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Forward and Backward Acoustic Waves in Crystals with High Piezoactivity and Dielectric Permittivity

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Abstract—Results are presented from studying the characteristics of acoustic waves of different types in plates of ceramic materials with high piezoactivity and dielectric permittivity (e.g., $0.95(Na_{0.5}Bi_{0.5})TiO_3$–$0.05BaTiO_3$, $(K,Na)(Nb,Ta)O_3$, and $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$). The dependences of the phase velocities and electromechanical coupling coefficients of these waves on parameter hf (where h is the thickness of a plate, and f is the frequency of a wave) are calculated for directions XY and YX of propagation. It is found that the investigated materials are characterized by frequency ranges of the existence of backward acoustic waves whose phase and group velocities are oriented in different directions. The existence of extremely broad frequency ranges that depend very weakly on a change in the electrical boundary conditions on the surface of a plate is established for waves with negative group velocity in the case of a $0.95(Na_{0.5}Bi_{0.5})TiO_3$–$0.05BaTiO_3$ single crystal. It is shown that the electromechanical coupling coefficient of acoustic waves in the investigated materials is greatest for an SH_1-wave in YX $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$, and can be as high as 7–30% in the range hf = 1330–2000 m/s.

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INTRODUCTION

One trend in the study of acoustoelectronics is the search for materials with high piezoelectric constants and dielectric permittivity. Such materials can be used to create more sensitive biological, physical, and chemical acoustic sensors and signal processors, due to the increased efficiency of the excitation of acoustic waves in such materials as a result of the strong piezoelectric effect.

A great many papers devoted to the creation of new materials (ferroelectric crystals, perovskites, melilite, and piezoceramic materials) with enhanced piezoelectric and dielectric constants and to studying their properties have been published in recent years [1–7]. It seems clear that studying the characteristics of different types of acoustic waves in these materials is of interest.

As is well known, waves in plates are characterized by a higher electromechanical coupling coefficient than surface acoustic waves in the same material [8–11]. This means the characteristics of these waves depend more strongly on the electrical boundary conditions on the surface of a plate than the characteristics of surface acoustic waves [12–15]. Studying the properties of these waves is therefore of great interest.

In addition, studies of acoustic waves propagating in such strong piezoelectrics as potassium niobate [16, 17] have demonstrated the possibile existence of such new effects as the hybridization of fundamental acoustic waves in plates [18] and the structural transformation of a surface acoustic wave upon a change of electrical boundary conditions [19]. It is obvious that the study of new materials will help develop our understanding of effects revealed earlier.

It should also be noted that the study of higher-order waves in piezoelectric plates has demonstrated the possible existence of not only forward, but also backward acoustic waves characterized by oppositely oriented phase and group velocities [20, 21]. Study of the specific features of the propagation of these waves in strong piezoelectrics was continued in [22, 23]. The application of higher-order waves for the development of acoustic sensors was described in [24].

The study of zero- and higher-order acoustic waves in new materials with increased piezoelectric constants and dielectric permittivity is thus a relevant scientific problem. In this work, we report results from analyzing acoustic waves propagating in lead-free $0.95(Na_{0.5}Bi_{0.5})TiO_3$–$0.05BaTiO_3$, $(K,Na)(Nb,Ta)O_3$, and $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$ piezoceramics.

THEORETICAL CALCULATIONS

Let us consider the propagation of forward and backward acoustic waves in a piezoelectric plate. The geometry of this problem is illustrated in Fig. 1. A wave propagates along axis x_1 of a piezoelectric plate bounded by planes $x_3 = 0$ and $x_3 = h$. The regions with

$x_3 < 0$ and $x_3 > h$ represent a vacuum. We consider a two-dimensional problem in which all mechanical and electrical variables are assumed to be constant along axis x_2. To solve the problem, we write the motion equation, the Laplace equation, and the material equations for a piezoelectric medium [25]:

$$\rho\,\partial^2 U_i/\partial t^2 = \partial T_{ij}/\partial x_j\,,\ \partial D_j/\partial x_j = 0\,, \quad (1)$$

$$\begin{aligned} T_{ij} &= C_{ijkl}\,\partial U_l/\partial x_k + e_{kij}\,\partial\Phi/\partial x_k\,, \\ D_j &= -\varepsilon_{jk}\,\partial\Phi/\partial x_k + e_{jlk}\,\partial U_l/\partial x_k\,. \end{aligned} \quad (2)$$

Here, U_i is a component of the mechanical displacement of particles; t is time; T_{ij} is a component of the mechanical stress tensor; x_j is the coordinates; D_j is a component of the electrical inductance vector; Φ is the electrical potential; and ρ, C_{ijkl}, e_{ikl}, and ε_{jk} are the density and elastic, piezoelectric, and dielectric constants of a piezoelectric, respectively.

