Modelling of the Concentration Fields in Metal Films under Irradiated with High-Intensive Pulse Beams of Charged Particles

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Abstract – We consider a space-time nonlocal mass transfer model to discuss some properties and solutions of an universal diffusion equation, which describes the space-time evolution of substance concentration and mass flux in thin films under highly intensive pulse beams irradiation. The model identifies two internal parameters – the delay times of flux and concentration gradient. Employing the method of Laplace transform, the present work derives the analytical expressions for mass flux. An influence of the initial fluxe rate on mass transfer is investigated.

1. Introduction

Among the known anomalous phenomena mass transfer in metals and alloys under influence of concentrated flows of energy (ion, electron and laser beams of nanosecond duration) [1–4] take place such as step-like distribution of concentrations of impurity, and non-monotone of concentration profiles. As one of the possible reasons, explaining various kinds of anomalous migration of atoms of impurity under fast-transient processes in small spatial volumes, is, probably, local-nonequilibrium heat and mass transfer. In the given work the role space nonlocal, given by arise and relaxation of viscoelastic mechanical pressure, on shaping the concentration fields in metal films under pulsed influences by powerful beams of particles are estimated.

2. Mathematical Model

Within the framework of extended irreversible thermodynamics [5, 6] one dimensional equation for flow of particles $J(x, t)$ (or concentrations of impurity atoms $c(x, t)$) in binary system under fast-transient processes in isothermal approach has the form [7, 8]

$$\frac{\partial J}{\partial t}+\tau_1\frac{\partial^2 J}{\partial t^2}=D\frac{\partial^2 J}{\partial x^2}+\tau_2\frac{\partial^3 J}{\partial t\partial x^2}. \qquad (1)$$

Here D is diffusion coefficient, which is taken constant; τ_1 and τ_2 – relaxation time of flow and gradient of concentration, respectively. Equation (1) is nonlocal in both time and space. Spatial nonlocal means that specific flow of mass and concentration gradient are connected between one another not in one spatial point with coordinate x, as in classical Fick's law, but in a certain neighbourhood of this point with characteristic size h. Time nonlocal appears due to take in to account relaxation processes (the gradient of concentration in point x systems initiates the flow of mass not in same moment of time t, as in local-irreversible approach, but for time of relaxations τ_1 later). The equation of transfer (1) contains partial derivative third order. It combines the characteristics of wave equation (under $\tau_2 = 0$), describing transport of concentration waves with final velocity in system, as well as diffusion equations (under $\tau_1 = \tau_2 = 0$), corresponding to dissipative mass transfer.

Let us construct the solution of equation (1) for flow on metal film $0 < x < l$ with following initial

$$J(x,0)=0,\ \partial J(x,0)/\partial t=\dot{J}_0 \qquad (2)$$

and boundary conditions

$$J(0,t)=J_0,\ \partial J(l,t)/\partial x=0 \ \text{at}\ t>0. \qquad (3)$$

I further introduce the dimensionless flow

$$\chi(\xi,\tau)=J(\xi,\tau)/J_0 \qquad (4)$$

and following dimensionless variables $\tau=t/(l^2/D)$ and $\xi=x/l$.

The dimensionless form of eq. (1) with initial and boundary conditions (2)–(3) then can be rewritten as

$$\frac{\partial\chi}{\partial\tau}+\alpha_j\frac{\partial^2\chi}{\partial\tau^2}=\frac{\partial^2\chi}{\partial\xi^2}+\alpha_c\frac{\partial^3\chi}{\partial\xi^2\partial\tau}, \qquad (5)$$

$$\chi(\xi,0)=0,\ \partial\chi(\xi,0)/\partial\tau=\dot{\chi}_0, \qquad (6)$$

$$\chi(0,\tau)=1,\ \partial\chi(1,\tau)/\partial\xi=0, \qquad (7)$$

where $\alpha_c=\tau_2/(l^2/D)$, $\alpha_j=\tau_1/(l^2/D)$ are dimensionless relaxation time; $\dot{\chi}_0=\dot{J}_0(l^2/D)/J_0$ is dimensionless initial mass flux rate.

