Original Paper

phys. stat. sol. (b) **244**, No. 2, 529 – 544 (2007) / **DOI** 10.1002/pssb.200642078

Influence of flexoelectricity on the propagation of nonlinear strain waves in solids

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Received 20 February 2006, revised 21 July 2006, accepted 14 August 2006
Published online 27 September 2006

PACS 46.70.De, 61.72.Ji, 62.30.+d

A system of equations is formulated to describe the self-consistent behavior of elastic displacement fields and the concentration field of nonequilibrium point atomic defects (vacancies, interstitial atoms) in irradiated crystals with a symmetry center (germanium, silicon). In accordance with the values of the defect relaxation times, the model equations are derived, describing the propagation of nonlinear 1D longitudinal strain waves, with regard to the flexoelectric effect. The effect is due to the dielectric polarization induced by nonuniform elastic deformations of the lattice. For a particular relationship between the coefficients of these equations, i.e., between the parameters of the subsystem of defects and those of the nonlinear elastic medium, the exact solutions are obtained, which describe both the shock-wave structures of low-intensity and the evolution of solitary strain waves. The contributions of the strain-defect interaction and the flexoelectric effect to the linear and nonlinear elastic modulus and the dispersion and dissipation properties of the medium are estimated.

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1 Introduction

The processes of generation and propagation of nonlinear (both surface and bulk), localized, strain waves (solitons, cnoidal and shock waves, etc.) in elastic media were investigated in a large body of theoretical and experimental research [1 – 10]. The study of the behavior of such waves is important for an assessment of the durability of elastic materials and structures, determination of the physical properties of both standard and new elastic materials [1, 7]. Other possible applications of strain nonlinear waves come from the dependence of their amplitude, phase velocity, etc. upon the material properties and elasticity of the solids.

Strain waves of permanent forms may propagate in crystals due to the balance between nonlinearity and dispersion. Dispersion of the medium can be caused by the finiteness of the crystal-lattice period or by the sample thickness. Nonlinearity is provided by both the elastic features of a material (physical nonlinearity) and by a nonlinear relationship between displacements and strains [1].

In a solid exposed to external energy fluxes, specifically to laser pulses, the structural distortions of the crystal lattice, such as point defects (PDs) (vacancies, interstitial atoms) generated from the atoms at the lattice sites, can be of considerable importance. The nonequilibrium PDs produce a noticeable deformation of the lattice due to the difference between the covalent radii of the atoms and defects. The role of lattice defects can also be played by PD clusters available in the crystal or formed at high concentration of PDs. Other type of defects are individual impurity atoms that can enter the initial crystal during

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growth or be introduced a priori, impurity complexes, and by complexes involving vacancies or interstitial atoms of the initial crystal and impurity atoms.

Dynamic studies of nonlinear elastic waves with regard to their interaction with structural defects are of indubitable theoretical and practical interest. Specifically, such investigations are important for analyzing the mechanisms of anomalous mass transfer revealed on laser-assisted implantation and ion implantation of materials [11], as well as for studying the mechanical activation processes in solid-phase chemical reactions. When propagating through a condensed medium with defects, the wave of elastic deformation carries information on the distortions of the shape and velocity of the defects and the energy losses associated with the defect structure. Such information is required for optoacoustical diagnostics of various parameters and structures of solids. Specifically, knowledge of the velocity dependence of longitudinal elastic waves on the structural parameters of a crystal allows the use of these dependences for controlling the real structural parameters of the medium.

Manifestations of local atomic defects in the acoustic properties of crystals can be rather diverse. A large variety of the interaction mechanisms of elastic waves with a field of defect concentration can be divided into the two groups: direct interactions and indirect interactions. The first-group mentioned includes the interactions that induce changes in the intrinsic characteristics of the defects. For example, deformations in the elastic wave induce defect motion in the crystal (deformation-induced drift) and modulate the probability of the generation and recombination of thermal-fluctuation defects by changing the energy parameters of the defect subsystem, in accordance with the activation energies of formation and migration of the PDs [12].

In semiconductor crystals with a symmetry center, such as germanium and silicon, along with the nonlinearities listed above, the flexoelectric effect induced by the dielectric lattice polarization proportional to the elastic deformation gradient [13–18] can be of paramount importance. The flexoelectric effect produces extra local currents of PDs, i.e., barocurrents similar to the deformational currents, thus affecting the kinetics of the currents. In addition, a flexoelectric potential is generated, which modifies the activation energies of the formation and migration of defects, with consequent changes in the local defect concentration and, hence, spatial rearrangements of the defects.

The flexoelectric effect was predicted theoretically by Tolpygo et al. [13] and then treated by other authors [14–16]. Experimentally, this effect was studied in [18]. In contrast to the piezoelectric effect, the flexoelectric effect involves polarization, which can appear in a nonpiezoelectric crystal as a result of nonelectric factors. Consideration of the flexoelectric effect is found to be essential in studies of the interaction of free carriers (electrons) with a field of deformations in nonpiezoelectric crystals. According to [16], the flexoelectric effect and the deformation potential yield the same energy of interaction between the charge carriers and acoustic waves. The study of the flexoelectric effect in irradiated semiconductors (germanium, silicon) has shown that the electrostatic potential induced by this effect is rather noticeable in magnitude and exerts an influence (comparable to that of free carriers) on the electrical properties of the defect formation regions and, in some cases, totally controls these properties [17].

By the indirect mechanisms, the mechanisms in which the wave of elastic deformation interacts with collective excitations (phonons, excitons, etc.) in a crystal medium rather than with PDs themselves is meant. In these mechanisms, the role of the defects is reduced to changes in the parameters of these interactions [19].

At high concentrations of nonequilibrium lattice defects ($n = 10^{19} - 10^{20}$ cm^{-3}), the nonlinearities related to these interactions may become essential for the propagation of elastic nonlinear perturbations in solids and can give rise to radically new physical effects. Thus, physical nonlinearities related to defects can lead to renormalization of the lattice parameters (of both linear and nonlinear elastic modulus). The presence of PDs with a finite recombination rate in the medium can give rise to dissipative terms, which are absent in conventional equations for elastic nonlinear waves.

The dynamics of the wave can be substantially influenced by the dispersion caused by the finite crystal-lattice period [19] or sample thickness and by the dispersion associated with the generation and recombination in the system of nonequilibrium defects, as well as with the motion of defects in the field of deformations [20]. In such systems, the waves of elastic deformations can propagate as shock waves [20,

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21] or solitons (or sequence of solitons) [22]. In this case, the effect of the generation and recombination is found to be similar to the dissipation of the energy of elastic vibrations in a viscoelastic medium with an aftereffect and relaxation.

Previously [20–22], we considered the propagation of nonlinear longitudinal waves in solids with a quadratic elastic nonlinearity, taking into account the deformation-induced generation, recombination, and motion of PDs.

In this paper we formulate the system of equations that describes the propagation of nonlinear strain waves in irradiated solids with a center of symmetry (for example, germanium and silicon) with allowance for electrostatic and elastic interaction of nonequilibrium defects. We derive the model equations that describe the stationary one-dimensional (1D) longitudinal strain waves with allowance for flexoelectricity related to origination of electric polarization as a result of inhomogeneous deformations of the lattice. It will be shown that the flexoelectricity can give rise to an additional contribution to the linear and nonlinear elastic modulus, the dispersion parameter and also to a variation in the dissipative properties of the medium.

