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On diffusion–elastic instabilities in a solid half-space

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ABSTRACT

A model of the diffusion–elastic instability that appears in an ensemble of non-equilibrium atomic defects in unbounded condensed media as well as on the free surface of a half-space is introduced and studied. The dynamical model developed here is based on coupled evolution equations for the elastic displacement of the medium and atomic defect density fields. The idea of an instability model is related to a drift of atomic defects under the influence of elastic fields. It is shown that the development of this instability creates ordered structures of coupled strain and defect-concentration fields. Dispersion relationships for the growth increment of these structures are derived and their characteristic scales are obtained.

1. Introduction

During the last few years, several attempts have been made to describe the generation of various ordered structures formed by elastic strains and non-equilibrium atomic defects within the framework of the self-organization theory of a non-equilibrium condensed system. The formation of non-equilibrium lattice defects may occur as a result of the action of intense external energy fluxes (laser and corpuscular radiations) on condensed media or as a result of mechanical, thermal, and electric treatments of materials. Examples of such defects are interstitial atoms, vacancies, color centers, electron–hole pairs, impurity atoms, etc. Depending on the conditions and on the material, atomic defects can either condense to form pores and dislocation loops or can join in periodic structures of the defect density field (or of different phases) [1]. The ordered structures are observed both on the surfaces (and in thin films) and in the bulk of solids, and are retained after the end of a pulse [1–6]. These structures appear in many forms—one and two-dimensional lattices, concentric rings, radial and radial-ray structures, spirals, and mazes [6–8]. The spatial orientation of such structures is unrelated to the polarization of the laser radiation and, in the case of crystals, it is governed by the crystallographic symmetry (superlattices) or by the symmetry of distribution of the laser field intensity. The lattice parameter (micron and submicron) is not related directly to the exciting radiation wavelength.

The formation of various defect-strain structures especially under laser irradiation is a problem of great technological importance, since ordered structures influence key material properties such as mechanical strength, electrical conductivity, magnetic susceptibility, etc. in a significant way. They can alter qualitatively both the process of interaction of radiation with condensed matter and the general pattern of modification of a material. Furthermore, phenomena such as laser annealing, fast recrystallization, and the laser-assisted thin-film deposition process also proceed through the formation of ordered structures on the surface of the matter, and laser–surface interaction is evidently a field where patterning phenomena are overwhelming. Thus, the understanding and control of the formation of ordered structures in solids is very important for laser surface modification technologies.

Spatial self-organization within defect ensembles on the surface of the material occurs as a result of the development of various instabilities. Instabilities appear at certain critical values of the parameters and the process of formation of dissipative structures is the result of competition between a large number of unstable growing modes, which results in selection of the amplitude of one or several modes. The amplitudes of the dominant modes determine the type and degree of ordering, i.e. they are the order parameters. In principle, if we know and control the parameters that represent the system and create conditions favourable for the dominance of specific modes, we can control the formation of various structures [1].

Control of the formation of ordered structures in solids requires prior knowledge of the mechanism of the relevant instabilities, development of their models, and calculations of critical conditions for the appearance of instabilities.

Much effort has been devoted to understand the mechanisms of various instabilities. The instabilities that appear in a solid under the action of external fluxes can be classified in accordance with the nonlinear interactions that give rise to feedback. The early investigations have been concerned with a number of specific

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mechanisms—nonlinear interaction in the course of recombination of atomic defects at the centers in the form of defect–impurity complexes [9]; loss of stability of a homogenous state for the subsystem of atomic point defects associated with their upward diffusion along a concentration gradient of substitutional impurity [10]; a mechanism due to the vacancy 'wind' effect and deviations from local neutrality on appearance of fluctuations of the impurity concentrations [11]. Although the stability mechanisms are realized under certain conditions, they are of very special nature.

In Refs. [1,2,12] the problem has been analyzed from a more general standpoint. The spatial self-organization of various coupled strain-defect structures in laser-irradiated crystals as a result of concentration–elastic instabilities has been discussed. A mechanism on the development of these instabilities is due to the coupling between defect dynamics and the elastic field of the solids [1,2]. Laser radiation (or, in general, a flux of particles) generates high concentrations of atomic defects in the surface layer of the irradiated material. When a fluctuation harmonic of the elastic deformation field appears in a medium because of the generation of atomic defects, the activation energies of formation and migration of the defects are modulated and a strain-induced drift of atomic defects occurs. This is a consequence of defect–strain interaction. The associated modulation of the rates of defect generation (recombination) and strain-induced flux of defects gives rise to periodic spatial–temporal fields of the defect concentration. The redistribution of defects creates forces proportional to their gradients. These forces lead in turn to additional growth of strain fluctuations. When the defect density or a critical rate of defect generation exceeds the critical value, concentration–elastic instabilities develop as a result of positive feedback, which result in the formation of ordered concentration–strain structures. The limiting case of these instabilities, when the spatial inhomogeneity of the defect distribution is the result solely of the strain-induced fluxes, can be called the diffusion–elastic instability (in short DEI) and the case in which only modulation of the defect generation rate is important can be considered as the generation–elastic instability (GEI). It follows that the system of atomic defects with the elastic interaction is internally unstable against a transition to a spatially inhomogeneous state.

