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 modifying 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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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

\[
\Phi_{ij}(r) = \frac{Z_i^* Z_j^* e^2}{r_{ij}} + \frac{Q_0}{\pi} \int_0^\infty \varphi_{bs}(g) \sin \frac{g r_{ij}}{r_{ij}} g dg.
\]

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

\[
\Delta a / a = \zeta_0^{Gr} \alpha^{Gr} \Omega_R^{Gr}.
\]