ISSN 1063-7826, Semiconductors, 2006, Vol. 40, No. 3, pp. 262–269. © Pleiades Publishing, Inc., 2006.
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Nonlinear Longitudinal Waves of Interacting Fields of Deformation and Defect Concentration in Germanium and Silicon

F. Kh. Mirzade

Institute for Laser and Information Technologies, Russian Academy of Sciences, Shatura, 140700 Russia
e-mail: fmirzade@rambler.ru

Submitted February 9, 2005; accepted for publication July 5, 2005

Abstract—A system of equations is formulated to describe the self-consistent behavior of elastic displacement fields and the concentration field of point defects in irradiated crystals with a symmetry center (germanium, silicon). In accordance with the values of the defect relaxation times, the model evolution equations are derived, describing the steady-state nonlinear longitudinal 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 the generation of solitons and low-intensity shock waves. The contributions of the strain-defect interaction and the flexoelectric effect to the linear velocity of sound and the dispersion properties of the medium are estimated.

PACS numbers: 71.55.Cn, 62.30.+d

DOI: 10.1134/S1063782606030031

1. INTRODUCTION

The processes of generation and propagation of nonlinear, (both surface and bulk) localized, deformation waves (solitons, cnoidal and shock waves, etc.) in elastic media were investigated in a large body of theoretical and experimental research [1–6]. In studies of the physical mechanisms of nonlinear wave generation, the inharmonious vibrations of the crystal lattice, which describe the deviation of the elastic properties of the medium from Hooke's law, are considered as the major contributor to nonlinearity. 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 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, individual impurity atoms that can enter the initial crystal during 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 [7], 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 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 group first-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 [8, 9].

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 [10–15] 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.* [10] and then treated by other authors [11–14]. Experimentally, this effect was studied in [15]. 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 [13], 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 [14].

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.

Under certain conditions, the nonlinearities caused by these interactions can be essential for the propagation of nonlinear elastic perturbations in solids, basically resulting in new physical effects. For example, the physical nonlinearities caused by the defects can yield a renormalization of the lattice parameters (both linear and nonlinear coefficients of elasticity). For a medium in which the PDs have a finite recombination rate, the equations describing nonlinear elastic waves can involve dissipative components lacking in the conventional equations for nonlinear elastic waves [16–19].

The dynamics of the wave can be substantially influenced by the dispersion caused by the finite crystal-lattice period [20] 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 [16]. In such systems, the waves of elastic deformations can propagate as shock waves [18, 19] or solitons (or sequence of solitons) [16, 17]. 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 [16–19], 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 study, an attempt to extend results of [16–19] to the processes that flexoelectric effects, is taken into account.

2. BASIC EQUATIONS

Let us consider a crystal in which the PDs are formed under the exposure of laser pulses. Let the volume concentration of the PDs be n_j, where the subscript $j = V$ refers to vacancies, and $j = I$ refers to interstitial atoms. 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

$$\frac{\partial H_i}{\partial x_i} = 4\pi\rho(\mathbf{r}), \quad \rho_0\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ik}}{\partial x_k}, \tag{1}$$

where ρ_0 is the density of the underformed; u_i is a component of the vector of displacements; σ_{ik} is the stress tensor; H_i is the component of the electrical induction vector; $\rho(\mathbf{r})$ is the charge density, and x_i is the Lagrangian coordinate.

To determine σ_{ik} and H_i, we use the expression for the free energy density F 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 nonuniform.

In the case of nonuniform 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 here). The corresponding contribution of the polarization to the free energy of the system can be represented as

$$F_{\text{fl}} = \frac{1}{2}P_i\mu_{ijkl}\left(\frac{\partial^2 u_j}{\partial x_k \partial x_l} + \frac{\partial^2 u_k}{\partial x_j \partial x_l}\right).$$

