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DEVELOPMENT OF COMBINED METHODS OF HIGH-INTENSITY WORKPIECE SURFACING. III. DESIGN OF ION MODIFICATION*

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Design of combined vacuum ion modification is considered. The structural stability of various stages of the process is investigated in subjecting workpieces to surfacing and during their operation. Basis ways of rational design of production and operation processes are outlined.

1. Ion Implantation with Ion Deposition of Coatings. Combined vacuum ion modification or ion implantation followed by ion deposition of coatings is a method for developing quality parameters in the process of both ion modification and subsequent operation of the surface. As a result of high-intensity surfacing, atoms can be implanted at a rather high concentration in the modified transitional surface layer (Fig. 1). However, since bombarding ions experience many elastic collisions with atoms of the crystal lattice, a large number of radiation defects, usually two or three orders of magnitude larger than the number of implanted atoms, are produced in the implantation layer. These two processes have a substantial effect on physicomechanical and physicochemical properties of the surface, which in some cases results in chemical conversions (Fig. 2). A layer of composite material formed in this way ensures operation in which the friction system is self-organized toward low intensity of the normal-wear area [1]. The initial conditions of formation and reorganization of the modified layers are determined by the chemical, phase, and structural composition of the base, the species and energy of the ions and atoms involved in implantation and deposition, and the energy of friction interaction of the surfaces [2]. The boundary conditions depend on the design of the modified layers and the relative motions of the surfaces in operation.

1.1. Methods. In order to reveal the mechanism of dissipation and absorption of the energy of thermomechanical fluxes by barriers formed in previous treatments, computer simulation [3] of the behavior of atoms of the modifing element (in the present example it is chromium) in the crystal lattice of martensite of hardened RGM5 high-speed tool steel was carried out. Immediately after implantation these atoms (ions) are at the position of introduction. They are located at interstitial sites (tetrahedral or octahedral) or form asymmetric dumbbell-shaped structures. These configurations of chromium atoms are nonequilibrium due to substantial elastic distortions of the lattice around them. Meanwhile, these configurations should be highly mobile because of the energy introduced into the system. In migration of implanted atoms it is possible that they: (1) interact with vacancies and enter into stable substitution configurations; (2) interact with each other or with other impurities in a solid solution (for example, with carbon) to produce complexes; (3) escape into the sinks (dislocations, grain boundaries, and phase interfaces).

As was mentioned above, in the implantation process the vacancy concentration in the modified surface layer is substantially increased due to the introduced radiation damage. Therefore, one of the most probable diffusion-controlled reactions is entry of the implanted chromium atoms into substitution positions (Fig. 3).

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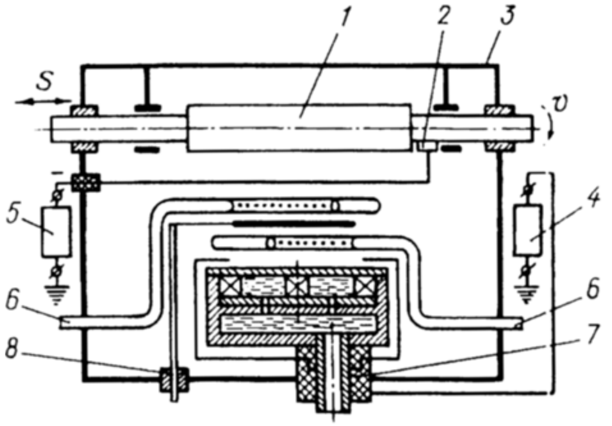


