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Mass transfer in field of fast-moving deformation disturbance

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Abstract

The mass transfer of interstitial impurities in a crystalline lattice under the influence of the fast-moving deformation disturbance of the type of a shock wave is considered. The velocity of the movement of the disturbance is supposed to be compared with the characteristic velocity of the relaxation of the diffusion flux to its local equilibrium value determined by the Fick's law. The similar situation occurs in a number of experiments on the exposure of a solid to dynamical external loads giving rise to such fast hydrodynamical processes in a sample that the local equilibrium assumption, normally assumed for the macroscopic description of transport processes, is no longer valid. Considering the diffusion flux among the set of independent variables we have derived a set of coupled hydrodynamic equations describing nonequilibrium behavior of a solid in the absence of local equilibrium in the system. Within the scope of the proposed model it has been shown that in comparison with the local equilibrium system an enhanced mass transfer occurs under local nonequilibrium conditions.

1. Introduction

In recent experiments [1,2] on the irradiation of the thin-film metal samples by high power ion beams (HPIB) thin films of aluminium and silver on the niobium and copper substrates were irradiated by carbon ions. The considerable penetration depth of the film atoms into the substrate, exceeding the length of the projective path of carbon atoms, has been revealed in the irradiated samples. The estimation of the effective diffusion coefficients has given the anomalously high magnitudes [1–3] $D \sim 10^{-2}$–10^{-4} sm^2 s^{-1}. The effect of the intensive mass transfer by HPIB irradiation has been registered earlier in work [4]. A similar effect has also been observed at electron and laser irradiation of solids [5–7] and at shock loading of the samples [8,9]. The complete explanation of this phenomenon within the scope of the known diffusion mechanisms has not yet been found.

One of possible causes responsible for the accelerated mass transport is the shock wave, generated by irradiation, which is able to induce the enhanced migration of atoms on large depths [2]. In investigating this mechanism of diffusion within the scope of the hydrodynamic description usually one starts from the known diffusion equation in which, according to Fick's law, the diffusion flux is defined by gradients of the concentration of a diffusing substance, a pressure and a temperature. Such approach is well justified if the disturbances occurring in a system change slowly enough in comparison with the characteristic rate at which the given system approaches the local equilibrium. Meanwhile the interaction of particle beams with a solid induces in the latter rather fast hydrodynamic processes with the characteristic times of order or less than 10^{-8} s and the shock velocity can reach several kilometers per second. Under these conditions one should expect a significant deviation of the system state from local equilibrium and the violation of Fick's law and take into account an influence of the relaxation of the system on the process of mass transport.

In this paper we want to study within a simple model basic features the impurity transfer in the relaxating solid medium. More specifically the purpose of the work is to research the interstitial diffusion in the field of the fast moving deformation disturbance of the type of the shock wave. The velocity of the movement of this disturbance is supposed to be compared with the velocity of

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Nomenclature

c	mass concentration of interstitials
E	energy density
$\mathbf{J}$	diffusion flux density of interstitials
p	pressure
$\mathbf{Q}$	energy flux density
$\mathbf{q}$	heat flux density
S	entropy density of the medium
T	temperature
t	time
$\mathbf{u}$	displacement vector
u_{ij}	infinitesimal strain tensor
V	velocity of the deformation disturbance
V_D	speed of the propagation of concentration perturbations
$\mathbf{v}$	mass velocity
x_i	coordinate

Greek symbols

δ	width of the transition region
μ	chemical potential of the medium
ν	chemical potential of the interstitials per unit of volume
ξ	dimensionless coordinate
Π_{ik}	the tensor momentum flux density
π_{ij}	viscous pressure tensor
ρ	total mass density
σ_{ij}	elastic stress tensor
τ	relaxation time of the diffusion flux
$\varphi = V/V_D$	constant value

the propagation of concentration disturbances in the medium. The latter condition just defines the condition of absence of local equilibrium in the system [11]. The task is also interest in connection with shock-compression experiments with metals containing considerable atomic concentrations of interstitial hydrogen [12,13].

The description of the fast hydrodynamical processes requires an extended number of independent variables, defining the nonequilibrium state of a medium, in comparison with conventional hydrodynamics. During the course of short enough the characteristic time intervals, in particular, the diffusion flux may not have time to relax to its local equilibrium value, defined by Fick's law and it should be considered as independent variable obeying some relaxation equation. The dissipative fluxes (diffusion flux, viscous pressure tensor, heat flux) included in the local conservative laws of mass, momentum and energy are frequently exploited as additional independent variables [10,11].

In Section 2 we determine the total set of the independent variables suitable for the description of the fast hydrodynamical processes in the crystalline solid with interstitials. For these variables the derivation of the set of the coupled hydrodynamical equations, including a relaxation equation for the diffusion flux is given. Section 3 is devoted to the investigation of the mass transport in the field of fast-moving deformation disturbance of the crystal in the absence of local equilibrium in the system. Resume and concluding remarks are given in Section 4.

