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Influence of heterogeneous external fields on propagation of bulk acoustic waves in crystals

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Abstract — Formulas describing the influence of non-homogeneous mechanical pressure on propagation of bulk acoustic waves in crystals have derived. Phase velocity dependence for small amplitude waves in $Bi_{12}SiO_{20}$ crystal subjected the action of non-homogeneous pressure has been investigated. Under those conditions the behavior of the wave front has researched. Numerical calculation of phase velocity of waves and their directions propagation changing have obtained.

Keywords - bulk elastic wave, non-homogeneous mechanical loading, phase velocity, wave surface.

I. INTRODUCTION

Propagation of bulk acoustic waves in crystals is defined by the well-known Green-Christoffel equation:

$$\left(\Gamma_{il} - \rho_0 v^2 \delta_{il}\right) U_l = 0. \tag{1}$$

Propagation of acoustic waves in the finite deformed crystalline medium becomes complicated one. It is convenient to introduce three configurations of the crystal:

1) *Initial* or *natural* state with density ρ_0 and coordinates X_A.

2) The *intermediate* state with density $\bar{\rho}$ and coordinates ξ_α.

3) *Present* state with density $\tilde{\rho}$ and coordinates x_i.

Such representation allows to consider the displacement of particles as a result of superposition of static strain and the field of acoustic wave for which it is necessary to present following vectors:

$\bar{U}(X_B)$ - displacement vector from the initial state to the intermediate one. This vector features the displacement caused by external finite influence and has stationary values;

$\tilde{U}(\xi_\beta, t)$ - displacement vector from the intermediate to the present state. This vector features the small dynamic variations of particle displacement caused by acoustic wave propagating in the crystal.

Vectors of displacement allow to connect mentioned states of crystalline medium by means of relations:

$$\xi_\beta = \delta_{\beta A}\left(X_A + \bar{U}_A\right), \tag{2}$$

$$x_i = \delta_{i\beta}\left(\xi_\beta + \tilde{U}_\beta\right). \tag{3}$$

The solution of problem of bulk acoustic wave propagation under the condition of finite strain has in mind the application of expanded elasticity theory. So Green-Christoffel tensor from (1) should be redefine as follows

$$\Gamma_{BA} = (C^*_{FBLE}\bar{C}_{LA} + \delta_{BA}\bar{\tau}_{FE})\, N_F N_E, \tag{4}$$

where $\bar{C}_{LA} = \delta_{LA} + 2\bar{\eta}_{LA}$ is Green tensor of finite deformation; $\bar{\eta}_{LA}$ is the tensor of static strain, $C^*_{FBLE} = C^{II}_{FBLE} + C^{III}_{FBLEPQ}\bar{\eta}_{PQ}$ are effective elastic constants; C^{II}_{FBLE} and C^{III}_{FBLEPQ} are second and third order elastic constants; $\bar{\tau}_{FE} = C_{FELM}\bar{\eta}_{LM}$ is the tensor of thermodynamic stress; N_F are components of the unit vector of bulk acoustic wave propagation.

The form of Green–Christoffel tensor (4) takes into account both the homogeneous and non-homogeneous possibilities of the crystal deformation. But in the homogeneous case components of the tensor (4) have stationary values independent from the time and coordinates of crystal space. If non-homogeneous case is considered these quantities become dependent from coordinate of the point of observation.

II. BASIC EQUATIONS

A. Linearization of a Green-Christoffel tensor

A lot of applied tasks allows the presentation of a Green-Christoffel tensor (4) in the linearized approximation. It can be received if the strain tensor has a form

$$\bar{\eta}_{LA} = S^*_{LAKS}\bar{\tau}_{KS}. \tag{5}$$

As a result we shall receive the following relation

$$\begin{aligned}\Gamma_{BA} = [C^{II}_{FBAE} + \big(\delta_{BA}\delta_{KF}\delta_{SE} + \\ + 2C^{II}_{FBLE}S^{II}_{LAKS} + C^{III}_{FBAEPQ}S^{II}_{PQKS}\big)\bar{\tau}_{KS}]N_F N_E.\end{aligned} \tag{6}$$

For instance we will consider the influence of the non-homogeneous pressure on wave propagation in $Bi_{12}SiO_{20}$ crystal belonging to the cubic point symmetry 23.

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B. Model of non-homogeneous deformation

Let's consider a crystal sample in the shape of a rod which edges coincide with axes of crystal orthogonal coordinate system. External force is attached to sides of rod which are parallel to (001) plane. The force value is changed along the X_1 axis under the linear law. As a result uniaxial non-homogeneous mechanical squeezing appears (Fig. 1). Other rod sides except for specified ones are free from loading.

