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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

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

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

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