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 anharmonicity). Thus, with regard to the generation of PDs and the flexoelectric effect, we can write the expression for free energy density of the elastic continuum as follows:

$$\begin{aligned} F - F_0 &= \frac{1}{2}\lambda_{iklm}u_{ik}u_{lm} + \frac{1}{3}\beta_{klmns}u_{ik}u_{lm}u_{ns} \\ &+ g_{iklmns}u_{ik}\frac{\partial^2 u_{lm}}{\partial x_n \partial x_s} - \sum_{j = V, I} K\Omega^j_{ik}u_{ik}n_j - \frac{1}{8\pi}\varepsilon_{ij}E_iE_j \\ &- \frac{1}{2}E_i\left(\mu_{iklm}\frac{\partial u_{kl}}{\partial x_m} + \mu_{ilkm}\frac{\partial u_{lk}}{\partial x_m}\right), \end{aligned} \tag{3}$$

where F_0 is the free energy of the undeformed crystal; u_{ik} is the strain tensor; λ_{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; E_i is a component of the electric field vector; ε_{ij} is the dielectric tensor, and Ω^j_{ik} is the symmetric tensor characterizing the lattice deformation due to the appearance of an individual PD of type j ($\Omega^j_{ik} > 0$ for interstitial atoms and $\Omega^j_{ik} < 0$ for vacancies). The first three terms on the right-hand side of expression (3) describe the elastic energy, while the fourth term describes the energy of the interaction of PDs with the field of elastic deformation. The last two terms refer to the contribution of the flexoelectric effect to free energy.

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

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

Since the stress tensor is $\sigma_{ik} = (\partial F/\partial u_{ik})_{E, T, n}$, we obtain, with regard to (3), the following expression:

$$\begin{aligned} \sigma_{ik} &= \lambda_{iklm}u_{lm} + \beta_{iklmns}u_{lm}u_{ns} + g_{iklmns}\frac{\partial^2 u_{lm}}{\partial x_n \partial x_s} \\ &- \frac{1}{2}(\mu_{iklm} + \mu_{ilkm})\frac{\partial^2 \varphi}{\partial x_l \partial x_m} - \sum_{j = V, I} K\Omega^j_{ik}n_j. \end{aligned} \tag{4}$$

On the right-hand side of formula (4), the second, third, fourth, and fifth 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.

Then, using expression (3) and the relation between H_i and F in the form $H_i = -4\pi(\partial F/\partial E_i)_{u_{kl}, T, n}$, we obtain an equation for the potential of φ as follows:

$$-\varepsilon_{ij}\frac{\partial^2 \varphi}{\partial x_i \partial x_j} = 4\pi\left(\rho - \mu_{iklm}\frac{\partial^2 u_{kl}}{\partial x_i \partial x_m}\right). \tag{5}$$

The right-hand side of Eq. (5) is defined by charge-carrier density and the flexoelectric effect.

Equations (4) and (5) should be supplemented by the equation for the PD concentration. In the context of the thermal fluctuations model for the formation of defects, the generation rate of the defects at the crystal lattice sites is controlled by temperature and elastic stresses, therefore it can be changed under the effect of propagating elastic waves. In other words, the defects can appear and recombine. We considered long-wavelength elastic waves, so that the scattering effects are not essential. The deformation in the elastic wave and the flexoelectric phenomenon affect the characteristics of the PDs themselves. In fact, when longitudinal wave perturbations of elastic deformation propagate through a medium, the formation energy of PDs in the stretched and compressed regions is modulated. In linear approximation, with respect to deformation, the activation energy of PDs formation, $\tilde{E}^j_f$, renormalized by a deformation and flexoelectric effect can be represented as $\tilde{E}^j_f = E^j_{f0} - \vartheta^j_{ik}\mathbf{u}_{ik} + Z^j\varphi$; where E^j_{f0} is the formation energy of the PD of type j in the undeformed crystal, ϑ^j_{ik} is the deformation potential. The energy modulation of the formation of defects brings about the corresponding modulation of the source function of the defects, Q_j,

$$Q_j = Q_{j0} + Q_{ju_{ik}}u_{ik} + Q_{j\varphi}\varphi$$

(Q_{j0} is the source function if there is no deformation and the subscript u_{ik} designates the derivative with respect to u_{ik}); as a consequence, changes in the local concentration and, correspondingly, by spatial rearrangement of the PDs over a crystal lattice are observed. In this case, the PDs can move over macroscopic or microscopic distances (on the order of the wavelength or lattice constant, respectively) [20].

