EFFECT OF STRESSES AND STRAINS ON IMPURITY REDISTRIBUTION IN A PLATE UNDER UNIAXIAL LOADING

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A model for the saturation of the surface layer of a thin metal plate with an impurity from the environment under uniaxial mechanical loading is proposed and investigated. The effect of stresses and strains on the diffusion process is analyzed. It is shown that, first, due to the deformation of the crystal lattice of the base, stresses that occur in local volumes lead to a change in the diffusion activation energy; second, stresses influence impurity transfer (this effect is similar to mass transfer by pressure diffusion in liquids). The joint effect of the two types of influences of stresses and strains on the behavior of the system at various geometrical and physical sample parameters is numerically investigated.

Key words: diffusion, uniaxial loading, plane stress state, activation volume.

Introduction. As is known, stresses and strains occurring in the zone where diffusion takes place (diffusion zone) have an impact on diffusion processes. Many studies have been devoted to the investigation of this phenomenon (for instance, see [1-3]).

The appearance of concentration stresses in the case of a binary system is due, first, to the difference between the atomic sizes of the diffusing substance and the base, and, second, to the inequality of the partial diffusion coefficients of the impurity and base, which leads to inequality of the opposite partial fluxes and the appearance of redundant vacancies causing stresses [4]. The stresses caused by the appearance of atoms of another substance in the lattice of the base are called concentration stresses, and the stresses due to the difference in diffusion mobility between the atoms of the base and the impurity atoms are called diffusion stresses. It is difficult to separate one type of stresses from the other. Stresses and strains in the diffusion zone eventually occur due to heterogeneity of concentration fields. From now on, concentration stresses and strains will be considered from this perspective.

The dependence of diffusion processes on stresses has motivated the Development of methods for controlling impurity redistribution. One of these methods is the use of an additional external load. To investigate the role of external loading in the presence of internal stresses, it is necessary to solve the problem of mechanical equilibrium of the sample taking into account the possible feedback between diffusion and mechanical processes. In the case where inertia forces may be neglected (due to the low rate of diffusion processes) under quasistatic loading, the problem is divided into two parts: the problem of mechanical equilibrium and the nonlinear diffusion problem. The purpose of this work is to investigate the impact of various physical factors on the parameters of the diffusion zone under quasistatic uniaxial loading.

Problem of Mechanical Equilibrium. Let us consider a plate of length L, width h, and depth δ $(L \gg h \gg \delta)$ which is subjected to uniaxial mechanical loading. The magnitude of the external load p is specified. Impurity from the environment or impurity from a previously applied layer containing an excess of the diffusing element can penetrate deep into the sample through one of the plate surfaces (z = 0). Impurity redistribution is possible due to both diffusion and mechanical equilibrium.

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Fig. 1. Diagram of the problem.

If there is no diffusion in the z direction (i.e., the composition of the sample is homogeneous) and if the external load is uniformly distributed over the surfaces of the plate $y = \pm L/2$, we may assume that the sample is in a plane stress state.

If the impurity which is nonuniformly distributed over the surface layer z = 0 penetrates into the sample, the stress field becomes three-dimensional $\sigma_{ij} = \sigma_{ij}(x, y, z)$. Just as in the previous case, the stress state can be characterized by the components σ_{xx} , σ_{yy} , and τ_{xy} . In this case, a generalized plane stress state takes place [5] and boundary conditions on the surfaces are formulated for mean magnitudes:

$$\bar{\sigma}_{xx} = \frac{1}{\delta} \int_{0}^{\delta} \sigma_{xx}(x, y, z) \, dz, \qquad \bar{\sigma}_{yy} = \frac{1}{\delta} \int_{0}^{\delta} \sigma_{yy}(x, y, z) \, dz, \qquad \bar{\tau}_{xy} = \frac{1}{\delta} \int_{0}^{\delta} \tau_{xy}(x, y, z) \, dz$$