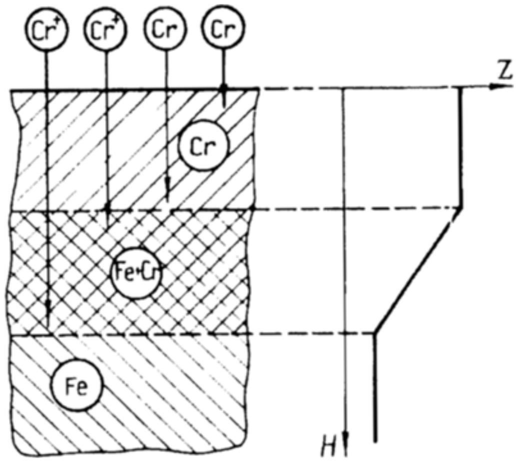


Fig. 1. Scheme of ion implantation with ion deposition of a coating: 1) surfaced workpiece; 2) sliding contact; 3) vacuum chamber; 4) power source of magnetron; 5) constant-voltage power source; 6) gas supply; 7) magnetron; 8) shutter.

Fig. 2. Schematic formation of a modified surface layer and changes in its properties Z over the depth H.

The method of molecular dynamics was used for analysis of the behavior of chromium atoms in the martensite lattice and estimation of the possibility and probability of formation of chromium atomic complexes. Application of this method requires knowledge of interatomic-interaction potentials [4] in the iron-chromium system. It is difficult to determine empirical paired central potentials with a set of constants that is fixed for each metal. Moreover, interatomic interaction potentials for the same species of atoms may be different in alloys and in the pure metal.

Therefore, in the present work, interaction potentials in the iron-chromium system were calculated within the theory of pseudopotentials [5, 6]. According to this theory, an interatomic pair potential is expressed in the form

$$\Phi_{ij}(r) = \frac{z_i^* z_j^* e^2}{r_{ij}} + \frac{\Omega_0}{\pi^2} \int_0^\infty \varphi_{bs}^{ij}(g) \frac{\sin g r_{ij}}{r_{ij}} g dg .$$

The first term in this expression describes direct interaction of ion skeletons, which can be reduced to repulsion of ions due to Coulomb interaction. The second term accounts for indirect interionic bonds that appear as a result of the dependence of the energy of the ion structure on the configuration of the ion subsystem.

For construction of interatomic-interaction potentials in the iron-chromium system, the Heine–Abarenkov–Animalou model in the quasilocal formulation (the Fermi sphere approximation) was chosen. To test the program microscopic characteristics such as energy of formation and vacancy migration, self-diffusion energy, etc. were calculated. From analysis of the data obtained the conclusion was made that the calculated values of the microscopic parameters chosen agreed well with reported experimental data, which indicates that the model chosen is correct.

The effect of chromium atoms on the martensite crystal lattice parameter was calculated by the procedure of artificial dissipation of kinetic energy (the quasidynamic method) [7]) using a set of programs.

The relative change in the martensite crystal lattice parameter caused by implantation of chromium atoms was found from the formula

$$\Delta a / a = C_0^{\mathrm{Gr}} \alpha^{\mathrm{Gr}} \Omega_R^{\mathrm{Gr}} .$$

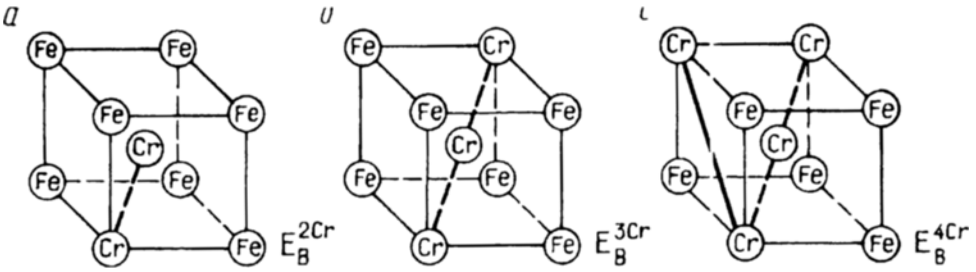


Fig. 3. Energetically most favorable configurations of two (a), three (b), and four (c) chromium atoms in a tool steel martensite lattice.