In addition to the modulation of generation rates, the interaction of the PDs with field of elastic deformations and the flexoelectric effect induce drift motion of the PDs, resulting in their additional spatial rearrangement. If $U_j = K\Omega^j_{ik}u_{ik}$ is the energy of the interaction of the PDs of type j with the deformation field [20], the force of the deformation field $F_j = -\nabla U_j$ causes the defects to move with the velocity $\mathbf{V}_j = \mathbf{F}_j D_j/kT$ (D_j is the diffusion coefficient for the PDs of type j; T is the temperature). Consequently, the total flux of the PDs is $\mathbf{J}_j = \mathbf{J}_{j1} + \mathbf{J}_{j2} + \mathbf{J}_{j3}$, where $\mathbf{J}_{j1} = -D_j\nabla n_j$ is the conventional diffusion flux, $\mathbf{J}_{j2} = n_j\mathbf{V}_j$ is the deformation-induced flux of the PDs, and $\mathbf{J}_{j3} = n_j\mathbf{V}_{j\varphi}$ is the flux induced by the flexoelectric effect.

With regard to the consideration above, we can write in the linear approximation with respect to the strain, the balance equation of diffusion for the concentration n_j as

$$\frac{\partial n_j}{\partial t} + \operatorname{div} J^j_\alpha = Q_{j0}\left(\frac{\vartheta^j_{ik}u_{ik}}{kT} - \frac{Z^j\varphi}{kT}\right) - \frac{n_j}{\tau_j}, \quad (6)$$

$$J^j_\alpha = -D^j_{\alpha m}\nabla_m n - \frac{Zn_{j0}D^j_{\alpha m}}{kT}\nabla_m\varphi + \frac{n_{j0}D^j_{\alpha m}K\Omega^j_{ik}}{kT}\nabla_m u_{ik}. \quad (7)$$

Here, $D^j_{\alpha m}$ is the tensor of the diffusion coefficients for the PDs of type j; τ_j is the relaxation time of the PDs of type j; T is the temperature; k is the Boltzmann constant, and $n_{j0} = Q_{j0}\tau_j$ is the spatially uniform steady-state concentration of the PDs. On the right-hand side of Eq. (6), the first and second terms in the parenthesis describe the contributions to the generation of PDs that refer, correspondingly, to the deformation potential ϑ_{ik} and to the flexoelectric effect. The last term in Eq. (6) describes the relaxation of the PDs controlled by recombination at neutral sinks. Expression (7) defines the α component of the PDs flux of type j, J^j_α. In this component, the first, second, and third terms describe the conventional diffusion, deformation-induced drift, and flexoelectric effect, respectively. The mutual recombination of the PDs of different types in the bulk is disregarded.

In order to simplify further presentations, we consider isotropic crystals with cubic symmetry. In addition, we assume that there is only one type of mobile PDs in the crystal (e.g., vacancies) and set $n_j = n$, $D^j_{\alpha m} = D_{\alpha m}$, and $\Omega^j_{ik} = \Omega_{ik}$ in relations (3)–(7). With respect to the system of crystal axes, the permittivity tensor is diagonal: $\varepsilon_{ij} = \varepsilon_0\delta_{ij}$. The diffusion tensor and the dilatation tensor are diagonal as well: $D_{\alpha m} = D\delta_{\alpha m}$ and $\Omega_{ik} = \Omega\delta_{ik}$. Then, from (1)–(7), we obtain the following system of equations:

$$\frac{\partial^2 u}{\partial t^2} = c_\tau^2\Delta\mathbf{u} + (c_l^2 - c_\tau^2)\nabla\operatorname{div}\mathbf{u} + N(\mathbf{u}) + g\nabla(\Delta\operatorname{div}\mathbf{u}) - \mu\nabla(\Delta\varphi) - \frac{K\Omega}{\rho}\nabla n, \quad (8)$$

$$\Delta\varphi = -\frac{4\pi}{\varepsilon_0}(\rho(r) - \mu\Delta\operatorname{div}\mathbf{u}), \quad (9)$$

$$\frac{\partial n}{\partial t} = Q_e\operatorname{div}\mathbf{u} + Q_\varphi\varphi - \frac{nDK\Omega}{kT}\Delta\operatorname{div}\mathbf{u} + \frac{nZD}{kT}\Delta\varphi + D\Delta n - \frac{n}{\tau}. \quad (10)$$

