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MODELING OF CONDITIONS OF PHASE TRANSFORMATIONS IN MICRO-AREAS OF METAL MATERIALS WITH EXTREME PENETRATION OF MICROPARTICLES

The stability of chemical bonds under the action of shock waves and free electrons in the thickness of metal targets is modeled on the basis of quantum mechanical calculations. At the same time, analytical solutions of the Schrödinger equation in ellipsoidal coordinates are made and the dependences of the energy of chemical bonds under different conditions are obtained, which clearly show the conditions of their stability. The conditions of ultra-deep penetration of microparticles have been experimentally established and it has been shown that the physical state during ultra-deep penetration can vary from the plasma to the amorphous or crystalline state.
***Keywords**: mathematical modeling; ultra-deep penetration; physical state; stability of chemical bonds.*

Проведено моделювання стійкості хімічних зв'язків під дією ударних хвиль та вільних електронів в товщі металічних мішеней на основі квантово-механічних розрахунків. При цьому проведені аналітичні розв'язки рівняння Шредингера в еліпсоїдальних координатах та отримані залежності енергії хімічних зв'язків при різних умовах, які наглядно показують умови їх стійкості. Експериментально встановлені умови надглибокого проникання мікрочастинок та показано, що агрегатний стан під час надглибокого проникання може змінюватися від плазмового до аморфного або кристалічного стану.
***Ключові слова**: математичне моделювання; надглибоке проникання; агрегатний стан; стійкість хімічних зв'язків.*

Problem's Formulation

The creation of functional materials with improved operational and technological properties, as well as to reduce the cost of their production, is one of the most promising tasks of modern materials science. Impulse and periodic impact on the processed material with high-speed and high-energy macro- and microparticles leads to a change in its structural and phase characteristics. One of these methods is high-speed bombardment of targets with microparticles using the energy of a cumulative explosion, which is capable of providing particles with a wide range of velocities and energies. Surface treatment of materials with high-speed flows of microparticles is widely used in mechanical engineering to obtain superhard alloys.

Depending on the speed, temperature, properties of particles and the surface to be treated, coatings are formed and implantation into the surface layer takes place. In this case, particle streams can be used with a wide range of velocities — from tens to several thousand meters per second and pressures up to tens of GPa. The study of high-speed collisions of microparticles is widely used for research purposes.

The method of surface doping with high-speed microparticles makes it possible to form shock waves in a wide range of pressures and velocities, which radically change the characteristics of the target material under study [1—4]. One of the problems that arises when bombarding materials with microparticles at supersonic speeds is their abnormally deep penetration deep into the metal (Usherenko's method). As a result of numerous experiments, it was found that anomalously deep penetration of

microparticles into the matrix occurs — up to 1000 of their diameters, instead of the classical 5—6 [1]. In addition to anomalous penetration, new chemical elements were discovered in the passage channel, which were not observed before the bombardment, and a change in the state of aggregation of the material is also observed [5—6]. Classical thermodynamic calculations, the theory of phase transitions, experimental studies of phase and structural transformations in a solid using various physical methods of influencing the microstructure indicate that such influences as impact, heating, compression, the passage of an electric current, etc. new results. The question also remains open: where does the energy come from two to four orders of magnitude more than the energy of a microparticle? A comprehensive study of superdeep penetration of microparticles into metals and their alloys is the most appropriate way to create a theory of superdeep penetration.

Research should be carried out in the field of physics of micro- and nanosecond time intervals, since all registrations of data from experiments on superdeep penetration occur for sufficiently long time intervals and are average statistical. Therefore, the description of individual acts of interaction, decay processes and the formation of chemical bonds, they must be carried out using quantum mechanics.

Analysis of recent research and publications

To clarify the conditions for superdeep penetration of microparticles into metal obstacles, the idea of destabilizing the microstructure of metal materials in limited microvolumes during the action of external physical factors is proposed. Among such methods of destabilization may be: synthesis of single crystals of metastable diamond under shock compression, previously destabilized graphite-metal systems [1—2]; transitions of graphite and zirconium to the amorphous state under the simultaneous action of high pressure and irradiation with heavy ion fluxes [5]; abnormally deep penetration of microparticles into metals with the formation of chemical elements that were absent before the interaction [6]. When using classical experimental methods of metal processing, the above results were not obtained. As a result of numerical experimental studies, it has been established that the mechanism of collective interactions of ultrafast microparticles with metal obstacles is significantly different from the interactions of single microparticles with them. Dynamic interactions of the particle flow radically change the physical, chemical and mechanical properties of materials [1]. The process of penetration of microparticles has a complex mechanism, and their movement is difficult to describe with known physical models. As a result of experimental studies, it was found that the effect of superdeep penetration is absent for single particles [1,7—8], but is observed only in the case of acceleration of a very large number of microparticles [8]. In addition, it was found that superdeep penetration of microparticles occurs if the size of microparticles is within certain limits, the so-called "scale factor", and the speed of their collisions does not go beyond the speed range (0.5 ... 3.0 km / s) [9 —11]. As the microparticles pass, the formed channels are filled with new phases, which are formed from obstacle elements, microparticle elements and new chemical elements that were not observed in the initial materials.

Formulation of the study purpose

Establishment of conditions for the occurrence of the phenomenon of superdeep penetration of micron-sized microparticles and changes in their state of aggregation.

