

Interrelation Between The Reaction And Diffusion During Gradient Structure Formation Of Surface Layer Under Particle Beam Action

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Abstract— The simple models are discussed for new phase formation in surface layer during ion implantation. The model of new phase formation for same conditions taking into account the finiteness of relaxation time is suggested. The parameters containing in the model were evaluated using literature data. The stresses and strains in diffusion zone are calculated. It was shown that the concentration distribution and stresses values depend on the relation between time scales of various physical processes.

Keywords— Ion Implantation, surface layer modification, finiteness of relaxation time, phases formation.

I. INTRODUCTION

The particle beam action on the materials leads to surface activation and surface diffusion structure change [1, 2]. It connects not only with mass transfer process, but also with chemical reactions occurring in surface layer. The diffusion immediately takes a participation in chemical reactions. Complex heterogeneous structure of materials and surface activation phenomena allow speak on other mass transfer mechanisms no corresponding to Fick's law. It can effect on chemical reaction course during ion implantation. Ion implantation assists the reaction between two different atomic species implanted in the inert matrix [3]. The conditions of reactions implementation are irreversible, and their kinetics is not obvious. Especially it relates to the intermetallic systems [4-6], when the chemical reactions have own features. Intermetallides are the compounds between metals. Corresponding reactions are called as intermetallic ones. At the conditions of ion implantation, the reaction initiation could possible when temperature is not very high, because the molecules and atoms in surface layer are activated by external action [7,8].

Usually, the Monte-Carlo and molecular dynamics methods are used for particle redistribution during plasma treatment or ion implantation. To describe irreversible processes there are many ways in science, which are used depending on object of specific investigation. For example, there are different media models with internal parameters and models of comprehensive thermodynamics which make up to describe irreversible phenomena associated with the formation of material properties during their surface treatment and at the condition of mechanical loading. Taking into account the remixing of the particles in molecular level, we could use for chemical conversion description the traditional laws of chemical kinetics and diffusion-kinetic models. Examples of enough complex similar models one can find in [9,10]. In contrast to these papers, here we will try reflecting the irreversible conditions for the reactions. The work is devoted to chemical reaction description during ion

implantation taking into account the finiteness of relaxation time for diffusion flux in isothermal approximation. Firstly we stop on the simple problems in classical diffusion approximation (Sect.1). Then we formulate the problem on new phase formation in surface layer during particle beam action for irreversible conditions. We will show the difference between reaction dynamics accompanying reversible diffusion and irreversible one using simple models (Sect.2). We describe the diffusion and reaction zone change when the source type varies (Sect.1 and 2). Finally we demonstrate the stresses and strains evolution in treated surface layer with constant and changing properties (Sect.3) varying the radiation dose.

II. ANALYSIS OF THE SIMPLEST PROBLEMS

A. Diffusion and Reaction at Equilibrium Conditions

We can come to irreversible process description step by step starting from simple problems. When particle beam acts on the material surface, chemical reactions are absent, and the particle rate is uniform along it, we can restrict the problem by one-dimensional formulation (Fig. 1)

$$\begin{aligned} \frac{\partial y_A}{\partial t} &= D_A \frac{\partial^2 y_A}{\partial x^2} \\ x = 0 : \mathbf{J}_A &= -D_A \frac{\partial y_A}{\partial x} = q_m \\ x \rightarrow \infty : \mathbf{J}_A &= 0 \\ t = 0 : y_A &= 0, \end{aligned} \quad (1)$$

where y_A is mole concentration of the diffusing particles, t is the time, x is the space coordinate in the direction of particle beam action, D_A - is diffusion coefficient, q_m - is particle beam density. This problem has exact solution. It is contained in many reference books.

We could find the solution using any classical methods and it has the form:

$$y_A = \frac{q_m}{\sqrt{D_A}} \sqrt{\frac{t}{\pi}} \left[\operatorname{erfc} \left(\frac{x}{\sqrt{4D_A t}} \right) - \frac{x}{\sqrt{D_A}} \left(\frac{x}{\sqrt{2D_A t}} \right) \right] \quad (2)$$

That is the particle concentration distribution along the coordinate perpendicular to treated surface is monotonic singularity-free function. It is shown on the Fig.2.

Concentration y_A changes in the point $x = 0$ as \sqrt{t} .

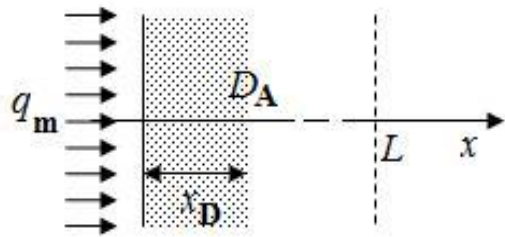


Fig. 1

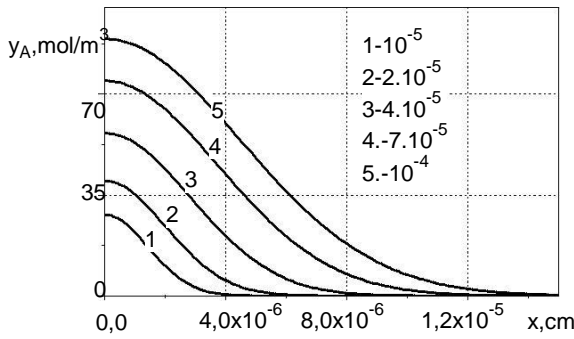
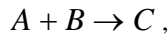


Fig. 2

$q_m = 1.5 \text{ mol} / (\text{m}^2 \text{ s})$; $D_A = 10^{-7} \text{ cm}^2/\text{s}$ When the chemical reaction is possible in surface layer, the particles are consumed for new phase formation. Assume the chemical reaction occurs by the simplest scheme



where the letter B corresponds to the substance contained in initial specimen and C – to the reaction product.