In this case, the loading conditions are formulated in the following way:

$$\bar{\sigma}_{yy} = p, \qquad \bar{\sigma}_{xx} = 0.$$

Since only stresses in the diffusion zone remote from loading surfaces are investigated in this work, we assume that $\sigma_{ij} = \sigma_{ij}(z)$ and $\varepsilon_{ij} = \varepsilon_{ij}(z)$. Then, the loading conditions take the form

$$p = \frac{1}{\delta} \int_{0}^{\delta} \sigma_{yy}(z) dz, \qquad 0 = \frac{1}{\delta} \int_{0}^{\delta} \sigma_{xx}(z) dz.$$
(1)

Using the conditions

$$0 = \frac{1}{\delta} \int_{0}^{\delta} \sigma_{yy}(z) z \, dz, \qquad 0 = \frac{1}{\delta} \int_{0}^{\delta} \sigma_{xx}(z) z \, dz, \qquad (2)$$

shear stresses and strains may be neglected. From the Duhamel–Neumann relation and the theory of mass elasticity [6], it follows that

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \delta_{ij}(\varepsilon_{kk}\lambda - Kw),$$

where

$$w = 3\Big(\sum_{k=i}^{n} \alpha_k (\eta_k - \eta_{k_0})\Big),$$

 λ and μ are the Lamé coefficient, K is the isothermal bulk compression modulus, η_k is the concentration of component k, α_k are the concentration expansion coefficients, k is the component number, and n is the total number of components; the subscript zero refers to the undeformed state. In this case, for the required components of the stress and strain tensors, we obtain

$$\varepsilon_{zz} = -\frac{\lambda}{\lambda + 2\mu} \left(\varepsilon_{xx} + \varepsilon_{yy} \right) + \frac{K}{\lambda + 2\mu} w,$$
(23)

$$\sigma_{xx} = -\frac{2\mu}{\lambda + 2\mu} [2(\lambda + \mu)\varepsilon_{xx} + \lambda\varepsilon_{yy} - Kw], \qquad (3)$$
$$\sigma_{yy} = -\frac{2\mu}{\lambda + 2\mu} [2(\lambda + \mu)\varepsilon_{yy} + \lambda\varepsilon_{xx} - Kw].$$

Just as in problems of thermoelasticity [5], to determine the components of the stress and strain tensors, we use compatibility equations because, in this case, the equilibrium equations are satisfied identically and they do not allow us to solve the problem of determining all components of the stress and strain tensors. In the problem under consideration, there are only two equations left (the remaining compatibility conditions are satisfied identically)

$$\frac{\partial^2 \varepsilon_{yy}}{\partial z^2} = 0, \qquad \frac{\partial^2 \varepsilon_{xx}}{\partial z^2} = 0,$$

the solutions of which are

$$\varepsilon_{xx} = Az + B, \qquad \varepsilon_{yy} = Cz + D.$$
 (4)

Substituting (4) into (3), we obtain

$$\sigma_{xx} = \frac{2\mu}{\lambda + 2\mu} [2(\lambda + \mu)(Az + B) + \lambda(Cz + D) - Kw],$$

$$\sigma_{yy} = \frac{2\mu}{\lambda + 2\mu} [2(\lambda + \mu)(Cz + D) + \lambda(Az + B) - Kw].$$

Using conditions (1) and (2) we obtain the system of linear equations for the integration constants A, B, C, and D:

$$\alpha A + \beta B + \gamma C + \lambda \delta D - F_1 = 0, \qquad \frac{2\mu}{\lambda + 2\mu} \left[\alpha C + \beta D + \gamma A + \lambda \delta B - F_1 \right] = p\delta,$$

$$\omega A + \alpha B + 2\delta \gamma C/3 + \gamma D - F_2 = 0, \qquad \omega C + \alpha D + 2\delta \gamma A/3 + \gamma B - F_2 = 0,$$

(5)

where

$$\begin{split} \alpha &= (\lambda + \mu)\delta^2 = \beta \delta/2, \quad \beta = 2(\lambda + \mu)\delta, \quad \omega = 2(\lambda + \mu)\delta^3/3 = \beta \delta^2/3, \quad \gamma = \lambda \delta^2/2, \\ F_1(t) &= K \int_0^{\delta} w \, dz, \qquad F_2(t) = K \int_0^{\delta} wz \, dz. \end{split}$$

