DOI:
UDC 621.7539.64
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MODELING THE INFLUENCE OF SHOCK WAVES ON THE STABILITY OF CHEMICAL LINKS DURING SUPER-DEEP PENETRATION OF MICROPARTICLES

In this paper, we simulate the effect of shock and Coulomb wave centers on the binding energy of metal targets with ultra-deep penetration of microparticles up to 500 microns in size. To calculate the chemical bond, a quantum-mechanical model of the influence of external factors on a separately selected chemical bond is developed. The calculations were carried out using the solution of the Schrödinger equation in ellipsoidal coordinates, which made it possible to reduce its solution to the Whittaker equation. As a result of the calculations, it was found that the influence of external factors leads to a decrease in the binding energy, and this in turn leads to a decrease in the viscosity of the target material during microsecond time intervals. This fact well explains the ultra-deep penetration of microparticles.
***Keywords**: mathematical modeling; super deep penetration; chemical bonding; metal viscosity.*

У цій роботі ми моделюємо вплив ударних та кулонівських хвильових центрів на енергію зв'язку металевих мішеней із надглибоким проникненням мікрочастинок розміром до 500 мкм. Для обчислення хімічного зв'язку розроблена квантово-механічна модель впливу зовнішніх факторів на окремо вибраний хімічний зв'язок. Розрахунки проводилися за допомогою рішення рівняння Шредінгера в еліпсоїдальних координатах, що дозволило звести його рішення до рівняння Віттакера. В результаті розрахунків було встановлено, що вплив зовнішніх факторів призводить до зниження енергії зв'язування, а це, в свою чергу, призводить до зниження в'язкості цільового матеріалу протягом мікросекундних часових інтервалів. Цей факт добре пояснює надглибоке проникнення мікрочастинок.
***Ключові слова**: математичне моделювання; супер глибоке проникнення; хімічне з'єднання; в'язкість металу.*

Formulation of the problem

Modeling of physicochemical processes caused by the interaction of microparticles flying at supersonic speeds with metal obstacles is fundamental and requires clarification of the conditions for superdeep penetration, and as a result of changes in the physicochemical properties of solids. In the study of amorphous materials, there are several approaches to the study of the structure and properties of liquids based on the use of laws and concepts of both gaseous and solid states. At first, based on the works of Van der Waals, the liquid was considered as a compacted gas and sought to apply modified equations of state of gases to it. Ya. I. Frenkel first drew attention to the fact that the structure and properties of liquids, at least far from the critical point, correspond more to a crystalline state than to a gaseous one.

Many scientists have created various theories of the liquid state, which ascribed the entire liquid or its individual regions to a quasicrystalline structure. In some theories of the liquid state, the concepts of gas and crystalline states are not used: a liquid is considered as a form of existence of matter, has a structure peculiar only to it [1,2]. The need for research in this direction has ripened due to the fundamental contradictions that have arisen in the physical interpretation of the detected phenomena of super deep penetration from the point of view of using not only the laws of mechanics, hydrodynamics, thermodynamics, etc. Numerous studies of super deep penetration into metal barriers do not give an answer due to what physical phenomena occur this effect. Microstructural changes, phase

transformations, synthesis of new elements and many other phenomena can be combined with one idea — a change in the energy of chemical bonds. Calculations of changes in the energies of chemical bonds using quantum mechanics will allow us to establish the influence of various physical factors on their stability.

Analysis of recent research and publications

The use of explosive alloying of the surface with microparticles of various compositions with highly concentrated energy flows is a promising method for increasing the physicochemical properties of the surface layer. When using this method, the phenomenon of super deep penetration of a substance (SGBP) occurs [3—5]. One of the most effective ways of restructuring the structure of metals is the effect of pulsed loads on them. Ultimate impulse loads during processing lead to the appearance of metastable structural complexes that cannot be unambiguously evaluated from the standpoint of static and long-term processes. The study of the phenomenon of SHPW showed that finely dispersed solid microparticles with a diameter of 1—200 μm, which move at a speed of 1—3 km / s, penetrate solid metal obstacles (targets) to depths of up to 10,000 their diameters, and the lengths of the filiform channels in steels reach 200 mm and even more. Calculations showed that the kinetic energy of the particle is enough to penetrate the target to a depth of no more than 6—10 diameters of the microparticle itself. Assessment of the energy necessary for the penetration of microparticles established an abnormal release of energy, which is $10^2...10^4$ times more than the kinetic energy of microparticles at the time of their impact on an obstacle [6—8]. Therefore, it is necessary to look for new mechanisms conducive to SHPV.