Beyond the plate, the electrical inductance in the regions with $x_3 < 0$ and $x_3 > h$ must satisfy the Laplace equation

$$\partial D_j^{\mathrm{V}}/\partial x_j = 0, \quad (3)$$

where $D_j^{\mathrm{V}} = -\varepsilon_0\partial\Phi^{\mathrm{V}}/\partial x_j$. Here, superscript V denotes the parameters that characterize a vacuum, and ε_0 is the vacuum's dielectric permittivity.

Acoustic waves propagating in a plate must also satisfy the mechanical and electrical boundary conditions. At the boundary with a vacuum ($x_3 = 0$, and $x_3 = h$), these conditions have the form

$$T_{3j} = 0, \quad \Phi^{\mathrm{V}} = \Phi; \quad D_3^{\mathrm{V}} = D_3. \quad (4)$$

When one or both sides of a plate are metallized, potential Φ becomes zero when $x_3 = 0$ or $x_3 = 0$, $x_3 = h$, respectively.

The above boundary problem was solved by presenting the solution as a set of plane inhomogeneous waves [26, 27] that had the form

$$Y_i(x_1, x_3, t) = Y_i(x_3)\exp\left[j\omega\left(t - x_1/V\right)\right], \quad (5)$$

where $i = 1$–8 for a piezoelectric and $i = 1, 2$ for a vacuum. V is the phase velocity, and ω is the angular velocity of an acoustic wave. The normalized variables introduced here are

$$\begin{aligned} &Y_i = \omega C_{11}^{*} U_i/V\,,\ Y_4 = T_{13},\ Y_5 = T_{23}, \\ &Y_6 = T_{33},\ Y_7 = \omega e^{*}\Phi/V\,,\ Y_8 = e^{*}D_3/\varepsilon_{11}^{*}\,, \end{aligned} \quad (6)$$

where $i = 1, 2, 3$; C_{11}^{*} and ε_{11}^{*} are the normalizing material constants of a piezoelectric medium in a crystallophysical coordinate system; and $e^{*} = 1$ and has the same units of measurement as the piezoelectric constant.

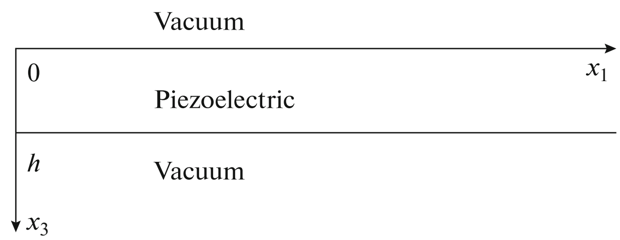

Fig. 1. Problem geometry.

Substituting Eq. (5) into Eqs. (1)–(4), we obtain sets of 8 and 2 ordinary differential linear equations for a piezoelectric medium and a vacuum, respectively. Each set can be written in matrix form:

$$[A][dY/dx_3] = [B][Y]. \quad (7)$$

Here, $[dY/dx_3]$ and $[Y]$ are eight-dimensional vectors for a medium and two-dimensional vectors for a vacuum with components determined using Eqs. (6). Matrices $[A]$ and $[B]$ are squares with sizes of 8×8 for a piezoelectric medium and 2×2 for a vacuum.

Since matrix $[A]$ is not singular ($\det[A] \neq 0$), we can write for each contacting medium that $[dY/dx_3] = [A^{-1}][B][Y] = [C][Y]$.