The additional term appears in this case in diffusion equation, and we come to the second simple problem

$$\frac{\partial y_A}{\partial t} = D \frac{\partial^2 y_A}{\partial x^2} - k y_A$$

$$x = 0 : \mathbf{J}_A = -D \frac{\partial y_A}{\partial x} = q_m$$

$$x \rightarrow \infty : \mathbf{J}_A = 0$$

$$t = 0 : y_A = 0$$

The exact solution of this problem has the form:

$$y_A = \frac{q_m}{2\sqrt{Dk}} \left[\exp\left(-x\sqrt{\frac{k}{D}}\right) \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}} - \sqrt{k}t\right) - \frac{q_m}{2\sqrt{Dk}} \left[\exp\left(-x\sqrt{\frac{k}{D}}\right) \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}} + \sqrt{k}t\right) \right] \right] \quad (3)$$

The previous formula (2) is limit of this solution for $k_A \rightarrow 0$.

Because the entered particles are consumed for new phase formation, the diffusion concentration decreases in the volume.

The product concentration changes by equation

$$\frac{\partial y_C}{\partial t} = \omega, \quad \omega = k y$$

For simple reaction of first order we can evaluate the product concentration. Using Laplace integral transform method, we shall find

$$y_C = \frac{q_m}{2\sqrt{Dk}} k_C \left[\exp\left(-x\sqrt{\frac{k}{D}}\right) \int_0^t (t-\tau) \operatorname{erfc}\left(\frac{x}{2\sqrt{D\tau}} - \sqrt{k\tau}\right) d\tau \right] - \frac{q_m}{2\sqrt{Dk}} k_C \left[\exp\left(-x\sqrt{\frac{k}{D}}\right) \int_0^t (t-\tau) \operatorname{erfc}\left(\frac{x}{2\sqrt{D\tau}} + \sqrt{k\tau}\right) d\tau \right] \quad (4)$$

The reagent and product concentrations behavior with time is shown on the Fig.3, a, b at the point $x = 0$. since the substance A is consumed for new phase formation, the reagent concentration grows slowly.

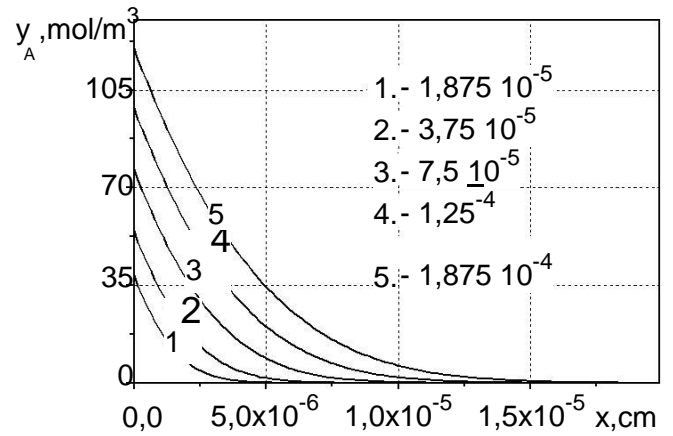


Fig.3 (a)

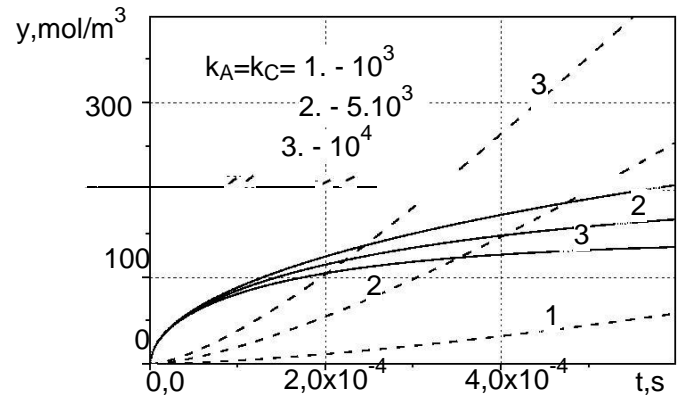


Fig.3 (b)

Fig.3. The dynamics of concentration change. $q_m = 2,5 \text{ mol} / (\text{m}^2 \text{ s})$; $D_A = 10^{-7} \text{ cm}^2/\text{s}$; (a) $k_C = k_A = 10^3 \text{ 1/s}$; (b) Solid line - y_A ; dotted line y_C .

B. Diffusion and Reaction for Mass Flux Depending on Time

At the condition of surface treatment the mass flux changes in time by various ways. It depends on technology and in significant extent determines the irreversible conditions for diffusion and reactions.

For example, we assume in second problem, that

$$\mathbf{J}_A = -D_A \frac{\partial y_A}{\partial x} = q_m \exp(-At). \quad (5)$$

Then, the solution of new problem (it can be found by Laplace's integral transform method, for example) gets the form

$$y_A = \frac{q_m}{\sqrt{D_A}} \int_0^t \frac{A \exp(-A(t-\tau)) - k_A \exp(-k_A(t-\tau))}{A - k_A} \left[\frac{1}{\sqrt{\pi\tau}} \exp\left(-\frac{x^2}{4D_A\tau} + k_A\tau\right) \right] d\tau + \frac{\sqrt{k_A}}{2} \left[\exp\left(-x\sqrt{\frac{k_A}{D_A}}\right) \operatorname{erfc}\left(\frac{x}{2\sqrt{D_A\tau}} - \sqrt{k_A\tau}\right) - \exp\left(-x\sqrt{\frac{k_A}{D_A}}\right) \operatorname{erfc}\left(\frac{x}{2\sqrt{D_A\tau}} + \sqrt{k_A\tau}\right) \right] d\tau$$

In this case the concentration distribution depends essential on relations between different physical scales analogous to diffusion rate, reaction rate, and reactant intake. Because the mass flux diminishes quickly with time, it is indispensable to large reaction rate constant to product appearance would appreciably.

The form of ions source could be different in time. For example, we can write

$$\mathbf{J}_A = -D_A \frac{\partial y_A}{\partial x} = q_m (\alpha + \beta t) \text{ or}$$

$$\mathbf{J}_A = -D_A \frac{\partial y_A}{\partial x} = q_m (1 - \cos(\gamma t)) \text{ or } \mathbf{J}_A = -D_A \frac{\partial y_A}{\partial x} = \frac{q_m}{1 + \delta t}.$$

For these cases, analytical solutions are not possible or are obtained very cumbersome and do not handy for using. Hence, we will use numerical methods. All problems which will describe below were solved using implicit difference scheme and double-sweep method.