In our publications [13–19], the self-organization models of formation of nonlinear localized concentration–strain structures in laser-excited free thin metal plates were considered with allowance for interaction with non-equilibrium atomic defects. We derived nonlinear evolutionary equations for the self-consistent strains in a solid caused by laser-induced atomic defects. The influence of strain-induced diffusion, generation, and recombination of atomic defects on the evolution of strain wave structures (as also concentration wave structures) was analyzed. We found exact solutions to the nonlinear equations, described nanoscale localized strain–concentration structures.

A mechanism of the generation of linear periodic strain–concentration structures due to GEI was revealed in Ref. [20]. The dynamical model developed here was based on coupled evolution equations for the elastic and atomic defect density fields. It was shown that the development of this instability creates various periodic surface structures of coupled strain and defect-concentration fields. Dispersion relationships were derived for the growth increment of these structures and their characteristic scales are obtained. The characteristic scale of surface defect–strain structures predicted by the GEI theory usually ranges from 1 to 10 μm (large-scale structures).

Self-organization of defect-strain structures due to DEI related to a drift motion of defects under the influence of elastic fields was previously investigated for the thin plates (see Refs. [1,2,8]. The present paper is devoted to further development of the DEI theory for the generation of plane harmonic elastic wave structures in unbounded media as well as Rayleigh's surface wave structures on the free surface of a half-space with non-equilibrium atomic defects. We will derive dispersion relationships for the growth increment of periodic structures. We will specify the conditions for the formation of ordered structures and determine their characteristic scales, such as period of a structure and concentration of defects in concentration–strain structures.

The paper runs as follows. The formulation of problems and constitutive equations are presented in Section 2. Section 3 is devoted to the derivation of the dispersion equations of an instability. The generation of plane harmonics wave structures in unbounded media and Rayleigh's surface waves are discussed in Sections 4 and 5. The last section contains the main results.

2. Basic equations

Let us consider an isotropic solid that occupies the half-space $z>0$. Due to thermal heating induced by an external energy flux (e.g., laser irradiation), an increased atomic defect density is created in the surface layer. The corresponding defect density profile results in a force that may induce a strain field in the medium. Let $n_j(x,z,t)$ be the concentration of these defects of jth type ($j=v$ for vacancies (v-defects) and $j=i$ for interstitials (i-defects). We shall consider two-dimensional structures in the x,z-plane, and denote the corresponding displacement components by u and v, respectively.

The dynamical model that can describe the evolution of such a system should be based on (i) the evolution of atomic defect density in a strained solid and (ii) the strain field of a solid in the presence of a non-uniform defect density field.

We use the expression for the energy density of the interaction between atomic defects and strain in the form

$$H=-\sum_{j=i,v} n_j \vartheta_d^{(j)} u_{ll}, \tag{1}$$

where $\vartheta_d^{(j)}=K\Omega_d^{(j)}$ [21] is the acoustic potential of the strain–defect interaction, where K is the bulk modulus and $\Omega_d^{(j)}$ is the volume elastic strain caused by the relaxation of the jth-type defect volume. For v-defects, $\Omega_d^{(v)}=-\delta^{(v)}\Omega<0$ (here, the coefficient is $\delta^{(v)}=0.2-0.4$ and Ω is the atomic volume), whereas, for i-defects, $\Omega_d^{(i)}=\delta^{(i)}\Omega>0$ (the coefficient is $\delta^{(i)}=1.7-2.2$). v- and i-defects are represented as a substitutional atom whose volume is smaller or greater than the volume of the matrix atoms.

The concentration of atomic defects is dependent on temperature of the medium. One thus needs to know how the laser radiation affects the local temperature field of the surface at the laser spot. We will consider here situations where the laser irradiation only heats the crystal (the light energy absorbed by the medium is transformed into heat) and that an equilibrium between laser radiation and the temperature field (T) is reached on time scales much shorter than the characteristic time scale of defect density evolution. Usually, the characteristic time scale for equilibration between photon absorption and defect generation is of the order of picoseconds, while that for defect diffusion is of the order of microseconds or milliseconds. We also assume that the contribution of thermal strains to deformation fields is negligible compared to lattice dilatation due to atomic defects and phase changes and chemical reactions in the medium are absent.

In this paper, we will analyze the problem of DEI in a solid irradiated over a large area by CW or pulsed lasers. Furthermore, we will assume that the temperature profile has reached its equilibrium value. Its evolution is sufficiently slow compared to atomic defect generation, and can be considered as quasi-stationary. The solution of the heat conduction equation for this case is given by Duley [22].

Then, using Eq. (1), we obtain the field equation in a linear solid of isotropic symmetry with the generation of atomic defect of the form

$$\frac{\partial^2 \vec{u}}{\partial t^2}-c_T^2\Delta\vec{u}-(c_L^2-c_T^2)\nabla\left(div\,\vec{u}\right)=-\rho^{-1}\sum_{j=i,v}\vartheta_d^{(j)}\nabla n_j. \tag{2}$$

Here $\vec{u}$ is the displacement vector of the medium, $\Delta=\partial_{xx}+\partial_{zz}$; c_L $(=\sqrt{(\lambda+2\mu)/\rho})$ is the sound velocity for longitudinal acoustic waves and c_T $(=\sqrt{\mu/\rho})$ is the sound velocity for transverse acoustic waves [23] (λ and μ are the Lame coefficients; ρ is the density of the medium).

