

The influence of some model parameters on the impurity distribution implanted into substrate surface

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Abstract. The model for description of the initial stage of ion implantation into the surface layer of the metal is presented. The interdependence of embedded impurity concentration and deformations arising from the impact of particles on the surface is investigated. The model takes into account the particle diffusion, the finite time of mass flux relaxation; the stress appearance due to a composition change of the surface layer and a mass transfer phenomenon under a stress gradient action. It is established that the interaction of mechanical waves and concentration leads to a distribution of concentration not corresponding to a pure diffusion process. The examples of coupled problems solution for different sets of model parameters are presented.

1. Introduction

Researches of the surface treatment process of materials by beams of charged particles are carried out by many authors [1-4]. The composition and structure, and, consequently, the surface properties of materials can be controlled owing to these methods. In spite of extensive experimental and theoretical data, possibilities of the implantation method are not fully exhausted. This is connected with a lack of understanding of physical processes in solids under irradiation [5] for small time moments.

In the process of implantation into the surface substrate, different phenomena occur simultaneously with the diffusion process. For example, mechanical disturbances appear and propagate, structural and phase changes happen, point defects are generated as a result of the particles impact on the surface and appearing mechanical stresses etc. All these phenomena influence each other. Therefore the interrelation between different processes must be considered during modeling [6]. In the literature, the thermoelastic waves caused by exposure to high-energy sources on the surface of materials attract the basic attention. However, it should be noted that there are coupled models of ion implantation which take into account the processes associated with the difference in the properties of the base material and introduced elements; in this case diffusion and physico-chemical phenomena are a rarity. In [7] it was shown that the interrelation between mechanical and diffusion waves leads to a distortion of the deformation (and stress) wave profile, and the concentration distribution does not correspond to a pure diffusion process. The purpose of this work consists in the study of the initial stage of the ion implantation.

2. The mathematical formulation

In the present paper, model [7] is used. This model is built with account that temperature is constant. It is assumed that the occurring stresses are elastic and deformations are small. Also this model takes



into account the fact that transfer coefficients can be change due to changes in the activation diffusion volume. In the dimensionless variables, the model under deformations takes the form:

$$\tau_r \frac{\partial^2 C}{\partial \tau^2} + \frac{\partial C}{\partial \tau} = \frac{\partial}{\partial \xi} \left[g(C) f_2(\Pi) \frac{\partial C}{\partial \xi} \right] - \omega \gamma \frac{\partial}{\partial \xi} \left[C f_2(\Pi) \frac{\partial e}{\partial \xi} \right], \quad (1)$$

$$\frac{\partial^2 e}{\partial \tau^2} = \frac{\partial^2 e}{\partial \xi^2} - \gamma \frac{\partial^2 C}{\partial \xi^2}, \quad (2)$$

$$S = e - \gamma(C - C_0), \quad (3)$$

$$\mathbf{J} = - \left[g(C) \frac{\partial C}{\partial \xi} - C \omega \gamma \frac{\partial e}{\partial \xi} \right] f_2(\Pi) - \tau_r \frac{\partial \mathbf{J}}{\partial \tau}, \quad (4)$$

$$\xi = 0: \mathbf{J} = \beta \varphi(\tau), \quad S = S_0 \varphi(\tau), \quad (5)$$

$$\xi \rightarrow \infty: C = 0, \quad e = 0, \quad (6)$$

$$\tau = 0: C = 0, \quad e = 0, \quad \frac{\partial C}{\partial \tau} = 0, \quad \frac{\partial e}{\partial \tau} = 0, \quad (7)$$

where $S = \frac{\sigma}{\sigma_*} = \frac{\sigma}{3E\alpha_0}$, $\tau = \frac{t}{t_*} = \frac{tE}{\rho D_0}$; $\xi = \frac{x\sqrt{E}}{D_0\sqrt{\rho}}$; $e = \frac{\varepsilon}{3\alpha_0}$ – are dimensionless variables, \mathbf{J} – is

the mass flux, S , e – are components of the stress and strain tensors in irradiation direction ($O\xi$), τ – is the time, C – is the mass concentration of the implanted component, $g(C) = f_1(C) + \omega\gamma^2 C$ – is the function of concentration, $f_2(\Pi) = -\kappa e S$ – is the function of stress work, the form of function $f(C)$ depends on the "solute" structure formed in the process of implantation, in this paper we used function $f_1(C) = a + bC + dC^2$, ω , γ , τ_r , β – are parameters of the model:

$$\omega = \frac{3mE\alpha_0^2}{RT\rho}, \quad \gamma = \frac{(\alpha - \alpha_0)}{\alpha_0}, \quad \tau_r = \frac{t_r E}{\rho D_0}, \quad \beta = m_0 \sqrt{\frac{\rho}{E}}, \quad \kappa = \frac{kE\alpha_0}{RT}$$

here ρ – is the density of the base material; α – is the concentration expansion coefficients of the implanted elements, α_0 – is the concentration expansion coefficients of the base material, τ_r – is the relaxation time of the mass flux, D_0 – is the self-diffusion coefficient, R – is the universal gas constant, T – is the temperature, m – is the molar mass, m_0 – is the velocity of the particles in the flux, E – is the elastic module, k – is the constant with the dimension of activation volume.

3. Results and discussions

System (1)-(7) was solved numerically with the help of the explicit difference scheme and a double - sweep method. Below we present examples of calculation.

Values of model parameters are presented in Table 1. Figure 1 shows distributions of impurity concentration (a) and deformations (b) in depth. By the time of $\tau = 1.225$ the concentration wave slightly lags behind the wave of deformations. By the time of $\tau = 3.67$ the deformations wave runs away far forward, and by the time of $\tau = 5.88$ the sloping plot on the wave appears between the extremes, which increases with time. This is a reflection of the weak influence of waves on each other for a long time. During these moments of time the pulse has already no effect on the substrate material. It can be seen from trailing edges of waves.