The distributions of reagent (diffusion) and product concentrations depend on source form. We can compare the curves presented on the Fig.4. The maximum position in the

curve 3 connects with diminishing of \mathbf{J}_A in time and new phase formation. Note, that it is not possible to recognize the curves 1 and 3 for product concentration for constant and periodic particle beam, because the diffusion leads to particle redistribution.

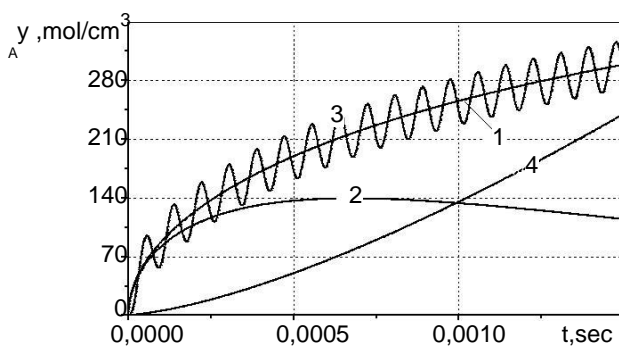


Fig.4 (a)

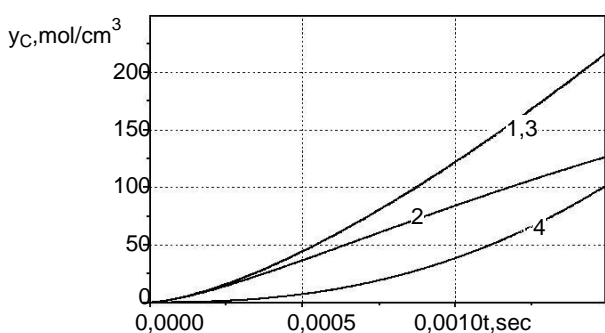


Fig.4 (b)

Fig.4. Reagent and product concentration in time for different types of particle beams:

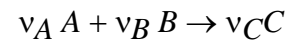
- (1). q_m (2). $-q \exp(-At)$; $A=10^3$;
- (3). $qm(1 - \cos(\gamma t))$; $\gamma=7.5 \cdot 10^4$ (4). $-qm(\alpha + \beta t)$;
- $\alpha=10^{-2}$; $\beta=7.5 \cdot 10^2$. $q_m = 2.5 \text{ mol} / (\text{m}^2 \text{ s})$;
- $k_C = k_A = 10^3 \text{ 1/s}$.

For all earlier figures $y_B \approx \text{const}$, that is correct when $y_C \ll y_B$; $y_A \ll y_B$, that is observation time is small, or mass source intensity is low. Go to more rigorous problem formulation.

III. SURFACE LAYER MODIFICATION MODEL FOR IRREVERSIBLE CONDITIONS

A. Total Problem Formulation for Irreversible Conditions

We have the body, the surface of which is treated uniformly by particle beam with given intensity and given time structure. In treated zone the chemical reaction of type



can proceed, where ν_A, ν_B, ν_C are stoichiometric coefficients.

The implanted particles concentration can change in surface layer due to diffusion and reaction. The balance equation reproduces

$$\frac{\partial y_A}{\partial t} = -\frac{\partial \mathbf{J}_A}{\partial x} + \omega_A \quad (6)$$

The implantation process is irreversible, the specific time is very small, and hence we could use for diffusion flux the generalized equation

$$\mathbf{J}_A = -D_A \frac{\partial y_A}{\partial x} - t_A \frac{\partial \mathbf{J}_A}{\partial t} \quad (7)$$

The boundary and initial conditions take the form

$$x = 0 : \mathbf{J}_A = q_m f(t) \quad (8)$$

$$x \rightarrow \infty : y_A = 0 \text{ or } \mathbf{J}_A = 0 \quad (9)$$

$$t = 0 : y_A = 0 ; \frac{\partial \mathbf{J}_A}{\partial t} = 0 \quad (10)$$

Here: y_A - concentration of A-substance (implanted particles, mol/m^3), \mathbf{J}_A - is the substance flux ($\text{mol}/(\text{m}^2 \text{ sec})$); $\omega_A = -k_A y_A$

$y_A = -\omega y_A$ (1/sec); $k_A = \nu_A k$ - rate constant for chemical reaction, t_A - is relaxation time; D_A - is diffusion coefficient, (m^2/sec).

From equation (7) we have

$$\frac{\partial \mathbf{J}_A}{\partial z} = -D_A \frac{\partial^2 y_A}{\partial z^2} - t_A \frac{\partial \mathbf{J}_A}{\partial t},$$

and from (6)

$$\frac{\partial^2 y_A}{\partial t^2} = -\frac{\partial \mathbf{J}_A}{\partial z} + \frac{\partial \omega}{\partial t}.$$

Hence

$$\frac{\partial \mathbf{J}_A}{\partial z} = -D_A \frac{\partial^2 y_A}{\partial z^2} + t_A \left(\frac{\partial^2 y_A}{\partial t^2} - \frac{\partial \omega_A}{\partial t} \right)$$

Using the flux derivative from (6), we shall find

$$t_A \left(\frac{\partial^2 y_A}{\partial t^2} - \frac{\partial \omega_A}{\partial t} \right) + \frac{\partial y_A}{\partial t} = D_A \frac{\partial^2 y_A}{\partial z^2} + \omega_A \quad (11)$$

In general case, correspondingly to mass action law, the chemical reaction rate could be written as $\omega = k y_A^{\nu_A} y_B^{\nu_B}$, where y_B - is concentration of basic substance. But, in many situations we can assume. Then the substance is in excess supply and its concentration does not change practically. Then

$$\omega = k' y_A.$$

This linearization was allowed above using analytical methods.