The right-hand side of Eq. (2) takes into account the forces applied to the lattice because of defect–deformation interaction. Eq. (2) represents the generalization of the known equation for the elastic waves in a solid [23] to the case of a system with concentration-related stresses [21], which are caused by generation–recombination processes in the non-equilibrium atomic defect subsystem.

The concentration of the non-equilibrium atomic defects $n^{(j)}(x,z,t)$ obeys the kinetic-diffusion equation. With allowance for the effect of the elastic strain field, this equation can be represented in the form

$$\frac{\partial n_j}{\partial t}=G_j-div\vec{Q}_j(r,t)-\gamma n_i n_v-n_j\tau_j^{-1}, \tag{3a}$$

$$\vec{Q}_j(r,t)=-D_j\nabla n_j-\vec{v}_j n_j(r,t). \tag{3b}$$

Here $G_j=g_0\exp[-w_f^{(j)}/k_BT]$ is the rate of generation of atomic defects by an external source ($w_f^{(j)}$ is the energy formation of defects, T the absolute temperature, k_B the Boltzmann constant, and g_0 the constant of defect generation). The defect flux $Q_j(r,t)$ is described by Eq. (3b), where the first term represents diffusion with coefficient D_j; the second term corresponds to the drift of defects at velocity $\vec{v}_j=(D_j/k_BT)\vec{F}_j$ under the influence of the force $F_j=-\nabla U_{int}$ resulting from the interaction of defects with an inhomogeneous strain field ($U_{int}=-K\Omega_d^{(j)}div\vec{u}$ is the energy of the interaction between one defect and the strain field). In Eq. (3a) the last two terms describe the mutual recombination of defects ($\gamma=4\pi R(D_i+D_v)$ is the recombination rate and R the recombination radius) and their absorption at sinks (τ_j is the relaxation time of defects of the jth type).

Eqs. (2) and (3) must be supplemented by the following boundary conditions at the surface $z=0$:

$$\frac{\partial u}{\partial z}+\frac{\partial v}{\partial x}=0, \tag{4}$$

$$c_L^2\frac{\partial v}{\partial z}+(c_L^2-2c_T^2)\frac{\partial u}{\partial x}=\rho^{-1}\sum_{j=i,v}\vartheta_d^{(j)}n^{(j)}, \tag{5}$$

$$\frac{\partial n^{(j)}}{\partial z}=0. \tag{6}$$

The condition at infinity requires that the solutions be bounded as z becomes large.

If the viscosity of the medium is taken into account the field equation has the form

$$\frac{\partial^2\vec{u}}{\partial t^2}-c_T^2\Delta\vec{u}-(c_L^2-c_T^2)\nabla\left(div\vec{u}\right)-\eta_T\frac{\partial}{\partial t}\left(\Delta\vec{u}\right)-(\eta_L-\eta_T)\frac{\partial}{\partial t}\nabla\left(div\vec{u}\right)=-\rho^{-1}\sum_{j=i,v}\vartheta_d^{(j)}\nabla n^{(j)}, \tag{2a}$$

where $\eta_T=\eta$, $\eta_L=4\eta/3+\zeta$; η and ζ are the first and second viscosity coefficients. The boundary condition (5) becomes

$$c_L^2\frac{\partial v}{\partial z}+(c_L^2-2c_T^2)\frac{\partial u}{\partial x}+\eta_L\rho^{-1}\frac{\partial^2 v}{\partial z\partial t}+(\eta_L-2\eta_T)\rho^{-1}\frac{\partial^2 u}{\partial x\partial t}=\rho^{-1}\sum_{j=i,v}\vartheta_d^{(j)}n^{(j)}. \tag{5a}$$

The system of Eqs. (2) and (3) is closely coupled. $\partial^2\vec{u}/\partial t^2$ in Eq. (2) depends on the defect-concentration field (n) and $\partial n/\partial t$ in Eq. (3) depends on the elastic displacement field ($\vec{u}$). The system of equations thus becomes highly nonlinear.

Below, we will demonstrate that the set of Eqs. (2) and (3), in combination with the conditions represented by expressions (4)–(6) describes the evolution of DEI with the self-organization of atomic defects interacting through the elastic field of the continuum. Such self-organization processes result in the formation of cluster and periodic defect–strain structures.

We shall consider the following two classes of solutions of these equations: (a) plane harmonic wave structures in an unbounded medium and (b) Rayleigh's surface wave structures on the free surface of a half-space.

From this point on, we limit our consideration to the case of only one type of atomic defect and drop the superscript j in Eqs. (2)–(6), i.e. we assume that $\vartheta_d^{(j)}=\vartheta_d$, $\Omega_d^{(j)}=\Omega_d$, $n_j(x,z,t)\equiv n(x,z,t)$, $\tau_j\equiv\tau_d$, $D_j=D$, etc.