The solution of system (5) is given by

$$A = \frac{\lambda p}{K\mu\delta} + \frac{4}{\delta^3 K} F_2 - \frac{2}{K} \frac{1}{\delta^2} F_1, \qquad B = -\frac{2}{3} \frac{p}{K\mu} \lambda - \frac{2}{\delta^2 K} F_2 + \frac{4}{3} \frac{1}{K\delta} F_1,$$
$$C = -\frac{2}{K\delta} \frac{\lambda + \mu}{\mu} p + \frac{4}{\delta^3 K} F_2 - \frac{2}{\delta^2 K} F_1, \qquad D = \frac{4}{3} \frac{\lambda + \mu}{K\mu} p - \frac{2}{K\delta^2} F_2 + \frac{4}{3\delta K} F_1.$$

Thus, the problem of mechanical equilibrium is solved. It is obvious that all coefficients are dependent upon the magnitude of the external load and the character of distribution of the diffusing substance.

Diffusion Problem. There are two possible types of stress effect on the diffusion process: 1) change in the diffusion coefficient due to changing activation volume [7]; 2) change in the mobility of impurity atoms in the stress field.

Let us consider in detail the concept of activation volume. Activation volume, which is one of the most important thermodynamic characteristics of diffusion, plays an important role in the case where it is necessary to investigate the effect of pressure or stresses on the behavior of the system. By definition, the activation volume equals the difference between the local volumes of the system in the basic state and in an activated state [8]. The magnitude of the activation volume makes it possible to judge the mechanism of the process; this is often used in experimental and theoretical works.

There are various ways to determine activation volume. In [9], in thermodynamic relations, for instance, in the Gibbs equation, volume change is identified with activation-volume change. Apparently, in [9] it is considered that the amount of substance is at least no less than 1 mole. A simple thermodynamic system obeys the Gibbs equation

$$dU = T \, dS - P \, dV,$$

where U is the internal energy, S is the entropy, T is the temperature, P is the pressure, and V is the volume. As in [9], we will assume that all quantities refer to 1 mole of substance Using the relation

$$G = U - TS + PV,$$

we find

$$dG = dU - T \, dS - S \, dT + P \, dV + V \, dP$$

or

$$dG = -S \, dT + V \, dP,$$

i.e.,

$$V = \left(\frac{\partial G}{\partial p}\right)_T.$$
(6)

Assuming that the sum of all particles of a multicomponent system also corresponds to 1 mole of substance, we write the following equation for the internal energy change of this system:

$$dU = T \, dS + P \, dV + \sum_{k=1}^{n} g_k \, dN_k$$

It is obvious that definition (6) does not change:

$$V = \left(\frac{\partial G}{\partial p}\right)_{T,N_k},\tag{7}$$

but the volume happens to be a function of composition. Expression (6) or (7) may be considered as a formal definition of the activation volume for 1 mole of substance.

Assuming that the temperature dependence of the self-diffusion coefficient obeys the Arrhenius equation [10]

$$D^* = D_0 \exp\left(-\Delta G/(RT)\right),$$

we obtain

$$\Delta G = -RT \ln \left(D^* / D_0 \right).$$

Hence,

$$V = -RT \left(\frac{\partial \ln D^*}{\partial p}\right)_T + RT \left(\frac{\partial \ln D_0}{\partial p}\right)_T,\tag{8}$$

where D_0 is the preexponential factor that contains the entropic factor. As a rule, the contribution of the second summand to Eq. (8) is no less than 10% of the contribution of the first one; therefore, the second summand is often neglected [10] or is included in the preexponential factor. For this reason, the activation volume is defined as

$$V = -RT \left(\frac{\partial \ln D^*}{\partial p}\right)_T.$$

 $D^* = D_1 \exp\left(-\Delta F/(BT)\right)$

In view of the aforesaid, the equation for the self-diffusion coefficient can be written as

where
$$F = U - TS = G - PV$$
 and $dF = -S dT - P dV - \sum_{k=1}^{n} g_k dN_k$. Then,
 $D^* = D_1 \exp\left(-\frac{(\Delta F)_V - P dV}{RT}\right).$