It is known that the structure of metals and alloys changes under the influence of shock waves formed during the collisions of a high-speed flow of micro particles, taking into account thermodynamic, hydrodynamic, and quantum-mechanical phenomena. The change in the structure of the target is local in nature, since close to 1% of the micro particles are involved in the GBSW phenomenon. Particles that penetrate the target form a system of partially healed channels. Channels have a complex structure. The established effect cannot be explained from the standpoint of modern thermodynamics, electrodynamics, hydrodynamics and mechanics, since the mechanisms of ultrafast interactions and chemical reactions must be described from the point of view of quantum mechanics. To explain the processes of superdeep penetration of microparticles into metals, it is necessary to consider penetration based on the known laws of physics. The main idea is to establish the influence of physical factors on the previously destabilized microstructure of materials. One of such destabilizing factors is the effect of shock waves and electric charges of ions on the chemical bond [9].

The purpose and objectives of research

The purpose of the work is to quantum-mechanical modeling of the influence of shock waves and Coulomb centers on the stability of chemical bonds inside metal targets with ultra-deep penetration of microparticles. When a microparticle moves in the volume of a metal target, a change in the energy of the chemical bond occurs under the influence of high pressure, the influence of ions surrounding the given chemical bond, the effect of shock waves, etc. To clarify these facts, it is necessary to construct quantum-mechanical models and solve the corresponding equations. The solution to the problem of the interaction of molecular systems with the structures of condensed matter is based on a quantum-mechanical model of the motion of an electron in the field of two Coulomb centers. The Born-Oppenheimer adiabatic approximation was used (the motion of electrons is considered separately from the motion of nuclei, the distances between which are considered fixed). To solve the two-center problem, a model equation is selected from the Schrödinger equation, the solution of which is obtained in an analytical form. Taking into account the boundary conditions made it possible to determine the quantum states of the valence electron in the field of two Coulomb centers. The obtained solution is approximate, since it is a solution of the shortened Schrödinger equation and, taking into account the perturbation, can be considered the first approximation to the exact solution. Using this solution, one can establish a qualitative picture of the processes occurring in a metal during ultra-deep penetration.

The Schrödinger equation for an electron located in the field of two Coulomb centers, which has the following form [10,11]:

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

where $U(r_a, r_b)$ — potential energy operator, Δ — Laplace operator in ellipsoidal coordinate systems, expressed using Lame coefficients [8]:

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

where r_a and r_b — distance from the electron to the centers a and b. We denote by R the distance between potential centers, then equations (1) in ellipsoidal coordinates will have the form:

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

where E — electron energy.

To solve equation (2), it is necessary that the variables in potential functions are separated, and the condition:

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

This class of separable functions includes functions of the type:

$$U(\lambda,\mu) = \frac{F_1(\lambda,\mu)}{\lambda-\mu} + \frac{F_2(\lambda,\mu)}{\lambda+\mu}. \tag{3}$$

The most common types of potentials include:

а) $U(\lambda,\mu) = \dfrac{2Z_a}{R(\lambda-\mu)} + \dfrac{2Z_b}{R(\lambda+\mu)}$ — potential of the Coulomb interaction of an electron with two charges Z_a and Z_b;

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

в) any superposition of previous potentials.

The listed potentials can serve as a test for approximate calculation methods. For the Coulomb potential, we present the solution $\Psi = X(\lambda)Y(\mu)\Phi(\varphi)$ equation (2), which is divided into three ordinary differential equations of the second order [8]:

$$\left[\frac{\partial^2}{\partial\varphi^2} + \Lambda^2\right]\Phi(\varphi) = 0; \tag{4}$$

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

$$\left[\frac{\partial}{\partial\lambda}(\lambda^2-1)\frac{\partial}{\partial\lambda} - \frac{\Lambda^2}{\lambda^2-1} + \lambda^2\varepsilon + \lambda Z^+ - A\right]X(\lambda) = 0, \tag{6}$$

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

$\varepsilon = \dfrac{ER^2}{2}$; $Z^{(\pm)} = (Z_a \pm Z_b)R$; $A(R)$ — separation constant.