2. Derivation of hydrodynamic equations

In this section we want to derive the set of equations relevant for the description of fast hydrodynamical processes in the crystalline solid with interstitial impurities. The complete set of the hydrodynamical equations has to contain the local conservation laws of mass, momentum and the equation for the entropy production

$$\frac{\partial\rho}{\partial t} + \operatorname{div}\rho\mathbf{v} = 0, \tag{1}$$

$$\frac{\partial(\rho v_i)}{\partial t} + \frac{\partial\Pi_{ik}}{\partial x_k} = 0, \tag{2}$$

$$\frac{\partial S}{\partial t} + \operatorname{div}\left(S\mathbf{v} + \frac{\mathbf{q}}{T} - \frac{\nu}{\rho T}\mathbf{J}\right) = \frac{R}{T}. \tag{3}$$

Here ρ is the total mass density of the medium (lattice plus interstitials), $\mathbf{v}$ is the mass velocity, S is the entropy density of the medium, Π_{ik} is the tensor momentum flux density, $\mathbf{q}$ is the heat flux density, $\mathbf{J}$ is the diffusion flux density of interstitials, ν and T are the chemical potential of the interstitials per unit of volume and the absolute temperature, respectively, and R ($R > 0$) is the dissipative function of the medium; summation over repeated Latin indices is implied.

Further we suppose that a concentration of vacancies is negligible or their mobility is significantly less than the mobility of interstitials so that the mass transport occurs mainly by the interstitial motion. Introducing the mass concentration of the interstitial particles c we write down the continuity equation for the interstitial density $c\rho$ as follows:

$$\frac{\partial(c\rho)}{\partial t} + \operatorname{div}(c\rho\mathbf{v} + \mathbf{J}) = 0. \tag{4}$$

It should be noted that the diffusion flux $\mathbf{J}$, appearing in Eqs. (3) and (4), is determined in a rest frame (moving with velocity $\mathbf{v}$ relative to the laboratory frame). Meanwhile for a crystal it is convenient to determine the diffusion flux $\mathbf{J}_{\mathrm{L}}$ relative to a lattice. It is easy to see that both fluxes are related by $\mathbf{J} = (1 - c)\mathbf{J}_{\mathrm{L}}$. As the mass concentration $c \sim m_{\mathrm{p}}/m_{\mathrm{L}}$, where m_{p} and m_{L} are masses of an impurity particle and a host atom, then for light impurities (type of hydrogen), occurring into a matrix of heavy atoms, $c \ll 1$ even for the finite atomic concentration. Because of this $\mathbf{J} \simeq \mathbf{J}_{\mathrm{L}}$.

The variables ρ, $\mathbf{v}$, c, S, (or T) define conventional set of the independent hydrodynamical variables for a "fluid-like" medium. A solid with point defects has the extra independent hydrodynamical variable. This is a displacement vector $\mathbf{u}$ defining displacement of lattice sites [14]. In addition, according to above said, in the case of fast processes the dissipative fluxes–diffusion flux $\mathbf{J}$, heat flux $\mathbf{q}$ and viscous pressure tensor π_{ik} must be included among the set of independent variables. For simplicity we shall assume that the relaxation times of fluxes $\mathbf{q}$ and π_{ik} are considerably less than the relaxation time of diffusion flux and during characteristic time of the process under consideration the fluxes $\mathbf{q}$ and π_{ik} have time to relax to their local equilibrium values [11]. In this case diffusion flux $\mathbf{J}$ is the only new independent variable.

Thus we assume that quantities ρ, $\mathbf{v}$, c, S, $\mathbf{u}$, $\mathbf{J}$ completely define the nonequilibrium state of the system. For such set variables the set of the hydrodynamical equations (1)–(4) has to be supplemented by the equations for the displacement vector $\mathbf{u}$ and the diffusion flux $\mathbf{J}$. To derive these equations and define the still unknown Π_{ik}, $\mathbf{q}$ and R, appearing in Eqs. (1)–(4), we use the method originally applied in the theory of the superfluids for the derivation of the equations of the two-fluid hydrodynamics [15]. The main idea, in the given case, is as follows. We shall find these quantities so that the conservation energy law

$$\frac{\partial E}{\partial t} + \operatorname{div}\mathbf{Q} = 0, \tag{5}$$

would follow from Eqs. (1)–(4) and the equations for $\dot{\mathbf{u}}$, $\dot{\mathbf{J}}$ (an upper dot denotes the time derivative). In Eq. (5) E and $\mathbf{Q}$ are the energy density and the energy flux density of the medium, respectively.

The energy E is related by the Gallilean transformation to its value E_0 in the frame, where a given element of the volume of the medium rests, by the relationship

$$E = E_0 + \frac{\rho v^2}{2}. \tag{6}$$

Let us now write down the differential of E_0, considered as a function of S, ρ, c, $\mathbf{J}$ and the infinitesimal strain tensor u_{ij} in the form

$$\mathrm{d}E_0 = T\,\mathrm{d}S + \mu\,\mathrm{d}\rho + \nu\,\mathrm{d}c + \tilde{\sigma}_{ij}\,\mathrm{d}\tilde{u}_{ij} + \mathbf{w}\cdot\mathrm{d}\mathbf{J}, \tag{7}$$

here μ is the chemical potential of the medium, $\mathbf{w} = \partial E_0/\partial\mathbf{J}$ is the conjugate variables with $\mathbf{J}$, and σ_{ij} is the symmetric, elastic stress tensor; here and further the tilde is used to denote the traceless part of a tensor. In Eq. (7) it has been taken into account that the variation du_{ii} of sum of diagonal components of the strain tensor u_{ij} is determined by the variation of the density $\mathrm{d}\rho$.