Here, c_l and c_τ are the longitudinal and transverse velocities of linear sound in the crystal, respectively [21]; $g = Kd_0^2/\rho$ (d_0 is the lattice period); and $N(\mathbf{u})$ is the force density caused by anharmonicity of elastic displacements. For longitudinal waves, we have $N(u) = (\beta/2\rho)\nabla(u_{ll})^2$ [21], where $\beta = 3\rho c_l^2 + 2(A + 3B + C)$ (A, B, and C are the third-order constants of elasticity) and $\operatorname{div}\mathbf{u} = u_{ll} = e$ is the strain of the medium.

In deriving the system of equations (8)–(10), we took into account the relations

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

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

valid for isotropic media [14]. Here, δ_{ij} is Kronecher's symbol, λ and G are the coefficients of elasticity Lamé, μ_1 and μ_2 are the flexoelectric coefficients, and $\mu = \mu_1 + 2\mu_2$.

System of equations (8)–(10) are close and completely define the intercorrelated behavior of the fields of elastic displacements, flexoelectric potential, and PD concentration in the nonlinear elastic media.

3. ONE-DIMENSIONAL STEADY-STATE NONLINEAR LONGITUDINAL WAVES

In the case of longitudinal waves, the system of equations (8)–(10) takes the following form:

$$\frac{\partial^2 u}{\partial t^2} - c_l^2\frac{\partial^2 u}{\partial x^2} - \frac{\beta}{\rho}\frac{\partial^2 u}{\partial x^2}\frac{\partial u}{\partial x} - g\frac{\partial^4 u}{\partial x^4} + \frac{K\Omega}{\rho}\frac{\partial n}{\partial x} + \mu\frac{\partial^3\varphi}{\partial x^3} = 0, \quad (11)$$

$$\frac{\partial n}{\partial t} - D\frac{\partial^2 n}{\partial x^2} + \frac{n}{\tau} = Q_e\frac{\partial u}{\partial x} + Q_\varphi\varphi - q_D\frac{\partial^3 u}{\partial x^3} + q_F\frac{\partial^2\varphi}{\partial x^2}, \quad (12)$$

$$\varepsilon_0\frac{\partial^2\varphi}{\partial x^2} = -4\pi\rho(x) + 4\pi\mu\frac{\partial^3 u}{\partial x^3}, \quad (13)$$

where $u = u_x$ is the x component of the vector of displacements; $q_F = DZn_0/kT$, and $q_D = Dn_0K\Omega/kT$.

Let us now consider the steady-state solutions to the system of equations (11)–(13). For one-dimensional gradual perturbations propagating along the x axis with velocity v = const, the system of equations (11)–(13) can be rewritten as

$$(v^2 - c_l^2)\frac{d^2u}{d\xi^2} - \frac{\beta}{\rho}\frac{d^2u}{d\xi^2}\frac{du}{d\xi} - g\frac{d^4u}{d\xi^4} = -\frac{K\Omega}{\rho}\frac{dn_1}{d\xi} - \mu\frac{d^3\varphi}{d\xi^3}, \tag{14}$$

$$-v\frac{dn_1}{d\xi} - D\frac{d^2n_1}{d\xi^2} + \frac{n_1}{\tau} = Q_e\frac{du}{d\xi} + Q_\varphi\varphi - q_D\frac{d^3u}{d\xi^3} + q_F\frac{d^2\varphi}{d\xi^2}, \tag{15}$$

$$\varepsilon_0\frac{d^2\varphi}{d\xi^2} = -4\pi\rho(\xi) + 4\pi\mu\frac{d^3u}{d\xi^3}, \tag{16}$$

where $\xi = x - vt$.