3. Dispersion equation of DEI

If we assume that $n=n_0+n_1$ and $\vec{u}=\vec{u}_1$ ($n_0=G\tau$ is a spatially homogeneous solution along the surface; n_1 and $\vec{u}_1$ are small perturbations) we find that our basic equations become

$$\frac{\partial^2 u}{\partial t^2}=c_L^2\frac{\partial^2 u}{\partial x^2}-(c_T^2-c_L^2)\frac{\partial^2 v}{\partial x\partial z}+c_T^2\frac{\partial^2 u}{\partial z^2}-\rho^{-1}\vartheta_d\frac{\partial n_1}{\partial x}, \tag{7}$$

$$\frac{\partial^2 v}{\partial t^2}=c_L^2\frac{\partial^2 v}{\partial z^2}-(c_T^2-c_L^2)\frac{\partial^2 u}{\partial x\partial z}+c_T^2\frac{\partial^2 v}{\partial x^2}-\rho^{-1}\vartheta_d\frac{\partial n_1}{\partial z}, \tag{8}$$

$$\frac{\partial n_1}{\partial t}-D\left(\frac{\partial^2 n_1}{\partial x^2}+\frac{\partial^2 n_1}{\partial z^2}\right)+\frac{n_1}{\tau_d}=g\left(\frac{\partial^3 u}{\partial x^3}+\frac{\partial^3 v}{\partial z^3}\right). \tag{9}$$

Here $g=Dn_0\vartheta_d/k_BT$.

It is necessary to note that, at the account of the strain-stimulated generation of defects, on the right part of Eq. (9), the term $\overline{g}_0(\vartheta_G/k_BT)(u_x+v_z)$ ($\overline{g}_0=g_0\exp(-w_{f0}/k_BT)$, w_{f0} is the defect formation energy in an unstrained crystal, ϑ_G is the deformation potential characterizing the variation of the formation activation energy of defects under lattice deformation) also appears additionally, leading to GEI [18]. The relation between strain-induced generation and drift terms is given by $4\pi^2(\vartheta_d/\vartheta_G)(D\tau/d_{latt}^2)$, where d_{latt} is the characteristic scale of the structures, arising due to the instabilities. Thus, the generation term dominates during the formation of "large-scale" structures ($d_{latt}\geq 2\pi(\vartheta_d/\vartheta_G)^{1/2}\sqrt{D\tau}$) and the drift term dominates during the generation of "small-scale" structures ($d_{latt}<2\pi(\vartheta_d/\ \vartheta_G)^{1/2}\sqrt{D\tau}$). As $\sqrt{D\tau}=\bar{l}$ ($\bar{l}$ is the average distance between sinks) and the scale of structures is always supposed to be greater than $\bar{l}$, the choice of drift or generation terms depends on the ratio ϑ_d/ϑ_G. In this paper we believe that $\vartheta_d/\vartheta_G>1$.

For the Rayleigh surface wave structures, we shall deal with the half-space defined by $z\geq 0$, where we assume that both the surface tractions and the concentration gradient vanish on the plane $z=0$.

The general solution of Eqs. (7)–(9) can be written as

$$(u,v,n)=\sum_{r=1}^{3}(d_{1r},d_{2r},d_{3r})\times\exp(-\gamma_r z)\times\exp i(kx+\omega t), \tag{10}$$

where for the unbounded medium we set $\gamma_r\equiv 0$, and for the Rayleigh's waves we require γ_r to have positive real parts; d_{1r}, d_{2r}, and d_{3r} are the amplitudes, k is the wave number of the perturbations, and ω the complex increment of the instability. Harmonic strain disturbances will be stable when $\mathrm{Im}(\omega)>0$ and unstable when $\mathrm{Im}(\omega)<0$; the wave speed is given by $v=\mathrm{Re}(\omega)/k$, where $\mathrm{Re}(\omega)$ and $\mathrm{Im}(\omega)$ denote the real and the imaginary part of ω, respectively. Let us note that in a non-stationary case, when T depends on time, d_r and $\omega=\psi(t)$ are slow functions of time $|\psi^{-1}\partial\psi/\partial t|\ll\omega$.

Substitution of expressions (10) in Eqs. (7)–(9) gives the following relationship between coefficients:

$$d_{21}=-\frac{i\gamma_1 k}{k^2-\omega^2 c_L^{-2}}d_{11},\quad d_{22}=-\frac{\gamma_2}{ik}d_{12},$$

$$d_{23}=-\frac{\gamma_3}{ik}d_{13},\quad d_{31}=0,$$
$$d_{32}=-\frac{k^2-\omega^2c_L^{-2}-{\gamma_2}^2}{i\vartheta_d\rho^{-1}c_L^{-2}k}d_{12},$$
$$d_{33}=-\frac{k^2-\omega^2c_L^{-2}-{\gamma_3}^2}{i\vartheta_d\rho^{-1}c_L^{-2}k}d_{13}. \tag{11}$$

Here

$${\gamma_1}^2=k^2-\omega^2/c_T^2, \tag{12}$$

and γ_2 and γ_3 are the roots of equation

$$\gamma^4(1+\delta_dD^{-1})-\gamma^2\left[2k^2-\omega^2c_L^{-2}+(\tau^{-1}+i\omega)D^{-1}\right]+(Dc_L^2)^{-1}\times\left\{(c_L^2k^2-\omega^2)(i\omega+Dk^2+\tau^{-1})-\delta_d\ c_L^2k^4\right\}=0, \tag{13}$$

where $\delta_d=g\vartheta_d/\rho c_L^2$ is a defect–strain coupling coefficient. As, $sign[g]=sign(\vartheta_d)$, we have $\delta_d>0$.