To complete the problem formulation, we add to the problem (11), (9) and (10) the kinetic equation for reaction product:

$$\frac{\partial y_C}{\partial t} = \omega_c,$$

where $\omega_C = k_C \omega = \nu_C k \omega$, and equation for basic material (because the moles are not conserved during the reaction). When the species B is mobile and could diffuse also in the mixture from three component $A + B + C$, we could assume that

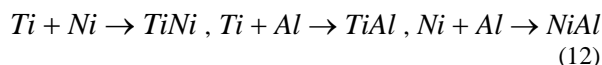
relaxation time for this element t_B is not equal to t_A . The mole number is not conserved in the reaction. Hence, we obtain the second equation for diffusion flux

$$\mathbf{J}_B = -D_B \frac{\partial y_B}{\partial z} - t_B \frac{\partial \mathbf{J}_B}{\partial t}$$

and second diffusion equation

$$t \left(\frac{\partial^2 y_B}{\partial t^2} - \frac{\partial \omega_B}{\partial t} \right) + \frac{\partial y_B}{\partial t} = D_B \frac{\partial^2 y_B}{\partial x^2} + \omega_B$$

For example, for reactions (which are observed during ion implantation [7])



absolute values of stoichiometric coefficients equal to unity:

$$v_A = v_B = v_C = 1,$$

we have

$$\omega = ky_A y_B,$$

and

$$\frac{\partial y_C}{\partial t} = ky_A y_B. \quad (13)$$

The diffusion equations take the form

$$t_A \frac{\partial^2 y_A}{\partial t^2} + (1 + t_A k y_B) \frac{\partial y_A}{\partial t} = D_A \frac{\partial^2 y_A}{\partial x^2} - ky_A \left[y_B + t_A \frac{\partial y_B}{\partial t} \right] \quad (14)$$

$$t_B \frac{\partial^2 y_B}{\partial t^2} + (1 + t_B k y_A) \frac{\partial y_B}{\partial t} = D_B \frac{\partial^2 y_B}{\partial x^2} - ky_B \left[y_A + t_B \frac{\partial y_A}{\partial t} \right] \quad (15)$$

Assuming $f(t) = \exp(-At)$, from (7) and (8) we shall find

$$q_m (1 - t_A A) \exp(-At) = -D_A \frac{\partial y_A}{\partial x}, \quad x = 0. \quad (16)$$

At this point $\mathbf{J}_B = 0$

The last boundary and initial conditions:

$$x \rightarrow \infty: y_A = 0, y_B = 0 \text{ or } \mathbf{J}_A = 0; \mathbf{J}_B = 0 \quad (17)$$

$$t = 0: y_A = 0; \frac{\partial \mathbf{J}_A}{\partial t} = 0; y_B = y_{B0}; \frac{\partial \mathbf{J}_B}{\partial t} = 0; y_C = 0. \quad (18)$$

The problem (13)-(18) was solved numerically.

The implicit difference scheme for diffusion equations was used.

B. Parameters Evaluation

Firstly we evaluate some parameters. According to

periodic table, for the Ti-Ni -system we have $m_A = 48$;

$$m_B = 59; m_C = m_A + m_B = 107 \text{ g/mol.}$$

We can determine partial densities of species

$$\rho_i = y_i m_i, \quad i = A, B, C$$

and calculate density change

$$\rho = \rho_A + \rho_B + \rho_C$$

during implantation accompanied by chemical reaction.

Assuming $\rho_B = 8.9 \text{ g/cm}^3$, we shall find $y_{B0} \approx 0.151 \text{ mol/cm}^3$.

Impulse source could be characterized by impulse duration $t_i =$

$$(2 \div 4) \cdot 10^{-4} \text{ sec}; q_m = (0.1 \div 2) \cdot 10^{-8}$$

$\text{mol}/(\text{cm}^2 \text{ sec})$. Relaxation time depends on material structure, but

for majority of substances it is unknown. It is interested for

investigation the parameters region, when various physical

processes could effect on each other. In this model there are

several specific times. Relaxation times t_A, t_B , impulse duration

t_i , chemical reaction time t_{ch} , specific diffusion time tD

different for substances A and B. The correlations between these

times will determine the concentration distributions.

Analysis of dimensionality allows writing $t_{ch} = y_{B0}/k$.

$$\text{Taking } k = k_0 \exp\left(-\frac{E_R}{RT}\right) \quad / \quad ; k_0 = 2 \cdot 10^{16} \text{ 1/sec;}$$

$$E_R = 1.181 \cdot 10^5 \text{ J/mol} \quad [7], \quad \text{we find}$$

$$t_{ch} = 0.135; 1.1 \cdot 10^{-4}; 9.7 \cdot 10^{-7} \text{ Sec for temperature}$$

$$T = 400, 500, 600 \text{ K.}$$

The reaction constant could differ from pure thermo dynamical evaluation due to activation phenomena [8], but it changes in wide limits when the temperature varies.

Diffusion coefficients depend on temperature in accordance with Arrhenius's law also

$$D_i = D_{i0} \exp\left(-\frac{E_{Di}}{RT}\right), \quad k = A, B.$$

It is not difficult to find in literature the data concerning self-diffusion. The diffusion coefficients in complex media are proportional to self-diffusion coefficients. Diffusion data depend essential on structure material, impurity presence and conditions of measurement

Since [11] for Nickel and for Titanium we have

$$D_{Ni} = 1.9 \exp\left[-\frac{279700}{RT}\right] \text{ and } D_{Ti} = 1.0 \exp\left[-\frac{251200}{RT} + 3.58 \cdot 10^{-4} \frac{130600}{RT}\right] \text{ cm}^2/\text{sec},$$

For temperature $T = 500, 550, 600 \text{ K.}$

We obtain $D_A = 8 \cdot 10^{-18}; 1.39 \cdot 10^{-16}; 1.51 \cdot 10^{-15}$ and

$$D_B = 1.1 \cdot 10^{-29}; 5.03 \cdot 10^{-27}; 8.2 \cdot 10^{-25} \text{ cm}^2/\text{sec}$$

correspondingly. Hence it is impossible to expect diffusion zone

formation during times t_A, t_B and t_i without additional

acceleration of diffusion.

Experimental data indicate that the materials activation happens under irreversible conditions of particle beam action. It leads to diffusion acceleration and changes many physical properties [8]. Diffusion acceleration could be connected with activation energy reduction. Kinetics of this physical process would be investigated especially.