Differentiating Eq. (6) with respect to time and using Eq. (7), one obtains

$$\frac{\partial E}{\partial t} = \frac{\partial}{\partial t}\left(\frac{\rho v^2}{2}\right) + T\frac{\partial S}{\partial t} + \mu\frac{\partial \rho}{\partial t} + \nu\frac{\partial c}{\partial t} + \tilde{\sigma}_{ij}\frac{\partial \dot{u}_i}{\partial x_j} + w_i\dot{J}_i. \tag{8}$$

Employing Eqs. (1)–(4) we can write down the time derivatives as

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{\rho v^2}{2}\right) &= -\frac{v^2}{2}\frac{\partial\rho}{\partial t} + v_i\frac{\partial(\rho v_i)}{\partial t}\\ &= -\operatorname{div}\left(\frac{\rho v^2}{2}\mathbf{v}\right) - v_i\frac{\partial}{\partial x_k}(\Pi_{ik} - \rho v_i v_k),\end{aligned} \tag{9}$$

$$\begin{aligned}T\dot{S} &= -T\operatorname{div}\left(S\mathbf{v} + \frac{\mathbf{q}}{T} - \frac{\nu}{\rho T}\mathbf{J}\right) + R\\ &= -\operatorname{div}\left(TS\mathbf{v} + \mathbf{q} - \frac{\nu}{\rho}\mathbf{J}\right) + \mathbf{v}\cdot\nabla(TS) - T\mathbf{v}\cdot\nabla S\\ &\quad - \mathbf{J}\cdot\nabla\left(\frac{\nu}{\rho}\right) + R + \mathbf{q}\cdot\frac{\nabla T}{T} + T\mathbf{J}\cdot\nabla\left(\frac{\nu}{\rho T}\right),\end{aligned} \tag{10}$$

$$\nu\dot{c} = -\nu\mathbf{v}\cdot\nabla c - \operatorname{div}\left(\frac{\nu}{\rho}\mathbf{J}\right) + \mathbf{J}\cdot\nabla\left(\frac{\nu}{\rho}\right), \tag{11}$$

$$\mu\dot{\rho} = -\operatorname{div}(\mu\rho\mathbf{v}) + \mathbf{v}\cdot\nabla(\mu\rho) - \mu\mathbf{v}\cdot\nabla\rho, \tag{12}$$

$$\tilde{\sigma}_{ij}\frac{\partial\dot{u}_i}{\partial x_j} = \frac{\partial}{\partial x_j}(\tilde{\sigma}_{ij}\dot{u}_i) - \dot{u}_i\frac{\partial\tilde{\sigma}_{ij}}{\partial x_j}. \tag{13}$$

Inserting Eqs. (9)–(13) into Eq. (8) and taking into account that

$$\nabla E_0 = T\nabla S + \mu\nabla\rho + \nu\nabla c + \tilde{\sigma}_{ij}\nabla\left(\frac{\partial u_i}{\partial x_j}\right) + w_i\nabla J_i,$$

after long, though simple, transformations, one has

$$\begin{aligned}\dot{E} &= -\operatorname{div}\left\{\frac{\rho v^2}{2}\mathbf{v} + TS\mathbf{v} + \mu\rho\mathbf{v} + \mathbf{q} - \dot{\mathbf{u}}\cdot\tilde{\sigma}\right\}\\ &\quad + v_k\tilde{\sigma}_{ij}\frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_k}\right) - v_i\frac{\partial}{\partial x_k}(\Pi_{ik} - \rho v_i v_k + \tilde{\sigma}_{ik})\\ &\quad + \mathbf{v}\cdot\nabla(-E_0 + TS + \mu\rho) + R + \mathbf{q}\cdot\frac{\nabla T}{T}\\ &\quad + T\mathbf{J}\cdot\nabla\left(\frac{\nu}{\rho T}\right) + (v_i - \dot{u}_i)\frac{\partial\tilde{\sigma}_{ij}}{\partial x_k} + w_i(\dot{J}_i + \mathbf{v}\cdot\nabla J_i).\end{aligned} \tag{14}$$

Finally Eq. (14) can be rewritten as

$$\begin{aligned}&\dot{E} + \operatorname{div}\left\{\frac{\rho v^2}{2}\mathbf{v} + TS\mathbf{v} + \mu\rho\mathbf{v} + \mathbf{q} - \dot{\mathbf{u}}\cdot\tilde{\sigma} + \mathbf{v}\cdot\pi\right\}\\ &\quad = R + \mathbf{q}\frac{\nabla T}{T} + \pi_{ik}\frac{\partial v_i}{\partial x_k} + T\mathbf{J}\cdot\nabla\left(\frac{\nu}{\rho T}\right)\\ &\qquad + \left(v_i - \frac{\mathrm{d}u_i}{\mathrm{d}t}\right)\frac{\partial\tilde{\sigma}_{ik}}{\partial x_k} + w_i\frac{\mathrm{d}J_i}{\mathrm{d}t},\end{aligned} \tag{15}$$

where the viscous pressure tensor π_{ik} is defined from the equality

$$\Pi_{ik} = \rho v_i v_k + p\delta_{ik} - \tilde{\sigma}_{ik} + \pi_{ik} \tag{16}$$

and the notations have been introduced

$$p = -E_0 + TS + \mu\rho, \tag{17}$$

and for the material derivative $\mathrm{d}/\mathrm{d}t = \partial/\partial t + \mathbf{v}\cdot\nabla$.

In the derivation Eq. (16) we have neglected the term of the second order of infinitesimal in strains $\tilde{\sigma}_{jk}\partial u_i/\partial x_j$ in comparison with the linear term $\tilde{\sigma}_{ik}$.