Presenting main material

The movement of a microparticle in a metal target along the channel is accompanied by high pressure, the influence of microsecond high-energy shock waves that lead to the destruction of chemical bonds. Fig. 1 shows the schemes of the cumulative charge of microparticles (Fig. 1, a) and the model of penetration of a microparticle into the target (Fig. 1, b). Fig. 2 shows a diagram of the motion of a single microparticle and shock waves inside the target after a cumulative explosion. If in the zone of passage of a microparticle there is a superposition of shock waves arising both upon impact on the surface of a metal target and reflections from obstacles inside the metal itself, then a shock wave front and a strip of a shock wave provoked by other microparticles appear (Fig. 2). Dislocations, crystallites, and impurities can be considered as obstacles. The interaction of shock waves, ultrahigh pressures with valence and free electrons leads to an increase in their vibrational energy. The reduced viscosity will be as long as the microparticle is in the area of the shock wave [11, 12]. If we assume that a microparticle after a cumulative shot moves before colliding with a target at a speed of 1000 m / s, then after hitting a metal surface, the propagation velocity of a shock wave will increase to 5100 m / s (for steel). Therefore, the depth of the penetration channel depends on the front and the stripe of the shock

wave in the direction of motion and the thickness of the metal target h (Fig. 2). Also, the size of the particle (the so-called "size factor") has an important place [11]. Taking into account reflected waves, we take the average time of passage of shock waves to be twice the time of passage of shock waves through a metal target $t_{прох}=2h/v$, and the penetration depth is statistical in nature. The collective motion of many particles leads to the fact that they become electrified, and when they collide with a metal surface, excess negative charges go to the metal surface, and then into the microparticle passage channel. Charges entering the channel of passage of microparticles interact with chemical bonds, contributing to their destruction. As a result, the molecules disintegrate, losing valence electrons and electrons of the outer electron shells. In connection with such a development of the situation, in a limited space at micro- and nanosecond time intervals, a limited volume of cold plasma appears, and the viscosity of the metal sharply decreases. The calculations show that the viscosity of the metal is comparable to the viscosity of water at temperatures from 55°C to 80°C [11]. If the motion of shock waves in the plasma stops, then the formation of chemical bonds begins. Moreover, the rate of formation of chemical bonds is about 10^{-5}—10^{-6} °/s, which, under certain conditions, leads to the formation of amorphous phases [12]. As an example, we present photographs of the surface morphology (Fig. 3) and electron diffraction patterns of the channel of passage of the SiC microparticle in steel (Fig. 4, point A).

The processes of decomposition and formation of new phases are confirmed by X-ray microscopic, X-ray phase, electron microscopic analyzes. It can be seen from Fig. 3 that the morphology of the target surface has changed greatly due to the passage of the microparticle through the channel. Electron microscopic microdiffraction data indicate the presence of an amorphous component. Fig. 4 shows three diffusion halos, which are inherent only in the amorphous phase. On the other hand, the formation of an amorphous phase according to classical laws is possible only from a liquid state by ultrafast cooling [12]. However, the energy for melting a microparticle and metal inside the microparticle passage channel is not enough [4].

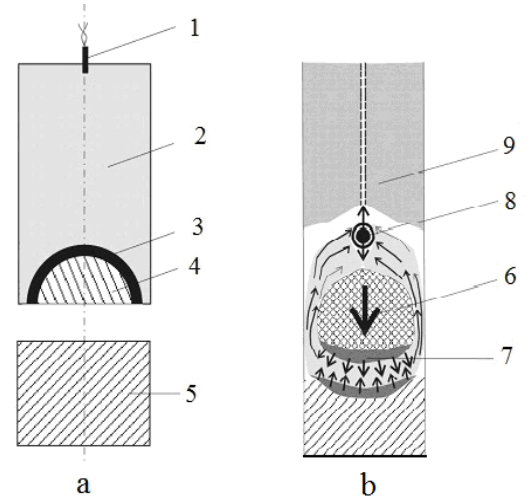

Fig. 1.a. Explosive accelerator diagram for throwing microparticles: 1 — detonator; 2 — explosive charge; 3 — metal shell of the cumulative recess; 4 — microparticles; 5 — target

Fig. 1.b. Model of particle penetration into the target [1]: 6 — microparticle; 7 — plasma; 8 — area of collision of plasma flows; 9 — channel structure

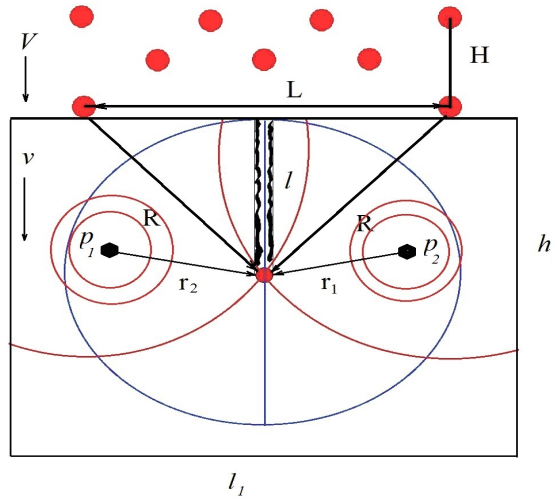

Fig. 2. Model of the passage of microparticles in a metal target: H is the average thickness of the layer of microparticles, R and r_1, r_2 — the radii vectors of sound shock waves of microparticles, H and L — dimensions of the flow of microparticles after a cumulative explosion, h and l_1 — dimensions of the target, V and v- velocity of microparticles in air and sound waves in the target, p_1 and p_2 — obstacles in the way of shock waves