Then γ_2^2 and γ_3^2 are defined from Eq. (13) as

$$\gamma_2^2+\gamma_3^2=\left[2k^2-\omega^2c_L^{-2}+(\tau^{-1}+i\omega)D^{-1}\right](1+\delta_dD^{-1})^{-1},$$
$$\gamma_2^2\gamma_3^2=(1+\delta_dD^{-1})^{-1}\left\{(k^2-\omega^2c_L^{-2})\left[k^2+(i\omega+\tau^{-1})D^{-1}\right]-\delta_dD^{-1}k^4\right\}. \tag{14}$$

In order to obtain the dispersion equation in the presence of viscosity of the medium, in Eqs. (12)–(14), the following replacement is necessary according to Eqs. (2a) and (5a)

$$c_{L,T}^2\to c_{L,T}^2(1+i\omega\eta_{L,T}/\rho c_{L,T}^2). \tag{15}$$

4. Ordered structures in unbounded medium

In this section as a special case we consider the generation of plane harmonic structures in an unbounded medium. Setting $\gamma_r=0$, $r=1, 2, 3$ in Eqs. (12) and (14) we obtain the following:

$$\omega^2=c_T^2k^2, \tag{16a}$$

$$(\omega^2-c_L^2k^2)(i\omega+Dk^2+\tau^{-1})+\delta_dc_L^2k^4=0. \tag{16b}$$

Eq. (16a) corresponds to transverse waves that are independent of δ_d, having speed of propagation c_T. Eq. (16b) pertains to the coupled strain–concentration waves.

To explore and delineate the strain and defect generation effects, we shall seek solutions of (16b) for small values of δ_d. For $\delta_d=0$, Eq. (16b) admits the following solutions: $\omega_{1,2}^{(0)}=\pm c_Lk$ (acoustical mode) and $\omega_3^{(0)}=i(Dk^2+\tau^{-1})$ (diffusion mode). Now, for small $\varepsilon=\delta_dk^2/c_Lk\ll1$, we may write

$$\omega_{1,2}=\omega_{1,2}^{(0)}+\varepsilon\omega_{1,2}^{(1)}+\varepsilon^2\omega_{1,2}^{(2)}+\cdots,$$

$$\omega_3=\omega_3^{(0)}+\varepsilon\omega_3^{(1)}+\varepsilon^2\omega_3^{(2)}+\cdots,$$

substituting into Eq. (16b) and retaining only terms of $O(\varepsilon)$, we finally arrive at the following equations:

$$\omega_{1,2}=\omega_{1,2}^{(0)}-\frac{\delta_dk^2}{2}\frac{c_L^2k^2(Dk^2+\tau^{-1}-i\omega_{1,2}^{(0)})}{\omega_{1,2}^{(0)}(c_L^2k^2+(Dk^2+\tau^{-1})^2)}, \tag{17}$$

$$\omega_3=\omega_3^{(0)}-\frac{i\delta_dc_L^2k^4}{c_L^2k^2+(Dk^2+\tau^{-1})^2}. \tag{18}$$

From Eq. (17) we obtain

$$\mathrm{Re}(\omega_{1,2})=\omega_{1,2}^{(0)}-\frac{\delta_dk^2}{2}\frac{c_Lk(Dk^2+\tau^{-1})}{c_L^2k^2+(Dk^2+\tau^{-1})^2}, \tag{19}$$

$$\mathrm{Im}(\omega_{1,2})=\frac{\delta_dk^2}{2}\frac{c_L^2k^2}{c_L^2k^2+(Dk^2+\tau^{-1})^2}. \tag{20}$$

If $c_L\gg Dk^2+\tau^{-1}$ and the viscosity is taken into account, the dispersion equation (20) describes attenuation of the amplitude of acoustic waves

$$\mathrm{Im}(\omega_{1,2})=(1/2\rho)\eta k^2+\frac{\delta_d}{2}k^2. \tag{21}$$

For the frequency spectrum of acoustic waves we have

$$\mathrm{Re}(\omega_{1,2})=\omega_{1,2}^{(0)}\left[1-\frac{\delta_d}{2}\frac{(Dk^2+\tau^{-1})}{c_L^2}\right]\approx\omega_{1,2}^{(0)}.$$

Note that the frequency of acoustic waves hardly changes. But the additional contribution to attenuation coefficient of waves arises. Since the attenuation decrement of acoustic waves is proportional to k^2, according to Eq. (21) short waves fade rapidly.

From Eq. (18) we receive

$$\omega_3=-i((\delta_d-D)k^2-\tau^{-1}). \tag{22}$$

It follows from the expression (22) that if

$$\delta_d\geq\delta_{cr}=D,\quad \text{i.e. } n\geq n_{cr}=\rho c_L^2kT/\vartheta_d^2,$$

there is a range of wave numbers

$$k>k_0=\sqrt{\tau^{-1}/(\delta_d-D)},$$

such that $\mathrm{Im}(\omega_3)<0$, i.e. the amplitudes of the Fourier harmonics of the small perturbations increase with time without a limit.