Here we assume that the activation energies reduction in four times takes place. That gives for $T = 500, 550, 600 \text{ K}$ the diffusion coefficients near to previous simple problems

$$D_A = 4.36 \cdot 10^{-7}; 1.46 \cdot 10^{-6}; 4.21 \cdot 10^{-6} \text{ and } D_B = 9.33 \cdot 10^{-8}; 4.31 \cdot 10^{-7}; 1.54 \cdot 10^{-6} \text{ cm}^2/\text{sec.}$$

IV. RESULTS ANALYSIS

The example of concentration distributions for $t_A = t_B = 0$ is presented in the Fig.5 for $q_m = 12.5 \cdot 10^{-4}$

$\text{mol}/(\text{m}^2 \text{ s})$; $T = 500$ and $A = 0$. In this case we have $t_{ch} = 1.1 \cdot 10^{-4} \text{ s.}$

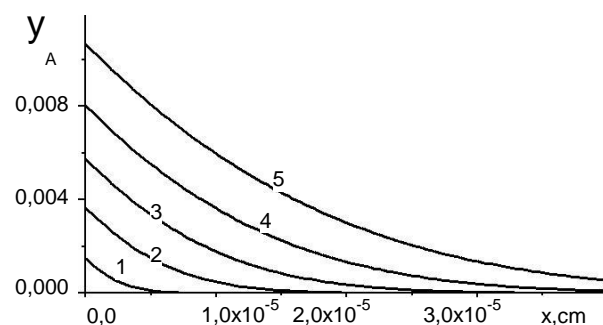


Fig.5 (a)

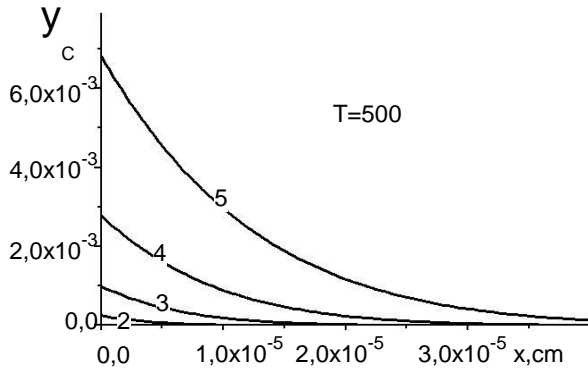


Fig.5 (b)

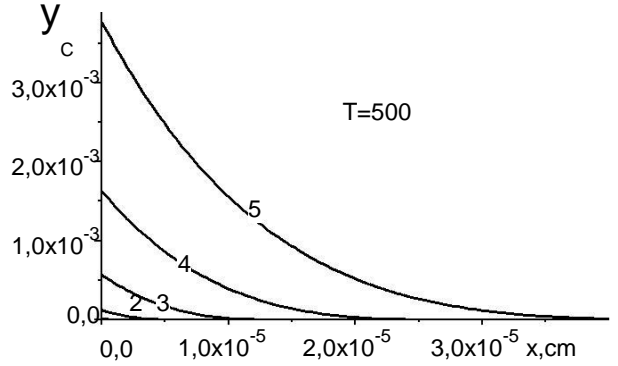


Fig.6 (b)

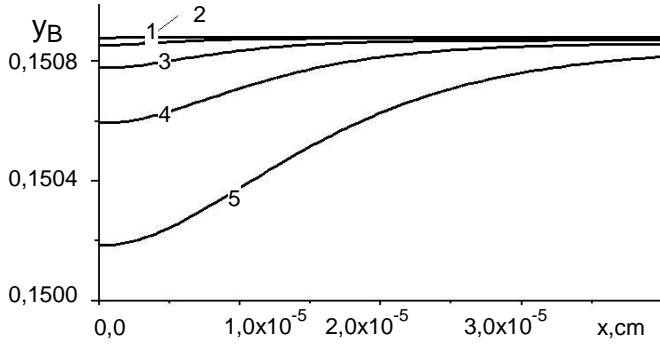


Fig.5 (c)

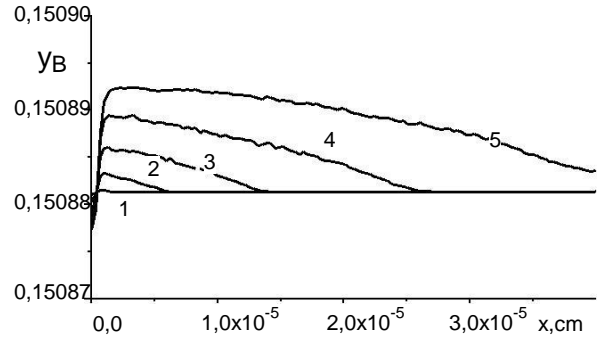


Fig.6 (c)

Fig.5. The concentration distribution in specimen for implanted element (a), reaction product (b) and initial substance (c) for

different time moment; $t_A = t_B = 0$; $T = 500$ K; $A = 0$; $t = 1.$

1. $2.5 \cdot 10^{-5}$ 2. $7.5 \cdot 10^{-5}$ 3. $1.875 \cdot 10^{-4}$ 4. $3.75 \cdot 10^{-4}$

5. $6.875 \cdot 10^{-4}$ Sec

It is shown that in this case we can actually neglect the initial substance concentration change for small times, less than specific

reaction time t_{ch} . When we evaluate the temperature to 550 K, the reaction time decreases to $t_{ch} = 8.36 \cdot 10^{-6}$ sec, and the concentration change for B-substance will more visible. The temperature leads to diffusion acceleration and diffusion zone increase (it is not shown on the pictures).

When we take into account the finiteness of relaxation time, we shall obtain some interested result (Fig.6 and 7).

If $t < t_i$, the implanted particles are distributed practically linearly (Fig.6,a). The type of concentration curves for reaction product does not change (Fig.6, b). Redistribution of initial substance is observed (Fig.6, c) in diffusion zone, that leads to density evaluation.

Fig.6. The concentration distribution in specimen for implanted element (a), reaction product (b) and initial substance (c) for

different time moment; $t_A = 10^{-4}$; $t_B = 10^{-5}$ sec;

$T = 500$ K; $A = 0$; $t = 1. 1.25 \cdot 10^{-5}$ 2. $7.5 \cdot 10^{-5}$ 3. $1.875 \cdot 10^{-4}$

4. $3.75 \cdot 10^{-4}$ 5. $6.875 \cdot 10^{-4}$ Sec.

When mass source acts only during $t_i = 2 \cdot 10^{-4} > t_A$, no monotonic concentration curves appear for implanted

particles after t_i (Fig.7.a) that propagates into the depth and leads to new phase formation acceleration (Fig. 7,b). In this case, the extreme is observed in initial substance concentration (Fig.7, c). The evaluation of mass flux density allows seeing the stepped concentration curves for small times (Fig.7.a).