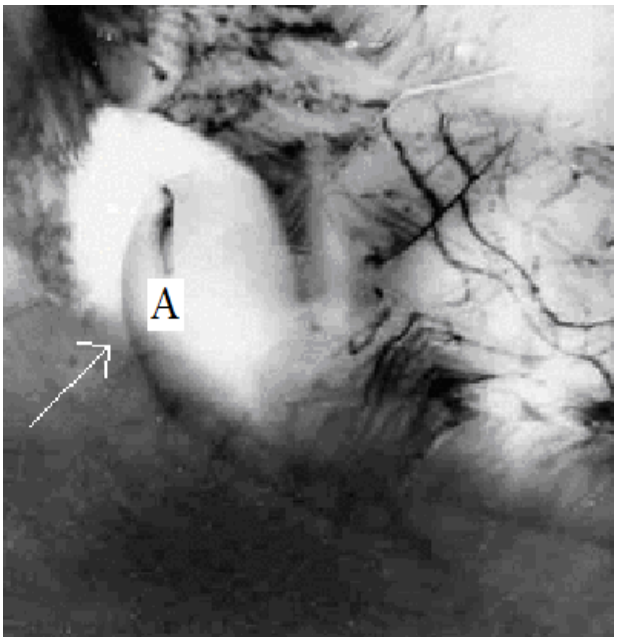

Fig. 3. Surface morphology of the sample in the region of the microparticle passage channel

Fig. 4. Electron diffraction pattern of the sample At point A

The assumption that the phase composition changes during the interaction of shock waves with chemical bonds that destroy them is evidenced by the fact that the formation of new chemical elements occurs in the collapse zone (Fig. 1b, point 8), where local nuclear fusion occurs. and there is a transmutation of chemical elements. In addition, mass spectrometric X-ray spectral analyzes recorded the presence of new chemical elements that were not present in the starting materials (Tabl. 1) [1, 6]. No new elements were found at the front of the microparticle movement (Fig. 1, b, point 7).

Table 1. Chemical composition of a steel target after treatment with a stream of lead microparticles

Sample No.	CHEMICAL ELEMENTS, %							
	Ti	Cr	Fe	Al	Mn	S	Cu	Pb
Ref. target composition in points	0,00	0,0013	99,98	0,00	0,00	0,007	0,00	0,00
Ref. particle composition								100
A		0,00	52,99	0,04	28,83	18,14	0,900	
B			28,61	13,99	39,17		0,55	17,68
V	0,31	0,18	43,83	0,00	30,39	25,01	0,28	
G			41,64	0,22	45,74		0,12	12,27
D			43,32	0,03	40,00		0,54	16,11
E			46,50	0,14	36,22		0,43	16,71

Fig. 5 shows the visible spectrum, reflecting the radiation during the transition of electrons from one shell to another in the processes of decay and the formation of chemical bonds during superdeep penetration of lead microparticles in steel. It can be seen from the figure that the set of emission lines has an almost continuous spectrum, and this indicates an infinite number of transitions of electrons from one state to another, both during the ramp and during the formation of new phases.

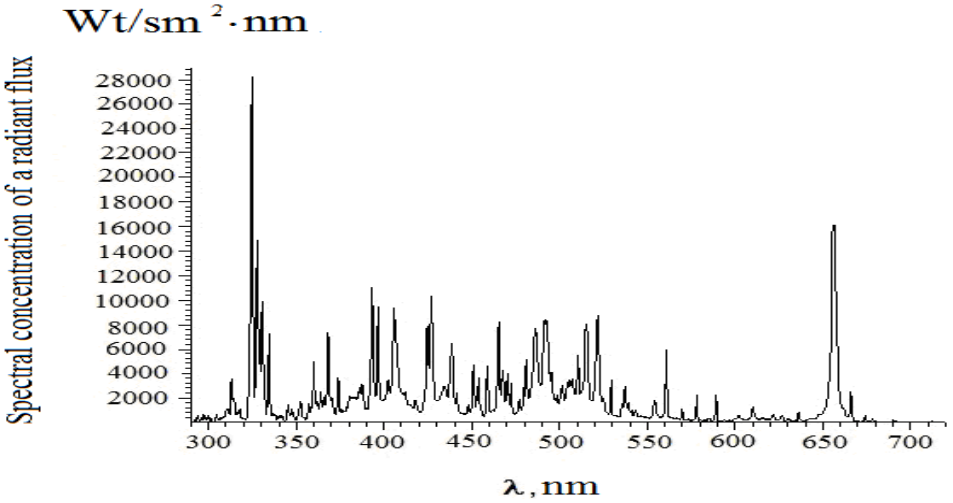

Fig. 5. Spectrogram of visible radiation obtained by bombarding a steel target with lead microparticles

As an example, let us give the results of bombardment of a steel target with lead microparticles. Results of X-ray spectral microanalysis at several points in the canal area. The table shows that transmutation of chemical elements is taking place and, obviously, local nuclear reactions are taking place [4].