If $Z_b = 0$, then the equations for the functions $X(\lambda)$ and $Y(\mu)$ exactly coincide, and the solution of the hydrogen-like problem has the form:

$$\Psi = \mathrm{X}(\lambda)\mathrm{Y}(\mu)\cdot\Phi(\varphi) \tag{7}$$

is the Whittaker equation whose solutions are quantum numbers: $k = \dfrac{1}{2}$, $\Lambda = 0$, $n = 0$. We will calculate some states using the formula with allowance for perturbation [8]:

$$E_{k,\Lambda,n} = \frac{\left\langle \Psi_{k,\Lambda,n} \middle| H_0 + W_{k,\Lambda,n} \middle| \Psi^*_{k,\Lambda,n} \right\rangle}{\left\langle \Psi_{k,\Lambda,n} \middle| \Psi^*_{k,\Lambda,n} \right\rangle}, \tag{8}$$

where H_0 — hamiltonian of a one-center problem, $W_{k,\Lambda,n}$ — indignation to the two-center problem:

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

a $\Psi_{k,\Lambda,n}$, $\Psi^*_{k,\Lambda,n}$ — conjugate wave functions that are solutions of the Whittaker equation [8,9]:

$$E_{\frac{1}{2},0,0} = \frac{4\left[\frac{1}{2}(a - Z^+) + e^{4a}E_i(-4a)(a^2 - aZ^+ - \frac{1}{4}a\right]}{R^2\left[\frac{1}{2a} - \frac{4}{3}ae^{4a}E_i(-4a)\right]}, \tag{9}$$

where $a = -1 + \sqrt{0.5 + Z^+}$ If a chemical bond has more than one electron, then electron-electron interactions must be taken into account. We calculate electron-electron interactions using the Slater determinant [12]:

$$\Psi_{\det} = \begin{vmatrix} u_1(1) & u_2(1) \\ u_2(2) & u_2(2) \end{vmatrix}, \tag{10}$$

here $u_1 = \alpha\varphi^{(\mathrm{mod})}$; $u_2 = \beta\varphi^{(\mathrm{mod})}$, т.е. as the basis, the model two-center field functions used are used H_2^+, and $\frac{1}{r_{1,2}}$ we represent it in the form of a Neumann expansion:

$$W_1(\lambda,\mu,\varphi,Z) = \frac{2Z}{R}\sum_{p=0}^{\infty}\sum_{m=-p}^{p}(-1)^m(2p+1)\left[\frac{(p-|m|)!}{(p+|m|)!}\right]P_p^{|m|}(\lambda_<)Q_p^{|m|}(\lambda_>)P_p^{|m|}(\mu_3)Q_p^{|m|}(\mu_3)e^{im(\varphi-\varphi_3)}, \tag{11}$$

where Z — electron charge, $\lambda_3 = \frac{R_2 + R_3}{R_1}$; $\mu_3 = \frac{R_2 - R_3}{R_1}$; $\lambda_{\substack{< \\ >}}$ — larger or smaller of; $P_p^{|m|}(\lambda_<)$ and $Q_p^{|m|}(\lambda_>)$ associated functions of Legendre I and II kind. Then the electron — electron interaction energy will be [10,11]:

$$E_{(e-e)\frac{1}{2},0,0} = \left\langle \psi_{\det} \middle| \frac{1}{r_{1,2}} \middle| \psi^*_{\det} \right\rangle = \frac{4}{R\left[\frac{1}{2a} - \frac{4}{3}a\cdot e^{4a}\cdot E_i(-4a)\right]^2}\cdot$$

$$\cdot\left[\left(\frac{3}{40a^2} + \frac{1}{20a^2}\right)\cdot(C + \ln 2a) + e^{8a}E_i^2(-8a)\left(\frac{3}{40a^2} + \frac{11}{20a} + \frac{7}{5} + \frac{8a}{15}\right) + e^{4a}E_i^2(-8a)\frac{4a^2}{15} + \right.$$

$$\left. + e^{4a}E_i^2(-4a)\left(-\frac{3}{20a^2} + \frac{1}{2a} - \frac{1}{5}\right) + \frac{1}{8a} - \frac{1}{10}\right], \tag{12}$$