In the deformed system, we have

$$dG = -S \, dT + \varepsilon_{ij} \, d\sigma_{ij} \, \frac{m_{\text{mean}}}{\rho} + \sum_{k=1}^{n} g_k \, dN_k,$$
$$dF = -S \, dT + \sigma_{ij} \, d\varepsilon_{ij} \, \frac{m_{\text{mean}}}{\rho} + \sum_{k=1}^{n} g_k \, dN_k,$$

where all quantities are functions of coordinate and time. Then,

$$D^* = D_1 \exp\left(-\frac{E_a + \sigma_{ij} \, d\varepsilon_{ij}}{RT} \, \frac{m_{\text{mean}}}{\rho}\right) = D'_0 \exp\left(-\frac{\sigma_{ij} \, d\varepsilon_{ij}}{RT} \, \frac{m_{\text{mean}}}{\rho}\right)$$
$$\approx D'_0 \exp\left(-\frac{k_0 \sigma_{kk} \, d\varepsilon_{kk}}{RT} \, \frac{m_{\text{mean}}}{\rho}\right). \tag{9}$$

Here m_{mean} is the mean molar mass and ρ is the density of the system. The first invariant of the stress tensor is the local pressure, and the quantity $(m_{\text{mean}}/\rho) d\varepsilon_{kk}$ is the local volume change per 1 mole of substance. In Eq. (9), k_0 is the proportionality coefficient which shows what part of the work is used to decrease the diffusion activation energy. This coefficient (we call it the sensitivity coefficient of diffusion to stress work) is a structurally dependent quantity, i.e., its value depends on the structure and physical features of the deformed medium. This allows us to take into account the effect of stresses and strains on the diffusion coefficient. The generalization (9) corresponds to the equation

$$D^* = D'_0 \exp\left(-k\Pi/(RT)\right),$$
(10)

where $k = k_0 m_{\text{mean}} / \rho$ and $\Pi = -(\sigma_{xx} \varepsilon_{xx} + \sigma_{yy} \varepsilon_{yy} + \sigma_{zz} \varepsilon_{zz})$.

The second type of effect of stresses on the deformation involves a direct change in the mobility of impurity atoms in the stress field, which is similar to the phenomenon of pressure diffusion in liquids.

According to thermodynamic theory [12], the flux of a component in a binary system under isothermal conditions can be represented as

$$J = -D_2 \frac{\partial \eta}{\partial z} + B_2 \eta \frac{\partial}{\partial z} \sigma_{kk}, \tag{11}$$

where the subscript 2 refers to the diffusing substance, η is the mass concentration of the diffusing substance, and $\sigma_{kk} = \sigma_{xx} + \sigma_{yy} + \sigma_{zz}$. To represent the coefficient D_2 , we use formula (10) and the definition which relates it to the self-diffusion coefficient:

 $D_2 = D_2^* f(\eta), \qquad D_2^* = D_0' \exp(-k \Pi/(RT)).$

The coefficient of transfer due to the stresses B_2 for the diffusing substance is given by the equality

$$B_2 = \alpha_2 D_2^* m_2 / (\rho RT),$$

where α_2 is the coefficient of concentration expansion of the diffusing substance and m_2 is the molar mass of the diffusing substance.

In fact, Eq. (11) is an extension of the Fick law to a deformable medium. Using the second Fick law

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial z} J$$

and the equation for the flux (11), we obtain

$$\frac{\partial \eta}{\partial t} = \frac{\partial}{\partial z} D_2 \frac{\partial \eta}{\partial z} - \frac{\partial}{\partial z} B_2 \eta \frac{\partial}{\partial z} \sigma_{kk}$$

Using the above solution of the problem of mechanical equilibrium to complete the formulation of the diffusion problem, we have the equation

$$\frac{\partial \eta}{\partial t} = \frac{\partial}{\partial z} \left[\left(D_2 + B_2 \eta \, \frac{12\mu K \,\Delta \alpha}{\lambda + 2\mu} \right) \frac{\partial \eta}{\partial z} - B_2 \eta \, \frac{6\mu K}{\lambda + 2\mu} \left(A + C \right) \right] \tag{12}$$

 $(\Delta \alpha = \alpha_2 - \alpha_1)$ is the difference between the coefficients of concentration expansion of the diffusing substance and the base material) with the boundary conditions

$$z = 0; \qquad \eta = \eta_0,$$

$$z = \delta; \qquad J = 0 \quad \text{or} \quad D_0 \frac{\partial \eta}{\partial z} = B_0 \eta \frac{\partial \sigma_{kk}}{\partial z}.$$

At the initial time, $\eta = 0$.