2 Basic equations

Let us consider a crystal in which the mobile PDs are formed under the exposure of laser pulses. Let the volume concentration of nonequilibrium PDs be $n^{(j)}(x, t)$, where the subscript $j = V$ refers to vacancies, and $j = I$ refers to interstitial atoms. Let $D^{(j)}$ is the diffusion coefficient for the PDs of type j. The propagation of slightly nonlinear perturbations of elastic deformation in irradiated crystals with a symmetry center should be studied by solving a coupled system of equations, which describes the interaction between the electromagnetic oscillations, elastic vibrations, and fields of PD concentration. This system involves the nonlinear equation of the theory of elasticity (written taking into account both the PD-produced forces acting on the lattice and the flexoelectric effect), the Maxwell equation, and the balance equation for the PD concentration.

In the approximation of an anisotropic elastic continuum, the dynamic equations for the elastic displacements in the lattice can be written, with regard to generation of PDs, as

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ik}}{\partial x_k}, \qquad \frac{\partial D_i}{\partial x_i} = 4\pi \rho_c (x_i), \tag{1}$$

here ρ is the density of the medium, u_i are the components of the displacement vector ($\boldsymbol{u}$) of the medium, σ_{ik} is the stress tensor, D_i is the component of the electrical induction vector, $\rho_c(x_i)$ is the charge density, and x_i is the cartesian coordinate.

To determine σ_{ik} and D_i we use the expression for the free energy density Φ of the system. The energy of the interaction between the PDs involves two contributions, namely, the contributions of deformational and electrostatic interactions.

In addition to the Coulomb attraction of the PDs to each other, the electrostatic interaction involves an interaction via the polarization of the medium. The electrostatic interaction can be important, if one of the PDs is charged or the fields of the crystal lattice deformations around the PDs are non-uniform.

In the case of non-uniform deformation of the medium, the dielectric polarization (P_i) can be represented as

$$P_i = \frac{1}{2} \mu_{ijkl} \left(\frac{\partial^2 u_j}{\partial x_k \, \partial x_l} + \frac{\partial^2 u_k}{\partial x_j \, \partial x_l} \right), \tag{2}$$

where μ_{ijkl} is the tensor of flexoelectric coefficients (piezoelectric semiconductors are not considered).

Assuming that the strains in the medium are fairly small, we restrict the expansion of free energy in terms of the invariants of the deformation tensor to the third-order quantities (the third-order anhar-

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monicity). Thus, with regard to the generation of PDs and the flexoelectric effect, we can write the expression for the density of the free energy in a crystal as follows:

$$\Phi = U - TS\,, \tag{3}$$

where U is the density of the potential energy of the elastic continuum with defects, S is the entropy density, and T is the temperature.

Let us represent U in the form:

$$\begin{aligned} &U = U_{\mathrm{elas}} + U_d + U_f + U_{\mathrm{el}}\,,\\ &U_{\mathrm{elas}} = \frac{1}{2}\, c_{iklm} u_{ik} u_{lm} + \frac{1}{3}\, \beta_{iklmns} u_{ik} u_{lm} u_{ns} + g_{iklmns} u_{ik}\, \frac{\partial^2 u_{lm}}{\partial x_n\, \partial x_s}\,,\\ &U_d = -\sum_{j=V,I} \vartheta_{ik}^{(mj)} u_{ik} n^{(j)}\,,\\ &U_f = -\frac{1}{2}\, E_i \left(\mu_{iklm} \frac{\partial u_{kl}}{\partial x_m} + \mu_{ilkm} \frac{\partial u_{lk}}{\partial x_m} \right),\\ &U_{\mathrm{el}} = -\frac{1}{8\pi}\, \varepsilon_{ij} E_i E_j\,, \end{aligned} \tag{4}$$

where U_{elas} is the energy density of the elastic continuum with allowance for anharmonicity (u_{ik} is the strain tensor; c_{iklm} and β_{iklmns} are the tensors of linear and nonlinear coefficients of elasticity defined in terms of the second- and third-order elastic constants; g_{iklmns} is the tensor of the dispersion constants of the lattice characterizing the spatial dispersion of the linear coefficients of elasticity); U_d and U_f are the energy densities corresponding to the interaction of PDs with elastic continuum and the flexoelectric effect; E_i is a component of the electric field vector; $\vartheta_{ik}^{(mj)} = K\Omega_{ik}^{(mj)}$ is the deformation potential. The dilatation parameter $\Omega_{ik}^{(mj)}$ characterizes the lattice deformation due to the appearance of a single point defect of the j-type in the lattice. By an order of magnitude, with $\Omega_{ik}^{(mV)} = -\delta^{(V)} a_0^3 < 0$ ($\delta^{(V)} = 0.2 - 0.4$, a_0 is the lattice period) for $j = V$, and $\Omega_{ik}^{(mj)} = \delta^{(I)} a_0^3 > 0$ ($\delta^{(I)} = 1.7 - 2.2$) for $j = I$. In the above formula, K is the bulk modulus. U_{el} is energy density of an electromagnetic field (ε_{ij} is the dielectric tensor).

The strain tensor is related to the components of elastic displacements by the expression

$$u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} + \frac{\partial u_l}{\partial x_i} \frac{\partial u_l}{\partial x_k} \right).$$

In order to simplify further presentations, we consider isotropic crystals with cubic symmetry. With respect to the system of crystal axes, the permittivity tensor is diagonal $\varepsilon_{ij} = \varepsilon_0 \delta_{ij}$. The diffusion tensor ($D_{ik}^{(j)}$) and the dilatation tensor ($\Omega_{ik}^{(mj)}$) are diagonal as well: $D_{ik}^{(j)} = D_d^{(j)} \delta_{ik}$ and $\Omega_{ik}^{(mj)} = \Omega^{(mj)} \delta_{ik}$.

Then using expressions (3) and (4), and the relation between σ_{ik} and Φ in the form

$$\sigma_{ik} = (\partial \Phi / \partial u_{ik})_{E_i, T, n}\,,$$

the equation of motion in view of the PD generation and the flexoelectric effect we shall write down as

$$\frac{\partial^2 \boldsymbol{u}}{\partial t^2} = c_t^2\, \Delta \boldsymbol{u} + \left(c_l^2 - c_t^2\right) \nabla\, \mathrm{div}\, \boldsymbol{u} + \frac{1}{\rho}\, N(\boldsymbol{u}) + g \nabla\, \Delta\, \mathrm{div}\, \boldsymbol{u} - \frac{\mu}{\rho}\, \nabla\, \Delta \varphi - \frac{1}{\rho} \sum_{j=I,V} \vartheta^{(jm)} \nabla n^{(j)}. \tag{5}$$

