture of the surface layers materials

The combined effect of thermal and deformation factors describes the destruction of the surface layer of the material and reflects self-organization of the processes of wear and destruction of machine parts and their conjugations [7, 9, 11].

The process of deterioration has an aftereffect if the magnitude and direction of the vector wear $\varphi(X, t)$ at a time instant t depends not only on the magnitude and direction of the load vector X at a given time, but also on the magnitude and direction of the vector X in the past time $\tau < t$ as well as on the wear value U of the rubbing surfaces in the time interval $[0, t]$. *The wear process without aftereffects* is characterized by the fact that the magnitude and direction of vector $\varphi(X, t)$ at a time instant t depends on the magnitude and direction of vector X only at this instant of time [12].

Depending on time τ_p during which the changes in the process of operating capacity loss associated with the prehistory of the product use are saved, there are two kinds of aftereffects: those *of the first and the second kind* [11, 18]. The aftereffect of the first kind is characterized by the fact that changes in the process of product operating capacity loss due to the prehistory of the load effect X are retained throughout the lifetime of the product τ_d that is $\tau_p \geq \tau_d$. If $\tau_p < \tau_d$, the process with the "fading memory" takes place – the aftereffect of the second kind.

Dependences of wear and material fracture of machine parts surfaces on the duration of operation (Fig. 6) differ from each other by the type of relations between the control parameter – *load effect X* – and *wear intensity* J conjugate with it. The choice of H – the order parameter – is caused in each case by the type of relations between the determining parameter H, used to estimate resource operating capacity of the investigated products, and *accumulated wear U* [11, 12].

Let's analyze the relations between external influences and parameters of the thermodynamic system f_H as well as between the characteristics of the process of working capacity loss g_H.

Provided wear intensity J conjugated with the order parameter H depends only on the amount of the load effect X (see Fig. 6, *a*):

$$\begin{cases} J(t) = f_H(X(t)), \\ H(t) = g_H(X(t), U(t), t) \end{cases}$$

If the wear process is considered as a continuous stochastic process [13], a condition of wear *without aftereffects* can be obtained. Under constant conditions of friction the wear increment $U(\Delta t) = U(t + \Delta t) - U(t)$ does not depend on time (a process with independent increments), therefore, the rate of wear is stationary during the time period τ [18, 19]. Hence, such a wear process is described by the mode with *memorizing* ($\tau_O^p \ll \tau_C^p$ and $\tau_O^p \ll \tau_F^p$) characterized by UN state.

The processes of the parts working capacity loss in the running-in period and the catastrophic destruction of the surface layers can not be described by the above equations, as the wear intensity J in these periods is not constant and depends on the value of accumulated wear *U* of rubbing surfaces.

When the load effect in the wear of rubbing surfaces [12] changes in the form of a special transition period $[t_0, t_1]$ wear intensity *J* differs from the values which it took at the previous level of load effect X_{i-1} and from the value corresponding to the new level X_i (see Fig. 6, *b*):

$$J(t) = \begin{cases} f_H(X_i, X_{i-1}, ..., X_{i-n}, t), t_0 \le t \le t_1, \\ f_H(X_i, t), t > t_1. \end{cases}$$

The emergence of transition periods with *an aftereffect of the second kind* is explained by several reasons [18, 19]: a change in specific pressures in the parts contact zone in the transition from one level of load effect to another and associated "secondary running-in" of rubbing surfaces; gradual recovery of the correspondence between the amount of load effect and distribution of lubrication and wear products on the rubbing surfaces.

Therefore, the wear processes in transition periods $[t_0, t_1]$ are characterized by a strong correlation between wear increments $U_i(\Delta t)$ и $U_{i+1}(\Delta t)$ [12, 18]. In this context they should be regarded as *relaxation* ($\tau_O^p >> \tau_C^p$ and $\tau_O^p >> \tau_F^p$) tending to SF mode with a characteristic period $[t_0, t_1]$.

When wear intensity *J* depends on the amount of both load effect *X* and the amount of the accumulated wear *U*, to the considered moment in time *t* (see Fig. 6, *c*):

$$\begin{cases} J(t) = f_H(X(t), U(t), t), \\ H(t) = g_H(X(t), U(t), t); \end{cases}$$

and with explicitly taking into account the feedback of the load effect X^* with wear *U*:

$$\begin{cases} J(t) = f_H(X^*(t), U(t), t), \\ H(t) = g_H(X^*(t), U(t), t), \\ X^*(t) = q_H(X(t), U(t), t). \end{cases}$$