For solving of boundary problem (5)–(7) the Laplace transformation is used. This transformation reduces equation (5) to an ordinary differential equation involving only ξ-derivatives:

$$\frac{\partial^2\overline{\chi}}{\partial\xi^2}-\left(\frac{p(1+\alpha_j)}{1+p\alpha_c}\right)\overline{\chi}+\frac{\alpha_j}{1+\alpha_j p}\overline{\chi}_0=0. \qquad (8)$$

The initial and boundary conditions in physical space should be transformed into corresponding ones in Laplace space

$$\bar{\chi}(0) = 1/p\,,\ \partial\bar{\chi}(1)/\partial\xi = 0\,. \qquad (9)$$

The Laplace transform solution satisfying (8)–(9) is easily obtained:

$$\bar{\chi}(\xi, p) = \frac{1}{p}\left(z_1 + (1 - z_1)\frac{ch\left((1-\xi)z_2\right)}{ch\left(z_2\right)} \right), \qquad (10)$$

where

$$z_1 = \alpha_j \dot{\chi}_0 / (1 + \alpha_j p)\,,\ z_2 = \sqrt{p(1+\alpha_j p)/(1+\alpha_c p)}\,.$$

In order to obtain the solution for $\chi(\xi,\tau)$ invers Laplace transfer is used:

$$\chi(\xi,\tau) = 1/2\pi i \int_{\gamma - i\infty}^{\gamma + i\infty} \bar{\chi}(\xi, p)\exp(p\tau)dp\,. \qquad (11)$$

The quantity γ is the real value of straight cut contour of integration. To obtain solution for non-dimensional flow the variable transformation $p = \gamma + i\omega$ is introduced and integral (11) is approximated by its Riemann sum

$$\chi(\xi,\tau) = \frac{\exp(\gamma\tau)}{\tau}\left[\frac{\bar{\chi}(\xi,\gamma)}{2} + \right.$$

$$\left. + \mathrm{Re}\sum_{n=1}^{N}(-1)^n \bar{\chi}\left(\xi, \gamma + in\pi/\tau\right)\right], \qquad (12)$$

where “Re” represents the real part of the summation. Accuracy of aproximation of integral by Riemann sum is defined by value of parameter γ and number *N*. Under fixed γ one must choose *N* such that inaccuracy of truncation less forward given to accuracy.

For turning from flow $J(x, t)$ to particles concentration $c(x, t)$ the equation of balance of mass $\partial c/\partial t = -\partial J/\partial x$ is used. Then for dimensionless function $V(\xi,\tau) = \left(c - c_i\right)D/\left[J_0 l\right]$, where c_i is initial concentration of impurity in sample, we shall have

$$V(\xi,\tau) = -\int_0^\tau \left(\frac{\partial\chi(\xi, y)}{\partial\xi}\right)dy\,, \qquad (13)$$

here *y* is dummy integration variable for time. Numerical calculation can now be applied to determine the dimensionless concentration.

3. Results of Modeling

We shall assume a zero initial mass flux rate for the time to study mechanisms associated with influence space nonlocality on mass transfer in terms of τ_1 and τ_2. Inserting Eq. (10) with $\dot{\chi}_0 = 0$ into Eq. (12), flux distributions in the physical space are obtained by the finite sum of the series. Fig. 1,a shows modeling results with the error norm being controlled below 10^{-5} (for achievement which enough there was take $N = 2000$) for all cases. A small value of time ($\tau = 0.05$) is selected for avoiding the effect of wave reflection from the boundary at $\xi = 1$. The value of α_j is fixed at 0.04 while the value of α_c is changed. The curve 1 with $\alpha_c = 0$ corresponds to the wave model with a mass transport speed of $(D/\tau_1)^{1/2}$ and a diffusion damping effect. A sharp wavefront exists at $\xi = \tau/(\alpha_j)^{1/2}$. As the value of α_c deviates slightly