Here, $c_l = \sqrt{(\lambda + 2G)/\rho}$ and $c_t = \sqrt{G/\rho}$ are the longitudinal and transverse velocities of linear sound in the crystal, respectively [23]; λ and G are the Lame coefficients of elasticity; $g = K a_0^2/\rho$; $K = \lambda + 2/3G$;

div $\boldsymbol{u} = \partial u_l/\partial x_l = e$ is the strain of the medium; $N(\boldsymbol{u})$ is a bulk force caused by anharmonicity of elastic displacements. According to [23] for a component of this force we have:

$$N_i(\boldsymbol{u}) = \left(G + \frac{1}{4}A\right)\left(\frac{\partial^2 u_l}{\partial x_k^2}\frac{\partial u_l}{\partial x_i} + \frac{\partial^2 u_l}{\partial x_k^2}\frac{\partial u_i}{\partial x_l} + 2\frac{\partial^2 u_i}{\partial x_l\,\partial x_k}\frac{\partial u_l}{\partial x_k}\right)$$
$$+\left(K + \frac{1}{3}G + \frac{1}{4}A + B\right)\left(\frac{\partial^2 u_l}{\partial x_i\,\partial x_k}\frac{\partial u_l}{\partial x_k} + \frac{\partial^2 u_k}{\partial x_l\,\partial x_k}\frac{\partial u_i}{\partial x_l}\right) - \left(K + \frac{2}{3}G + B\right)\frac{\partial^2 u_i}{\partial x_k^2}\frac{\partial u_l}{\partial x_l},$$
$$+\left(\frac{1}{4}A + B\right)\left(\frac{\partial^2 u_k}{\partial x_l\,\partial x_k}\frac{\partial u_l}{\partial x_i} + \frac{\partial^2 u_l}{\partial x_i\,\partial x_k}\frac{\partial u_l}{\partial x_l}\right) + (B + 2C)\frac{\partial^2 u_k}{\partial x_i\,\partial x_k}\frac{\partial u_l}{\partial x_l}$$

where A, B, and C are the third-order elastic moduli. In this expression the terms with A, B, and C account for the physical nonlinearity, and other terms describe the geometrical nonlinearity.

On the right-hand side of Eq. (5), the third, fourth, fifth and sixth terms account for the anharmonicity of the medium, the spatial dispersion, the flexoelectric effect on the lattice, and the stresses produced by the PDs, respectively; φ is the electrostatic potential induced by the flexoelectric effect ($E = -\nabla\varphi$).

Using expression (3) and the relation between D_i and Φ in the form

$$D_i = -4\pi(\partial\Phi/\partial E_i)_{u_{kl},\,T,\,n}\,,$$

we obtain an equation for the potential of φ as follows:

$$\varepsilon_0\,\Delta\varphi = -4\pi\left(\rho_c(r) - \mu\,\Delta\,\mathrm{div}\,\boldsymbol{u}\right). \tag{6}$$

The right-hand side of Eq. (6) is defined by charge-carrier density and the flexoelectric effect.

In deriving the system of Eqs. (5) and (6), we took into account the relations [23]

$$c_{iklm} = \lambda\delta_{ik}\delta_{lm} + G\left(\delta_{il}\delta_{mk} + \delta_{im}\delta_{kl}\right),$$

$$\mu_{iklm} = \mu_1\delta_{ik}\delta_{lm} + \mu_2\left(\delta_{il}\delta_{mk} + \delta_{im}\delta_{kl}\right),$$

valid for isotropic media.

Here, δ_{ij} is Kronecker's symbol, μ_1 and μ_2 are the flexoelectric coefficients, and $\mu = \mu_1 + 2\mu_2$.

Equations (5) and (6) should be supplemented by the equation for the PD concentration. In the context of thermal-fluctuation model of the PD production, the rate of defect generation from the lattice sites is governed by temperature (or intensity of laser radiation) and stresses. Therefore, this rate may vary under the effect of propagating elastic wave, i.e., thermofluctuation-related defects may be generated and annihilate. Strain wave propagation and flexoelectricity affect the characteristics of the defects. Thus, when the longitudinal strain wave propagates, the formation energy ($w_q^{(j)}$) of PDs changes in the compression and dilatation zones. The renormalized formation energy of PDs can be represented as

$$\tilde{w}_q^{(j)} = w_q^{(j)}(0) - \vartheta^{(dj)}u_{ll} + Z^{(j)}\varphi$$

($w_q^j(0)$ is the formation energy for the j-th type of defect in an unstrained crystal, $Z^{(j)}$ is the change of defects). If there is a deformation-related perturbation of the lattice, not only the formation energy of defects decreases, but also the activation energy for the defect migration

$$\tilde{w}_m^{(j)} = w_m^{(j)}(0) - \vartheta^{(mj)}u_{ll} + Z^{(j)}\varphi$$

($w_m^{(j)}(0)$ is the migration energy of defects in the absence of deformation) decreases; this results in an increase in the diffusion coefficient.

We will consider here situations where the laser only heats the material, and that an equilibrium between laser radiation and the temperature field (T) is reached on time scales much shorter than the char-

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acteristic time scale of defects density evolution. Typically, the time scale for equilibration between photon absorption and defects generation is on the order of picoseconds, while that for PD diffusion is of the order of microseconds. We will also assume that the contribution of thermal strains to deformation fields is negligible compared to lattice dilatation due to PDs.

Modulation of the formation and migration energies brings about the corresponding modulations of the source function ($q^{(j)}$) and recombination rate ($r^{(j)}$) of defects of the j-type,

$$q^{(j)} = q^{(j)}(0) + q_1^{(j)} u_{ll} + q_2^{(j)} u_{ll}^2 + q_{1f}^{(j)} \varphi + q_{2f}^{(j)} \varphi^2 ,$$

$$r^{(j)} = r^{(j)}(0) + r_1^{(j)} u_{ll} + r_2^{(j)} u_{ll}^2 + r_{1f}^{(j)} \varphi + r_{2f}^{(j)} \varphi^2 ,$$

where $q^{(j)}(0)$ and $r^{(j)}(0)$ are the values of the source function and recombination rate in the absence of deformation ($u_{ll} = 0$, $\varphi = 0$);

$$q_1^{(j)} = q_{u_{ll}}^{(j)}(0) , \qquad q_2^{j} = \tfrac{1}{2}\, q_{u_{ll}u_{ll}}^{j}(0) , \qquad q_{1f}^{(j)} = q_{\varphi}^{(j)}(0) , \qquad q_{2f}^{(j)} = \tfrac{1}{2}\, q_{\varphi\varphi}^{(j)}(0) ,$$

$$r_1^{(j)} = r_{u_{ll}}^{(j)}(0) , \qquad r_2^{(j)} = \tfrac{1}{2}\, r_{u_{ll}u_{ll}}^{(j)}(0) , \qquad r_{1f}^{(j)} = r_{\varphi}^{(j)}(0) , \qquad r_{2f}^{(j)} = \tfrac{1}{2}\, r_{\varphi\varphi}^{(j)}(0)$$

(the subscripts "u_{ll}" and "φ" denotes the derivative with respect to u_{ll} and φ).

As a consequence, the local concentration of defects changes; correspondingly, the defects become spatially redistributed in the crystal lattice over macroscopic (on the order of the wavelength) or microscopic (on the order of the lattice constant) distances [19]. The corresponding changes of defect concentration results in a force on the lattice that may induce longitudinal deformation.

As a longitudinal strain wave propagates through the medium, defects interact with the strain field; as a result, not only do the rates of generation-recombination processes modulated but also strain-induced drift of defects arises, which gives rise to their additional spatial redistribution. If

$$W^{(j)} = U/n^{(j)} = \vartheta^{(mj)} u_{ll}$$

is the energy of the defect interaction with the strain field, the force exerted on defects by the strain field $F^{(j)} = \nabla W^{(j)}$ causes the defects to move with the velocity

$$\boldsymbol{V} = \frac{D_d^{(j)}}{k_{\mathrm{B}} T} \boldsymbol{F}^{(j)} .$$

Consequently, the total flux of defects is given by

$$\boldsymbol{J} = \boldsymbol{J}_1 + \boldsymbol{J}_2 + \boldsymbol{J}_3 ,$$

where

$$\boldsymbol{J}_1 = -D_d^{(j)} \nabla n^{(j)}$$

is the conventional diffusive flux,

$$\boldsymbol{J}_2 = n^{(j)} \boldsymbol{V}^{(j)} = \frac{n^{(j)} D_d^{(j)} \vartheta^{(mj)}}{k_{\mathrm{B}} T} \nabla u_{ll}$$

is the strain-induced flux of the PDs,

$$\boldsymbol{J}_3 = n^{(j)} \boldsymbol{V}_f^{(j)} = -\frac{n^{(j)} D_d^{(j)} Z^{(j)}}{k_{\mathrm{B}} T} \nabla \varphi$$

is the flux induced by the flexoelectric effect.