Table 1 – Values of model parameters.

Parameter	Numerical value
ω	10
τ_r	1.0
β	0.01
γ	-0.09
κ	2.9
$\varphi(\tau)$	$\sin(R \cdot \tau)$, where $R = \frac{\pi}{t_{imp}}$
$f_1(C)$	$0.05 + 0.01C + 0.8C^2$

A change of the sign of the strain corresponds to the depth of impurity penetration. This phenomenon is related to the fact that the impurity is introduced at a smaller depth than the mechanical wave. Thus, the maximum range of ions is the distance where compressive deformation converts into tensile (or vice versa, it depends on properties of used materials).

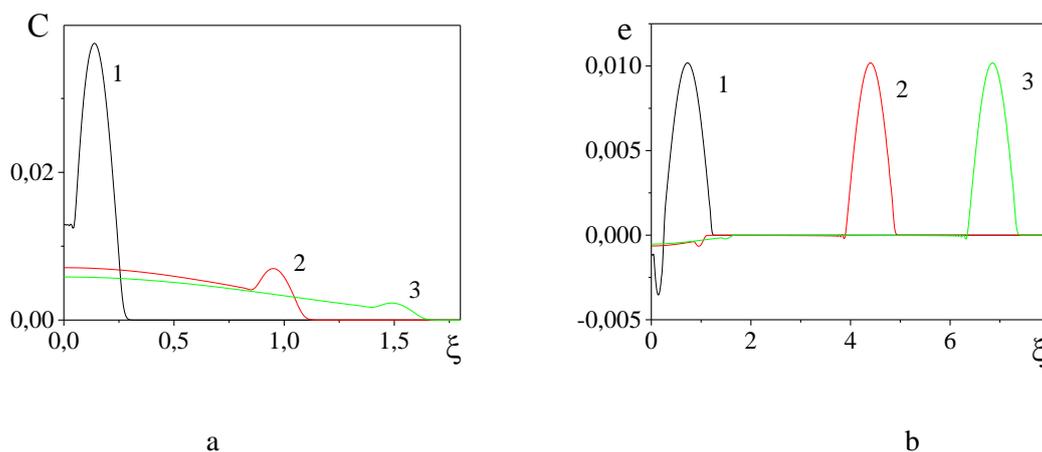


Figure 1. Distributions of impurity concentration and deformations in depth. Pulse time $t_{imp} = 1.0$.
Times, τ : 1 – 1.225; 2 – 3.675; 3 – 5.88.

Figure 2 shows the influence of model parameters on distributions of impurity concentration. The increase of the relative relaxation time leads to a significant increase in the amplitude of impurity concentration. The reduction of τ_r reduces the penetration depth. The increase of κ leads to decreased values of impurity concentration on the surface (for earlier moments this phenomenon is more significant), the maximum value decreases, the penetration depth of the impurity increases slightly. The change of connectedness coefficient ω results in a significant distortion of wave profiles, in particular the area of waves near extreme. The value of impurity concentration on the sample surface increases. Increase γ leads to augmentation of the maximum and to a decrease of the concentration value on the surface

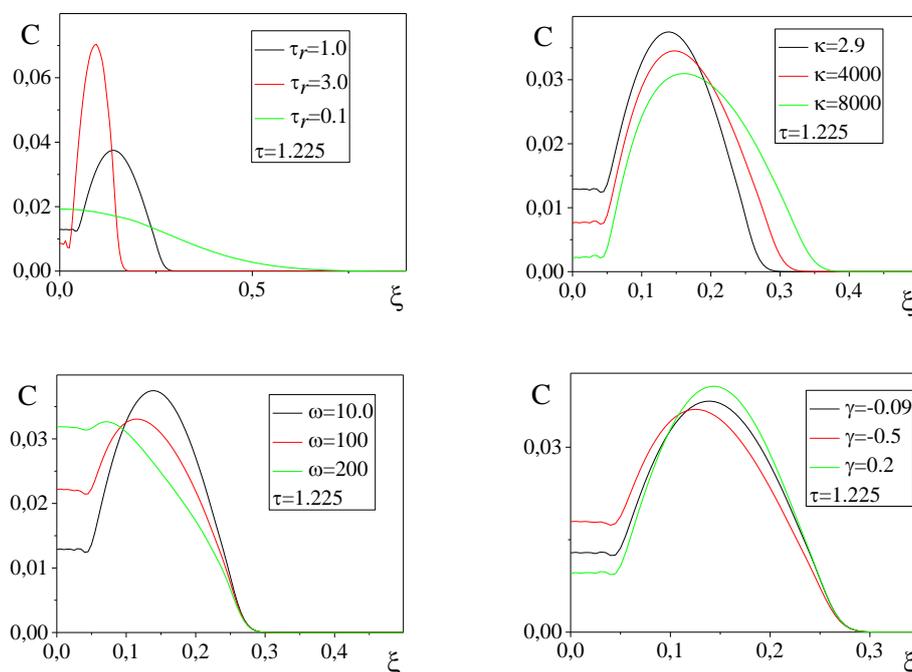


Figure 2. The influence of model parameters on distributions of impurity concentration.

Thus, the variation of model parameters results in qualitative and quantitative changes of the impurity concentration profile. It is necessary to accurately calculate these parameters for obtaining a result corresponding to experimental observations.

4. Conclusion

Thus, in this work the mathematical model of the initial stage of ion implantation is described. Concentration and strain distribution in the waves are strongly dependent on the relations among the parameters of the model.

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