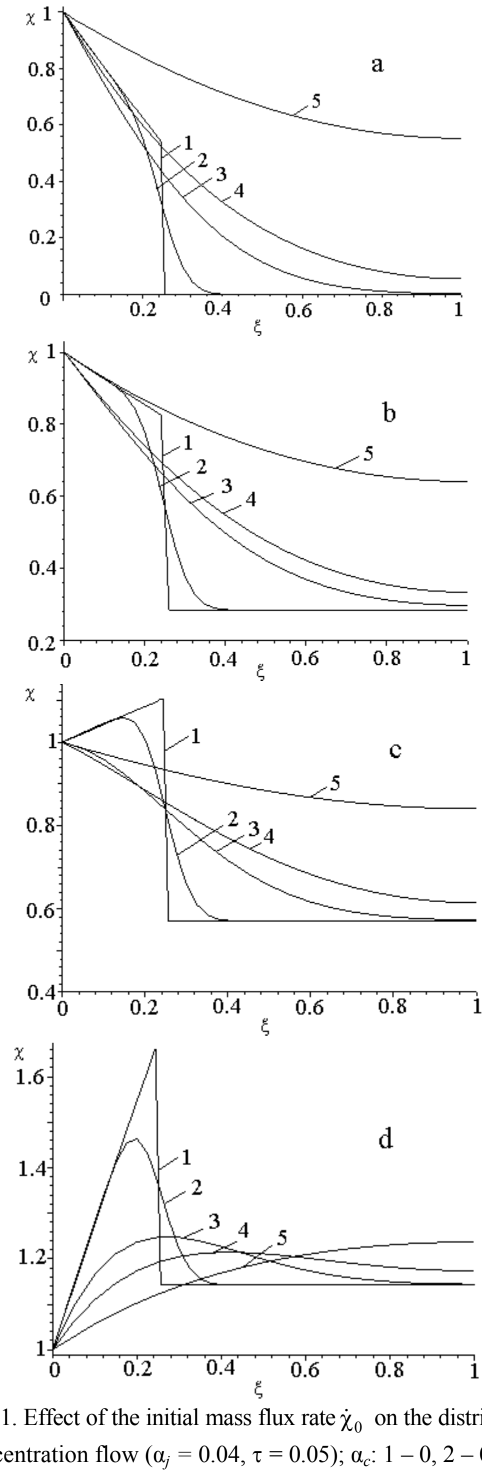

Fig. 1. Effect of the initial mass flux rate $\dot{\chi}_0$ on the distribution concentration flow ($\alpha_j = 0.04$, $\tau = 0.05$); α_c: 1 – 0, 2 – 0.002, 3 – 0.04, 4 – 0.1, 5 – 0.5; $\dot{\chi}_0$: a – 0, b – 10, c – 20, d – 40

from zero to 0.002, implying the gradual activation of the microscale effect, the sharp wavefront is destroyed and the mass-affected zone extends deeper into the medium. For the case of $\alpha_c = \alpha_j$, i.e. $\tau_1 = \tau_2$ and not necessarily equal to zero (the curve 3), the flux distribution approaches the result of diffusion, since Eq. (5) is equivalent to the diffusion equation (known as Fick's law).

The mass flux level exceeds those of diffusion and wave as the value of α_c becomes large that of α_j. The amount increases with the value of α_c and the mass-affected zone significantly extends to a large distance from the wall. Large deviations from the classical wave theory shown in Fig. 1(a) indicate that the small-scale response in space and time cannot be separated and must be accommodated as an entirety. Although the wave theory aims to capture the small-scale response in time (in terms of τ_1), it does not seem to be complete until the microscale response in space (in terms of τ_2) is implemented.