In view of the above experimental data, let us consider the quantum-mechanical aspects of changes in the stability of chemical bonds under the action of various external disturbances, since atomic transitions, decay and formation of chemical bonds have nanosecond time intervals. To confirm this hypothesis, we will use the solution of the Schrödinger equation in ellipsoidal coordinates. This formulation of the problem most fully corresponds to the real orbits of valence electrons. The Schrödinger equation for an electron moving in the field of two stationary Coulomb centers (Z_a and Z_b), located at a distance in ellipsoidal coordinates, has the following form [13, 14]:

$$\Delta\Psi + 2\left[E + U(r_a, r_b)\right]\Psi = 0, \tag{1}$$

where $U(r_a, r_b)$ — operator of potential energy, r_a and r_b — distance from the electron to the charges Z_a and Z_b; E — energy of the electron; Δ — Laplace operator in an ellipsoidal coordinate system, expressed using the Lamé coefficients [15]:

$$\Delta = \left\{ \frac{4}{R^2(\lambda^2 + \mu^2)} \left[\frac{\partial}{\partial\lambda}(\lambda^2 - 1)\frac{\partial}{\partial\lambda} + \frac{\partial}{\partial\mu}(1 - \mu^2)\frac{\partial}{\partial\mu} \right] + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial^2}{\partial\varphi^2} \right\},$$

then the Schrödinger equations (1) in ellipsoidal coordinates will have the form:

$$\left\{ \frac{4}{R^2(\lambda^2 + \mu^2)} \left[\frac{\partial}{\partial\lambda}(\lambda^2 - 1)\frac{\partial}{\partial\lambda} + \frac{\partial}{\partial\mu}(1 - \mu^2)\frac{\partial}{\partial\mu} \right] + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial^2}{\partial\varphi^2} \right\} \Psi + 2\left[E + U(\lambda, \mu)\right]\Psi = 0. \tag{2}$$

The solution to equation (2) is possible by separating the variables λ and μ in the potentials, and the condition is satisfied:

$$U(\lambda, \mu)(\lambda^2 - \mu^2) = \varphi_1(\lambda) - \varphi_2(\mu).$$

This class of separating functions includes potentials:

a) $U(\lambda, \mu) = \frac{2Z_a\alpha}{R(\lambda - \mu)} + \frac{2Z_b\alpha}{R(\lambda + \mu)}$; — is the potential of the Coulomb interaction of an electron with two charges Z_a and Z_b, α — coefficient that depends on the nature of the Coulomb forces;

b) $U = A(\lambda^2 - \mu^2)$ — potential created by an isotropically oscillating two-center spatial oscillator;

c) any superposition of the previous potentials.

In expression (1), it is enough to pass to ellipsoidal coordinates in order to use the potential (a) and (b) for approximate methods of solving two-center problems with a basis that depends on R. For the Coulomb potential, we represent the solution of equation (1), which is divided into three ordinary differential equations order [15]:

$$\left[\frac{\partial^2}{\partial\varphi^2}+\Lambda^2\right]\Phi(\varphi)=0, \tag{3}$$

$$\left[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu}+\frac{\Lambda^2}{1-\mu^2}-\mu^2\varepsilon+\mu Z^{+}+A\right]Y(\mu)=0, \tag{4}$$

$$\left[\frac{\partial}{\partial\lambda}(\lambda^2-1)\frac{\partial}{\partial\lambda}-\frac{\Lambda^2}{\lambda^2-1}+\lambda^2\varepsilon+\lambda Z^{+}-A\right]X(\lambda)=0, \tag{5}$$

where $\Phi(\varphi)=\exp(i\Lambda\varphi)$, $|\Lambda|$ — integer.

$\varepsilon=\frac{ER^2}{2}$; $Z^{(\pm)}=(Z_a\pm Z_b)R/\alpha$; *A(R)* — constant separation of variables.

Equations (4) and (5) have two regular singular points with coordinates (± 1), and one regular at infinity (+). Many general theorems are applicable to this equation, which are valid for ordinary differential equations of the second order, in particular, the discrete spectrum of these boundary value problems will be nondegenerate [16]. Equations (4) and (5) contain functions of depending on parameters Λ, E, R, Z_a, Z_b, which are entire functions of parameters, therefore, by Poincaré's theorem, the solutions will be entire functions of parameters. If $Z_b=0$, then the equations for the functions $X(\lambda)$ and $Y(\mu)$ exactly coincide, and the solution to the hydrogen-like problem has the form

$$\Psi=\mathrm{X}(\lambda)\mathrm{Y}(\mu)\cdot\Phi(\varphi). \tag{6}$$

The analysis carried out for equations (3—5) makes it possible to distinguish a model equation:

$$\left\{\frac{\partial}{\partial t^2}+\frac{1-\Lambda^2}{4t^2}+\frac{C}{t}+\varepsilon+\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu}-\frac{\Lambda^2}{1-\mu^2}+n(n+1)+\frac{\partial^2}{\partial\varphi^2}+\Lambda^2\right\}F^0(t,\mu,\varphi)=0, \tag{7}$$

whose solutions will be:

$$F^0(t,\mu,\varphi)=M_{k,\frac{\Lambda}{2}}(2\sqrt{-\varepsilon})P_n^{\Lambda}(\mu)e^{-i\Lambda\varphi}. \tag{8}$$