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Using the above-mentioned assumptions we can write the following kinetic equation if the inhomogeneous perturbations in the defect density $n_1^{(j)} = n^{(j)} - n_0^{(j)}$ are slight ($n_1^{(j)} \ll n_0^{(j)}$, where $n_0^{(j)} = q_0\tau^{(j)}$ is the steady-state uniform distribution of defects):

$$\frac{\partial n_1^{(j)}}{\partial t} + \nabla \boldsymbol{J}^{(j)} = (q_1^{(j)} + q_2^{(j)} u_{ll})\, u_{ll} + (q_{1f}^{(j)} + q_{2f}^{(j)}\varphi)\, \varphi - r_1^{(j)} n_0^{(j)} u_{ll} - r^{(j)}(0)\, n_1^{(j)}\,, \tag{7}$$

$$\boldsymbol{J}^{(j)} = -D_d^{(j)} \nabla n + q_D^{(j)} \nabla u_{ll} - q_f^{(j)} \nabla \varphi\,, \tag{8}$$

where

$$q_D^{(j)} = \frac{n_0^{(j)} D_d^{(j)} \vartheta^{(mj)}}{k_B T}\,, \qquad q_f^{(j)} = \frac{n_0^{(j)} D_d^{(j)} Z^{(j)}}{k_B T}\,.$$

Two first terms in the round brackets on the right-hand side of Eq. (7) accounts for the contributions to the generation of PDs that refer to the deformation potential, the two following terms describe the contributions to the generation of PDs that refer to the flexoelectric effect. The fourth accounts for the deformation-induced recombination of defects $r_1^{(j)} = r^{(j)}(0)\vartheta^{(mj)}/k_B T$, and the fifth term accounts for the losses of defects due to recombination in the absence of deformation ($r^{(j)}(0) = 1/\tau^{(j)}(0) = \rho_s^{(j)} D_d^{(j)}(0)$ is the recombination rate at the sinks, $\rho_s^{(j)}$ is the density of sinks, $D_d^{(j)}(0) = D_{d0} \exp(-w_m^{(j)}(0)/k_B T)$ is the diffusion coefficient for a defect of type j, k_B is the Boltzmann constant, and $\tau^{(j)}(0)$ is the relaxation time). Expression (8) defines the PDs flux of type j, $J^{(j)}$. In this expression the first, second, and third terms describe the conventional diffusion, deformation-induced drift, and flexoelectric effect, respectively.

According to experimental results [24] the values of defect-relaxation times can to vary over a wide range: from 10^{-3} s (for low temperatures) to 10^{-8} s (for high temperatures). The mutual recombination of the PDs of different types in the bulk is neglected. For the thermal mechanism of the PD generation, we have:

$$q_1^{(j)} = q(0)\,\frac{\vartheta^{(dj)}}{k_B T}\,, \qquad q_2^{(j)} = \frac{1}{2}\, q(0) \left(\frac{\vartheta^{(dj)}}{k_B T}\right)^2, \qquad q_{1f}^{(j)} = q(0)\,\frac{Z^{(j)}}{k_B T}\,,$$

$$q_{2f}^{(j)} = \frac{1}{2}\, q(0) \left(\frac{Z^{(j)}}{k_B T}\right)^2, \qquad q(0) = d_0^3 \omega_0 N_0^2 \exp\left(-\frac{w_q(0)}{k_B T}\right).$$

Here, ω_0 is the atomic vibrational frequency ($\omega_0 \sim 10^{14}\ \mathrm{s}^{-1}$); N_0 is the density of lattice sites.

As can be seen from Eqs. (5)–(8), within the framework of the above-specified approximation, the entropy density (S), with is involved in (3), does not enter into the equations of motion.

In what follows, we restrict ourselves to a system with a single type of defects and set $n_1^{(j)}(x,t) \equiv n_1(x,t)$, $\tau^{(j)}(0) \equiv \tau$, $D_d^{(j)} = D_d$, $\vartheta^{(dj)} = \vartheta^{(d)}$, etc. in Eqs. (5)–(8).

System of Eqs. (5)–(8) are close and completely define the self-consistent behavior of the fields of elastic displacements, flexoelectric potential, and PD concentration in the nonlinear elastic media.

3 One-dimensional longitudinal strain waves

Below, we will consider a one-dimensional crystal where the strain tensor has a single x-component,

$$u_{xx} = \frac{\partial u_x}{\partial x} \equiv e(x)\,.$$

Here, $u_x \equiv u$ is the component of the vector of medium displacement.

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For 1D smooth perturbations propagating the system of Eqs. (5)–(8) can be written as

$$\frac{\partial^2 u}{\partial t^2} - c_l^2 \frac{\partial^2 u}{\partial x^2} - \frac{\beta}{\rho}\frac{\partial^2 u}{\partial x^2}\frac{\partial u}{\partial x} - g\frac{\partial^4 u}{\mathrm{d}x^4} + \frac{\vartheta^{(m)}}{\rho}\frac{\partial n_1}{\partial x} + \frac{\mu}{\rho}\frac{\partial^3 \varphi}{\partial x^3} = 0\,, \tag{9}$$

$$\frac{\partial n_1}{\partial t} - D_d \frac{\partial^2 n_1}{\partial x^2} + \frac{n_1}{\tau} = (q_1 - r_1 n_0)\frac{\partial u}{\partial x} + q_2\left(\frac{\partial u}{\partial x}\right)^2 + q_{1f}\varphi + q_{2f}\varphi^2 - q_D\frac{\partial^3 u}{\partial x^3} + q_f\frac{\partial^2 \varphi}{\partial x^2}\,, \tag{10}$$

$$-\varepsilon_0 \frac{\partial^2 \varphi}{\partial x^2} = 4\pi\left(\rho_c(x) - \mu\frac{\partial^3 u}{\partial x^3}\right). \tag{11}$$

In Eq. (9) we have taken into account that for 1D longitudinal waves, $N(u) = (\beta/\rho)\,u_x u_{xx}$ [23], where $\beta = 3\rho c_l^2 + 2(A + 3B + C)$.

3.1 Linear waves

Let us consider the set of Eqs. (9)–(11) in the absence of quadratic non-linearity of an elastic continuum ($\beta = 0$). Then the solutions of this system can be presented as flat waves

$$n_1, u, \varphi \sim \exp\left[i(kx - \omega t)\right] \tag{12}$$

(k is the wave number and ω is the frequency of a wave). Substituting (12) into Eqs. (9)–(11), we obtain the following dispersion equation

$$(D_d k^2 + \tau^{-1} - i\omega)\,(c_l^2 k^2 - \omega^2 - \bar{g}_f k^4) = \frac{\vartheta^{(m)}}{\rho}\,\bar{q}_D k^4\,, \tag{13}$$

where

$$\bar{g}_f = g - \frac{4\pi}{\rho\varepsilon_0}\mu^2\,, \qquad \bar{q}_D = q_D - \frac{4\pi}{\varepsilon_0}\mu q_f\,,$$

c_l^2 is a square of velocity of a longitudinal sound in absence of the PDs and the flexoelectric effect. In arriving of Eq. (13) we have neglected by modulation of the rate of generation of defects due to the deformation potential and the flexoelectric effect ($q_1 = q_2 = q_{1f} = q_{2f} = 0$).