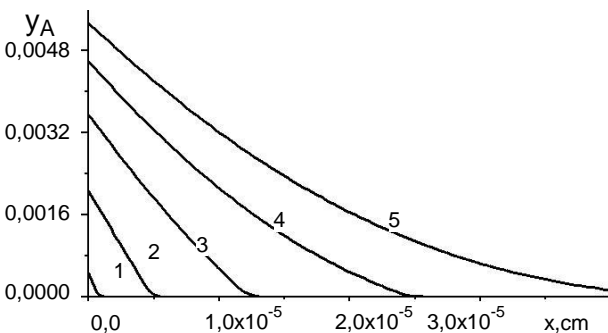


Fig. 6 (a)

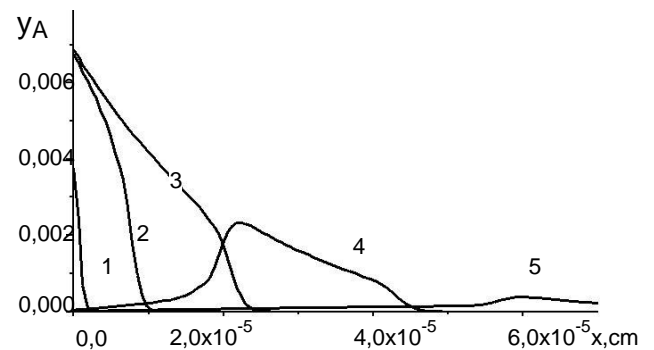


Fig.7 (a)

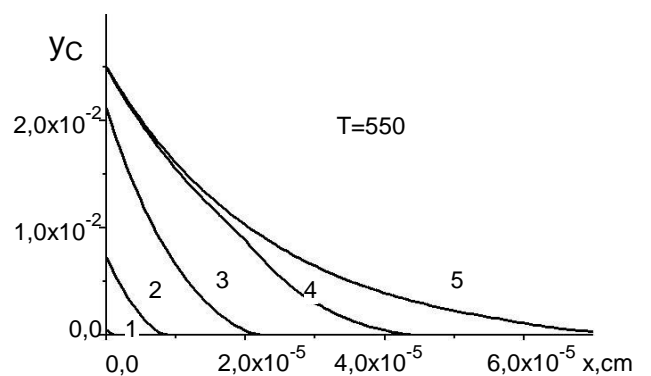


Fig.7 (b)

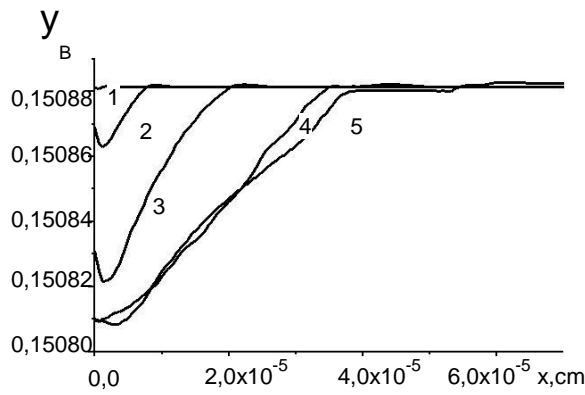


Fig.7 (c)

Fig. 7 The concentration distribution in specimen for implanted element (a), reaction product (b) and initial substance (c) for different time moment; $t_A = 10^{-4}$; $t_B = 10^{-5}$ sec; $T = 500$ K;

$$A = 0; t_i = 2 \cdot 10^{-4} \text{ sec}; q_m = 5 \cdot 10^{-3} \text{ mol} / (m^2 s)$$

$$t = 1. 1.25 \cdot 10^{-5} \quad 2. 7.5 \cdot 10^{-5} \quad 3. 1.875 \cdot 10^{-4} \quad 4. 3.75 \cdot 10^{-4}$$

$$5. 6.875 \cdot 10^{-4} \text{ Sec}$$

V. STRESSES IN THE SURFACE LAYER

A. General Equations

Since the temperature is not too large, the stresses in diffusion zone are elastic and we can use known solutions of thermal elasticity theory, where some changing are permissible. According to Dugamel Neyman relations, we have connection between stress and strain tensor components and temperature in the form [12]

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \delta_{ij} [\lambda\varepsilon_{kk} - K\omega]$$

or

$$\sigma_{ij} = 2\lambda(1+\nu) \frac{\varepsilon + \delta}{ij} + \frac{E\nu}{(1-\nu)(1+\nu)} \varepsilon_{kk} - 3\lambda(1-\nu)(1+\nu) \omega$$

where $i, j = x, y, z$; λ, μ - Lamé coefficients, $K = \lambda + \frac{2}{3}\mu$ - is bulk module, connecting with technical values elastic module and Poisson coefficient by relations

$$K = \frac{E}{3(1-2\nu)}, \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \mu = \frac{E}{2(1+\nu)},$$

and

$$\begin{cases} \delta_{ij} = 1, \text{ if } i = j; \\ \delta_{ij} = 0, \text{ if } i \neq j, \end{cases}$$

$$\omega = 3\alpha_T(T - T_0)$$

α_T is thermal expansion coefficient, T_0 - initial temperature.

When the composition changes, we can write [13]

$$\omega = \alpha_T(T - T_0) + \sum_{k=1}^n \alpha_k (C_k - C_{k0})$$

where α_k are the concentration expansion coefficients; C_k are relative mass concentrations; index «0» relates to no deformed state n is species quantity (pure elements and chemical compounds).

Mass concentrations are determined by following way

$$c_k = \frac{\rho_k}{\rho} = \frac{m_k y_k}{\rho}, \rho = \sum_{k=1}^n \rho_k,$$

where m_k is molar mass of k -species, ρ_k - partial densities (see above).

Hence, we can write for $T = const$

$$\omega = 3 \sum_{k=1}^n \frac{\alpha_k m_k}{\rho_0} \left(y_k \frac{\rho_0}{\rho} - y_{k0} \right)$$

For coefficients α_k the simple evaluation takes a place

$$\alpha_k = \frac{1}{3} \frac{\omega_k}{\sum_{i=1}^n \omega_i}$$

where for pure substances ω_i - are atom volumes; for chemical compounds - molar volumes:

$$\omega_i = \frac{m_i}{\rho_{i0}}$$

ρ_{i0} is individual density of substance in standard state.