In deriving the expression for the potential involved in Eq. (16), 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 [14]) and, hence, can be disregarded. Then, for the relation between the flexoelectric field φ and the deformation field, we have the equation

$$\varphi = \frac{4\pi\mu}{\varepsilon_0}\frac{du}{d\xi}.$$

Using this expression to eliminate the potential φ, we can represent Eqs. (14) and (15) as

$$(v^2 - c_l^2)\frac{d^2u}{d\xi^2} - \frac{\beta}{\rho}\frac{d^2u}{d\xi^2}\frac{du}{d\xi} - \left(g - \frac{4\pi}{\varepsilon_0}\mu^2\right)\frac{d^4u}{d\xi^4} = -\frac{K\Omega}{\rho}\frac{dn}{d\xi}, \tag{17}$$

$$-v\frac{dn}{d\xi} - D\frac{d^2n_1}{d\xi^2} + \frac{n}{\tau} = \tilde{Q}_e\frac{du}{d\xi} - \tilde{q}_D\frac{d^3u}{d\xi^3}, \tag{18}$$

where $\tilde{Q}_e = Q_e - 4\pi\mu Q_\varphi/\varepsilon_0$ and $\tilde{q}_D = q_D - 4\pi\mu q_F/\varepsilon_0$.

The solution to Eq. (18) satisfying the boundary conditions ($n(\pm\infty) = 0$), which can be written as

$$n(\xi) = \int_{-\infty}^{+\infty} d\xi' z_{DF}(\xi')S(\xi - \xi'), \tag{19}$$

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

$$z_{DF}(\xi) = \tilde{Q}_e\frac{du}{d\xi} - \tilde{q}_D\frac{d^3u}{d\xi^3}.$$

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), we use (19) to obtain

$$n \approx \tau\tilde{Q}_e\frac{du}{d\xi} + v\tau^2\tilde{Q}_e\frac{d^2u}{d\xi^2} + \tau(\tilde{Q}_e\tau D - \tilde{q}_D)\frac{d^3u}{d\xi^3} - v\tau^2\tilde{q}_D\frac{d^4u}{d\xi^4} - D\tau^2\tilde{q}_D\frac{d^5u}{d\xi^5}. \tag{20}$$

Combining (17) and (20), we obtain the equation for the nonlinear wave of displacements

$$(v^2 - \tilde{c}_l^2)\frac{d^2u}{d\xi^2} - \frac{\beta}{\rho}\frac{d^2u}{d\xi^2}\frac{du}{d\xi} - \gamma\frac{d^3u}{d\xi^3} - \tilde{g}\frac{d^4u}{d\xi^4} - \sigma\frac{d^5u}{d\xi^5} = 0, \tag{21}$$

where

$$\tilde{c}_l^2 = c_l^2 - \frac{K\Omega}{\rho}\tau Q_e + \frac{4\pi\tau\mu ZK\Omega}{\varepsilon_0\rho kT},$$

$$\tilde{g} = g + g_D + g_Q + g_F,$$

$$g_D = q_D\frac{K\Omega\tau}{\rho}, \quad g_Q = -Q_e\frac{K\Omega\tau^2 D}{\rho},$$

$$g_F = -\frac{4\pi\mu^2}{\varepsilon_0} + \frac{4\pi\mu K\Omega\tau^2 DZ}{\rho\varepsilon_0 kT} - \frac{4\pi\mu K\Omega\tau q_F}{\rho\varepsilon_0},$$

$$\gamma = \gamma_Q + \gamma_F, \quad \gamma_Q = \frac{K\Omega}{\rho}v\tau^2 Q_e, \quad \gamma_F = \frac{v\tau^2 4\pi K\Omega Z}{\rho\varepsilon_0 kT},$$

$$\sigma = \tilde{q}_D\frac{\tau^2 K\Omega v}{\rho}, \quad \delta = v^2 - \tilde{c}_l^2.$$

In Eq. (21), 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. 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 rate by the deformation potential and the contribution γ_F of the flexoelectric effect. With the typical values of the parameters $K|\Omega_m| = 10^{-11}$ erg, $\varepsilon_0 = 6$, and $d_0 = 5 \times 10^{-8}$ cm, we obtain the estimate $\gamma_F/\gamma_Q = 4\pi Z^2/\varepsilon_0 K|\Omega_m|d_0 \approx 10$. Thus, the contribution of the flexoelectric effect is found to be prevalent.