In a limiting case $\bar{q}_D = 0$ (the interaction of PDs with the strain field and flexoelectric effect are absent), the Eq. (13) breaks up to two independent dispersive equations:

$$\omega = -i(D_d k^2 + \tau^{-1})\,, \qquad \omega^2 = c_l^2 k^2 (1 - a_0^2 k^2)\,. \tag{14}$$

The first in (14) describes the diffusion mode, the second corresponds to propagation of acoustic waves in the absence of defects and flexoelectric effect.

In studying Eq. (13) for the case $\bar{q}_D \neq 0$ the solution shall be presented as:

$$\omega(k) = c(k)\,k\,. \tag{15}$$

Then from (13) we shall obtain the following equation for the phase velocity of the sound wave

$$(c')^3 + ia_1(c')^2 - a_2 c' - ia_3 = 0\,. \tag{16}$$

Here, the following dimensionless variables have been introduced:

$$c' = c/c_l\,, \qquad a_1 = (D_d k^2 + \tau^{-1})\,(kc_l)^{-1}\,, \qquad a_2 = 1 - \bar{q}_D k^2 c_l^{-2}\,,$$

$$a_3 = (D_d k^2 + \tau^{-1})\,(c_l^2 - \bar{g}_f k^2)\,(c_l^3 k)^{-1} - \bar{q}_D \vartheta^{(m)} (c_l^3 \rho)^{-1}\,k\,.$$

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Taking into account that the parameters a_1, a_2, a_3 are small, we can receive the following solutions of Eq. (16):

$$c_1' = ia_3\ ,$$

$$c_{2,3}' = \pm\left[1 - \frac{1}{8}(a_1^2 + 2a_1a_3 - 3a_3^2)\,(a_1 - a_2)\right] - \frac{i}{2}\,(a_1 - a_3)\,.$$

Then we obtain the expressions for the frequencies (after transition to a dimensional variable) in the form

$$\omega_1 = -i\left[\bar{D}_d k^2 - D_d \bar{g}_f k^4 c_l^{-2} + \frac{1}{\tau}\,(1 - \bar{g}_f k^2 c_l^{-2})\right], \qquad (17)$$

$$\omega_{2,3} = \pm c(k)\,k - i\Gamma(k)\,. \qquad (18)$$

First of these solutions characterizes the diffusion mode with the diffusion coefficient ($\bar{D}_d$) renormalized due to the defect-deformation interaction and the flexoelectric effect,

$$\bar{D}_d = D_d\left(1 + n_0\,\frac{4\pi Z\mu\vartheta^{(m)}}{\varepsilon_0\rho c_l^2 k_{\mathrm{B}}T} - n_0\,\frac{(\vartheta^{(m)})^2}{\rho c_l^2 k_{\mathrm{B}}T}\right),$$

and other two solutions describe a dispersion of elastic waves propagating along and against the x-axis.

The attenuation coefficient of acoustic waves (Γ) is determined by the formula

$$\Gamma(k) = (D_d k^2 + \tau^{-1})\,\frac{\bar{g}_f k^2}{2c_l^2} + \bar{q}_D\,\frac{K\Omega^{(m)}k^2}{2\rho c_l^2}\,. \qquad (19)$$

Note that according to (16)–(19) both the attenuation, and the dispersion are determined by dilatation volume, the modulus of elasticity and the flexoelectric modulus, and also by the temperature and the concentration of defects.

3.2 Nonlinear waves

For the self-similar variable $\xi = x - vt$ (v is the velocity of nonlinear wave), Eqs. (9)–(11) transforms into the following equation

$$(v^2 - c_l^2)\,\frac{\mathrm{d}^2u}{\mathrm{d}\xi^2} - \frac{\beta}{\rho}\,\frac{\mathrm{d}^2u}{\mathrm{d}\xi^2}\,\frac{\mathrm{d}u}{\mathrm{d}\xi} - g\,\frac{\mathrm{d}^4u}{\mathrm{d}\xi^4} = -\frac{\vartheta^{(m)}}{\rho}\,\frac{\mathrm{d}n_1}{\mathrm{d}\xi} - \frac{\mu}{\rho}\,\frac{\mathrm{d}^3\varphi}{\mathrm{d}\xi^3}\,, \qquad (20)$$

$$-v\frac{\mathrm{d}n_1}{\mathrm{d}\xi} - D_d\,\frac{\mathrm{d}^2n_1}{\mathrm{d}\xi^2} + \frac{n_1}{\tau} = (q_1 - r_1n_0)\,\frac{\mathrm{d}u}{\mathrm{d}\xi} + q_2\left(\frac{\mathrm{d}u}{\mathrm{d}\xi}\right)^2 + q_{1f}\varphi + q_{2f}\varphi^2$$
$$-q_D\,\frac{\mathrm{d}^3u}{\mathrm{d}\xi^3} + q_f\,\frac{\mathrm{d}^2\varphi}{\mathrm{d}\xi^2}\,, \qquad (21)$$

$$\varepsilon_0\,\frac{\mathrm{d}^2\varphi}{\mathrm{d}\xi^2} = -4\pi\left(\rho(\xi) - \mu\,\frac{\mathrm{d}^3u}{\mathrm{d}\xi^3}\right). \qquad (22)$$

In deriving the expression for the potential involved in Eq. (22), we took into account that the potential of the charges localized at free carriers and the defects are small, in comparison to the flexoelectric potential (the corresponding estimations can be found in [17]) and, hence, can be disregarded. Then, for the relation between the flexoelectric field φ and the deformation field, we have the equation

$$\varphi = \frac{4\pi\mu}{\varepsilon_0}\,\frac{\mathrm{d}u}{\mathrm{d}\xi}\,.$$

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Using this expression to eliminate the potential φ, we can write Eqs. (20) and (21) as

$$(v^2 - c_l^2)\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - \frac{\beta}{\rho}\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2}\frac{\mathrm{d}u}{\mathrm{d}\xi} - \left(g - \frac{4\pi}{\rho\varepsilon_0}\mu^2\right)\frac{\mathrm{d}^4 u}{\mathrm{d}\xi^4} = -\frac{\vartheta^{(m)}}{\rho}\frac{\mathrm{d}n_1}{\mathrm{d}\xi}, \tag{23}$$

$$-v\frac{\mathrm{d}n_1}{\mathrm{d}\xi} - D_d\frac{\mathrm{d}^2 n_1}{\mathrm{d}\xi^2} + \frac{n_1}{\tau} = \tilde{q}_1\frac{\mathrm{d}u}{\mathrm{d}\xi} + \tilde{q}_2\left(\frac{\mathrm{d}u}{\mathrm{d}\xi}\right)^2 - \tilde{q}_D\frac{\mathrm{d}^3 u}{\mathrm{d}\xi^3}, \tag{24}$$

where

$$\tilde{q}_1 = q_1 - r_1 n_0 + \frac{4\pi\mu}{\varepsilon_0}q_{1f}, \qquad \tilde{q}_2 = q_2 + \frac{16\pi^2}{\varepsilon_0^2}\mu^2 q_{2f}, \qquad \tilde{q}_D = q_D - \frac{4\pi\mu}{\varepsilon_0}q_f.$$