Transformation to Dimensionless Variables. Since the purpose of this work is to investigate the role of various physical phenomena under changing loading conditions, we perform a detailed parametric investigation. For this, we transform to dimensionless variables:

$$\eta, \quad \tau = t \frac{D'_0}{\delta^2}, \quad \xi = \frac{z}{\delta}, \quad s_{ij} = \frac{\sigma_{ij}}{3K\alpha_2}, \quad e_{ij} = \frac{\varepsilon_{ij}}{3\alpha_2}.$$

Then, Eq. (12) with the boundary and initial conditions becomes

$$\frac{\partial \eta}{\partial \tau} = \frac{\partial}{\partial \xi} \left(\bar{D}_{\text{eff}} \frac{\partial \eta}{\partial \xi} \right) - \bar{V}_{\text{eff}} \frac{\partial \eta}{\partial \xi},$$

$$\xi = 0; \quad \eta = \eta_0, \qquad \xi = 1; \quad J = -\bar{D}_{\text{eff}} \frac{\partial \eta}{\partial \xi} - \bar{V}_{\text{eff}} \eta = 0, \qquad \tau = 0; \quad \eta = 0,$$
(13)

where

$$\begin{split} \bar{D}_{\text{eff}} &= \varphi(x) \Big(f(\eta) + \frac{2h_1}{2h_2 + 1} \eta \Omega \alpha_c \Big), \qquad \bar{V}_{\text{eff}} = \varphi(x) \Omega \frac{6}{2h_2 + 1} \left(-S^e - 2\alpha_c h_1 I_1 + 4\alpha_c h_1 I_2 \right), \\ \varphi(x) &= \exp\left(x \Omega \frac{3}{3 - h_1} \bar{\Pi}\right), \qquad \bar{\Pi} = s_{11} e_{11} + s_{22} e_{22}, \\ I_1 &= \int_0^1 \eta \, d\xi, \qquad I_2 = \int_0^1 \eta \xi \, d\xi, \\ h_1 &= \frac{2\mu}{\lambda + 2\mu}, \qquad h_2 = \frac{\lambda}{\lambda + 2\mu} = 1 - h_1, \qquad S^e = \frac{p}{3K\alpha_2}, \\ \Omega &= \frac{9\alpha_2^2 m_2 K^2}{RT \rho(\lambda + 2\mu)}, \qquad \alpha_c = \frac{\Delta \alpha}{\alpha_2}, \qquad x = k \frac{\rho}{m_2}. \end{split}$$
 Let us represent the nonzero components of the stress and strain tensors as

 $e_{11} = x_1\xi + y_1, \qquad e_{22} = x_2\xi + y_2,$

$$e_{33} = -h_2(x_1\xi + x_2\xi + y_1 + y_2) + \frac{1+2h_2}{3}\alpha_c\eta,$$

$$s_{11} = h_1\Big(\frac{1+h_2}{1+2h_2}(x_1\xi + y_1) + \frac{3h_2}{1+2h_2}(x_2\xi + y_2) - \alpha_c\eta\Big),$$

$$s_{22} = h_1\Big(\frac{1+h_2}{1+2h_2}(x_2\xi + y_2) + \frac{3h_2}{1+2h_2}(x_1\xi + y_1) - \alpha_c\eta\Big).$$

Here

$$h_{2} = 1 - h_{1}, \qquad x_{1} = \frac{2h_{2}}{h_{1}}S^{e} + 4\alpha_{c}I_{2} - 2\alpha_{c}I_{1}, \qquad y_{1} = \frac{4h_{2}}{3h_{1}}S^{e} - 2\alpha_{c}I_{2} + \frac{4}{3}\alpha_{c}I_{1}$$
$$x_{2} = -2\frac{1 + h_{2}}{h_{1}}S^{e} + 4\alpha_{c}I_{2} - 2\alpha_{c}I_{1}, \qquad y_{2} = 4\frac{1 + h_{2}}{3h_{1}}S^{e} - 2\alpha_{c}I_{2} + \frac{4}{3}\alpha_{c}I_{1}.$$