Eq. (16) defines the momentum flux density, where p can be interpreted as "pressure" in the medium. Comparing further Eq. (15) with the energy conservation law (5) we define the energy flux density $\mathbf{Q}$ and the dissipative function R as

$$\mathbf{Q} = \left(\frac{\rho v^2}{2} + E_0 + p\right)\mathbf{v} + \mathbf{q} - \dot{\mathbf{u}}\cdot\tilde{\sigma} + \mathbf{v}\cdot\pi \tag{18}$$

and

$$R = -\mathbf{q}\cdot\frac{\nabla T}{T} - \pi_{ik}\frac{\partial v_i}{\partial x_k} - T\mathbf{J}\cdot\nabla\left(\frac{v}{\rho T}\right) - \left(v_i - \frac{\mathrm{d}u_i}{\mathrm{d}t}\right)\frac{\partial\tilde{\sigma}_{ik}}{\partial x_k} - w_i\frac{\mathrm{d}J_i}{\mathrm{d}t}. \tag{19}$$

Since the energy E_0 is even under time reversal, the dependence between E_0 and J_i in the simplest approximation has the form

$$E_0 = \tfrac{1}{2}W_{ij}J_iJ_j + \cdots, \quad W_{ij} = W_{ji},$$

where W_{ij} is assumed to be constants and dots denote the terms of the highest order of infinitesimal in fluxes. In this case

$$w_i = \frac{\partial E_0}{\partial J_i} = W_{ik}J_k \tag{20}$$

and the dissipative function R can be rewritten as

$$R = -\mathbf{q}\cdot\frac{\nabla T}{T} - \pi_{ik}\frac{\partial v_i}{\partial x_k} - \left(v_i - \frac{\mathrm{d}u_i}{\mathrm{d}t}\right)\frac{\partial\tilde{\sigma}_{ik}}{\partial x_k} - J_iX_i, \tag{21}$$

where

$$X_i = T\frac{\partial}{\partial x_i}\left(\frac{v}{\rho T}\right) + W_{ij}\frac{\mathrm{d}J_j}{\mathrm{d}t}.$$

In the framework of the linear theory the positive definiteness of R leads to the linear relationships relating the dissipative fluxes to the thermodynamic forces. Taking into account Onsager's reciprocity relations for the transport coefficients and time-reversal property of dissipative effects [16], we can write these relationships in the form

$$\pi_{ik} = -\eta_{iklm}\frac{\partial v_l}{\partial x_m}, \tag{22}$$

$$q_i = -\frac{\kappa'_{ik}}{T^2}\frac{\partial T}{\partial x_k} - \alpha'_{ik}X_k - \beta'_{ik}\frac{\partial\tilde{\sigma}_{kj}}{\partial x_j}, \tag{23}$$

$$J_i = -\frac{\alpha'_{ik}}{T^2}\frac{\partial T}{\partial x_k} - \gamma'_{ik}X_k - \zeta'_{ik}\frac{\partial\tilde{\sigma}_{kj}}{\partial x_j}, \tag{24}$$

$$v_i - \frac{\mathrm{d}u_i}{\mathrm{d}t} = -\frac{\beta'_{ik}}{T^2}\frac{\partial T}{\partial x_k} - \zeta'_{ik}X_k - \chi'_{ik}\frac{\partial\tilde{\sigma}_{kj}}{\partial x_j}, \tag{25}$$

where the forth-rank tensor η is related to the effect of the viscosity and $\alpha'_{ik}, \beta'_{ik}, \ldots$ are tensor transport coefficients.

Let us eliminate the thermodynamic force X_k from Eqs. (23) and (25). Redenoting the transport coefficients and introducing the explicit definition of X_k into Eq. (24) one rewrites the set (23)–(25) for the case of the cubic lattice as

$$\mathbf{q} = \alpha\mathbf{J} - \kappa\frac{\nabla T}{T^2} - \beta\nabla\cdot\tilde{\sigma}, \tag{26}$$

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{v} - \zeta\mathbf{J} + \beta\frac{\nabla T}{T^2} + \chi\nabla\cdot\tilde{\sigma}, \tag{27}$$

$$\tau\frac{\mathrm{d}\mathbf{J}}{\mathrm{d}t} + \mathbf{J} = -\gamma T\nabla\left(\frac{v}{\rho T}\right) - \omega\frac{\nabla T}{T^2} - \lambda\nabla\cdot\tilde{\sigma}, \tag{28}$$

where $\alpha, \beta, \gamma, \ldots$ are the scalar transport coefficients. κ is connected with the heat conductivity, τ is the relaxation time of the diffusion flux. The coefficients β, χ, λ determine the relation between the dissipative effects and shear stresses. The remaining coefficients are due to the processes of diffusion, thermal diffusion and barodiffusion (owing to the pressure dependence of the interstitial chemical potential v in Eq. (28)).

Thus the complete set of the hydrodynamic equations of the system under consideration contains now Eqs. (1)–(4) and Eqs. (27) and (28), where the fluxes π_{ik}, $\mathbf{q}$ and the dissipative function R are given by Eqs. (22), (26) and (21). As it seen from (28) the equation for diffusion flux is the equation of a relaxation type. At $\tau = 0$, i.e. for slow processes, it determines directly the diffusion flux in terms of gradients of the basic hydrodynamic variables.

3. Mass transfer in field of fast-moving deformation disturbance

In this section we consider the diffusion of interstitial impurities in the field of the fast-moving deformation disturbance of the type of a shock wave. We assume that the stepped disturbance (kink), for which the displacement field (along the x-axis) has the form [17,18].

$$u(x,t) = u_0\left(1 - \tanh\frac{x - Vt}{\delta}\right), \tag{29}$$

where u_0 is the amplitude of the disturbance and δ is the width of the transition region, propagates along the

x-direction with the constant velocity V compared with the velocity of the propagation of concentration disturbances in the medium.