The solution to Eq. (24) supplemented by boundary conditions ($n_1(\pm\infty) = 0$) can be represented as

$$n_1(\xi) = \int_{-\infty}^{+\infty} \mathrm{d}\xi'\, L(\xi')\, S(\xi - \xi'), \tag{25}$$

where

$$S(\xi - \xi') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\,\frac{\exp[ik(\xi - \xi')]}{ikv - D_d k^2 - \tau^{-1}},$$

$$L(\xi) = \tilde{q}_D\frac{\mathrm{d}^3 u}{\mathrm{d}\xi^3} - \tilde{q}_1\frac{\mathrm{d}u}{\mathrm{d}\xi} - \tilde{q}_2\left(\frac{\mathrm{d}u}{\mathrm{d}\xi}\right)^2.$$

Eliminating the defect concentration and using expression (25), we obtain the following equation for the elastic displacement wave:

$$(v^2 - c_l^2)\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - \frac{\beta}{\rho}\frac{\mathrm{d}u}{\mathrm{d}\xi}\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - \left(g - \frac{4\pi}{\rho\varepsilon_0}\mu^2\right)\frac{\mathrm{d}^4 u}{\mathrm{d}\xi^4} + \frac{\vartheta^{(m)}}{\rho}\frac{\mathrm{d}}{\mathrm{d}\xi}\int_{-\infty}^{+\infty} S(\xi - \xi')\, L(\xi')\,\mathrm{d}\xi' = 0. \tag{26}$$

The Eq. (26) represents the integro-differential equation in which the occurrence of an integral term is caused by defect–strain interaction. Equations similar to (26) are characteristic of dissipative media with deformational memory (or relaxation) [1]. If there is no dispersion ($g = 4\pi\mu^2/\rho\varepsilon_0 = 0$) and the defects are not generated ($\vartheta^{(m)} = 0$), Eq. (26) has the same form as an equation for a longitudinal wave in free space. Eq. (26) can be used to analyze thoroughly the propagation of a nonlinear deformation wave in a solid with allowance for effects of both the dispersive properties of the medium and elastic properties of the lattice and of the point-defects' subsystem.

Let us consider the case of short relaxation times. At short relaxation times of the PDs, $\tau \ll t_0$, where $t_0 = \Lambda/c_l$ is the characteristic propagation time of the wave perturbations (Λ is the characteristic wavelength of the perturbations), the integral in Eq. (26) can be easily calculated, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\int_{-\infty}^{+\infty} \mathrm{d}\xi'\, S(\xi - \xi')\, L(\xi') \approx 2\tilde{q}_2\tau\frac{\mathrm{d}u}{\mathrm{d}\xi}\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} + \tilde{q}_1\tau\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} + \tilde{q}_1\tau^2 v\frac{\mathrm{d}^3 u}{\mathrm{d}\xi^3} + \tau(\tilde{q}_1\tau^2 v^2 - \tilde{q}_D)\frac{\mathrm{d}^4 u}{\mathrm{d}\xi^4} - \tilde{q}_D\tau^2 v\frac{\mathrm{d}^5 u}{\mathrm{d}\xi^5}. \tag{27}$$

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Combining (26) and (27), we obtain the equation for the nonlinear wave of displacements

$$\alpha \frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - \frac{\tilde{\beta}}{\rho} \frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} \frac{\mathrm{d}u}{\mathrm{d}\xi} - \gamma \frac{\mathrm{d}^3 u}{\mathrm{d}\xi^3} + \tilde{g} \frac{\mathrm{d}^4 u}{\mathrm{d}\xi^4} - \delta \frac{\mathrm{d}^5 u}{\mathrm{d}\xi^5} = 0 . \tag{28}$$

The sound velocity ($\tilde{c}_l$) and the nonlinearity ($\tilde{\beta}$), dissipation (γ), and dispersion ($\tilde{g}$) coefficients are expressed in the following form in terms of the generation-relaxation parameters of the PDs subsystem:

$$\alpha = v^2 - \tilde{c}_l^2 , \qquad \rho \tilde{c}_l^2 = \rho c_l^2 - \vartheta^{(m)} \tau (q_1 - r_1 n_0) - \frac{4\pi \vartheta^{(m)}}{\varepsilon_0} \tau \mu q_{1f} , \qquad \tilde{\beta} = \beta + \beta_q + \beta_f ,$$

$$\beta_q = -2\vartheta^{(m)} \tau q_2 , \qquad \beta_f = -\frac{32\pi^2 \vartheta^{(m)}}{\rho \varepsilon_0^2} \mu^2 q_{2f} , \qquad \gamma = \gamma_q + \gamma_f , \qquad \gamma_q = -\frac{\vartheta^{(m)}}{\rho} v \tau^2 (q_1 - r_1 n_0) ,$$

$$\gamma_f = -\frac{4\pi \vartheta^{(m)}}{\rho \varepsilon_0} v \tau^2 \mu q_{1f} , \qquad \delta = \delta_D + \delta_f , \qquad \delta_D = \frac{\vartheta^{(m)}}{\rho} v \tau^2 q_D , \qquad \delta_f = -\frac{4\pi \vartheta^{(m)}}{\rho \varepsilon_0} \mu v \tau^2 q_f ,$$

$$\tilde{g} = -(g + g_D + g_q + g_f) , \qquad g_D = \frac{\vartheta^{(m)}}{\rho} \tau q_D , \qquad g_q = -\frac{\vartheta^{(m)}}{\rho} \tau^3 v^2 (q_1 - r_1 n_0) ,$$

$$g_f = -\frac{4\pi}{\rho \varepsilon_0} \mu (\mu + \vartheta^{(m)} \tau^3 v^2 q_{1f} + \vartheta^{(m)} \tau q_f) .$$

In Eq. (28), the additives to sound velocity and to the dispersion coefficient are due to the interaction of the PDs with the deformation field and to the flexoelectrical effect. Since, $\rho = \mathrm{const}$, modulation of sound velocity means the corresponding modulation of the linear elastic moduli. The nonlinear coefficient ($\tilde{\beta}$) consists of three contributions, the contribution (β) associated with anharmonicity of elastic displacements of the medium, the contribution β_q associated with modulation of the defect generation rate by the deformation potential and the contribution β_f of the flexoelectric effect. The dissipative term appears due to the finite relaxation rate of the PDs, and the dissipation coefficient (γ) consists of two contributions, the contribution γ_q associated with modulation of the PD generation by the deformation potential and the contribution γ_f of the flexoelectric effect. With the typical values of the parameters $|\vartheta^{(m)}| = K|\Omega^{(m)}| = 10^{-11}$ erg, $\varepsilon_0 = 6$, and $a_0 = 5 \times 10^{-8}$ cm, we obtain the estimate:

$$\gamma_f / \gamma_q = 4\pi \mu Z / \varepsilon_0 K |\Omega^{(m)}| \approx 10 .$$

Thus, the contribution of the flexoelectric effect is found to be prevalent.