Using data [14] $\rho_A = 4.54 \cdot 10^3$ (Titanium); $\rho_B = 8.902 \cdot 10^3$ (Nickel) and $\rho_C = 6.44 \cdot 10^3 \text{ kg/m}^3$ ($TiNi$), we find

$$\alpha_A = 0.104; \alpha_B = 6.53 \cdot 10^{-2}; \alpha_C = 0.164.$$

B. Mechanical Equilibrium Problem

Let our specimen is thin plate that is the object the thickness of which is more less than the width and length. If for diffusion process the specimen thickness is infinite, so for mechanical stresses the specimen finiteness is principal. Using the solution of the problem on mechanical equilibrium of thick plate free on external mechanical loading, but absorbing the admixture from environment [12], and taking into account the presented above formulae, we write the expressions for stress and strain tensor components in the form

$$\begin{aligned} \varepsilon_{xx} &= \varepsilon_{xx}(x), \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon(x), \varepsilon_{xy} = \varepsilon_{xz} = \varepsilon_{zy} = 0 \\ \sigma_{yy} &= \sigma_{zz} = \sigma(x), \sigma_{xy} = \sigma_{xz} = \sigma_{zy} = 0 \\ \varepsilon_{xx} &= \frac{1}{3} \frac{1}{1-\nu} + \frac{\nu}{1-\nu} \frac{2}{1-\nu} (F_1 x + F_2) \\ \sigma &= \sigma_{yy} = \sigma_{zz} = -\frac{\omega}{3} \frac{E}{1-\nu} + \frac{E}{1-\nu} (F_1 x + F_2) \\ \varepsilon &= F_1 x + F_2, \end{aligned}$$

where

$$F_1 = \frac{N\beta - M\alpha}{\beta^2 - \gamma\alpha}, F_2 = -\frac{N\gamma - M\beta}{\beta^2 - \gamma\alpha}$$

$$N = \frac{1}{3} H \int_0^H \omega(z,t) \frac{E}{1-\nu} dz, M = \frac{1}{3} H \int_0^H \omega(z,t) z \frac{E}{1-\nu} dz$$

$$\alpha = H \int_0^H \frac{E}{1-\nu} dz, \beta = H \int_0^H \frac{E}{1-\nu} z dz, \gamma = H \int_0^H \frac{E}{1-\nu} z^2 dz$$

The similar solution has been used in many publications, for example [15, 16].

Because function ω equal to zero far from diffusion zone, $x_D \ll H$, the integrals differ from zero only in diffusion zone,

$x < x_D$. This value is determined numerically during solution of diffusion-kinetic problem.

The mechanical properties (modulus of elasticity and Poisson's ratio) can depend on composition.

We assume $E = E_A C_A + E_B C_B + E_C C_C$;

$\nu = \nu_A C_A + \nu_B C_B + \nu_C C_C$.

In accordance with literature data [14], we have $E_A = 116$;
 $E_B = 204$; $E_C = 200$ GPa; $\nu_A = 0.32$; $\nu_B = 0.28$;
 $\nu_C = 0.35$.

C. Stresses and Strains Analysis

The stress and strains distribution for described above cases are presented in Fig.8-10. The strains are small for

small q_m . The character of strains distribution is similar to the reaction product distribution. Stresses in the reaction zone in the direction perpendicular to particle beam action achieve the large values. The most of them correspond to the case with large q_m and short impulse (Fig.10). The Young module changes very quickly, because the properties of materials are near to each other. The E -curves repeat qualitatively the implanted particles curves (Fig.8-10, c).

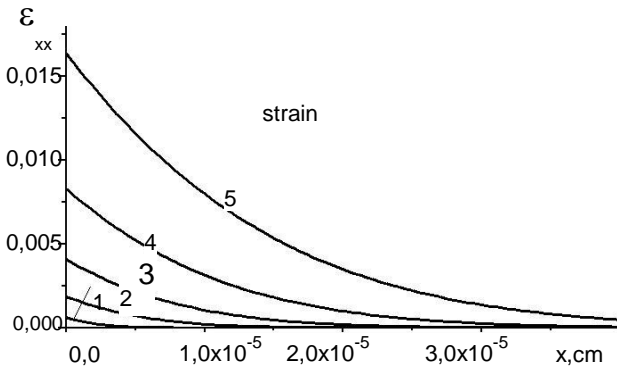


Fig.8 (a)

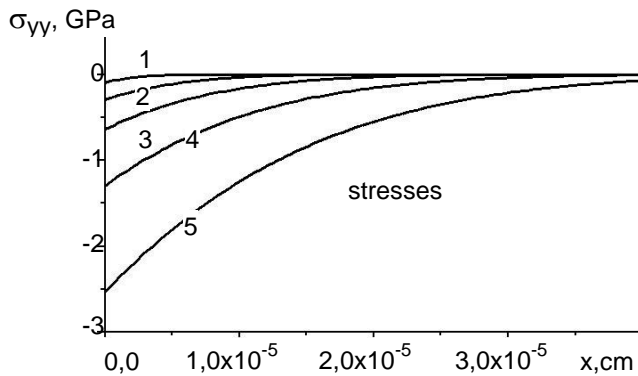


Fig.8 (b)

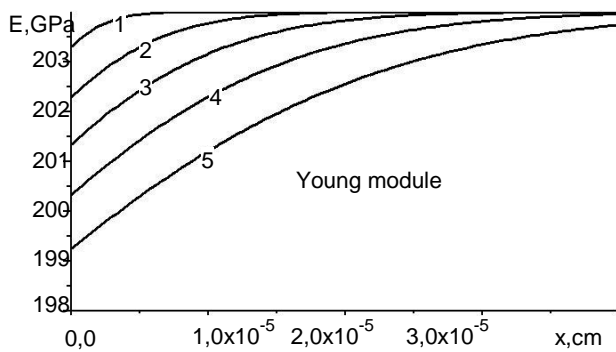


Fig.8 (c)

Fig. 8 Strains, stresses and Young module in surface layer for different time moment; $t_A = t_B = 0$; $T = 500$ K; $A = 0$
 $t = 1. 1.25 \cdot 10^{-5}$ 2. $7.5 \cdot 10^{-5}$ 3. $1.875 \cdot 10^{-4}$ 4. $3.75 \cdot 10^{-4}$
 5. $6.875 \cdot 10^{-4}$ Sec.