The nonzero initial mass flux rate produces additional effects in the short-time response. For the same values of τ and α_j used previously, results are displayed in Fig. 1,b–d for $\dot{\chi}_0 = 10$, 20, and 40. Under a moderate rate, $\dot{\chi}_0 = 10$, mass flux levels increase with α_c (curves 3–5 in Fig. 1,b). This is the same behavior as that in the absence of the initial flux rate shown in Fig. 1,a. When the initial rate increases to 20, Fig. 1,c, flux distribution with $\alpha_c = 0.5$ remains at the reference level while flux in the neighborhood of the $\xi = 0$ start to decrease when the value of α_c increases. The rate effect in this case dominates over the combined effect of damping and reverses the qualitative trend in Fig. 1,a where no initial rate is present. When the value of $\dot{\chi}_0$ further increases to 40, as shown in Fig. 1,d, the field flux may exceed the wall flux ($\chi = 1$). No matter how high the initial rate space nonlocality destroys the wave structure in mass propagation. A slight deviation of from zero, as shown in Fig. 1, destroys sharp wave front and reduced the peak value of flow. In the presence of an initial flux rate the result of diffusion is no longer retrieved by special case with $\tau_1 = \tau_2$, since the classical diffusion model is not compatible with the initial condition describing mass flux rate due to absence of a wave term in the mass continuity equation.

The three-dimensional dimensionless concentration maps of the mass transfer problem for two sets of parameters α_c and α_j are drawn in Figs. 2 and 3 in depending of an initial values of mass flux rate. For the small value of $\dot{\chi}_0$ (< 10) maximum of concentration is observed at a surface of a film which increase with time marching. When the value of $\dot{\chi}_0$ increases to 20 or 40, maximum of concentration are displaced deeper into the medium and decreases with increase of time. The non-monotone concentration profiles for the certain values of initial mass flux rate are observed.