Note that the coefficients γ and δ in Eq. (28) are always positive $\gamma > 0,\ \delta > 0$, since

$$\vartheta^{(m)} (q_1 - r_1 n_0) < 0 , \qquad \vartheta^{(m)} \mu q_{1f} < 0 , \qquad \vartheta^{(m)} q_D > 0, \qquad \vartheta^{(m)} \mu q_f < 0 .$$

The coefficients α, $\tilde{\beta}$ and $\tilde{g}$ may be of different signs depending upon the material properties of the condensed system, the PD subsystem, and the flexoelectric effect. For example, $\tilde{g} > 0$, when the flexoelectric effect dominates:

$$|g_f| > g + g_D + g_q .$$

Performing a single integration with respect to ξ and using the boundary conditions $\mathrm{d}u/\mathrm{d}\xi|_{\xi \to \pm\infty} = 0$ we obtain the following nonlinear equation for the self-consistent strain $e(\xi) = \mathrm{d}u/\mathrm{d}\xi$:

$$\delta \frac{\mathrm{d}^3 e}{\mathrm{d}\xi^3} - \tilde{g} \frac{\mathrm{d}^2 e}{\mathrm{d}\xi^2} + \gamma \frac{\mathrm{d}e}{\mathrm{d}\xi} + \frac{\tilde{\beta}}{2\rho} e^2 - \alpha e = 0 . \tag{29}$$

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Equation (29) appears as an extension of the Kuromoto–Sivashinsky model, describing the propagation of nonlinear concentrations waves at chemical reactions [25]. Equations similar to Eq. (29) appear in many other physical problems, such as concerning nonlinear longitudinal waves in viscoelastic rods and plates [5, 7], nonlinear gravitational waves in a shallow water [26].

Equation (29) admits under particular conditions exact analytical solutions. In order to find these solutions, we use the method of [27] that makes it possible to implement the Backlund transformations, which simplify the solution to a great extent.

Using Backlund's transformation [27]

$$e(\xi) = \frac{15}{76}\left(\frac{\tilde{g}^2}{\sigma} - 16\gamma\right)\frac{\partial}{\partial \xi}\ln F + 15\tilde{g}\frac{\partial^2}{\partial \xi^2}\ln F - 60\sigma\frac{\partial^3}{\partial \xi^3}\ln F\,,$$

we can obtain the exact analytical solutions of Eq. (29) of the type of solitary waves which can be represented as

$$e(\xi) = 15k^2\left(\frac{\tilde{g}}{4} + \sigma k\,\tanh\left(\frac{k}{2}\xi\right)\right)\cosh^{-2}\left(\frac{k}{2}\xi\right) + \frac{15k}{152}\left(\frac{\tilde{g}^2}{\delta} - 16\gamma\right)\left[1 + \tanh\left(\frac{k}{2}\xi\right)\right].$$

These solutions exist in the following three cases:

$$\text{a)}\ \ \tilde{g} = 4\sqrt{\gamma\sigma}\,, \qquad k^2 = \frac{\gamma}{\delta}\,, \qquad \alpha = -6\gamma\sqrt{\frac{\gamma}{\delta}}\,, \tag{30}$$

$$\text{b)}\ \ \tilde{g} = 19\sqrt{\frac{\gamma\sigma}{47}}\,, \qquad k^2 = \frac{\gamma}{47\delta}\,, \qquad \alpha = \frac{60}{47}\gamma\sqrt{\frac{\gamma}{47\delta}}\,, \tag{31}$$

$$\text{c)}\ \ \tilde{g} = 16\sqrt{\frac{\gamma\sigma}{73}}\,, \qquad k^2 = \frac{\gamma}{73\delta}\,, \qquad \alpha = \frac{90}{73}\gamma\sqrt{\frac{\gamma}{73\delta}}\,. \tag{32}$$

In case (a), the solution of Eq. (29) is a solitary wave

$$e(\xi) = e_0\frac{1 + \tanh\,(k\xi/2)}{\cosh^2\,(k\xi/2)}. \tag{33}$$

Here,

$$e_0 = -\frac{15\rho}{\tilde{\beta}}\gamma\sqrt{\frac{\gamma}{\delta}} = -\frac{15 n_0 \vartheta^{(m)}(\vartheta^{(m)} - \vartheta^{(d)})\,v}{\tilde{\beta}k_B T}\sqrt{\frac{\tau}{D_d}}$$

is the amplitude of the nonlinear wave.

At $\xi \to \pm\infty$, the solution decays. At $\xi = 0$ it has a single maximum:

$$e_{\max} = \frac{160}{9}\gamma\sqrt{\frac{\gamma}{\delta}}\,.$$

The width of the solitary wave is proportional to the of dissipation coefficient (γ) as defined by expression

$$\Delta_0 = \frac{12\gamma}{\tilde{c}_l^2 - v^2}\,.$$

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According to (30), the velocity of the nonlinear wave and its amplitude are interrelated by expression

$$v^2 = \tilde{c}_l^2 - 6\gamma\sqrt{\frac{\gamma}{\delta}} = -\frac{2\tilde{\beta}}{5\rho}\, e_0 \,. \tag{34}$$

Note that the type of the strain wave (33) (compressive or tensile) is defined only by the sign of the nonlinear coefficient $\tilde{\beta}$, which depends on the coefficients of elasticity and the flexoelectric coefficients of the lattice, as well as the parameters of the PD subsystem. The propagating wave is a dilatation wave ($e_0 > 0$) if $\tilde{\beta} < 0$ and a compression wave ($e_0 < 0$) if $\tilde{\beta} > 0$.

The solution to Eq. (24) for the defect concentration is given by the following formula in the case of solition (33):

$$n_1(\xi) = \tau\tilde{q}_2 e^2 + \tau\tilde{q}_1\left(e + \tau v\frac{\mathrm{d}e}{\mathrm{d}\xi} + \tau^2 v^2\frac{\mathrm{d}^2 e}{\mathrm{d}\xi^2}\right) + \tau\tilde{q}_D\left(\tau v\frac{\mathrm{d}^2 e}{\mathrm{d}\xi^2} + \frac{\mathrm{d}e}{\mathrm{d}\xi}\right). \tag{35}$$

It follows from (34) that the solitary waves of strain (and also the defect concentration) are fairly slow and their velocities are not higher than the longitudinal sound velocity in the crystal. Evidently, the waves with larger amplitudes propagate with higher velocities.

In the other two cases, ((b) and (c)), the solution represents a kink. If the coefficients of Eq. (29) are related by expressions (31), we substitute expression

$$e(\xi) = e_0\,(1 + \exp(-k\xi))^{-3} \tag{36}$$

directly into Eq. (29) and can verify that expression (36) is the exact solution of Eq. (29). The amplitude of the nonlinear wave:

$$e_0 = \frac{120}{47}\,\frac{\rho\gamma}{\tilde{\beta}}\sqrt{\frac{\gamma}{47\delta}} = -\frac{120}{47}\,\frac{n_0\vartheta^{(m)}(\vartheta^{(m)} - \vartheta^{(d)})\,v}{\tilde{\beta}k_{\mathrm{B}}T}\sqrt{\frac{\tau}{47D_d}}\,.$$

This solution describes the structure of a shock wave, since it continuously combines two asymptotically uniform states described as

$$e(\infty) = \frac{120}{47}\,\frac{\gamma}{\tilde{\beta}}\sqrt{\frac{\gamma}{47\delta}}\,, \qquad e(-\infty) = 0\,.$$

Let us now consider the behavior of solution (36) behind the wave front. Assuming that $e = e(\infty) + e_1$ and $|e_1| \ll 1$, from the Eq. (29) we obtain the third-order differential equation for deformational perturbation. By calculating the discriminant ($\mathit{\Delta}$) of the corresponding characteristic equation, we find that $\mathit{\Delta} < 0$, i.e., the roots of the equation are real quantities. Therefore, the perturbation e_1 cannot be an oscillatory quantity. This means that the shock wave described by expression (36) has a monotonic structure.