The possibility and probability of formation and growth of chromium atom complexes in the martensite lattice were estimated by calculation of the bond energy for various combinations of chromium atoms located at crystal lattice points. The calculation was conducted for two-, three-, and four-atom configurations. The possibility of formation of a complex was determined by the sign of its bond energy, and the probability of the appearance of a particular configuration was determined by the value of this energy. The bond energy of an n-atom complex was found from the expression

$$E_{\mathrm{B}}^{n1} = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}[\Phi_{\mathrm{GrGr}}(r_{ij}) - \Phi_{\mathrm{FeGr}}(r_{ij})] + E_R^n - nE_R^1 .$$

Relaxation energies are differences of the total potential energies of the crystallite containing a defect before and after relaxation.

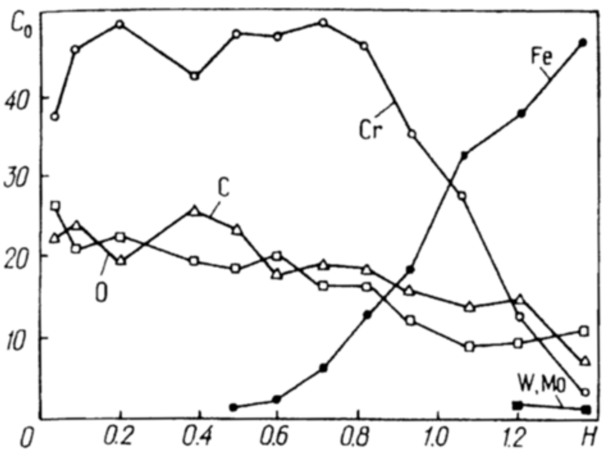
The equations of motion for mobile atoms of the crystallite were integrated by Nordsik's method using the adapted program implementing the quasidynamic method [6]. The structural defect studied (a chromium atom or a complex of n chromium atoms) was located at the crystallite center, and the surrounding atoms were located at ideal-lattice points. Each time the kinetic energy of the system that accumulated in the relaxation process reached a maximum, damping was performed, i.e., for all mobile atoms the velocities and their time derivatives were set equal to zero. The calculations were stopped if during two or three successive dampings the kinetic energy of the crystallite atoms remained at the level of 0.01 eV.

1.2. Results and Discussion. Analysis of the present calculations of equilibrium configurations of isolated chromium atoms in the substitution position in the martensite lattice showed that the lattice parameter should increase by $(4-14)\cdot 10^{-2}$, on the average, depending on the chromium concentration in the solid solution. In this case the calculated relaxation volume for one chromium atom should amount to $-0.11\ \Omega_0$. The minus sign in this expression predicts the appearance of compressive stresses in the modified surface layer, which are useful in operation under friction.

The calculations showed that in all possible versions of the relative positions of chromium atoms at martensite lattice points, it is energetically favorable for them to form complexes, especially in the case when chromium atoms are the nearest neighbors (Fig. 3). It should be noted that as the number of chromium atoms increases in the complex, the bond energy increases: for two atoms $E_{\mathrm{B}}^{2\mathrm{Cr}} = +0.09 \pm 0.01$ eV, for three atoms $E_{\mathrm{B}}^{3\mathrm{Cr}} = +0.17 \pm 0.01$ eV, and for four atoms $E_{\mathrm{B}}^{4\mathrm{Cr}} = +0.23 \pm 0.01$ eV. This fact also confirms that these compounds are energetically beneficial.

Experimental studies confirmed the calculations in general. Analysis of Auger spectra confirmed the presence of a modified transitional surface layer with a thickness of about 1 μm (Fig. 4). In this area the microhardness was found to increase from 5000 MPa in the initial state to 20,000 MPa after modification with a 10-g load on the indenter (Fig. 5).