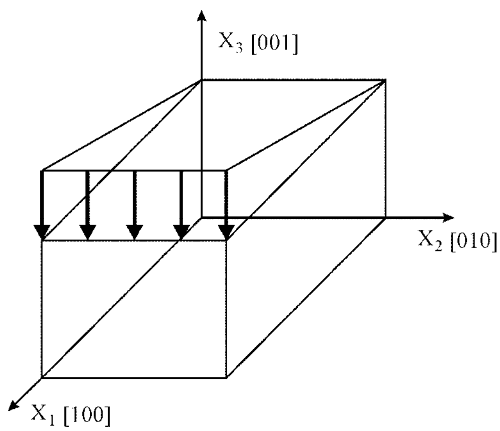

Figure 1. Coordinate system of crystal rod and profile of squeezing.

Using **m** unit vector parallel to X_3 axes, the force referred to unit area can be calculated as

$$\mathbf{p} = -p\mathbf{m},\ p = kX_1. \tag{7}$$

To such type of loading there is the tensor of strain in the form

$$\bar{\tau}_{CD} = -pm_C m_D, \tag{8}$$

satisfying to boundary conditions:

$$\bar{\tau}_{33} = 0\ (X_1 = 0),\ \bar{\tau}_{33} = -5 \cdot 10^7 \text{ Pa } (X_1 = l), \tag{9}$$

where l is the rod size along X_1 axes and $\mathbf{m} \leftrightarrow (0,0,1)$. Using (9) we find that coefficient $k = 5 \cdot 10^7 / l$.

C. Wave surface of an equal phase

For the analysis of behavior of the acoustic wave propagation in non-homogeneously deformed crystal it is enough to consider the equation of wave surface of equal phase in the intermediate state

$$\varphi = \omega\left[t - \frac{\delta_{P\alpha} n_\alpha X_P}{v_i(X_1)}\right] = \text{const}. \tag{10}$$

In general case the phase velocity in (10) depends on all spatial coordinates.

Writing down components of unit vector n_α in coordinates of the initial state we have obtained the calculated relation referred to the same coordinates

$$\frac{\delta_{P\alpha}\xi_{\alpha,S} X_P N_S}{\lambda_N v_i(X_1)} = t - \frac{\text{const}}{\omega}, \tag{11}$$

where $\xi_{\alpha,S} = \partial\xi_\alpha / \partial X_S$ are gradients of deformations and $\lambda_N = \sqrt{\bar{C}_{AB} N_A N_B}$ is the stretching of material line.

For considered example we shall take gradients of deformations as

$$\xi_{\alpha,S} = 0,\ \alpha \neq S\ (\alpha, S = 1,2,3); \tag{12}$$

$$\xi^2_{1,1} = \xi^2_{2,2} = 1 + 2S_{12}\bar{\tau}_{33}(X_1),$$
$$\xi^2_{3,3} = 1 + 2S_{11}\bar{\tau}_{33}(X_1), \tag{13}$$

where S_{11} and S_{12} are components of elastic compliances tensor.

III. NUMERICAL CALCULATIONS

A. Difference scheme

Using the local homogeneity of a Green-Christoffel tensor, the linear nonuniform problem can be reduced to a set of consecutive homogeneous ones.

For this purpose the crystal rod was dissected by planes which are parallel to X_2X_3 plane and they equally spaced by ΔX_1 distance. So each of such planes is satisfied the condition of homogeneous deformation. Then the approach well investigated earlier in the framework of the homogeneous theory can be used to define phase velocities of bulk waves.

Let's set the direction of wave propagation along [100] axis in the sample of a crystal and the direction of loading application along [001] axis. Then all modes existing under the such external influence and possessing eigenvectors with [100], [010] and [001] polarization were examined.

In calculation the rod with length l = 0.1 m has been dissected along X_1 axis by (100) planes with the step of 0.01 m. For each plane the Green-Christoffel tensor (6) with a stress tensor (8) has used. Eigen values of tensor (6) and wave velocities have found. Results for some propagation directions of acoustic wave in crystal sample have been presented below.

B. Phase velocites

In [100] direction of crystal under mentioned conditions three wave modes propagated. For each mode there is its own dependence of velocity distribution versus X_1 coordinate.

Fig. 2 is presented $\frac{\Delta v}{v} = f(X_1)$ dependences. Apparently from Fig. 2 the phase velocity of a longitudinal wave is decreasing linearly from the beginning to the end of rod and it is increasing for SF- and SS-waves. It means that the slowed and accelerated motion of waves in different parts of non-homogeneous deformed crystal is possible.