After integrating with respect to ξ and taking into account the boundary conditions $du/d\xi|_{\xi \to \pm\infty} = 0$, we obtain an equation for the deformation wave

$$\sigma\frac{d^3e}{d\xi^3} - \tilde{g}\frac{d^2e}{d\xi^2} + \gamma\frac{de}{d\xi} + \frac{\beta}{\rho}e^2 - \delta e = 0. \tag{22}$$

Here, the first, second, and third terms describe the energy transfer to the wave, the dispersion of the wave, and the dissipative processes, respectively. The equations similar to Eq. (22) are typical for nonlinear waves in a dissipative dispersion media with instabilities, e.g., for the waves of downslope flows of thin liquid films on sloped surfaces [22] and for the concentration waves in chemical reactions [23]. Such an equation has exact analytical particular solutions. As a rule for finding these solutions, the method based on the definition of Bäklund's transformation [24] is used.

Using Bäklund's transformation

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

we can obtain the exact analytical solutions of Eq. (22) of the type of solitary waves [24] which can be represented as

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

$$\Sigma(\xi) = \tanh\left(\frac{k}{2}\xi\right).$$

These solutions exist in the following three cases:

$$\text{(a) } \tilde{g}^2 = 16\gamma\sigma, \quad k^2 = \frac{\gamma}{\sigma}, \quad \delta = 6\gamma\sqrt{\frac{\gamma}{\sigma}}; \tag{23}$$

$$\text{(b) } 7\tilde{g}^2 = 144\gamma\sigma, \quad k^2 = \frac{\gamma}{47\sigma}, \quad \delta = -\frac{60}{47}\gamma\sqrt{\frac{\gamma}{47\sigma}}; \tag{24}$$

$$\text{(c) } 73\tilde{g}^2 = 256\gamma\sigma, \quad k^2 = \frac{\gamma}{73\sigma}, \quad \delta = \frac{90}{73}\gamma\sqrt{\frac{\gamma}{73\sigma}}. \tag{25}$$

In case (a), the solution of Eq. (21) is a solitary wave

$$e(\xi) = a\cosh^{-2}\left(\frac{k}{2}\xi\right)\left[1 + \tanh\left(\frac{k}{2}\xi\right)\right]. \tag{26}$$

Here, $a = -15\beta^{-1}\rho\gamma\sqrt{\gamma/\sigma}$ is the amplitude of the nonlinear wave.

At $\xi \longrightarrow \pm\infty$, the solution falls off. At $\xi = 0$, it has a maximum equal to $(160/9)\gamma\sqrt{\gamma/\sigma}$. The width of the solitary wave is proportional to the dissipation coefficient γ, as defined by expression

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

The solitary wave described by formula (26) elastically interacts with other perturbations [24], and hence, it is a soliton. According to (23), the velocity of the nonlinear wave and its amplitude are interrelated by expression

$$v^2 = \tilde{c}_l^2 - 6\gamma\sqrt{\frac{\gamma}{\sigma}} = -\frac{2\beta}{5\rho}a. \tag{27}$$

In the other two cases (cases (b) and (c)), the solution represents a kink. If the coefficients of Eq. (21) are related by expressions (24), we substitute expression

$$e(\xi) = \frac{120}{47}\frac{\rho\gamma}{\beta}\sqrt{\frac{\gamma}{47\sigma}}(1 + \exp(-k\xi))^{-3} \tag{28}$$

directly into Eq. (22) and can verify that expression (28) is the exact solution of Eq. (22). This solution describes the structure of a shock wave, since it continuously combines two asymptotically uniform states described as

$$e(\infty) = \frac{120}{47}\frac{\gamma}{\beta}\sqrt{\frac{\gamma}{47\sigma}}, \quad e(-\infty) = 0.$$

Let us now consider the behavior of solution (28) behind the wave front. Assuming that $e = e(\infty) + \varepsilon_1$ and $|e_1| \ll 1$, we obtain the third-order differential equation for deformational perturbation. By calculating the discriminant Δ of the corresponding characteristic equation, we find that $\Delta < 0$, 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 (28) has a monotonic structure.