It is evident from Eq. (22) that the evolution of concentration inhomogeneous in the presence of acoustic waves is determined by the renormalized diffusion coefficient of defects:

$$D_{eff}=D\left(1-n_0\frac{\vartheta_d^2}{kT\rho c_L^2}\right),$$

which at certain values of the defect concentration (n_0) or at the temperature field (T) is negative. Therefore in such conditions occurs growth of inhomogeneous fluctuations in defect-concentration and, as increment is proportional to k^2, the first turn grow the heterogeneity, characterized by smaller wave length.

This means that the homogeneous distribution of defects becomes unstable, beginning from a certain critical rate of their formation, which is governed by the temperature of a solid, the dilatation volume of a defect, the bulk modulus, and the concentration of sinks. A directional flux appears and this flux increases the defect concentration in the compressed region, causing super-saturation with defects and formation of nanometre-sized clusters. Typical value of the critical wave number at $T=700\ ^\circ$C ($\Omega=10^{-23}$ cm^3, $K=5\times10^{11}$ erg cm^{-3}, and $\tau=10^{-3}$ s) is $k_0^2=5\times10^7$ cm^{-2}.

This mechanism of the appearance of clusters is clearly analogous to the formation of a polaron representing a self-trapped electron state in ionic crystals [24]. The DEI causes self-trapping of atomic defects in the potential wells created by the defects themselves.

If $c_Lk\ll Dk^2+\tau^{-1}$ from Eqs. (19) and (20) we obtain

$$\mathrm{Re}(\omega_{1,2})=\omega_{1,2}^{(0)}\left(1-\frac{\delta_dk^2}{2(Dk^2+\tau^{-1})}\right), \tag{23}$$

$$\mathrm{Im}(\omega_{1,2})=\frac{1}{2}\eta k^2+\frac{\delta_dk^2}{2}\frac{c_L^2k^2}{(Dk^2+\tau^{-1})^2}. \tag{24}$$

Since $\delta_d>0$, in this case there is a softening of frequencies of acoustic waves (instability of frequencies $\mathrm{Re}(\omega_{1,2})\to0$, $\mathrm{Im}(\omega_{1,2})>0$) and this is related to taking into account the generation of atomic defects. Eq. (24) describes attenuation of the amplitudes of acoustic waves.

5. Surface defect-strain structures

Substituting expressions (10) into boundary conditions (4)–(6), and taking into account expressions (11), we find a set of three linear algebraic equations

$$(\omega^2 c_T^{-2}-2k^2)\gamma_1 d_{11}+2(k^2-\omega^2 c_T^{-2})\gamma_2 d_{12}-2(k^2-\omega^2 c_T^{-2})\gamma_3 d_{13}=0, \tag{25}$$

$$2k^2 d_{11}-(\omega^2 c_T^{-2}-2k^2)d_{12}-(\omega^2 c_T^{-2}-2k^2)d_{13}=0, \tag{26}$$

$$\gamma_2(\gamma_2^2-k^2+\omega^2 c_L^{-2})d_{12}+\gamma_3(\gamma_3^2-k^2+\omega^2 c_L^{-2})d_{13}=0. \tag{27}$$

The condition of existence of a non-trivial solution of this system yields the following dispersion equation for the diffusion–elastic instability on the surface of a semi-infinite medium:

$$\frac{(1-\omega^2/2c_T^2k^2)^2}{1-\omega^2/c_T^2k^2}=\frac{\gamma_2\gamma_3(\gamma_2+\gamma_3)}{\gamma_1\left[(\gamma_2+\gamma_3)^2-\gamma_2\gamma_3+\omega^2 c_L^{-2}-k^2\right]} \tag{28}$$

Eq. (28) is a transcendental equation for the determination of $\omega(k)$. The structure of Eq. (28) is identical to the structure of the dispersion equation for DEI considered in Ref. [18]. This equation can be readily solved numerically or graphically, but in some cases of interest it can also be solved analytically. We shall now consider this in the following special cases.

a) If $\delta_d=0$, from Eq. (14) we have

$$\gamma_{1,2}^2=k^2-\omega^2 c_{T,L}^{-2},$$

$$\gamma_3^2=k^2+(i\omega+\tau^{-1})D^{-1}.$$

Substituting these expressions with Eq. (28) we obtain the following equations:

$$R(\omega^2/k^2)\times(i\omega+Dk^2+\tau^{-1})=0,$$

$$R(\omega^2/k^2)=\left(1-\frac{\omega^2}{2k^2c_T^2}\right)^4-\left(1-\frac{\omega^2}{k^2c_L^2}\right)\left(1-\frac{\omega^2}{k^2c_T^2}\right),$$

which yields

$$R(\omega^2/k^2)=0,\quad w=i(Dk^2+\tau^{-1}). \tag{29a, b}$$

Eq. (29a) is equivalent to the classical Rayleigh's equation, while Eq. (29b) defines the attenuation constant for the concentration waves. With $c_R^2=\omega^2/k^2$ Eq. (29a) reduces to

$$(2-c_R^2c_T^{-2})^4=16(1-c_R^2c_T^{-2})(1-c_R^2c_L^{-2}). \tag{30}$$

b) $\delta\neq 0$: In this case it has solutions describing qualitatively different types of instability: (1) instability of frequencies of acoustic waves and (2) generation of ordered surface (static) structures.