In [16], the constructed Green's function for the operator of equation (7)

$$\int G(t,t',\mu,\mu',\varphi,\varphi')=\frac{1}{2\pi}\sum_{\Lambda}\sum_{n}\int G_n(t,t',k)\frac{(2n+1)}{2}\frac{(n-\Lambda)!}{(n+\Lambda)!}P_n^{\Lambda}(\mu)P_n^{\Lambda}(\mu')e^{-i\Lambda(\varphi-\varphi')}, \tag{9}$$

where $G_n(t,t',k)=\frac{\Gamma(-K+\frac{\Lambda}{2}+\frac{1}{2})}{\Gamma(\Lambda+1)}M_{k,\frac{\Lambda}{2}}(2at)\cdot W_{k,\frac{\Lambda}{2}}(2at)$, $t<t'$, $a=\sqrt{-\varepsilon}$, if $k=\frac{1}{2}$, $\Lambda=0$, then

$$G_n(t,t',k)=\frac{1}{4}e^{-at}e^{-at'}2att'\left[2at+2at'-3+C+\ln 2at+\ln 2at'+E_i(-2at)+E_i(-2at')\right].$$

At $t<t'$ and $k=\frac{\Lambda+1}{2}$ the singular term must be excluded from the expression. The presence of the Green's function makes it possible to find a solution with perturbation:

$$W(t,\mu)=W(t)+W(\mu)=\frac{C-Z^{+}}{t+2}+\frac{\Lambda^2-1}{4(t+2)^2}+\mu^2\varepsilon+\mu Z^{-} \tag{10}$$

Since the perturbation is a continuous and bounded function, the iterative process will be similar. If the solution of the model problem (7) at certain values k,Λ,n, can be expressed in terms of functions $f_{k,\Lambda}(t)Y_{\Lambda,n}(\mu)e^{i\Lambda\varphi}$, then the solution to a real problem will look like

$$\psi_{k,\Lambda,n}(\lambda,\mu,\varphi)=f_{k,\Lambda}(t)Y_{\Lambda,n}(\mu)\Phi(\varphi)-\int G(t,t',\mu,\mu',\varphi,\varphi')W(t',\mu',\varphi')\psi_{k,\Lambda,n}(t,\mu,\varphi)dt. \tag{11}$$

The presence of the Green's function makes it possible to find a solution of the Schrödinger equation with perturbation. After the first iteration

$$F_{k,\Lambda,n}(t,\mu,\varphi) = F^0(t,\mu,\varphi) - \int G(t,t',\mu,\mu',\varphi,\varphi')W(t',\mu',\varphi')dt \tag{12}$$

$$F_{k,\Lambda,n}(t,\mu,\varphi) = 4e^{-at}e^{\frac{1}{2}}\left\{A_1 t + A_2\ln(t+2) + A_3 + \sum_{r=1}^{\infty}\frac{A_r}{(t+2)^2} + (Z^-\mu + \varepsilon\mu^2)\cdot\right.$$

$$\left.\cdot\left[B_1 t + B_2\ln(t+2) + B_3 + \sum_{r=1}^{\infty}\frac{b_r}{(t+2)^2}\right]\right\},$$

where $A_1 = -Z^+ - 4ae^{4a}E_i(-4a) + \frac{3a}{2} + e^{4a}E_i(-4a)(6a^2 + \frac{a}{2})$; $A_2 = -2Z^+e^{4a}E_i(-4a) + 0.25$;

$$A_3 = -\frac{2}{3} - 2Z^+ - \frac{Z^+}{a} - 2(3+4a-C)e^{4a}E_i(-4a) - 3a + 2 - \frac{1}{4}\ln 2 - (11a + 12a^2 + \frac{1}{2} - \frac{C}{4} - 3aC)\cdot$$

$$\cdot e^{4a}E_i(-4a) - Z^+e^{4a}E_i(-4a)\left[-C - \ln 2 + \sum_{r=1}^{\infty}\sum_{l=1}^{r}\frac{(-1)^l b_r}{(4a)^r(r-l)!} - \right.$$

$$\left. - \sum_{r=-1}^{\infty}\sum_{l=1}^{r=1}\sum_{p=1}^{r-l}\frac{(-1)^{l+p-1}b_r}{(4a)^r(r-l)...(r-l)(r-l)(r-l-p+1)} + \sum_{r=1}^{\infty}\sum_{l=1}^{r}\frac{(-1)^l b_r}{(4a)^r(r-l)!}\right];$$

$$A_r = \sum_{r=1}^{\infty}\sum_{l=1}^{r}\frac{2(-1)^l b_r}{(2a)^r(r-l)!}\left[3a + 0.25 - Z^+\right];\ B_1 = -4ae^{4a}E_i(-4a);\ B_2 = 2e^{4a}E_i(-4a);$$

$$B_3 = -2 + 2(3+4a+C)e^{4a}E_i(-4a) - 2e^{4a}E_i(-4a)\left[-C - \ln 2 + \sum_{r=1}^{\infty}\sum_{l=1}^{r}\frac{(-1)^l b_r}{(4a)^r(r-l)!} - \right.$$

$$\left. - \sum_{r=-1}^{\infty}\sum_{l=1}^{r=1}\sum_{p=1}^{r-l}\frac{(-1)^{l+p-1}b_r}{(4a)^r(r-l)...(r-l)(r-l)(r-l-p+1)} + \sum_{r=1}^{\infty}\sum_{l=1}^{r}\frac{(-1)^l b_r}{(4a)^r(r-l)!}\right];$$

$$B_r = \sum_{l=1}^{r-1}\frac{(-1)^r b_r}{(4a)^r(r-l)\cdot 2^l}.$$

Let us calculate the wave function under the influence of the third center on it has the form (in this case, these are free electrons and positive ions