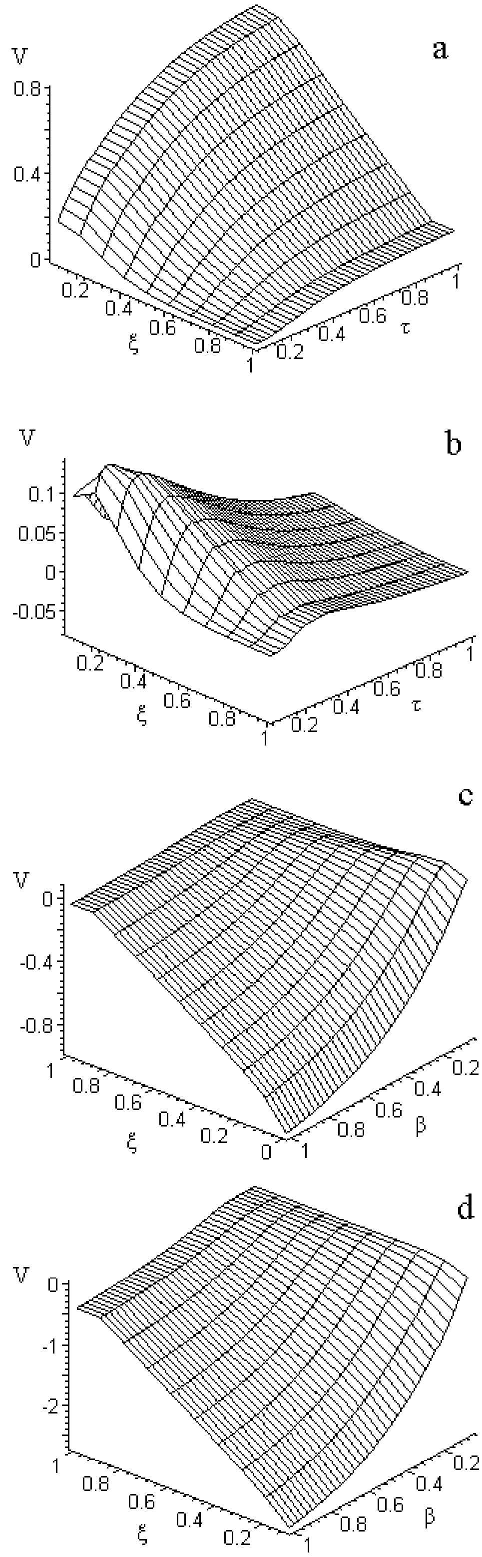

Fig. 2. Concentration fields of impurity atoms in film depending on initial mass flux $\dot{\chi}_0$: a – 0, b – 10, c – 20, d – 40; $\alpha_c = 0.1$, $\alpha_j = 0.5$

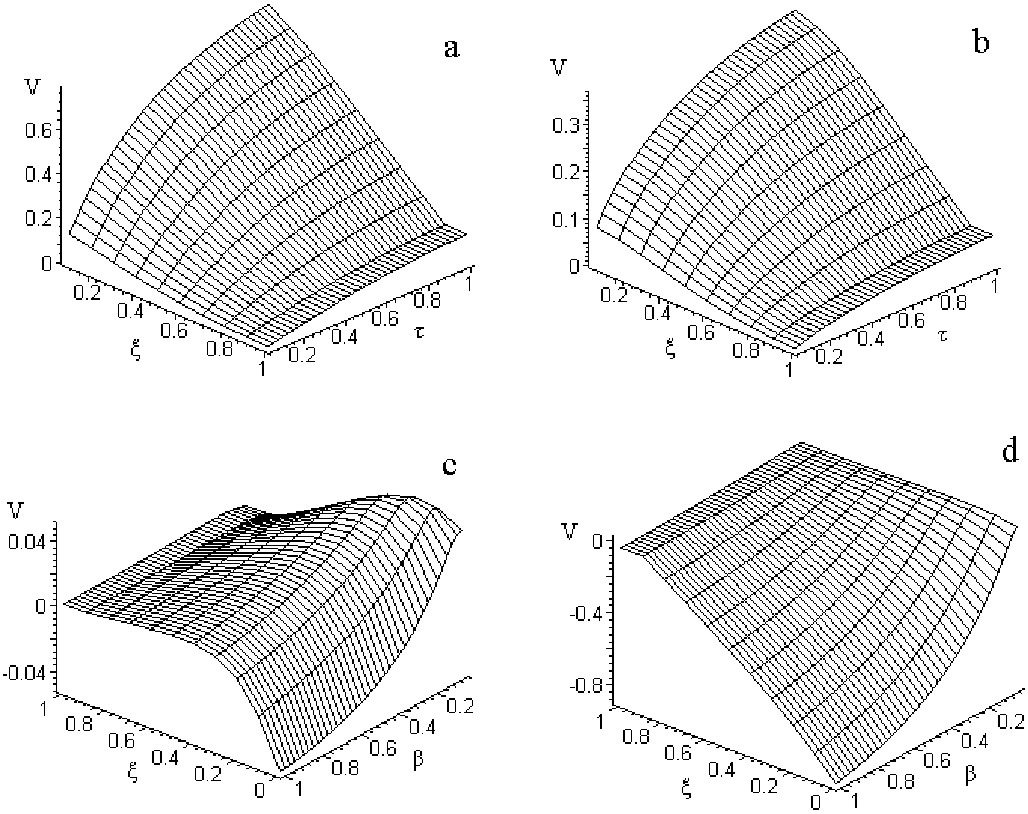

Fig. 3. Concentration fields of impurity atoms in film depending on initial mass flux $\dot{\chi}_0$: a – 0, b – 10, c – 20, d –40; $\alpha_c = 0.5$, $\alpha_j = 0.1$

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