Substitution of expressions (12), (14) and (15) in Eq. (28) gives the following relationship:

$$\frac{(1-\omega^2/2k^2c_T^2+i\omega^3\eta_T/2k^2\rho c_T^4)^4}{1-\omega^2/k^2c_T^2+i\omega^3\eta_T/k^2\rho c_T^4}=\frac{a\left[b+2\sqrt{a}/\sqrt{1+\delta_d D^{-1}}\right]}{k^2\left[b+(\omega^2c_L^{-2}-k^2)(1+\delta_d D^{-1})+\sqrt{a}/\sqrt{1+\delta_d D^{-1}}\right]^2}, \tag{31}$$

where

$$a(k,\omega)=(k^2-\omega^2c_L^{-2}+\eta_L i\omega^3(\rho c_L^4)^{-1})(k^2+(i\omega+\tau_d^{-1})D^{-1})-k^4\delta_d D^{-1},$$

$$b(k,\omega)=2k^2-\omega^2c_L^{-2}+(i\omega+\tau_d^{-1})D^{-1}+\eta_L i\omega^3/\rho c_L^4.$$

Assuming that $\varepsilon=\delta_d k^2/\omega_R$ is sufficiently small, set

$$\omega^2/k^2=c_R^2(1+\varepsilon\xi_1+\varepsilon^2\xi_2+\cdots), \tag{32}$$

where $c_R=\omega_R/k$ is the classical Rayleigh wave speed, which is a root of Eq. (30).

Substituting expression (32) with Eq. (31), and retaining only terms of $O(\varepsilon)$, we receive the following dispersion relation:

$$\omega^2=k^2c_R^2+ik^3\delta_d\frac{c_R(1-c_R^2c_T^{-2})}{c_L^2R'(c_R)}+ik^3\eta\frac{c_R^3c_T^{-2}}{\rho},$$

$$R'(c_R)=\frac{dR}{d(\omega^2/k^2)}\Big|_{\omega^2/k^2=c_R^2}, \tag{33}$$

where $\omega/k\ll c_R$ is the classical Raleigh wave speed, which is a root of Eq. (30).

Eq. (33) is derived on the assumption that

$$\omega_R^2\eta D\ll\rho c_T^4\quad\text{and}\quad c_Rk\gg Dk^2+\tau^{-1}.$$

After decomposition of Eq. (33) into real and imaginary parts, for the frequency of surface acoustic waves (SAW) we have the familiar expression $\omega_R=c_Rk$.

The attenuation constant $\Gamma=\mathrm{Im}(\omega)$ of SAWs obtained from Eq. (33) is as follows:

$$\Gamma=\eta k^2\frac{c_R^2c_T^{-2}}{2\rho}+\delta_d k^2\frac{(1-c_R^2c_T^{-2})}{2c_L^2R'(c_R)}.$$

If $\omega_R^2\eta D\ll\rho c_T^4$ and $c_Rk\ll Dk^2+\tau^{-1}$, substitution of expressions (32) in Eq. (31) gives the following relationship:

$$\mathrm{Re}(\omega)=\omega_R\left(1-\frac{\beta^2}{2(1-\beta^2)}\frac{\delta_d k^2}{(Dk^2+\tau^{-1})}\right),$$

where $\beta^2=c_T^2c_L^{-2}$.

Note that, as well as for the case of unbounded medium, there is a softening of frequencies of SAWs. The critical value of the pump parameter is found from the condition $\mathrm{Re}(\omega)=0$. It is noted that the reduction of acoustic frequencies occurs not up to zero, and up to a value $\Gamma\approx\eta k^2c_R^2c_T^{-2}/2\rho\ll\mathrm{Re}(\omega)$.

Eq. (28) leads to the dispersion equation for static structures (on condition that $\omega/c_{T,L}\ll k$, $\sqrt{(i\omega+\tau^{-1})/D}$) in the form

$$\Gamma=\frac{\delta_d k^2}{1-c_T^2c_L^{-2}}-Dk^2-\tau^{-1}. \tag{34}$$

From the expression (34) it follows that if

$$\delta_d\geq\delta_{cr}=(1-c_T^2c_L^{-2})D,$$

i.e.

$$G>G_{cr}=\frac{k_BT\rho c_L^2(1-c_T^2c_L^{-2})}{\tau\vartheta_d^2},$$

there is a range of wave numbers

$$k>k_0=\sqrt{\tau_d^{-1}/(\delta_d(1-c_T^2c_L^{-2})^{-1}-D)},$$

in which $\Gamma>0$, i.e. the amplitudes of the Fourier harmonics of the perturbations increase with time without limit. This gives rise to an instability and its growth results in the formation of coupled ordered structures of defect density and strain on surface. The scale of surface static structures is