At the given motion of the lattice (29) the diffusion process is largely governed by the set of two equations: the local conservation law of mass (4) and the relaxation equation for the diffusion flux (28). Let us now transform the right side of Eq. (28) to the alternative form. Combining Eqs. (7) and (17) and taking into account Eq. (20), one obtains

$$\rho\,\mathrm{d}\mu = -S\,\mathrm{d}T + \mathrm{d}p + v\,\mathrm{d}c + \tilde{\sigma}_{ij}\,\mathrm{d}\tilde{u}_{ij} + \frac{W}{2}\,\mathrm{d}J^2, \tag{30}$$

where $W = \frac{1}{3}W_{ii}$. It follows from Eq. (30) that one can consider the chemical potential v to be a function of the independent variables $T, p, c, \tilde{u}_{ij}, J^2$. Omitting essentially nonlinear terms, note that in the case of the cubic symmetry a scalar function can depend on the tensor $\tilde{u}_{ij}$ by convolution $\tilde{u}_{ii} = 0$ only. Consequently one can consider v to be a function of T, p, c only.

The available experimental data indicate that when a shock wave propagates in a solid the effect of thermodiffusion is neglected in comparison with barodiffusion [2,19]. Here we also assume that the main factor determining mass transfer in our system is the effect of barodiffusion. Then omitting the gradient of a temperature one rewrites Eq. (28) in the more simple form as

$$\tau\frac{\mathrm{d}\mathbf{J}}{\mathrm{d}t} + \mathbf{J} = -\gamma T\frac{\partial}{\partial c}\left(\frac{v}{\rho T}\right)\nabla c - \gamma\frac{\partial}{\partial p}\left(\frac{v}{\rho T}\right)\nabla p - \lambda\nabla\cdot\tilde{\sigma}, \tag{31}$$

It follows from Eq. (16) that $\sigma_{ik} = -p\delta_{ik} + \tilde{\sigma}_{ik}$, with $\sigma_{ii} = -3p$ is the elastic stress tensor. In the one-dimensional case one neglects the influence of shear stress on a diffusion mobility. [1] In addition, we assume that Hook's law $p = -kU$, relating the pressure p with the deformation $U = \partial u/\partial x$ of a material element, is valid. Redenoting the constants in Eq. (31) one writes down in the linear approximation the coupled set of the one-dimensional versions of Eqs. (4) and (31) as

$$\rho\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x}, \tag{32}$$

$$\tau\frac{\partial J}{\partial t} + J = -\rho D\frac{\partial c}{\partial x} + \rho G\frac{\partial U}{\partial x}, \tag{33}$$

where $G > 0$ has the meaning of the coefficient of the barodiffusion and $D = \gamma\rho^{-1}T\partial(v/\rho T)/\partial c$ is the diffusion constant. In addition, in obtaining of Eqs. (32) and (33) we have neglected the term $\mathbf{v}\cdot\nabla$, appearing in the material derivative that is small for fast processes in comparison with the time derivative $\partial/\partial t$.

After some algebra, Eqs. (32) and (33) are brought to the form

$$\frac{\partial c}{\partial t} + \frac{D}{V_D^2}\frac{\partial^2 c}{\partial t^2} - D\frac{\partial^2 c}{\partial x^2} = -G\frac{\partial^2 U}{\partial x^2}, \tag{34}$$

$$\frac{\partial J}{\partial t} + \frac{D}{V_D^2}\frac{\partial^2 J}{\partial t^2} - D\frac{\partial^2 J}{\partial x^2} = \rho G\frac{\partial^2 U}{\partial x\,\partial t}. \tag{35}$$

At $U = 0$ Eq. (34) (as well as Eq. (35)) is known as the telegrapher equation that, unlike to the classical diffusion equation, gives rise to the finite speed $V_D^2 = D/\tau$ of the propagation of concentration perturbations [10,11].

It is convenient to consider Eqs. (34) and (35) in the reference frame moving with velocity V together with the front of the disturbance (29). Passing to the dimensionless coordinate $\xi = (x - Vt)/\tau V_D$, one has

$$(\varphi^2 - 1)\frac{\mathrm{d}^2\bar{c}}{\mathrm{d}\xi^2} - \varphi\frac{\mathrm{d}\bar{c}}{\mathrm{d}\xi} = -\frac{\mathrm{d}^2\overline{U}}{\mathrm{d}\xi^2}, \tag{36}$$

$$(\varphi^2 - 1)\frac{\mathrm{d}^2\overline{J}}{\mathrm{d}\xi^2} - \varphi\frac{\mathrm{d}\overline{J}}{\mathrm{d}\xi} = -\varphi\frac{\mathrm{d}^2\overline{U}}{\mathrm{d}\xi^2}, \tag{37}$$

where $\varphi = V/V_D$, $\overline{U} = GU/c_0D$, $\bar{c} = (c - c_0)/c_0$, $\overline{J} = J/c_0\rho V_D$ and c_0 is the equilibrium interstitial concentration.