The model contains five parameters: Ω , α_c , \mathfrak{R} , S^e , and h_1 . Using the terminology adopted for the classical equation of mass transfer, we call \bar{D}_{eff} the effective diffusion coefficient, and \bar{V}_{eff} the convective velocity. The



Fig. 2. Dependence of the mass concentration on the parameter ξ for and $\alpha_c = 0.2$, and $S^e = 0$, $\omega = 0$ (a) and 100 (b), and various times: $\tau = 0.0001$ (1), 0.0004(2), 0.0008 (3), 0.0012 (4), 0.0016 (5), 0.0020 (6), and 0.0025 (7); solid curves refer to the numerical calculation and dash-dot curves to the distributions (14).

relative coefficient of concentration expansion α_c characterizes the difference between the atomic volumes of the diffusing substance and matrix; therefore it can take both positive and negative values. The coefficient Ω , which is called the connectivity coefficient, can vary over a wide rage and increase with increasing temperature because of the dependence of the mechanical moduli on temperature [13]. The parameter h_1 characterizes the mechanical properties of the medium. The coefficient x is a dimensionless sensitivity coefficient, whose increase leads to an increase in the activation volume of the system.

The problem (13) was solved numerically with the use of an implicit difference scheme and the sweep method. In the numerical calculations, we investigated the effect of the sensitivity coefficient x on the behavior of the system by varying the external load S^e and the relative coefficient of concentration expansion α_c , which characterize the difference in atomic volume between the diffusing substance and the matrix. The coefficients Ω and h_1 are fixed ($\Omega = 10, h_1 = 0.41$).

Results of Numerical Calculations. Typical concentration distributions in the diffusion zone without external loading for $\alpha_c = 0.2$ (i.e., for the case where the atomic volume of the diffusing substance is greater than the atomic volume of the base) are presented in Fig. 2. If $\alpha = 0$ (see Fig. 2a), then, with this set of parameters, the concentration distribution is qualitatively similar to the solution of the simplest diffusion equation

$$\frac{\partial \eta}{\partial t} = \frac{\partial^2 \eta}{\partial \xi},$$

$$\xi = 0; \quad \eta = 1, \qquad \xi \to \infty, \quad \frac{\partial \eta}{\partial \xi},$$

$$\eta = \operatorname{erfc}\left(\xi/(2\sqrt{\tau}\,)\right). \tag{14}$$

which takes the form

ualitatively different profile (see Fig. 2b). Increasing the sensitivity coefficient affects

Setting x = 100, we obtain a qualitatively different profile (see Fig. 2b). Increasing the sensitivity coefficient affects the behavior of the system in the following way. Despite the fact that the effective diffusion coefficient \bar{D}_{eff} increases (Fig. 3a), the mean concentration of the diffusing substance in the plate (Fig. 3b), calculated by the formula

$$\langle \eta \rangle = \int_{0}^{1} \eta(\xi) \, d\xi,$$

decreases with increasing \hat{x} because of the compressive stresses occurring near the surface $\xi = 0$. This behavior of the integral characteristic may be due to an increase in the absolute value of the convective velocity \bar{V}_{eff} (Fig. 4a). 428



Fig. 3. Curves of the effective diffusion coefficient versus parameter ξ at $\tau = 0.0016$ (a) and curves of the mass concentration of the diffusing substance in the plate versus time (b) for $S^e = 0$ and $\alpha = 0$ (1), 10 (2), 50 (3), and 100 (4); solid and dashed curves refer to $\alpha_c = 0.2$ and -0.2, respectively.



Fig. 4. Curves of the convective velocity (a) and width of the diffusion front (b) versus time for $\alpha_c = 0.2$ and $S^e = 0$ (1), 0.01 (2), 0.05 (3), and 0.10 (4); solid curves refer to x = 100 and dot-dashed curves to x = 0.

The width of the diffusion zone Δ_{ξ} which is determined from the typical value of the concentration of the diffusing substance in the sample $\eta(\Delta_{\xi}, \tau) = 0.005$ also decreases (Fig. 4b) but not significantly.