$$d_{latt}=2\pi\sqrt{\tau_dD}\sqrt{\frac{G_{cr}}{G-G_{cr}}}. \tag{35}$$

6. Conclusions

A dynamical model is proposed for the development of the DEI theory, which predicted the generation of one-dimensional plane harmonic elastic wave structures in unbounded media as well as Rayleigh's surface wave structures on the free surface of a half-space with non-equilibrium atomic defects. Lattice defects are generated as a result of shallow absorption of concentrated energy fluxes. The underlying idea of the model of an instability considered in this paper is caused by occurrence of a drift of atomic defects under the influence of elastic fields. A drift of defects results in a strain-induced flux of defects. At small concentrations of atomic defects, a little of their return influence can also be ignored. However under strongly non-equilibrium conditions, when the pump parameter is $G > G_{cr}$ (or the density of atomic defects $n > n_{cr}$), it is necessary to take into account the fact that the processes of generation react on the stress fields. Typical values of the constants $\Omega = 10^{-23}$ cm^3, $K = 5 \times 10^{11}$ erg cm^{-3}, $\tau = 10^{-3}$ s, $T = 500$ °C give an estimate of the critical defect (vacancy type) concentration $n_{cr} = 2 \times 10^{19}$ cm^{-3}. The equation for the kinetics of atomic defects is then supplemented by an equation from the theory of elasticity.

The set of dynamical differential equations accounting for simultaneous action of mechanical deformation and concentration fields is formulated. The defect dynamics is based on defect transport, generation, and annihilation. In the linear approximation with respect to the amplitude the dispersion equations for DEI are derived and investigated. We have shown that the dispersion equations predict the following two types of instabilities: (1) instability of frequencies of acoustic waves and (2) generation of ordered surface (static) structures.

We have observed that if the pump parameter is above the critical value, due to elastic–defect interaction the homogeneous distribution of atomic defects and the strain field become unstable and a coupled stationary strain–defect ordered structure on the surface or in the interior of solids arises. The increment of these structures is proportional to the pump parameter. The criterion of self-organization of atomic defects and the dependence of a lattice period on temperature of medium are determined analytically. The growth in period with increase in temperature is related to a decrease in the life-time of atomic defects. For a fixed value of the temperature field the period of the lattice decreases with increase in pump parameter. The critical value of the pump parameter for self-organization of periodic structures is governed by the dilatation volume of defects, by the potential energy of elastic interaction, and the elastic parameters of the medium.

In addition to one-dimensional (or two-dimensional) lattices, the growth of DEI on the surface can also create structures of different types. If the laser field has the axial symmetry relative to the z-axis, then surface structures in the form of radial rays and rings are formed. Then, the substitution

$$\exp(ikx) \to J_m(kr)\cos(m\varphi)$$

is made in solutions (10); here J_m is a Bessel function of the first kind and of order m ($m \gg 1$ is an integer). The specific case of $m = 0$ corresponds to structures that are concentric rings; r and φ are the polar coordinates in the xy-plane. An analysis similar to that given in Section 5 leads to a dispersion equation that is identical to Eq. (28) and the increment is independent of the number of a harmonic.

The degeneracy in respect of m is lifted if the laser radiation intensity (I) in a laser spot has the Gaussian distribution $I = I_0 \exp(r^2/r_0^2)$. This leads to the appearance of structures in the form of radial rays and it is then found that

$$\exp(ikx) \to (r/r_{eff})^m \cos(m\varphi)\exp(-r^2/r_{eff}^2).$$

($r_{eff} = r_0\sqrt{k_B T_0/\varepsilon_g} \ll r_0$, T_0 is the temperature at the center of the laser spot ($r = 0$), and r_0 is the laser spot radius; $k_B T_0 \ll \varepsilon_g$).

The dispersion dependences for these structures are again described by Eq. (28), but with k^2 replaced by $\tilde{k}^2 = 4m/r_0^2$. The maximum number of rays in a structure deduced from the condition $k_m^2 = \tilde{k}^2$ is $m \approx \pi^2 r_{eff}^2/d_{latt}^2$. For typical parameters $r_{eff} = 4 \times 10^{-3}$ cm and $d_{latt} = 3 \times 10^{-4}$ cm, we find that $m = 2 \times 10^3$.

We considered the self-organization of atomic defects of same jth type due to the interaction of these defects through the self-consistent strain field. In an irradiated medium, defects are generated as pairs of interstitial atoms ($j = i$) and vacancies ($j = v$). Usually the inequality $\vartheta_i \gg \vartheta_v$ is met for such processes. Therefore, we kept only the term with $\vartheta_d^{(j)} \equiv \vartheta_d > 0$ in Eqs. (7) and (8) for self-consistent displacements. Interstitial atoms form self-consistent periodic structures with defect-concentration maxima within the regions where strain field $div\, u_{ll} = \zeta > 0$. Vacancy defects are accumulated within the regions where $\zeta < 0$. Thus, double interstitial atom–vacancy periodic structures are formed.

Clearly, the linear theory considered here describes the early stage of the development of an instability only. However, the nature of generated ordered structures (due to an instability) and the amplitudes of these structures as functions on material and irradiation conditions can only be determined by considering the influence of nonlinear effects in the model. In this connection, computer simulation of fluctuation development is needed.

It is worth noting that the model developed in this paper can also be used to study the generation of thermo-elastic wave structures in irradiated insulating and semiconducting wafers. In this case, the roles of formation energy and the defect-relaxation time can be played by the band gap of the semiconductor (or insulator) and by the characteristic time of heat exchange with the surrounding medium (the thermal-relaxation time), respectively.

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