The front width and velocity of the shock wave are defined by the formulas

$$\mathit{\Delta}_0 = \sqrt{\frac{47\delta}{\gamma}} = -\frac{60\gamma}{47(\tilde{c}_l^2 - v^2)}\,,$$

$$v^2 = \tilde{c}_l^2 + \frac{60}{47}\gamma\sqrt{\frac{\gamma}{47\delta}} = \frac{\tilde{\beta}}{2\rho}\, e_0\,. \tag{37}$$

If the coefficients in Eq. (29) satisfy relations (32), the exact solution of the equation is

$$e(\xi) = e_0\,\frac{3 + \exp(-k\xi)}{(1 + \exp(-k\xi))^3}\,, \tag{38}$$

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here

$$e_0 = \frac{60\gamma}{73\tilde{\beta}} \sqrt{\frac{\gamma}{73\delta}} = \frac{60}{73} \frac{n_0 \vartheta^{(m)} (\vartheta^{(m)} - \vartheta^{(d)})\, v}{\tilde{\beta} k_{\mathrm{B}} T} \sqrt{\frac{\tau}{73 D_d}} .$$

For long distances from the wave front $\xi = 0$, we use formula (38) to obtain the asymptotic values

$$e(\infty) = -\frac{60}{73} \frac{\gamma}{\tilde{\beta}} \sqrt{\frac{\gamma}{73\delta}} , \qquad e(-\infty) = 0 .$$

According to (32) and (38), the front width and velocity of the shock wave are defined by formulas

$$\Delta_0 = \frac{90\gamma}{73(\tilde{c}_l^2 - v^2)} ,$$

$$v^2 = \tilde{c}_l^2 + \frac{90}{73} \gamma \sqrt{\frac{\gamma}{73\delta}} = \frac{3\tilde{\beta}}{2\rho} e_0 . \tag{39}$$

As in previous case (33), the type of the strain waves (36) and (38) (compressive or tensile) is defined only by the sign of the nonlinear coefficient $\tilde{\beta}$.

The solutions to Eq. (24), which correspond to kink-type solutions (36) and (38), can be derived using formula (35).

The received solutions (36) and (39) describes the structures of shock waves, as continuously connect two homogeneous statuses $e(\infty)$ and $e(-\infty)$ of systems ahead and behind of wave front. The shock wave profiles obtained indicate that there are no oscillations ahead and behind the fronts, i.e., the wave structures are monotonic. It follows from formula (34) that the defect-strain solitary waves are fairly slow; their velocity is no higher than the linear-sound velocity. In contrast, the shock waves propagate with hypersonic velocities [see formulas (37) and (39)]. The front widths of both waves are proportional to the dissipation coefficient. The waves with higher amplitudes propagate with higher velocities.

Let us now consider the case of long relaxation times. For long relaxation times, i.e., $\tau \gg t_0$, by integrating by parts, we represent the integral term in Eq. (26) as an expansion in the powers of τ^{-1}:

$$\frac{\mathrm{d}}{\mathrm{d}\xi} \int_{-\infty}^{+\infty} \mathrm{d}\xi' \, S(\xi - \xi')\, L(\xi') \approx \frac{1}{v} \left(\tilde{q}_D \frac{\mathrm{d}^3 u}{\mathrm{d}\xi^3} - \tilde{q}_1 \frac{\mathrm{d}u}{\mathrm{d}\xi} \right) + \frac{1}{v^2 \tau} \left(\tilde{q}_D \frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} + \tilde{q}_1 u \right) + \frac{\tilde{q}_1}{v^3 \tau^2} \frac{\mathrm{d}u}{\mathrm{d}\xi} \cdots$$

Restricting ourselves to the leading terms in this expansion, we arrive at the equation

$$(v^2 - \tilde{c}_l^2) \frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - \frac{\beta}{\rho} \frac{\mathrm{d}u}{\mathrm{d}\xi} \frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - \tilde{g} \frac{\mathrm{d}^4 u}{\mathrm{d}\xi^4} = -\eta_1 u + \eta_2 \frac{\mathrm{d}u}{\mathrm{d}\xi} - \eta_3 \frac{\mathrm{d}^3 u}{\mathrm{d}\xi^3} . \tag{40}$$

Here,

$$\tilde{c}_l = c_l (1 - \tilde{q}_D \vartheta^{(m)} / \rho \tau c_l^{\,2})^{1/2}$$

is the sound velocity renormalized by the interaction of the defects with the field of elastic displacements;

$$\tilde{g} = g(1 - 4\pi \mu^2 / g \rho \varepsilon_0)$$

is the dispersion coefficient renormalized by the flexoelectric effect;

$$\eta_1 = \tilde{q}_1 \vartheta^{(m)} / \rho \tau v^2 , \qquad \eta_2 = \tilde{q}_1 \vartheta^{(m)} / \rho v \quad \text{and} \quad \eta_3 = \tilde{q}_D \vartheta^{(m)} / \rho v$$

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are the coefficients of the wave dissipation caused by the generation-recombination processes (η_1, η_2) and the strain-induced drift of lattice defects (η_3). Note, that all coefficients in Eq. (40) (with the exception of β) contain the contributions caused by the flexoelectric effect.

The right-hand side of Eq. (40) accounts for attenuation of nonlinear wave. In this case, the shock waves are not formed in the medium; rather, the strain perturbations propagate in the form of solitary waves (solitons). The presence of strain-induced drift of defects and the flexoelectric effect lead to the renormalization of both the velocity of the longitudinal sound wave and the dispersion and dissipation parameters of the medium. The analytical solution of the Eq. (40) can be obtained by a technique similar to that considered in [20, 28]. One may consider Eq. (40) as a slightly dissipation-perturbed KdV equation. Physically it responds to the propagation of solitary waves in medium with slowly varying parameters. Prominent feature of solutions of these equations is occurrence due to the dissipative terms of a “shelf” for perturbed solitary waves.

4 Conclusion

In crystals with a symmetry center, the deformation-induced modulation of the probabilities of defect generation, the motion of defects, and the flexoelectric effect result in an interaction between the field of deformations in the elastic wave and the PD subsystem. In the linear approximation the dispersion equation for the propagation of the linear waves in such systems is derived and investigated. The dispersive equation has three roots. First of these solutions characterizes the diffusion mode with the diffusion coefficient renormalized due to the defect-strain interaction and the flexoelectric effect, and other two solutions describe a dispersion of elastic waves propagating along and against the x-axis. The attenuation coefficient and the dispersion of the linear waves are determined by dilatation volume of PDs, the modulus of elasticity and the flexoelectric modulus, and also by the temperature and the concentration of defects.

The propagation of nonlinear strain waves can be described by the modified KdV-Burgers’s equation commonly applied to a media with dissipation and dispersion. At a particular relationship between the coefficients of this equation, i.e., between the parameters of the PD subsystem and the elastic nonlinear medium, both solitary and low-intensity elastic shock waves can develop in a medium. The contributions of the interaction between the PDs and deformations and of the flexoelectric effect to the linear and nonlinear elastic modulus and the dispersion and dissipation properties of the medium are estimated. The amplitude and velocity of the nonlinear waves considered in this study depend on the elastic and flexoelectric constants, temperature, and parameters of the PD subsystem of the medium. Consequently, the analytical predictions of this study make it possible to independently determine the coefficients of elasticity and the flexoelectric coefficients of the lattice, as well as the parameters of the PD subsystem (e.g., the recombination rates, the activation energies of migration and formation of PDs, etc.) in solids from the experimental data on nonlinear distortions of longitudinal deformation waves.

Acknowledgment The author would like to thank Professor L. A. Shelepin for stimulating and helpful discussions. The author would also like to thank the referees for valuable comments.

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