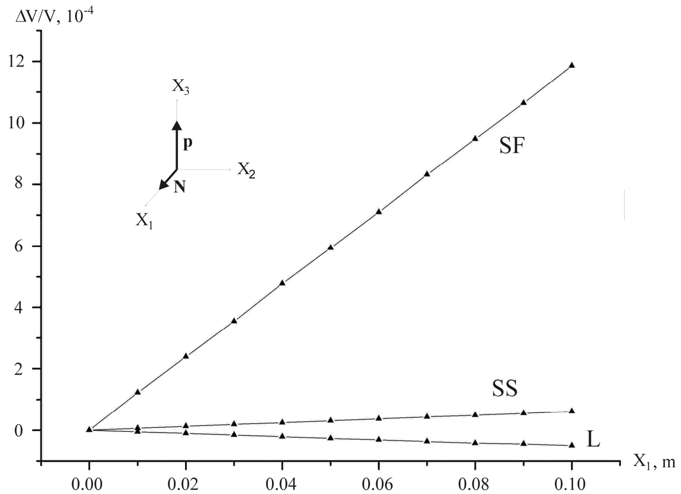

Figure 2. Distribution of $\frac{\Delta v}{v} = f(X_1)$ for $\mathbf{N} \parallel [100]$. L, SF and SS are designations of longitudinal, shear fast and shear slow waves respectively. **N** is unit vector of wave propagation and **P** is the vector of pressure force.

Let's introduce the quantity

$$\beta_{v_i} = \frac{1}{v_i(0)} \left(\frac{\Delta v_i}{\Delta X_1} \right) \tag{14}$$

describing the angle slope of curves shown on Fig. 2. Using (14) it can define the phase velocity as a function of coordinate as:

$$v_i(X_1) = v_i(0)[1 + \beta_{v_i} X_1]. \tag{15}$$

For various propagation directions and polarization vectors of acoustic wave coefficients β_{v_i} and initial velocities $v_i(0)$ are given in the table I.

TABLE I. VELOCITIES $v_i(0)$ AND COEFFICIENTS β_{v_i}.

Direction			**Wave**	$v_i(0)$, **m/s**	β_{v_i}, 10^{-4} m^{-1}
N	**U**	**P**			
100	100	001	L	3761.45	-5.05
100	010	001	SS	1635.44	6.11
100	001	001	SF	1635.44	118.62
010	100	001	SS	1635.44	6.11
010	010	001	L	3761.45	1.06
010	001	001	SF	1635.44	41.58
001	100	001	SF	1635.44	66.65
001	010	001	SS	1635.44	-9.78
001	001	001	L	3761.45	45.46
110	110	001	L	3373.57	-1.48
110	$1\bar{1}0$	001	SF	2332.84	1.29

C. Wavefronts

Let's look how it will be change the plane of an equal phase in consequence of velocity distribution for acoustic waves propagating along [010], [001] and [110] directions.

[010] and [001] propagation directions. Let's mark out $b_i^{-1} = v_i(0)(t - \text{const}/\omega)$. Then substituting (15), (12), (13) into (11), it can receive such equations:

$$-\beta_{v_i} X_1 + b_i X_2 = 1 \quad (\mathbf{N} \parallel [010]), \tag{16}$$

$$-\beta_{v_i} X_1 + b_i X_3 = 1 \quad (\mathbf{N} \parallel [001]). \tag{17}$$

Straight-line equations in X_1X_2 and X_1X_3 planes are given by (16) and (17) relations accordingly. Let the initial phase of a wave is equal to zero at the time moment t. For other time moments counted of zero with some step Δt we have received a set of lines which are projections of wavefronts to coordinate planes (Fig. 3).

For a [001] direction there are results which are analogous to the [010] direction with replacement of X_1X_2 plane on a X_1X_3 plane.

[110] propagation direction. In this case the equation of projections of the wavefront has a form

$$\left(\frac{\sqrt{2} b_i}{2} - \beta_{v_i} \right) X_1 + \frac{\sqrt{2} b_i}{2} X_2 = 1. \tag{18}$$

Relation (18) is the straight-line equation analogous (16), but there is the essential difference. Coefficient at X_1 coordinate depends from time and sets for each straight line its own intersection point with X_1 axis, while (16) has one point only (Fig. 4).