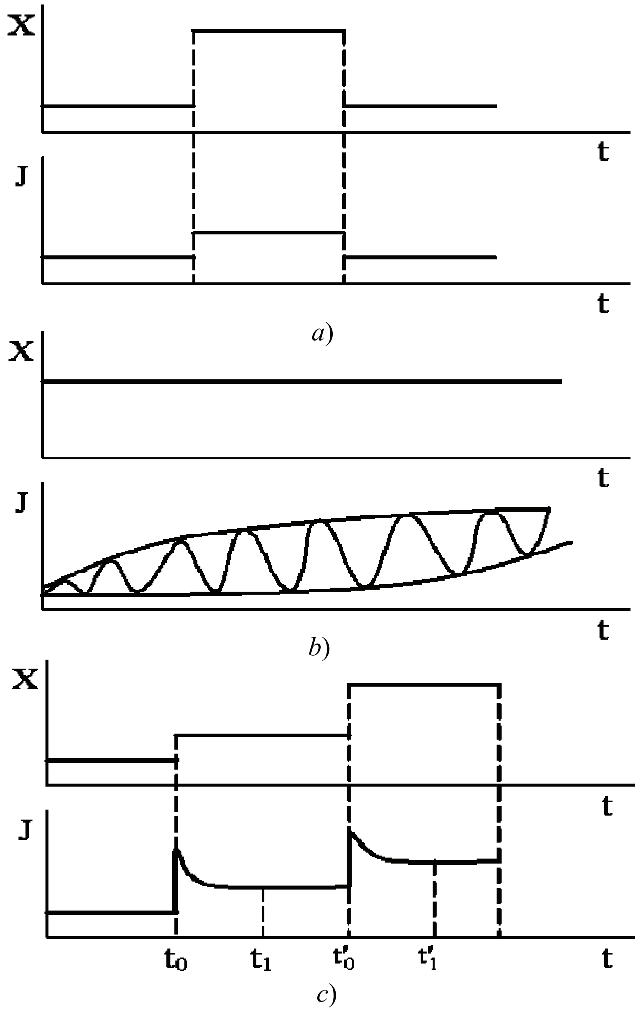


Fig. 6. Dependences of the wear intensity *J* of friction nodes on the operation time *t*:
a – the wear intensity depends only on the load intensity *X* at a time *t*; *b* – it depends on the operation time *t* at constant *X*; *c* – it depends on operation time *t* at a step change in *X* in time intervals $[t_0, t_1]$, $[t'_0, t'_1]$, etc

The changes in wear intensity *J* of rubbing conjunctions under constant load effect in time period τ at the inlet of a thermodynamic system *X* can be caused by two factor groups [18, 19].

The first group does not consider explicitly the feedback of load *X* with wear *U*. It includes such factors as differences in physico-mechanical properties along the depth of material surface layer of the product; an increase in the concentration of wear products in the process of operation; aging of lubricants resulting in the deterioration of their tribological properties, in a change in thermal mode of the conjugate and a change in the types of wear of rubbing surfaces, etc.

The second group considers changes in dependence q_H of load effect X^* on friction node parts due to conjugation wear *U*. These factors are related to an increase in gaps between rubbing conjugations; transformation of macrogeometry of friction surfaces in wear and warping of parts; a change in the contact stiffness of swivel joints, etc.

The processes of working capacity loss with the *aftereffect of the first kind* are referred to the processes with strong correlation, which have some relationship between values of the order parameter $H_i(\Delta t)$ and $H_{i+1}(\Delta t)$ even at relatively large $\tau = t_{i+1} - t_i$. Here $H_i(\Delta t) = H(t_i + \Delta t) - H(t_i)$, $H_{i+1}(\Delta t) = H(t_{i+1} + \Delta t) - - H(t_{i+1})$, $t_i < t_{i+1}$.

As a result of this, the processes of working capacity loss caused by the first and second groups of reasons, are described by the states of two or three degrees of freedom of a thermodynamic system characterized by *self-oscillating* $\left(\tau_O^p \gtrless \tau_C^p \text{ or } \tau_O^p \gtrless \tau_F^p\right)$ or tending to LC mode and *stochastic* $\left(\tau_C^p \gtrless \tau_O^p \gtrless \tau_F^p\right)$ tending to US mode.

Conclusion

Thus, from the standpoint of single formalism based on the synergetic approach, there are presented phase transitions and structure formation in metals and alloys under thermal and thermo-mechanical effects as well as pressure treatment in the process of wear and destruction [20].

It was found that relaxation time of the order parameters for the processes of materials cooling and stress relaxation, conjugate with structure formation processes governing heat and pressure parameters define the modes of behavior of the thermodynamic system.

On the basis of determining the characteristic relaxation time of the order parameters for materials cooling processes and stress relaxation there were defined groups of heat treatment operations, mechanical pressure treatment and groups of processes of working capacity loss related to structure formation in materials.

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