and indignation to the two-center problem:

$$\Delta W_{\frac{1}{2},0,0} = \left(C + Z^+\right)\left[\left[\frac{1}{a} + \frac{2}{3} + \left(4 + \frac{8a}{3}\right)e^{4a}E_i(-4a)\right] - \frac{\Lambda^2 - 1}{4}\left[\frac{11}{6} + \frac{2a}{3} + \left(2 + 8a + \frac{8a^2}{3}\right)e^{4a}E_i(-4a)\right] - \right.$$

$$\left. - \frac{1}{6} - \frac{4}{15}a^2e^{4a}E_i(-4a)\right]\cdot\frac{1}{R\left[\frac{1}{2a} - \frac{4}{3}a\cdot e^{4a}\cdot E_i(-4a)\right]^2}\cdot \tag{13}$$

Considering the fact that elementary acts of chemical reactions involve the interaction of chemical bonds with positive and negative charges, we will consider these charges as the influence of the third Coulomb center (Z_3) on a separately selected chemical bond. Let us represent the third Cou-

lomb center as a certain perturbation that acts on a chemical bond. Given these assumptions, we choose two Coulomb centers as the basis, and the perturbation caused by the influence of the third center is presented in the form of a Neumann expansion, taking into account the fact that, then $Z = Z_3$, the energy of the system of three particles, taking into account the influence of the third center, will be:

$$E_3(R_1,R_2,R_3) = \frac{\left\langle \Psi \left| H + W_{\frac{1}{2},0,0} \right| \Psi^* \right\rangle}{\left\langle \Psi \middle| \Psi^* \right\rangle} = E_0(R_1) +$$

$$+ \sum_{i=1}^{N} \frac{4aZ_i}{R_i\left[\frac{1}{2a} - \frac{4a}{3}e^{4a}E_i(-4a)\right]} \left\{ Q_0^0(\lambda_3)\left[\frac{2}{3}e^{4a}E_i(-4a) - \frac{1}{4a^2}\right] - \frac{1}{8a^2 e^{2a(\lambda_3-1)}}\left[P_2(\lambda_3)P_2(\mu_3) - 1\right]\cdot \right.$$

$$\cdot \left[e^{2a(\lambda_3+1)}E_i(-2a(\lambda_3+1) - e^{2a(\lambda_3-1)}E_i(-2a(\lambda_3-1))\right] - Q_2(\lambda_3)P(\mu_3)\left[\frac{2}{3}e^{4a}E_i(-4a) + \right.$$

$$+ (\lambda_3^2-1)e^{2a(\lambda_3-1)}E_i(-2a(\lambda_3-1)) + e^{-2a(\lambda_3-1)}\left(\frac{1}{2a} - \frac{1}{4a^2} - \frac{\lambda_3}{2a}\right) + \frac{1}{4a^2}\Bigg] +$$

$$+ Q_0(\lambda_3)P_2(\lambda_3)P_2(\mu_3)\left[(\lambda_3^2-1)e^{2a(\lambda_3+1)}E_i(-2a(\lambda_3+1)) - \left(\frac{1}{2a} - \frac{1}{4a^2} - \frac{\lambda_3}{2a}\right)\right]e^{-2a(\lambda_3-1)} \cdot$$

$$\left. \cdot P_2(\lambda_3)P_2(\mu_3)\cdot\left[e^{4a}E_i(\lambda_3+1)E_i(-2a(\lambda_3+1)) + \frac{1}{2a}e^{-2a(\lambda_3-1)}\right]\right\}. \qquad (14)$$

We will consider the shock wave as the influence of the potential $U = \gamma(\lambda^2 - \mu^2)$ to a chemical bond. Since this potential belongs to the class of separable potentials, we bring this problem to the solution of the two-center problem.