$$\Psi_{k,\Lambda,n}(\lambda,\mu,\varphi) = \Psi^0_{k,\Lambda,n}(\lambda,\mu,\varphi) + \int G\cdot W(t',\mu',\varphi')\Psi_{k,\Lambda,n}(t',\mu',\varphi')d\tau, \tag{13}$$

where $\psi^0_{k,\Lambda,n}(t,\mu,\varphi) = \sqrt{2at}e^{-at}$. After the first iteration we will have

$$\Psi^1_{k,\Lambda,n} = \sum_{i=1}^{n}\frac{2}{3}a^2Z_ie^{-at}t^2\left\{Q_0^0(\lambda_i)\left[\frac{17}{(2a)^4} + \frac{6}{(2a)^3} - \frac{t}{6a} - \left(\frac{6}{8a^2} + \frac{1}{2a}\right)t^2\right] + \right.$$

$$\left. + \left(Q_0^0(\lambda_i) - Q_0^0(0)\right)\cdot\left[\left(E_i(-2at) - 2C - 2at - \ln 2at\right)\xi^{(1)}(t_i) - \beta_i^{(1)}(t_i)\right]\right\},$$

where $\xi^{(1)}(t_i) = e^{-2at}\left[\frac{t_i^3}{2a} + \left(\frac{3}{2a^2} + \frac{1}{a}\right)t_i^2 + \left(\frac{3}{4a^2} + \frac{1}{a^3} - \frac{1-D}{2a}\right)t_i + \frac{3}{8a^4} + \frac{1}{2a^3} + \frac{1-D}{4a^2}\right]$.

$$\beta_i^{(1)}(t_i) = e^{-2at}\left[t_i^4 + \left(\frac{1}{2a} + 2\right)t_i^3 + \left(\frac{1}{a^3} + 1 - D\right)t_j^2 + \left(\frac{11}{8a^3} + \frac{1}{2a^2} + \frac{1-D}{2a}\right)t_i + \frac{17}{(2a)^4} + \frac{3}{4a^3}\right] +$$

$$+ e^{-2at}\ln 2at_i\left[\frac{t_i}{2a^2} + \left(\frac{3}{2a^3} + \frac{1}{a}\right)t_i^2 + \left(\frac{3}{4a^3} + \frac{1}{a^2} - \frac{1-D}{4a^2}\right)t_i + \frac{3}{8a^4} + \frac{1}{2a^3} + \frac{1-D}{4a^2}\right] +$$

$$+ \left[E_i(-2at_i) - C\right]\cdot\left(\frac{3}{8a^4} + \frac{1}{2a^3} + \frac{1-D}{4a^2}\right) - \frac{1}{16a^4} + \frac{1}{4a^3} + \frac{1-D}{4a^2}. \tag{14}$$

$$D = \frac{1}{2} P_2^0(\mu_i).$$

The influence of these interactions is due to the potential $\varphi_i(Z_i, \lambda, \mu, \varphi)$ and is taken into account by the perturbation theory with the Green's function

$$\Psi_{k,\Lambda,n} = \Psi^0_{k,\Lambda,n}(Z_a, Z_b, Z_i) + \int G(t, t', Z_a, Z_b, Z_i) W(t', Z_a, Z_b - Z_i) \Psi^0_{k,\Lambda,n}(t', Z_a, Z_b, Z_i) d\tau . \quad (15)$$

To return from a mathematical model to a real physical problem, we transform equation (7) by making the inverse change $\lambda=t+1$, then $f(\lambda)=[\lambda^2-1]^{-½}\cdot X(\lambda)$.

Since this transformation is nonlinear, we get an equation of the form

$$\left\{ \frac{4}{R^2(\lambda^2-\mu^2)} \cdot \left[\frac{\partial}{\partial\lambda}(\lambda^2-1)\frac{\partial}{\partial\lambda} - \frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} \right] + 2\cdot[E+U(\lambda,\mu)] + \frac{4}{R^2(\lambda^2-1)(1-\mu^2)}\frac{\partial^2}{\partial\varphi^2} - \right.$$
$$\left. - \frac{4(\lambda^2-2)Z^-\mu}{R(\lambda^2-\mu^2)} - \frac{2\mu^2 E(\lambda^2-2)}{\lambda^2-\mu^2} + \frac{4(\lambda^2-2)}{R^2(\lambda^2-\mu^2)} \left[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \frac{1}{1-\mu^2}\frac{\partial^2}{\partial\varphi^2} \right] \right\} \mathrm{X}(\lambda)\mathrm{Y}(\mu)\Phi(\varphi) = 0 . \quad (16)$$

We see that equation (16) includes the original equation, and the solution to the model problem takes the form

$$\Psi = F = [t(t+2)]^{-\frac{1}{2}} \cdot y^{\frac{\Lambda+1}{2}} \cdot e^{\frac{y}{2}} \cdot \Phi\left(\frac{\Lambda}{2}k + \frac{1}{2}, \Lambda+1, y\right) P_n^{\Lambda}(\mu) e^{i\Lambda\varphi} , \quad (17)$$

where Φ — degenerate hypergeometric function.