Supposing that far from the front of the wave ($\xi = 0$) the medium is not disturbed, we take the boundary conditions in the form

$$\xi \to \pm\infty, \quad \bar{c} \to 0, \quad \overline{J} \to 0. \tag{38}$$

The solution of the boundary value problem (36)–(38) can be presented as follows:

$$\bar{c}(\xi) = \begin{cases} b\overline{U}(\xi) - ab\int_{-\infty}^{\xi} \mathrm{e}^{-a(\xi-\xi')}\overline{U}(\xi')\mathrm{d}\xi', & \varphi < 1, \\ \dfrac{\mathrm{d}\overline{U}}{\mathrm{d}\xi}, & \varphi = 1, \\ b\overline{U}(\xi) + ab\int_{\xi}^{\infty} \mathrm{e}^{-a(\xi-\xi')}\overline{U}(\xi')\mathrm{d}\xi', & \varphi > 1, \end{cases} \tag{39}$$

Here $a = \varphi b$, $b = 1/(1 - \varphi^2)$ and the solution for the dimensionless flux $\overline{J}$ follows from (39) as a result of the replacement of b by a. Eq. (39) is the solution of boundary value problem for arbitrary deformation disturbance U, vanishing at $\xi \to \pm\infty$.

The transition to the local equilibrium theory occurs if in Eq. (33) one puts formally $\tau = 0$. Using the same dimensionless variables as in Eqs. (36) and (37) one has in this case the following equations:

$$\frac{\mathrm{d}^2\bar{c}_{\mathrm{leq}}}{\mathrm{d}\xi^2} - \varphi\frac{\mathrm{d}\bar{c}_{\mathrm{leq}}}{\mathrm{d}\xi} = -\frac{\mathrm{d}^2\overline{U}}{\mathrm{d}\xi^2}, \tag{40}$$

$$\frac{\mathrm{d}^2\overline{J}_{\mathrm{leq}}}{\mathrm{d}\xi^2} - \varphi\frac{\mathrm{d}\overline{J}_{\mathrm{leq}}}{\mathrm{d}\xi} = -\varphi\frac{\mathrm{d}^2\overline{U}}{\mathrm{d}\xi^2}. \tag{41}$$

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[1] In the one-dimensional case $\tilde{\sigma}$ is proportional to $\partial u/\partial x$. Therefore allowance for the term $\lambda\nabla\cdot\tilde{\sigma}$ in the right-hand side of Eq. (31) leads simply to redefinition of the constant G in Eq. (33).

The solution of this equations has the standard form and we shall not give it here.

For the disturbance (29) $\overline{U}(\xi) = -U_0/(\cosh^2\xi/\delta_1)$, where U_0 is the known constant and $\delta_1 = \delta/\tau V_D$, one rewrites Eq. (39) in the form

$$\bar{c}(\bar{\xi})/U_0 = \begin{cases} -\dfrac{b}{\cosh^2\bar{\xi}} + (a\delta_1)b\displaystyle\int_{-\infty}^{\bar{\xi}} \dfrac{\mathrm{e}^{-a\delta_1(\bar{\xi}-\xi)}}{\cosh^2\xi}\mathrm{d}\xi, & \varphi < 1, \\ \dfrac{2}{\delta_1}\dfrac{\sinh\bar{\xi}}{\cosh^2\bar{\xi}}, & \varphi = 1, \\ -\dfrac{b}{\cosh^2\bar{\xi}} - (a\delta_1)b\displaystyle\int_{\bar{\xi}}^{\infty} \dfrac{\mathrm{e}^{-a\delta_1(\bar{\xi}-\xi)}}{\cosh^2\xi}\mathrm{d}\xi, & \varphi > 1, \end{cases} \tag{42}$$

here $\bar{\xi} = \xi/\delta_1$. Eq. (42) is the solution of the given problem at arbitrary values of parameters. Here we are interested in values of the parameter $\varphi = V/V_D$ close to one for which $|a| \gg 1$, $|b| \gg 1$. At the same time the parameter δ_1, characterizing the width of the transition region of the disturbance, can take, generally speaking, any values. In what follows we confine ourselves to two limiting cases:

(1) *The wide transition region, $\delta_1 = \delta/\tau V_D \sim 1$:* Figs. 1–3 present the curves for the impurity concentration $\bar{c}/U_0$ (as well as for the diffusion flux $\overline{J}/\varphi U_0$) at different values of the parameter φ in the case of the propagating local compression ($U_0 > 0$). This figures also show the difference between the local equilibrium and the local nonequilibrium (presence of the relaxation process in the medium) theories. In all cases the deformation disturbance produces the enhanced impurity concentration immediately before the front of the deformation wave (the region of $\bar{\xi} > 0$), lowering it behind the front. In the region of the of the enhanced concentration the diffusion flux points in the direction of the disturbance propagation, while in the region of lowered concentration–in the opposite direction.

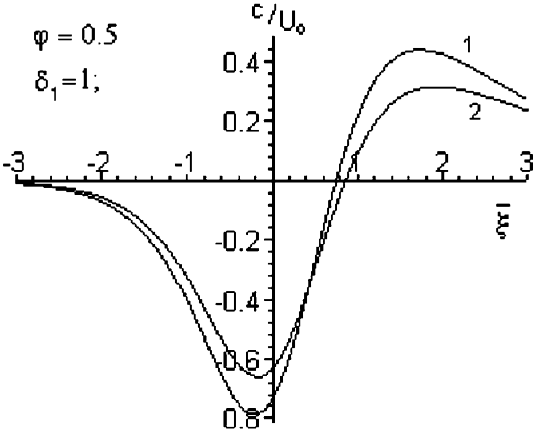

Fig. 1. Normalized interstitial concentration $\bar{c}/U_0$ (normalized dimensionless diffusion flux $\overline{J}/\varphi U_0$) vs. dimensionless coordinate $\bar{\xi}$ at $\varphi = 0.5$, $\delta_1 = 1$ and $U_0 > 0$. Local nonequilibrium system—curve 1; local equilibrium system—curve 2.