Due to the external loading, the width of the diffusion front increases and the effective velocity becomes almost zero when $S^e = 0.1$.

Dependences of the mass concentration on the parameter ξ for two values of x and $S^e = 0.1$ are presented in Fig. 5. One can see that the external load prevents the penetration of impurity into the material; if the atomic volume of the diffusing material is greater than the atomic volume of the base ($\alpha_c > 0$), the dependence of the sensitivity coefficient of diffusion on stress, in fact, leads to the occurrence of a solubility limit of the diffusing substance in the base (dash-dot curves in Fig. 5). If the atomic volume of the diffusing substance is smaller than that of the base ($\alpha_c = -0.2$), the effective diffusion coefficient increases with increasing sensitivity coefficient (dashed



Fig. 5. Mass concentration versus parameter ξ for $S^e = 0.1$ at various times: $\tau = 0.0001$ (1), 0.0012 (2), and 0.0025 (3); dash-dot curves refer to $\alpha = 80$ and $\alpha_c = 0.2$, solid curves to $\alpha = 20$ and $\alpha_c = 0.2$, and dashed curves to $\alpha = 20$ and $\alpha_c = -0.2$.

curves in Fig. 3); this, in turn, influences the behavior of $\langle \eta \rangle$ and the width of the diffusion zone. If $\alpha_c < 0$, then, for the chosen set of parameters, the concentration of the diffusing substance in the base increases (dashed curves in Fig. 3b) and the width of the diffusion zone for the same value of x exceeds the width of the diffusion zone for $\alpha_c > 0$ (cf. the solid and dashed curves in Fig. 5). The behavior of the convective velocity and the width of the diffusion zone remain unchanged, indicating the predominant role of the second type of effect of stresses and strains on diffusion under loading.

Conclusions. A model of impurity redistribution was proposed which takes into account the effect of stresses and strains on diffusion processes in a plate in a plane stress state. It was shown that the solubility limit of the diffusing substance in the base occurs because of the dependence of the sensitivity coefficient on stresses. The stress effect on the redistribution of impurities with various atomic volumes was considered.

REFERENCES

- 1. V. S. Eremeev, Diffusion and Stresses [in Russian], Énergoatomizdat, Moscow (1984).
- 2. J. P. Stark and S. J. Rothman, "Solid-state diffusion," Physics Today, 30, Issue 8, 53 (1977).
- K. P. Gurov, V. A. Kartashkin, and Y. A. Ugaste, *Interdiffusion in Multiphase Metal Systems* [in Russian], Nauka, Moscow (1981).
- 4. Ya. E. Geguzin, *Diffusion Zone* [in Russian], Nauka, Moscow (1979).
- 5. B. A. Boley and J. H. Weiner, *Theory of Thermal Stresses*, Wiley, New York (1960).
- 6. T. D. Shermergor, Elasticity Theory for Microinhomogeneous Media [in Russian], Nauka, Moscow (1977).
- J. Aziz Michael, "Thermodynamics of diffusion under pressure and stress: Relation to point defect mechan isms," Appl. Phys. Lett., 70, No. 21, 2810–2812 (1997).
- B. B. Straumal, L. M. Klinger, and L. S. Shvindlerman, "Indium diffusion in tin-germanium single interfaces at high pressures," *Fiz. Tverd. Tela*, 25, No. 7, 2085–2089 (1983).
- 9. H. Mehrer, Diffusion in Solids, Springer, Berlin (2007). (Springer Ser. in Solid-State Sci.; Vol. 155.)
- R. N. Jeffery and D. Lazarus, "Calculating activation volumes and activation energies from diffusion measurements," J. Appl. Phys., 41, 3186–3187 (1970).
- 11. B. Y. Lyubov, Diffusion Processes in Inhomogeneous Solid Media [in Russian], Nauka, Moscow (1981).
- A. G. Knyazeva, "Diffusion and rheology in locally equilibrium thermodynamics," in: Mathematical Modeling of System and Processes (collected scientific papers), No. 13 (2005), pp. 45–60.
- A. G. Knyazeva and Y. G. Donskaya, "A diffusion-deformation model for the growth of a spherical nucleus of a solid-state reaction product," *Combust., Expl., Shock Waves*, 33, No. 2, 168–182 (1997).