To solve the set of Eqs. (7), we must find eigenvalues $\beta^{(i)}$ of matrices $[C]$ and their corresponding eigen vectors $[Y^{(i)}]$ characterizing the parameters of partial waves for each contacting medium. The general solution will be a linear combination of all partial waves for each medium:

$$Y_k = \sum_{i=1}^{N} A_i Y_k^{(i)} \exp\left(\beta^{(i)} x_3\right)\exp\left(i\omega\left[t - x_1/V\right]\right), \quad (8)$$

where the number of eigenvalues is $N = 8$ for a piezoelectric medium and $N = 2$ for a vacuum, and A_i are unknown coefficients. To find coefficients A_i and velocity V, we use mechanical and electrical boundary conditions (4), which are also written in normalized form in light of Eqs. (6). Let the eigenvalues with negative and positive real parts be excluded from consideration for the vacuum in the areas with $x_3 < 0$ and $x_3 > 0$, respectively, since all variables in a vacuum must have an amplitude that falls as we move away from a piezoelectric plate.

Unknown coefficients A_i and velocity V can thus be determined from set of ordinary algebraic linear equations (4).

This technique allows us to estimate the phase velocity of a wave and the amplitudes of all electrical and mechanical variables, depending on the coordinate x_3.

Table 1. $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$ material constants [1] used in our calculations ($\rho = 5200$ kg/m^3)

Elasticity moduli C_{ij}^E (10^{10} N/m^2)					
C_{11}^E	C_{12}^E	C_{13}^E	C_{33}^E	C_{44}^E	C_{66}^E
13.6	8.9	8.5	11.3	2.66	2.44
Piezoelectric moduli e_{ij} (C/m^2)			Dielectric constants ε_{ij}^S (ε_0)		
e_{15}	e_{31}	e_{33}	ε_{11}^S	ε_{33}^S	
12.1	−5.7	22.4	1652	2930	

Table 2. (K,Na)(Nb,Ta)O_3 material constants [2] used in our calculations ($\rho = 5165$ kg/m^3)

Elasticity moduli C_{ij}^E (10^{10} N/m^2)								
C_{11}^E	C_{12}^E	C_{13}^E	C_{22}^E	C_{23}^E	C_{33}^E	C_{44}^E	C_{55}^E	C_{66}^E
23.1	9.88	3.33	28.1	11.9	19.7	7.8	1.9	7.7
Piezoelectric moduli e_{ij} (C/m^2)					Dielectric constants ε_{ij}^S (ε_0)			
e_{15}	e_{24}	e_{31}	e_{32}	e_{33}	ε_{11}^S	ε_{22}^S	ε_{33}^S	
4.76	12.96	4.9	−2.43	6.95	197	1187	181	

RESULTS AND DISCUSSION

Using the approach described above, we calculated the phase velocity of zero- and higher-order acoustic waves propagating in plates of new materials with high piezoelectric constants and dielectric permittivity. To calculate the electromechanical coupling coefficient, analysis was performed for plates that were electrically open and electrically short (metallized) on one side. The material constants for our crystals were taken from [1–3] and listed in Tables 1–3. Two directions of wave propagation, *XY* and *YX*, were studied with Euler angles of (90°, 90°, 0°) and (180°, 90°, 0°) [28], respectively.

Some typical dependences of the phase velocity of acoustic waves on parameter *hf* (where *h* is the thickness of the plate and *f* is the frequency of the wave) for a $0.95(Na_{0.5}Bi_{0.5})TiO_3$–$0.05BaTiO_3$ single crystal plate are shown in Fig. 2.

Analysis of our results shows that all of the studied plates were characterized by frequency ranges with backward waves, the phase and group velocities of which were oriented in different directions. For example, the investigated range of the $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$ plate contained a single backward Lamb mode whose characteristics remained constant after an electrical short-circuit of the surface of this plate. Forward waves were weakly piezoactive for this crystal, so the electromechanical coupling coefficients were small. Since the given material had a hexagonal symmetry system, it was transversally isotropic, so both studied cuts had identical shapes of their dispersion curves.