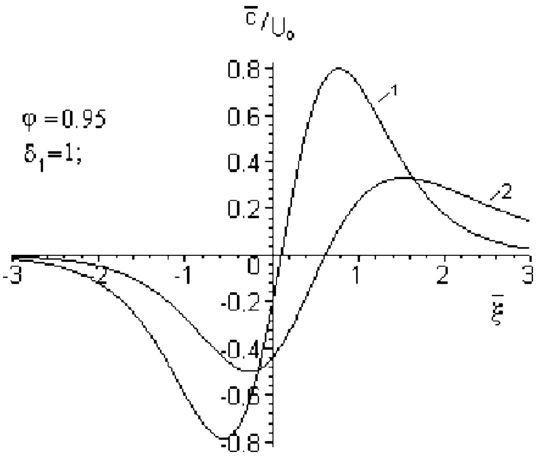

Fig. 2. Normalized interstitial concentration $\bar{c}/U_0$ (normalized dimensionless diffusion flux $\overline{J}/\varphi U_0$) vs. dimensionless coordinate $\bar{\xi}$ at $\varphi = 0.95$, $\delta_1 = 1$ and $U_0 > 0$. Local nonequilibrium system—curve 1; local equilibrium system—curve 2.

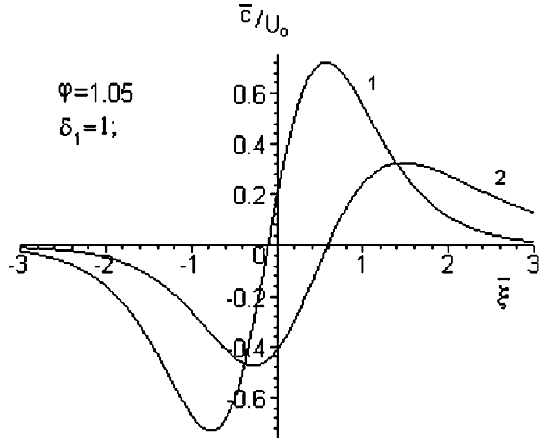

Fig. 3. Normalized interstitial concentration $\bar{c}/U_0$ (normalized dimensionless diffusion flux $\overline{J}/\varphi U_0$) vs. dimensionless coordinate $\bar{\xi}$ at $\varphi = 1.05$, $\delta_1 = 1$ and $U_0 > 0$. Local nonequilibrium system—curve 1; local equilibrium system—curve 2.

As Figs. 2 and 3 show, at $\varphi \approx 1$ the concentration perturbations are significantly greatly in the local nonequilibrium medium. In this case the diffusion flux is nearly twice as large as that for the local equilibrium system.

(2) *The narrow transition region, $\delta_1 = \delta/\tau V_D \ll 1$:* In what follows we consider the special case of $\delta_1 = 1/|a|$,

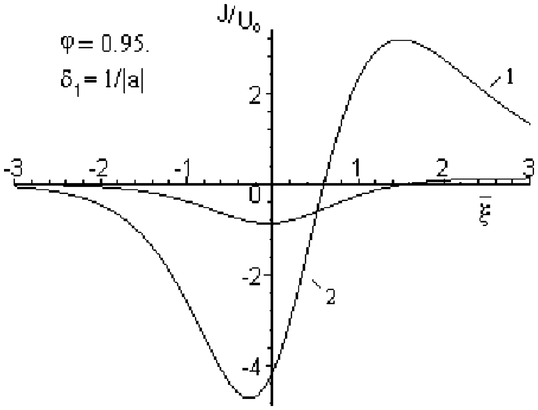

Fig. 4. Normalized dimensionless diffusion flux $\overline{J}/U_0$ (normalized interstitial concentration $\varphi\bar{c}/U_0$) vs. dimensionless coordinate $\overline{\xi}$ at $\varphi = 0.95$, $\delta_1 = 1/|a|$ and $U_0 > 0$. Local nonequilibrium system—curve 1; local equilibrium—curve 2.

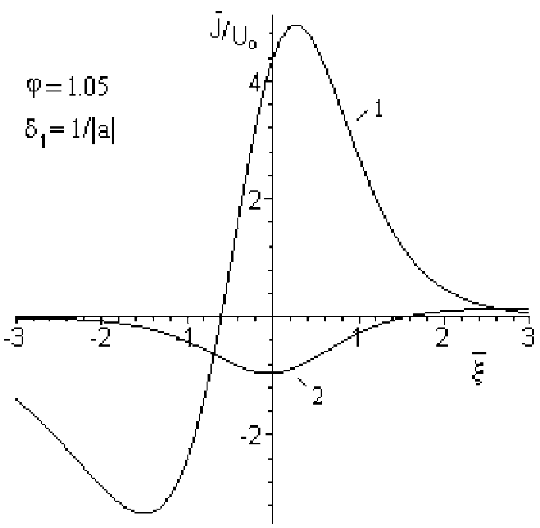

Fig. 5. Normalized dimensionless diffusion flux $\overline{J}/U_0$ (normalized interstitial concentration $\varphi\bar{c}/U_0$) vs. dimensionless coordinate $\overline{\xi}$ at $\varphi = 1.05$, $\delta_1 = 1/|a|$ and $U_0 > 0$. Local nonequilibrium system—curve 1; local equilibrium—curve 2.