Consider the first group of energy terms (for n = 0) for the case when Λ=0. Let's introduce $a_i = 2b_i = \sqrt{-\varepsilon_i}$. Then, from equation (17), we obtain an explicit form of the model wave functions $\psi_{k,\Lambda,n}$

$$\Psi_{\frac{1}{2},0,0} = \frac{\sqrt{a_1}}{\sqrt{t+2}} \cdot \exp\left(-\frac{a_1 t}{2}\right); \quad \Psi_{\frac{3}{2},0,0} = \frac{\sqrt{a_3}}{\sqrt{t+2}} \cdot (1-a_3 t) \cdot \exp\left(-\frac{a_3 t}{2}\right);$$

$$\Psi_{\frac{5}{2},0,0} = \frac{\sqrt{a_3}}{\sqrt{t+2}} \cdot \left(1 - a_5 t + 0{,}5 a_5^2 t^2\right) \cdot \exp\left(-\frac{a_3 t}{2}\right),$$

where b_i is found by the formula

$$b_i = -2k \pm \sqrt{4k_i + 2L} ,$$

$L = \frac{\Lambda^2 - 1}{4} + n(n+1) + \frac{Z^+}{2}$. Considering that b_i>0, for bound states, the "+" sign is chosen in the formula (…). Based on the solutions of the model problem, we obtain the energies of states corresponding to the quantum numbers k=1/2, 3/2, 5/2 и $\Lambda = 0$, $n = 0$.

Let us calculate some states by the formula

$$E_{k,\Lambda,n} = \frac{\left\langle \Psi_{k,\Lambda,n} \middle| H_0 \middle| \Psi^*_{k,\Lambda,n} \right\rangle}{\left\langle \Psi_{k,\Lambda,n} \middle| \Psi^*_{k,\Lambda,n} \right\rangle}, \quad (18)$$

where H_0 — hamiltonian of the two-center problem

$$\hat{H} = \sum_{i=1}^{\infty} \left(-\frac{1}{2}\Delta_i - \frac{Z}{r_i} \right) + \frac{1}{r_{12}},$$

$\Psi_{k,\Lambda,n}$, $\Psi^*_{k,\Lambda,n}$ — wave functions that are solutions of the Whittaker equation [17]

$$E_{\frac{1}{2},0,0} = \frac{4\left[\frac{1}{2}(a_1 - Z^+) + e^{4a_1} E_i(-4a_1)(a_1^2 - a_1 Z^+ - \frac{1}{4}a_1\right]}{R^2\left[\frac{1}{2a_1} - \frac{4}{3}a_1 e^{4a_1} E_i(-4a_1)\right]}, \quad (19)$$

where $a_1 = -1 + \sqrt{0.5 + (Z_a + Z_b)}$,

$$E_{\frac{3}{2},0,0} = \frac{1}{R^2\left[\frac{1}{2a_3} - 4a_3 - 16a_3^2 - 4a_3(1+4a_3)^2 e^{4a_3} E_i(-4a_3)\right]} \times$$

$$\times 12\left\{\left(\frac{3a_3}{4} - Z^+\left(\frac{1}{2} + a_3 + 4a_3\right) - e^{4a_3} E_i(-4a_3)\right) * \left[\frac{1}{4}a_3 + a_3^2 - 4a_3^2 + Z^+(16a_3^3 + 8a_3^2 + a_3\right]\right\}, \quad (20)$$

where $a_3 = -3 + \sqrt{8.5 + (Z_a + Z_b)}$,

$$E_{\frac{5}{2},0,0} = \left\{Z\left(16a_5^3 + 28a_5^2 + 14a_5 + \frac{3}{2} + \frac{0{,}5}{a_5}\right) - \frac{9}{8} - 4a_5 - 27a_5^2 - 40a_5^3 - 16a_5^4 + e^{4a_5} E(-4a_5) \cdot \right.$$

$$\left. \cdot\left(64a_5^4 + 128a_5^3 + 80a_5^2 + 16a_5 + 1\right) - 64a_5^5 + 176a_5^4 - 144a_5^3 - 36a_5^2 - a_5 + 0{,}25\right\} / \left\{R^2\left[\frac{5}{4a_5^2} - 1 - \right.\right.$$

$$\left.\left. - \frac{28}{3}a_5 - \frac{56}{3}a_5^2 - \frac{32}{3}^3{}_5 - \frac{8}{3}e^{4a_5} E(-4a_5)(16a_5^4 + 32a_5^3 + 20a_5^2 + 40a_5 + 0.25)\right]\right\}, \quad (21)$$

where $a_3 = -5 + \sqrt{24.5 + (Z_a + Z_b)}$.

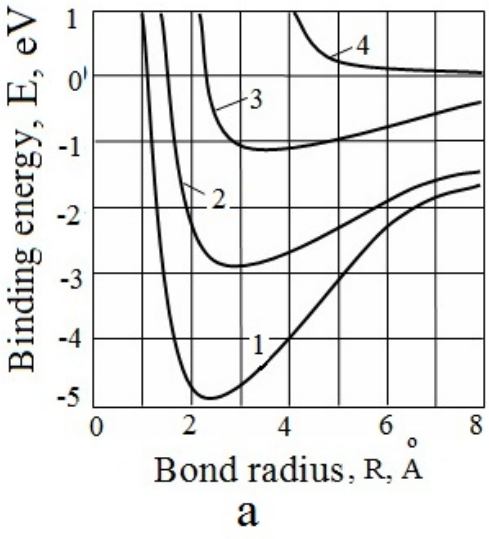

Fig. 6. The energies of chemical bonds of iron, depending on the interaction with free electrons (a): 1 — no interaction; 2 — with one electron; 3 — with two electrons; 4 — with three electrons.