Table 3. $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$ material constants [3] used in our calculations ($\rho = 5777$ kg/m^3)

Elasticity moduli C_{ij}^E (10^{10} N/m^2)					
C_{11}^E	C_{12}^E	C_{13}^E	C_{33}^E	C_{44}^E	C_{66}^E
15.9	9.5	7.5	8.1	7.5	7.8
Piezoelectric moduli e_{ij} (C/m^2)			Dielectric constants ε_{ij}^S (ε_0)		
e_{15}	e_{31}	e_{33}	ε_{11}^S	ε_{33}^S	
12.1	−1.7	12	877	489	

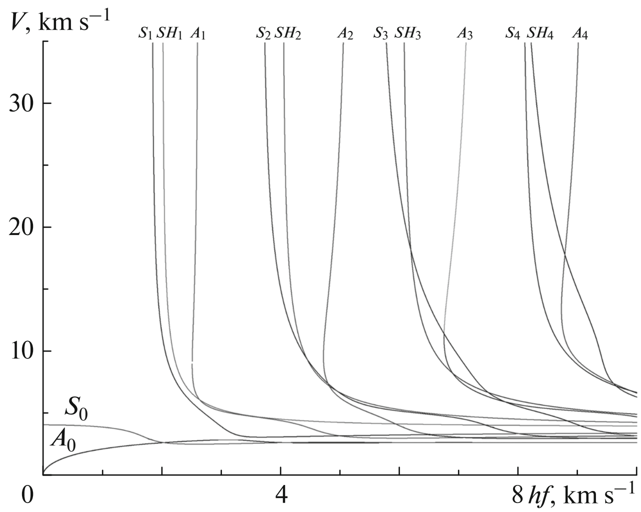

Fig. 2. Phase velocity of zero- and higher-order acoustic waves versus *hf* for a $0.95(Na_{0.5}Bi_{0.5})TiO_3$–$0.05BaTiO_3$ single crystal plate.

An odd feature of the $(K,Na)(Nb,Ta)O_3$ crystal plate with an *X*-cut was the simultaneous existence of two types of backward, transverse, and Lamb modes. Backward Lamb modes are not transformed after metallizing one side of this plate, but transverse waves disappear in the investigated range of velocities. This means the point with zero group velocity rose above this range. The *Y*-cut of the studied crystal was also characterized by the only backward Lamb wave that was not transformed after the change in boundary conditions within this range. Analysis shows that forward waves in this crystal were characterized by small electromechanical coupling coefficients.

The *X*- and *Y*-cuts for tetragonal $0.95(Na_{0.5}Bi_{0.5})TiO_3$–$0.05BaTiO_3$ single crystal plates were identical. An interesting feature in this case was very broad frequency ranges that remained virtually unchanged after an electrical short-circuit on the surface of a plate for waves with negative group velocity. For example, in the antisymmetric first-order Lamb mode, backward waves exist within the range of *hf* = 2.5–3 km/s (Fig. 2). Based on the qualitative theory developed in [22], we may state the existence of similar broad ranges for waves with oppositely oriented vectors of their phase and group velocities is associated with concavities in the slow surface of this crystal. As for forward modes, metallization also has no appreciable effect on the phase velocities of these waves, or for other crystals.

On the whole, analysis shows that the electromechanical coupling coefficient of acoustic waves in the studied materials is greatest for an SH_1 wave in *YX* $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$ and can be as high as 7–30% in the range of *hf* = 1330–2000 m/s.

Our results show that the studied materials could be of interest for the development of signal processors that operate on backward acoustic waves.

CONCLUSIONS

The characteristics of acoustic waves in plates of contemporary piezoelectric materials with high piezoelectric constants (ferroelectric crystals, perovskites, crystals of melilite class, piezoceramic $(K,Na)NbO_3$ based materials) were studied theoretically. Our analysis showed that all of the studied materials were characterized by frequency ranges of the existence of backward acoustic waves, the phase and group velocities of which were oriented in different directions. In the case of a $0.95(Na_{0.5}Bi_{0.5})TiO_3$–$0.05BaTiO_3$ single crystal, the existence of very broad frequency ranges that depended weakly on a change in the electrical boundary conditions on the surface of a plate was revealed for these waves. It was also shown that the electromechanical coupling coefficient of acoustic waves in the studied materials was greatest for SH_1 waves in *YX* $Ba(Zr_{0.2}Ti_{0.8})O_3$–$50(Ba_{0.7}Ca_{0.3})TiO_3$. This coefficient can be as high as 7–30% in the range of *hf* = 1330–2000 m/s. The possibility of backward waves disappearing after a change in the electrical boundary conditions was also demonstrated.

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