The Schrödinger equation for this problem can be written as:

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

$$+ 2\left[E - V_{кул} + V_A\right]\Psi = 0, \qquad (15)$$

where $V_{кул} = \frac{2Z_a}{R(\lambda-\mu)} + \frac{2Z_b}{R(\lambda+\mu)}$, $V_A = \gamma\left((\lambda^2+\mu^2)(R_1^2+R_2^2) + 2\lambda(R_1R_2^2 + R_1^2R_2) + 2R_1R_2\right)$,

R_1 and R_2 the amplitudes of the displacements of atoms 1 and 2. Now we can separate the variables:

$$\left[\frac{\partial^2}{\partial\varphi^2} + \Lambda^2\right]\Phi(\varphi) = 0, \qquad (16)$$

$$\left[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \frac{\Lambda^2}{1-\mu^2} - \left(\frac{R^2E}{2} + \frac{R^2R_1^3}{\gamma}\right)\mu^2 + \frac{R^2\gamma}{2}\mu^4 - A\right]\mathrm{Y}(\mu) = 0, \qquad (17)$$

$$\left[\frac{\partial}{\partial\lambda}(\lambda^2-1)\frac{\partial}{\partial\lambda} - \frac{\Lambda^2}{\lambda^2-1} - \left(\frac{R^2E}{2} + \frac{R^2R_1^3}{\gamma}\right)\mu^2 + \frac{R^2\gamma}{2}\mu^4 - A\right]\mathrm{X}(\lambda) = 0, \qquad (18)$$

for $k = 1/2$

$$a = -1 + \sqrt{0.5 + Z^+ + \left[2(R_1R_2^2 - R_1^2R_2) + R_1^2R_2^2\right]\frac{\gamma R_2}{4R_1R_2}}. \qquad (19)$$

For identical atoms, the last (19) reduces to $a = -1 + \sqrt{0.5 + Z^{+} + \frac{\gamma R_2}{4}}$, where γ — shock wave repetition rate (a function of wavelength).

It follows that, this solution of the Schrödinger equation under the influence of a shock wave can be reduced to the solution of the two-center problem, and the influence of the third center as an additive $E_3(R_1, R_2, R_3)$ to the sum of equations (9), (12) and (13) taking into account (8) and (19). The calculations of the chemical bond energy as the sum of perturbations of electric charges and shock waves on the Fe-Fe bond energy are shown in Fig. 1, 2.

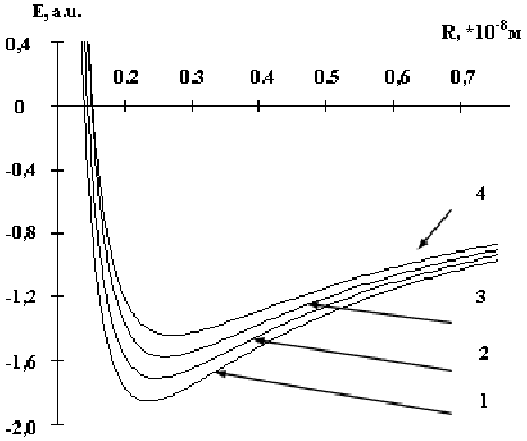

Fig. 1. The influence of a positive charge ($Z = +2$) on the Fe-Fe chemical bond if its normal distance from it is: 1 — $1 \cdot 10^{-8}$ m; 2 — $0{,}8 \cdot 10^{-8}$ m; 3 — $0{,}4 \cdot 10^{-8}$ m; 4 — $0{,}2 \cdot 10^{-8}$ m

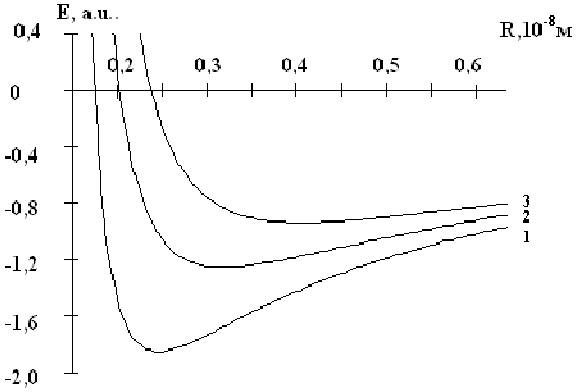

Fig. 2. Joint influence of shock waves and positive charge ($Z = +2$) on the chemical bond: 1 — chemical bond of Fe-Fe; 2 — chemical bond Fe-Fe + shock wave and Z at a normal distance of $0{,}4 \cdot 10^{8}$ m; 3 — chemical bond of Fe-Fe + shock wave and Z at a normal distance of $0{,}2 \cdot 10^{-8}$ m

It can be seen from the figures that the influence of positively charged ions and shock waves on chemical bonds significantly reduces their energy, and, accordingly, the viscosity coefficient of the metal in a limited space, namely, in the region of microparticle motion inside the metal target. It should be noted that a decrease in the viscosity coefficient occurs in a short period of time, less than 10^{-5} s. his is explained by the difference in the time of destruction of the chemical bond (10^{-12} c) и nd its relaxation (10^{-5} c). Thus, the assumption of a decrease in the viscosity coefficient made in [6—9] was qualitatively confirmed as a result of quantum-mechanical calculations.