Presence of singular point in (16), (17) which is the center of rotation of wavefront lines allows to receive the time dependence of rotation angle θ(t) on which the projection of a wavefront on X_1X_2 or X_1X_3 plane eventually turns. Let's represent (16) in the form

$$X_2 = \beta_{v_i} b_i (X_1 + \beta_{v_i}^{-1}). \tag{19}$$

Relation (19) is the straight-line equation too. Line passes through the fixed point with $(-\beta_{v_i}, 0)$ coordinates, and slope of such line is defined by $\tan\theta = \beta_{v_i} b_i^{-1}$. Using $b_i^{-1} = v_i(0)t$ it can be obtained

$$\theta(t) = \arctan[v_i(0)\beta_{v_i} t]. \tag{20}$$

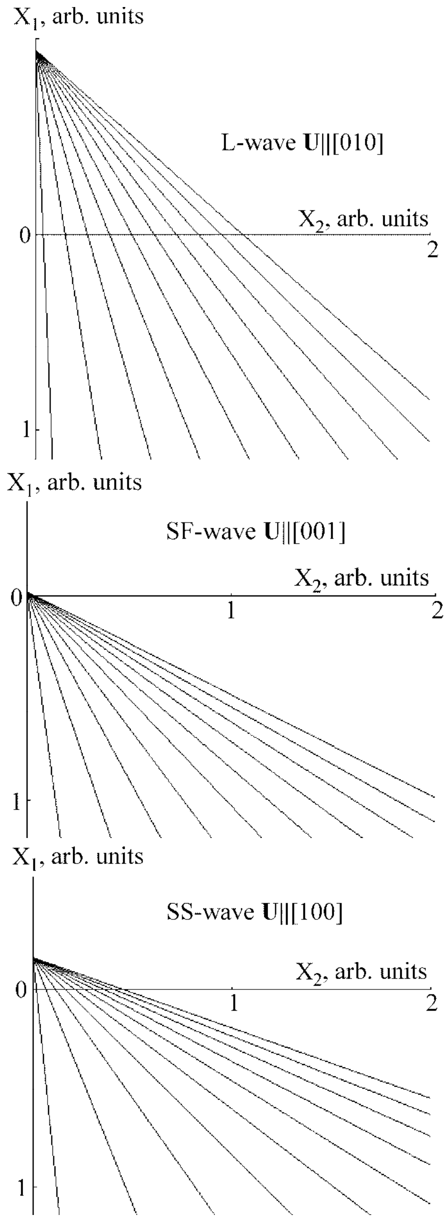

Figure 3. Projections of wavefronts of L-, SF- and SS- modes on coordinate plane X_1X_2 for $\mathbf{N} \parallel [010]$.

Let's estimate the time t_1 which wavefront of L mode ([010] propagation direction) is required for its rotation on one degree. Using values from the table I we can obtain

$$t_1 = \frac{\tan(1^\circ)}{1{,}06 \cdot 10^{-4}\ \mathrm{m}^{-1} \cdot 3761{,}45\ \mathrm{m/s}} = 4{,}38 \cdot 10^{-2}\ \mathrm{s}. \qquad (21)$$

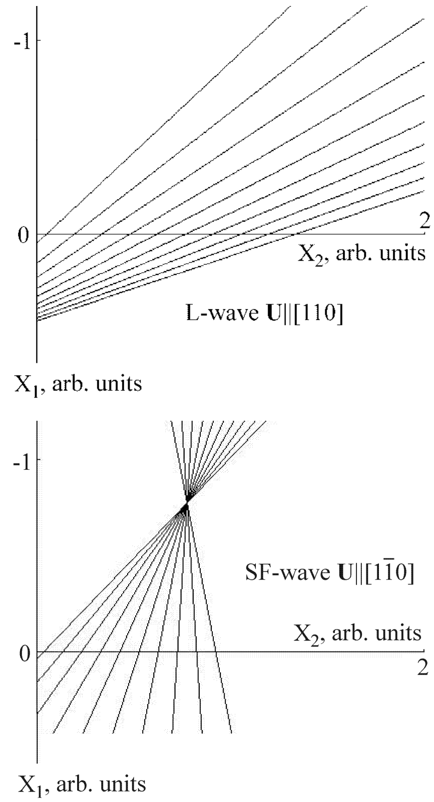

Figure 4. Projections of wavefronts of L-and SF- modes on coordinate plane X_1X_2 for $\mathbf{N} \parallel [110]$.

IV. Conclusion

Green–Christoffel equation taking into account non-homogeneous deformation of crystal has been presented. Deformation gradients have become functions of coordinates. Thus it can reduce the problem of the small amplitude acoustic wave's propagation in non-homogeneous deformed crystal to uniform propagation problem in small vicinity of the geometric point, i.e. to local uniform problem. If it is considered any other geometric point there are exist new values of the wave phase velocities and polarization vectors which are not equal to previous ones. Thereby it is possible to connect the movable trihedron of polarization vectors and vectors of the wave phase velocities with each point of crystal.

Account of non-homogeneity leads to the change in the position of time relative location of wave front which is conditioned by the variation of both wave phase velocity and directions of the wave propagation with the time.

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