X-ray diffraction analysis revealed a substantial increase in the martensite lattice parameter from 0.2879 nm to 0.2883 nm in the modified layer. Simultaneously, a shift in the main martensite reflections toward smaller diffraction angles for the (110) and (200) lines or a slight decrease in the halfwidths of the martensite reflection lines was observed. All these findings confirm calculations that predicted that the modified layer was hardened by



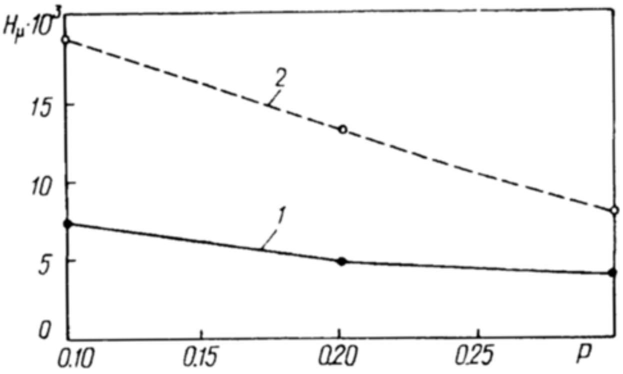


Fig. 4. Distribution of chemical elements in a surface layer of R6M5 high-speed steel after combined vacuum ion modification.

Fig. 5. Plot of the surface microhardness H_μ versus the load on the indenter for the initial state (1) and after modification (2) of R6M5 steel.

chromium and that the compressive stresses increased. Moreover, the present results indicate that the suggestion that the martensite lattice parameter changes due to distortion and the appearance of different kinds of stresses can be rejected and that only the statement about replacement of iron atoms by chromium atoms at lattice points, i.e., hard-alloy hardening, should be considered.

Microstructural studies showed that after vacuum ion modification the total number of microcracks in the surface layer decreases without substantial changes in the phase distribution pattern. The type of microstructure does not change in general. It can be suggested that the transitional zone formed becomes a barrier for emergence of microdefects on the surface. All these factors should increase the wear resistance of the steel.

Consequently, the combined vacuum chromium ion-modification of the surface of the high-speed tool steel hardened it, which was predicted by the computer simulation. This result is most probable both in the ion modification and in the energy dissipation in the friction process. The predicted formation and growth of chromium complexes in the martensite lattice are energetically favorable, and these complexes can be nuclei for advanced precipitation of the intermetallic phase, improving operational tribological properties of the surface.

As a result, it can be noted that in the modified surface layer a specific process is generated and takes place that suppresses development of microplasticity due to manifestation of difference defects in displacements upon motion of dislocations. This process is similar to formation of difference dislocations when the dislocations move through the interface with a low incoherence.

Both the energy of ions and atoms that they acquire by participating in ion implantation and deposition and the energy released in processes accompanying operation of the product in running-in, wear, and failure stages can be an external action that causes the system to be organized in the direction predicted by the calculation.

Thus, the following conclusions can be made:

1. During formation, modification, and operation of the surface the initial and boundary conditions can be changed by energy fluxes of different nature or by one source with a changing intensity and also by using the energy of running-in, wear, and failure processes.

2. It is expedient that the order of actions for forming the boundary conditions and placing the technological barriers along the depth from the surface be inverse to the order of operation of the surface layers: first the energy flux is applied that is the last to act in operation and is characterized by minimum deviations from the initial conditions of steady-state operation of the workpiece.

3. It is reasonable to form the structures studied both during surfacing and in operation stages, and it is expedient to connect these processes in such a way that the structures produced by surfacing are restored or reconstructed, depending on the conditions of operation of the surface layers.

TABLE 1. Number of Material Components C, Energy Fluxes F, Phases P, and Degrees of Freedom D in Different Stages of Technological Processes and Operation of Workpieces

Stages	Energy interaction zones		
Technological processes	I. Bulk	II. Many localized	III. One focused
	$C+F = P+C$	$C+F = P+C$	$C+P = P+D$
a) b) c)	$1+3 = 3+1$ $1+3 = 4+0$ $1+3 = 2+2$	$2+2 = 2+2$ $2+2 = 4+0$ $2+2 = 3+1$	$2+2 = 3+1$ $2+2 = 4+0$ $2+2 = 2+2$
Operation	$3+2 = 3+2$	$3+2 = 4+1$	$3+2 = 5+0$
	$C+P = F+D$	$C+P = F+D$	$C+P = F+D$
	III''. Failure	II''. Friction	I''. Running-in

2. Design of Combined Methods of High-Intensity Surfacing. In accordance with division according to energy concentration that allows us to describe interaction of energy fluxes with the modified and operated surface [8], combined high-efficiency methods were considered, in each of which one type of source was used (Table 1).