Conclusions

Thus, in the framework of the proposed quantum-mechanical model on the influence of shock waves and the third Coulomb center on a separately selected chemical bond, it was established:

– shock waves and positively charged Coulomb centers have a destructive effect on the chemical bond;

– destabilization of chemical bonds by shock waves is due to interaction with valence electrons;

– destabilization of chemical bonds by Coulomb charges occurs both due to the effect on valence electrons and due to Coulomb interaction with Coulomb centers of chemical bonds;

– the decrease in the binding energy is spasmodic and lasts in the period of passage of the shock wave in the region of motion of the microparticle and entails a decrease in the viscosity coefficient.

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МОДЕЛЮВАННЯ ВПЛИВУ УДАРНИХ ХВИЛЬ НА СТІЙКІСТЬ ХІМІЧНИХ ЗВ'ЯЗКІВ ПРИ НАДГЛИБОКОМУ ПРОНИКАННІ МІКРОЧАСТИНОК

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Реферат

Дана робота присвячена моделюванню впливу ударних хвиль і кулонівських центрів на енергію зв'язку атомів металевих мішеней при надглибокому проникненні мікрочастинок, що летять з надзвуковими швидкостями. Процеси при надглибокому проникненні мають фундаментальний характер і потребують пояснення фізико-хімічних властивостей твердих тіл. Необхідність досліджень в даному напрямку назріла в зв'язку з принципіальними протиріччями при фізичній інтерпретації виявленими явищами надглибокого проникання з точки зору використання класичних закономірностей механіки, гідродинаміки, термодинаміки та ін.

Під час руху мікрочастинки в об'ємі металевої мішені відбувається зміна енергії хімічного зв'язку під дією високого тиску, впливу іонів, що оточують цей хімічний зв'язок, під дією ударних хвиль і так далі. Для з'ясування цих фактів побудована квантово-механічна модель взаємодії хімічних з'вязків і розв'язані відповідні рівняння. В основу розв'язку задачі про взаємодію молекулярних систем із структурами конденсованих середовищ покладена квантово-механічна модель руху електрона в полі двох кулонівських центрів. Використовували адіабатичне наближення Борна-Опенгеймера (рух електронів розглядається окремо від руху ядер, відстані між якими вважаються вважали фіксованими). Під час розв'язку двоцентрової задачі з рівняння Шредінгера виділено модельне рівняння, а розв'язок якого отримано в аналітичному виді. Врахування граничних умов дозволило визначити квантові стани валентного електрона в полі двох кулонівських центрів.

Отримане рішення є наближеним, оскільки воно є розв'язком скороченого рівняння Шредінгера і з врахуванням збурення може вважатися першим наближенням до точного розв'язку. За допомогою такого розв'язку можна встановити якісну картину процесів, що відбуваються в металі при надглибокому проникненні.

Таким чином, у рамках запропонованої квантово-механічної моделі по моделюванню впливу ударних хвиль і третього кулонівського центру на окремо вибраний хімічний зв'язок встановлено:

– ударні хвилі і позитивно заряджені кулонівські центри чинять руйнівну дію на хімічний зв'язок;

– дестабілізація хімічних зв'язків ударними хвилями здійснюється за рахунок взаємодії з валентними електронами;

– дестабілізація хімічних зв'язків кулонівськими зарядами відбувається як за рахунок впливу на валентні електрони, так і за рахунок кулонівської взаємодії з кулонівськими центрами хімічного зв'язку;

– зменшення енергії зв'язку стрибкоподібне і триває в проміжку часу проходження ударної хвилі в області руху мікрочастки і спричиняє зниження коефіцієнту в'язкості.

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