$|a| \gg 1$. Figs. 4 and 5 demonstrate a pronounced difference between two approaches. The ejection of the major number of interstitials into the region before the front of the wave is observed in the absence of a local equilibrium in the medium. In the latter case the impurity concentration in the indicated region is nearly by an order greater than the local equilibrium concentration that does not change practically with the rising of φ. Figs. 4 and 5 also show the considerable deviation for diffusion fluxes demonstrating the acceleration of the

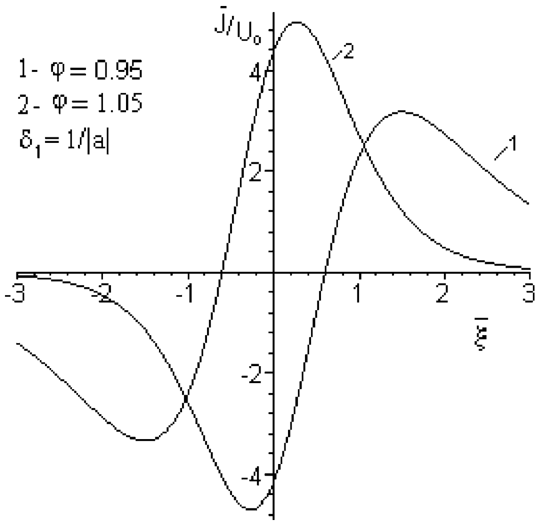

Fig. 6. Normalized dimensionless diffusion flux $\overline{J}/U_0$ (normalized interstitial concentration $\varphi\bar{c}/U_0$) vs. dimensionless coordinate $\overline{\xi}$ for the case of local nonequilibrium system at $\delta_1 = 1/|a|$, $U_0 > 0$ and $\varphi = 0.95$ (curve 1), $\varphi = 1.05$ (curve 2).

mass transfer under local nonequilibrium conditions. Note that at $\varphi > 1$ in the region of the front the diffusion fluxes referring to the different nonequilibrium states of the medium point in complete opposite directions. The difference between the local nonequilibrium curves at different magnitudes φ are shown in Fig. 6.

The reason of the enhanced impurity concentration before the front in the local nonequilibrium system is that when the velocity of the deformation wave is near to V_D, the concentration disturbances have no time to propagate on large distances from the front. This has the effect of accumulation of interstitials in the indicated region. Here is a complete analogy with the task about the motion of a thermal source in a relaxating medium [20].

It should be noted that in the case of the local tension ($U_0 < 0$) the concentration peaks will form behind the front of the wave ($\overline{\xi} < 0$) by the moving particles from the region $\overline{\xi} > 0$.

4. Summary and conclusion

In this work we have presented the investigation of mass transfer in the field of the fast-moving deformation disturbance of the type of a shock wave, propagating in the infinite lattice with interstitial impurities. The research is motivated by experiments on the exposure of solid to dynamical external loads [1–9].

For the description of fast hydrodynamical processes the extending of the set of the conventional variables, characterizing the nonequilibrium state of a solid is needed. In the given model the only extra variable is the diffusion flux, the relaxation time of which is assumed to be comparable to the timescale of the process under consideration. For the selected variables the set of the coupled hydrodynamical equations has been derived.

Having assumed that the main factor impacting on mass transfer in our case is the effect of barodiffusion [2,19], we reduce the diffusion task to the investigation of the set of two linear, one-dimensional equations. These are the equation for the interstitial concentration (36) and the relaxation equation for the diffusion flux (37). The solution of this set is defined by two dimensionless parameters $\varphi = V/V_D$ and $\delta_1 = \delta/\tau V_D$. At the different magnitudes $\varphi \sim 1$ we have considered two special cases $\delta_1 \simeq 1$ and $\delta_1 \ll 1$.

Figs. 1–5 show that the occurrence of the relaxation process in the medium leads to the significant deviation of the concentration profiles and the diffusion fluxes from the local equilibrium diffusion data. The ejection of interstitials into the region before the front enables to speak about the effect of the entrainment of impurity particles by the wave. This effect takes place in the local equilibrium system also (see [21] as well), however at $\delta_1 \ll 1$ to a largest measure it is displayed in the local nonequilibrium conditions (Figs. 4 and 5).

In the case of the local tension ($U_0 < 0$; the mirror reflection of the plots 1–6 relative to axis $\bar{\xi}$) the concentration peaks will form beyond the front of the wave by a "suction" of particles from the range before the front into the extended range.

The case of $\delta_1 \sim 1$ ($\delta \sim \tau V_D$) corresponds to the smooth enough behavior of the deformation disturbance. Here, in the region of the front, the local nonequilibrium diffusion flux is nearly twice as large as that for the local equilibrium system. The case of $\delta_1 \ll 1$ ($\delta \ll \tau V_D$) corresponds to the sharp deformation variations. From Figs. 4 and 5 it is seen that in this case one can speak about the significant acceleration of the mass transfer in the local nonequilibrium system. The all effects noted above are by an order less in the local equilibrium system.

Thus our investigation has shown that at the taken magnitudes of the parameters of the model an enhanced mass transfer takes place in local nonequilibrium system in comparison with the same process considered under the local equilibrium conditions.

Note in conclusion that the results presented here have been obtained within the scope of the linear theory. The set of the hydrodynamical equations derived in Section 2 can form the basis for the investigation of nonlinear effects.

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