2.1. Surface Formation Processes. I. A three-dimensional source was used for applying the coating and rotary cutting with plasma heating [9]. Since homogeneous materials were used, the number of components is $C = 1$. Plasma preheating and normal and tangential loads providing both translational and rotational deformation modes [10] determine the number of imposed fields $F = 3$. Rotation of the rotary tool over a wide range of velocities provides the degree of freedom $D = 1$ to the technological system and forms the phases $P = 3$: a coating of large thickness (3–4 mm) and zones of the thermal effect and deformation hardening (Table 1, Ia). In order to create an additional zone ($P = 4$) of thermodynamic hardening, it is necessary to fix the rotational velocity of the tool and deprive the technological system of the degree of freedom $D = 0$ (Table 1, Ib). By virtue of self-organization of thermal deformation processes in cutting and friction and by dissipation of excess energy, the system tends from this unsteady state $D = 0$ to the steady state $D = 2$ in which thermomechanical processes $P = 2$ occur over the entire depth (Table 1, Ic).

II. Many local sources were used for electromagnetic surfacing by superficial plastic deformation [11] with the use of ferromagnetic powders that were applied in a thin layer (up to 1 mm) to a steel substrate, so $D = 2$. Electromagnetic fields determine $F = 2$. Thermomechanical processes are provided by $D = 2$ degrees of freedom and form $P = 2$ phases, namely, the coating and the substrate (Table 1, IIa). An attempt to render the upper coating layer amorphous by intense heating failed, since the coating becomes (including partly) over its entire area of a small thickness under high-intensity heat removal to the substrate or it remains nonamorphous. At temperature gradients necessary for rendering the surface amorphous, the heat flux is directed to the substrate, which gives rise to a new zone of thermal effect, while the number of phases becomes $P = 4$, and the system loses the degrees of freedom $D = 0$ (Table 1, IIb). The surface becomes amorphous only over the entire depth of the coating at $P = 3$, and the coating formed acquires a mechanical degree of freedom of motions $D = 1$ (Table 1, IIc).

III. A single focused high-energy source was used in electron beam heating of a coated surface [12] and in combined ion modification of the surface [1]. In these methods $C = 2$ components are used, namely, the substrate material and the material of the implanted or deposited coating (3–6 μm in thickness). The number of energy fluxes is $F = 2$, namely, the flux of deposited ions and an electron or ion beam. A wide range of intensity of electron or ion radiation provides a degree of freedom $D = 1$ to the system and forms $P = 3$ phases, namely, the coating, the substrate, and the zone of the thermal effect or implantation (Table 1, IIIa). Layer-by-layer formation (as a result of thermocapillary convection with beam-induced fusion of the surface) of hexagonal and cylindrical cells [13] or formation of clusters of implanted ions gives rise to a new phase ($P = 4$) in the surface layer and deprives the system of the degree of freedom ($D = 0$) (Table 1, IIIb). The system tends from this unsteady state $D = 0$ to a state with D = 2 degrees of freedom. In the process of forming structures, intense mixing of components takes place in the liquid phase. At the walls and in the corners of the cells components that reduce the surface tension of the melt are concentrated [12]. In the case of intense formation of clusters followed by deposition of a coating, the phase interfaces are smeared [1]. The processes just described result in formation of a single phase of combined action that together with the substrate forms P = 2 phases and provides D = 2 degrees of freedom to the system for the intensities of both coating deposition and beam surfacing (Table 1, IIIc).