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

$$\Delta_0 = \sqrt{\frac{47\sigma}{\gamma}} = -\frac{60\gamma}{47(\tilde{c}_l^2 - v^2)},$$

$$v^2 = \tilde{c}_l^2 + \frac{60}{47}\gamma\sqrt{\frac{\gamma}{47\sigma}} = \frac{\beta}{2\rho}a. \tag{29}$$

If the coefficients in Eq. (21) satisfy relations (c), the exact solution of the equation is

$$e(\xi) = -\frac{60\gamma}{73\beta}\sqrt{\frac{\gamma}{73\sigma}}\frac{3 + \exp(-k\xi)}{(1 + \exp(-k\xi))^3}. \tag{30}$$

For long distances from the wave front ($\xi = 0$), we use formula (30) to obtain the asymptotic values

$$e(\infty) = -\frac{60}{73}\frac{\gamma}{\beta}\sqrt{\frac{\gamma}{73\sigma}}, \quad e(-\infty) = 0.$$

According to (28) and (30), the front width and velocity of the shock wave are defined by formulas

$$\Delta_0 = \frac{90\gamma}{73(\tilde{c}_l^2 - v^2)}, \quad v^2 = \tilde{c}_l^2 + \frac{90}{73}\gamma\sqrt{\frac{\gamma}{73\sigma}} = \frac{3\beta}{2\rho}a. \quad (31)$$

The solutions of Eq. (18) corresponding to the kink-type solutions (29) and (31) can be determined using formula (20).

The calculated profiles of the shock wave suggest that there are no oscillations behind and ahead of the wave fronts, i.e., the wave is monotonic in structure. From formula (29) it follows that the solitary defect-deformation waves are fairly slow and the velocity of these waves do not exceed the longitudinal velocity of linear sound. However, the shock waves propagate with a supersonic velocity (see formulas (29) and (31)). The front width of both types of waves is 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 part by part, we represent the integral in (19) as an expansion in the powers of τ^{-1}. Restricting the expansion to basic terms and substituting it into Eq. (17), we obtain the equation

$$(v^2 - \tilde{c}_l^2)\frac{d^2u}{d\xi^2} - \frac{\beta}{\rho}\frac{d^2u}{d\xi^2}\frac{du}{d\xi} - \tilde{g}_F\frac{d^4u}{d\xi^4} = -\eta_1 u + \eta_2\frac{du}{d\xi}.$$

Here, $\tilde{c}_l = c_l(1 - \tilde{q}_D K\Omega/D\rho c_l^2)^{1/2}$ is the velocity of sound renormalized by the interaction of the PDs with the field of elastic deformations; $\tilde{g}_F = g(1 - 4\pi\mu^2/g\varepsilon_0)$ is the dispersion coefficient renormalized by the flexoelectric effect; $\eta_1 = \tilde{Q}_e K\Omega/\rho D$ and $\eta_2 = \tilde{q}_D K\Omega v/\rho D^2$ are the coefficients of the wave dissipation caused, correspondingly, by the generation and recombination of the PDs and by the deformation-induced drift of the PDs.

In this case, no shock waves are formed in the medium, and deformational perturbations propagate as solitary waves (solitons) or as a sequence of solitons (moving periodic structures) [16]. The deformation-induced drift of PDs and the flexoelectric effect lead to the renormalization of both the velocity of the longitudinal sound wave and the dispersion parameters of the medium. It should be noted that, in this case, the renormalization of sound velocity does not involve a contribution related to the finite rate of recombination of the defects.

4. CONCLUSIONS

Thus, 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 such crystals, the propagation of nonlinear perturbations of elastic deformation can be described by the modified Korteweg–de Vries–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 solitons 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 velocity of sound are estimated. The amplitude and velocity of the nonlinear waves considered in this study depend on the elastic 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.

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Translated by É. Smorgonskaya