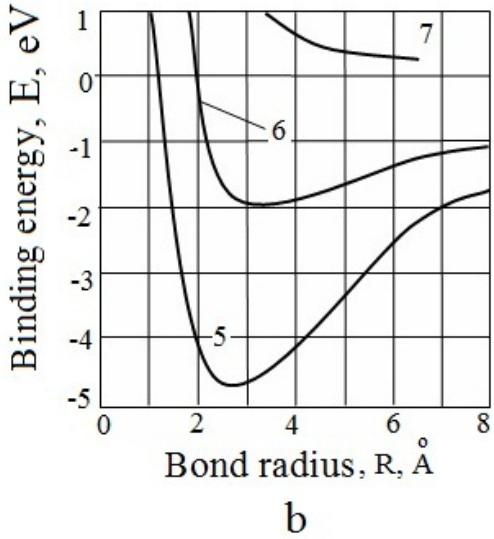

Fig. 7. The energies of the vibrating chemical bond of iron (5) without interaction with shock waves, with interaction with a single shock wave (6), with interaction with a superposition of several shock waves (7).

Since the solution of the Schrödinger equation with a vibrational potential is reduced to the solution of an equation with a Coulomb potential, then instead of the variable $a_1 = -1 + \sqrt{0.5 + (Z_a + Z_b)}$ we apply the variable in the wave function $a = -1 + \sqrt{0.5 + Z^+ + \frac{\gamma R_2}{4}}$, where γ — shock wave repetition rate (is a function of wavelength) [9, 10]. Let's calculate the bond energies for steel. The calculation of energies in different states is shown in Fig. 6, which shows the stability of chemical bonds when exposed to free electrons (Fig. 6). It can be seen from the figure that

with an increase in the number of free electrons, the chemical bond energy decreases (Fig. 6, curves 2 and 3), and when interacting with three electrons, the chemical bond is destroyed (Fig. 6, curve 4). Fig. 7 shows the interaction of vibrating chemical bonds (Fig. 7, curve 5) with single-amplitude shock waves (single wave (Fig. 7, curve 6) and with a continuous flow of shock waves (Fig. 7, curve 7). Analysis of Fig. 6 and 7 showed that free electrons and shock waves sharply decrease the energy of chemical bonds (Fig. 6, curves 2, 3 and Fig. 7, curve 6.) Such a change suggests that a phase transition is possible. shock waves lead to the destruction of chemical bonds (Fig. 6, curve 4 and Fig. 7, curve 7).

Conclusions

Thus, as a result of the conducted researches it is established:

Shock hypersonic shock waves and free electrons cause a decrease in the energy of chemical bonds, which leads to their decay in the micro- and nanosecond time intervals.

The movement of a microparticle in the thickness of the metal is possible only when the microparticle hits the front of the shock waves and when the scale factor of the microparticles is observed.

In a limited volume there is a decay of the crystalline state and its transition to the state of cold plasma, which is similar to the liquid state. This state is observed during the processes of decomposition and formation of chemical bonds.

Cooling of the plasma state occurs similarly to cooling of a liquid. In this case, if the cooling rate is greater than 105 deg / s, it is possible the formation of an amorphous state in the channel of the microparticle

Quantum-mechanical nanosecond processes are a special case of classical ideas about the theory of formation and transition of substances from one physical state to another.

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МОДЕЛЮВАННЯ УМОВ ФАЗОВИХ ПЕРЕТВОРЕНЬ В МІКРООБЛАСТЯХ МЕТАЛЕВИХ МАТЕРІАЛІВ ПРИ НАДГЛИБОКОМУ ПРОНИКАННІ МІКРОЧАСТИНОК

Баскевич О.С., Соболєв В.В., Середа Б.П., Середа Д.Б.

Реферат

Проведено моделювання стійкості хімічних зв'язків під дією ударних хвиль та вільних електронів в товщі металічних мішеней на основі квантово-механічних розрахунків. При цьому проведені аналітичні розв'язки рівняння Шредингера в еліпсоїдальних координатах та отримані залежності енергії хімічних зв'язків при різних умовах, які наглядно показують умови їх стійкості. Залежно від швидкості, температури, властивостей частинок та оброблюваної поверхні утворюються покриття та відбувається імплантація в поверхневий шар. При цьому можуть використовуватися потоки частинок, що мають широкий діапазон швидкостей — від десятків до декількох тисяч метрів в секунду та тисків до десятків ГПа. Для з'ясування умов надглибокого проникнення мікрочастинок у металеві перешкоди запропоновано ідею дестабілізації мікроструктури металевих матеріалів в обмежених мікрооб'ємах під час дії зовнішніх фізичних факторів. Рух мікрочастинки в металевій мішені вздовж каналу супроводжується високим тиском, впливом мікросекундних високоенергетичних ударних хвиль, що призводять до руйнування хімічних зв'язків. Рух мікрочастинки в товщині металу можливий тільки при попаданні мікрочастинки у фронт ударних хвиль і при дотриманні масштабного фактора мікрочастинок. В обмеженому обсязі відбувається розпад кристалічного стану і перехід його в стан холодної плазми, яка подібна до рідкого стану. Цей стан спостерігається протягом процесів розпаду та утворення хімічних зв'язків. Експериментально встановлені умови надглибокого проникання мікро-

частинок та показано, що агрегатний стан під час надглибокого проникання може змінюватися від плазмового до аморфного або кристалічного стану.

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