2.2. Surface Operation Stage. I″. Two counterbodies and the environment (C = 3) participate in operation of the surface. The processes are thermomechanical (F = 2). During running-in, oxygen-doped amorphous-crystalline alloys are produced on the surfaces of the counterbodies, and the number of phases increases to P = 5, which deprives the system of the degrees of freedom (D = 0) and makes the state unsteady (Table 1, I″).

II″. In the stage of developed wear an oxygen-doped alloy common for the counterbodies is produced in the friction process, the number of phases decreases to P = 4 and a degree of freedom (D = 1) appears that provides translational mutual displacements of the coupled bodies (Table 1, II″).

III″. When the surface is damaged, one more degree of freedom D = 2 appears due to rotation of pricked-out particles [15], and the number of phases P = 3 becomes equal to the number of components (Table 1, III″).

2.3. Design of Combined Methods. The present studies of dissipative structures and phases developing in open production and operation systems with additional degrees of freedom show the need to include the following in designing combined methods:

1. In technological systems heredity is composed of matter and energy fluxes via formation of phases in the surface layer: P = C + F − D.
2. The structural stability of the combined surfacing determines the phases of the layer formed and depends on the matter and energy sources used: D + P = C + F.
3. Due to additional degrees of freedom of the technological system, it is possible to control the structural stability of formation of phases in the surface layer with the aid of matter and energy fluxes: D = C + F − P.
4. In the operation stages the phases in the surface layer impose restrictions on the degrees of freedom of the system and determine the order of actions in technological operations and the possibility of combining or separating them: P + D = C + F.

Conclusions. Analysis of combined surfacing methods that use diverse energy sources and combine different operations and stages allow us to formulate the main principles for controlling the processes of formation and operation of workpiece surfaces.

1. Output, energy concentration, the number of additional degrees of freedom of the sources, tools, technological media and surfaced materials, and their interactions are increased by self-organization and this increase is evolutionary. Combined surfacing and operation of workpieces are determined by cooperative nonlinear phenomena and effects involved in interaction of the various matter and energy fluxes. Structures of the workpieces produced such as phases, layers, and surfaces are dissipative, self-organizing and are inherited during formation and operation.
2. The location of the structures is described by the boundary conditions and is determined by the position of technological and operational barriers, which can be defined as the second derivative of pulsed matter and energy transfer in time and space. The state of the structures is described by the initial conditions and is determined by the magnitude of the barriers, and transition from one state to another should be accompanied by pulsed matter and energy transfer that reorganizes the barriers. In the processes of formation and operation of workpieces the open production system can be controlled through interrelated boundary and initial conditions by changing the position and magnitude of the technological and operational barriers.
3. Dissipative self-organizing structures are inherited and reorganized during surfacing and operation of workpieces. It is useful that the structures be inherited or reorganized into a new state successively from operation to operation with minimum pulses of matter and energy transfer. It is reasonable that in forming the workpiece surface the technological barriers and surfacing operations be arranged in the order inverse to the order of the technological barriers and actions in the operation stages.

NOTATIONS

Z, properties of modified surface layer; H, depth of hardened layer; Φ_{ij}, potential of interaction of the i-th and j-th atoms; r_{ij}, distance between i-th and j-th atoms; z_i^* and z_j^*, effective valences of i-th and j-th ions; e, electron charge; Ω_0, average atomic volume of alloy; φ_{bs}^{ij}, characteristic function of band structure; g, magnitude of wave vector; a, crystal lattice parameter; C_0, concentration of chemical composition of modified layer; α, constant ($\alpha^{\mathrm{Cr}} = 1/300$); Ω_R, relaxation volume that represents the difference of equilibrium atomic volumes of ideal lattice and one foreign atom in lattice after relaxation; E_{B}^{n1}, bond energy of complex of n atoms; E_R^n and E_R^1, relaxation energy of complex of n atoms and one atom; H_μ, surface microhardness; P, load on identer of hardness gauge; P, number of phases; C, number of components; F, number of imposed variable fields; D, number of degrees of freedom of system.

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