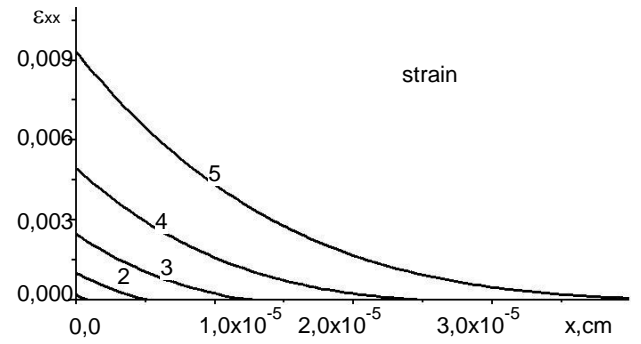


Fig.9 (a)

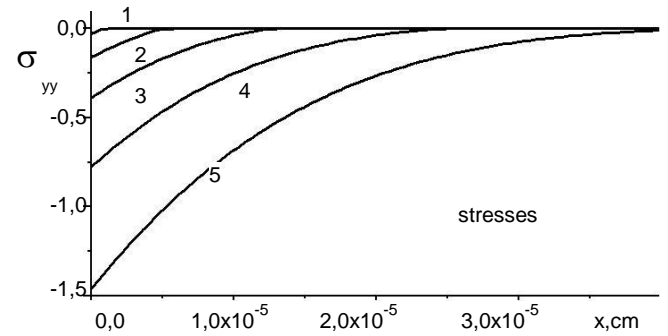


Fig.9 (b)

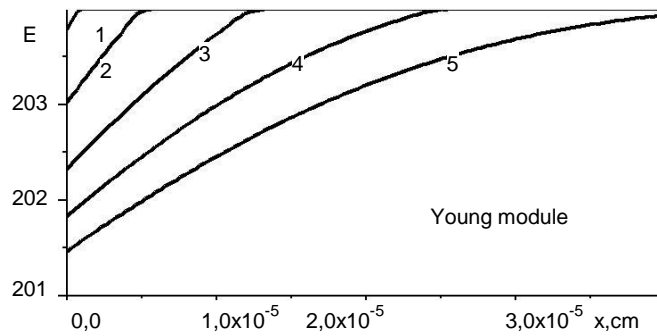


Fig.9 (c)

Fig. 9 Strains, stresses and Young module in surface layer for different time moment $t_A = 10^{-4}$; $t_B = 10^{-5}$ sec; $T = 500$ K; $A = 0$; $t = 1. 1.25 \cdot 10^{-5}$ 2. $7.5 \cdot 10^{-5}$ 3. $1.875 \cdot 10^{-4}$
 4. $3.75 \cdot 10^{-4}$ 5. $6.875 \cdot 10^{-4}$ Sec.

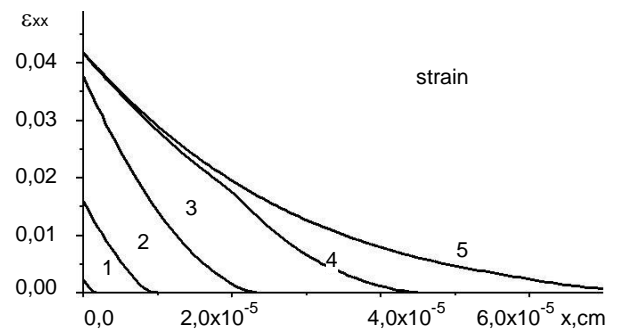


Fig.10 (a)

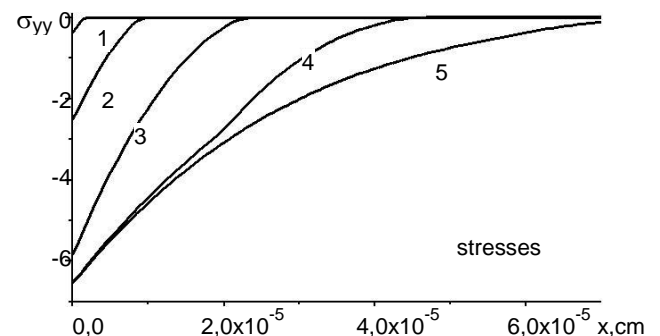


Fig.10 (b)

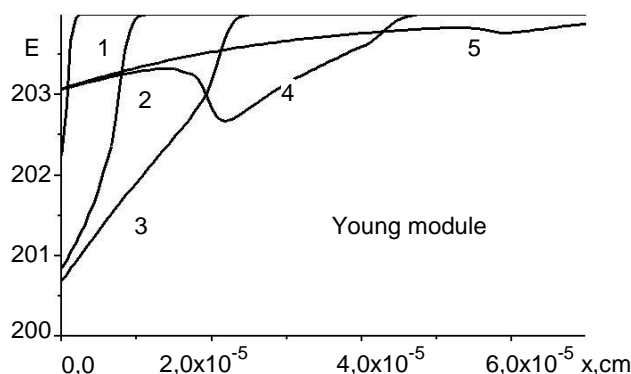


Fig.10 (c)

Fig. 10 Strains, stresses and Young module in surface layer for different time moment. $t_A = 10^{-4}$; $t_B = 10^{-5}$ Sec; $T = 500$ K; $A = 0$; $t_i = 2 \cdot 10^{-4}$ sec; $q = 5 \cdot 10^{-3}$; $t = 1.125 \cdot 10^{-5}$ m

2. $7.5 \cdot 10^{-5}$ 3. $1.875 \cdot 10^{-4}$ 4. $3.75 \cdot 10^{-4}$ 5. $6.875 \cdot 10^{-4}$ Sec

VI. CONCLUSION

Consequently, in this work the simple models of new phase formation at the initial stage of ion implantation are suggested. It is shown that relaxation time finiteness changes the concentrations distribution in diffusion zone in comparison with usual diffusion problems. The stresses and strains can achieve large values. The detected effects could be used at the discussion of experimental data. The model can be applied to various chemical systems.

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