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Spatial Anisotropy of Electromechanical Coupling in Li₂B₄O₇ Crystals

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In this research, we study electromechanical coupling coefficients in Li₂B₄O₇ crystals. For the spatial anisotropy research, we used an algorithm to construct indicative surfaces for a particular direction of the radius vector. The indicative surfaces for electromechanical coupling coefficients in Li₂B₄O₇ crystals have been obtained for the first time. These surfaces were constructed using piezoelectric stress constants, elastic constants, density and dielectric constants. On the basis of parameters from different articles, the directions of efficient use of Li₂B₄O₇ crystal for acoustic devices were determined. For transverse polarization, the maximum coefficient of electrical communication is from 0.16 to 0.3, and for longitudinal polarization from 0.36 to 0.42. For fast transverse acoustic waves, the maximum coefficient of electrical communication is observed along the X_1 axis, but with the slow of transverse acoustic waves, the maximum coefficient occurs on the plane X_1X_3 where the angle of deviation from the X_3 axis is from 20.34 to 25.38 depending on the referenced articles.

topics: the electromechanical coupling, spatial anisotropy, the indicative surfaces, Li₂B₄O₇ crystals

1. Introduction

The piezoelectric transducer is an important part of an acoustic or acousto-optical device. Acoustic and acousto-optical devices are widely used, for example in telecommunications networks [1–4]. The piezoelectric transducer is a device that uses a piezoelectric effect to convert mechanical energy into electrical energy and vice versa [5]. The most important parameters characterizing the energy efficiency of such devices are the electromechanical coupling coefficients. The coefficient of electromechanical coupling k expresses the degree of connection between the electrical and mechanical properties of piezoelectric material and characterizes its ability to convert electrical energy into mechanical and on the contrary [6]. Therefore,

$$k^2 = \frac{P_a}{P_e},\tag{1}$$

where P_a is power of the acoustic wave developed by the piezoelectric as a result of the piezoelectric effect, P_e is electric power consumed by the piezoelectric material from a source that generates voltage.

The only way to determine the effective cut of materials for a piezoelectric transducer is 3D analysis of the spatial anisotropy for the electromechanical coupling coefficient [7]. For the spatial anisotropy research, we used an algorithm constructing the indicative surfaces of electromechanical coupling coefficients [7–9]. $Li_2B_4O_7$ crystals show promise for use in various devices, including acoustic and acousto-optical devices. Consequently, $Li_2B_4O_7$ crystals are actively explored and there are many publications for various parameter [10–16], including the electromechanical coupling coefficients [15, 17]. For the theoretical determination of the coefficient, it is necessary to have information about the piezoelectric stress constants [10–13], elastic constants [10–12, 14], density [10, 15] and dielectric constants [10–13, 15, 16], which are different in different publications.

The aim of this paper is to theoretically determine the effective cut in $Li_2B_4O_7$ crystals for the electromechanical coupling on the basis of different information about piezoelectric stress constants, elastic constants, density and dielectric constants.

2. Algorithm for constructing the indicative surfaces of electromechanical coupling coefficients

In [18], the coefficient of electromechanical coupling k is defined as the ratio of the density of mutual elastic and electrical energies U_m (or energy of electromechanical interaction) to the geometric mean value of the density of elastic U_l and electrical energy U_d ,

$$k = \frac{U_m}{\sqrt{U_l U_d}}.$$
(2)

The coefficient of electromagnetic coupling is also determined by velocities [19] as

$$k = \sqrt{\frac{v^2}{v_0^2} - 1},\tag{3}$$

where v_0 and v are the speeds of sound for a given crystallographic direction without taking into account and including the piezoelectric connection, respectively.

The speeds of sound v_0 and v are found from the Green–Christoffel's equation, in accordance [6]

$$\rho v_0^2 \delta_{ik} - c_{ilkm} a_l a_m = 0, \tag{4}$$

and

$$\rho v^2 \delta_{ik} - c_{ilkm} a_l a_m - \frac{(e_{lmi} a_l a_m)(e_{pqk} a_p a_q)}{\varepsilon_{rs} a_r a_s} = 0,$$
(5)

where ρ is the density of the crystal, δ_{ik} is the Kronecker symbol, e_{lmi} is the piezoelectric tensor, ε_{rs} is the dielectric constant, \boldsymbol{a} is the unit vector along the direction of the sound propagation, and c_{ijkl} is the elastic stiffness tensor.

Now (4) and (5) have three solutions related to the velocities of the three waves, each of which has its own vector f(q). Here, the index q determines which of the three polarizations of the acoustic wave is considered [20]: when q = 1 — a transverse wave with a lower velocity; when q = 2 — a transverse wave with a higher velocity; when q = 3 — a longitudinal acoustic wave. The vector f(q) is the unit vector along the direction of acoustic wave polarization. The vectors f(1), f(2) and f(3) are mutually perpendicular.

In various reference books, for example [21] to assess the possible use of the crystal, the coefficients of electromechanical coupling k_{33} , k_{15} , k_{31} are given. In [6] those coefficients are defined as:

$$k_{jb} = \frac{e_{ia}}{\sqrt{\varepsilon_{jg}C_{ba} + e_{ig}^2}}.$$
(6)

Indices jb corresponds to 33, 15 and 31 for k_{33} , k_{15} , k_{31} respectively. Note that k_{33} , k_{15} , k_{31} define special cases, which are important for designing the piezo-transducers. Although (6) is presented in a matrix form, the indices j and b do not represent the tensor components of k, since k is a scalar value. Instead, here indices indicate the corresponding dielectric and elastic constants.

For the spatial anisotropy research, we used an algorithm constructing the indicative surfaces of electromechanical coupling coefficients for a particular direction of the radius vector [7, 20]. The algorithm is the following:

- 1. choose a particular direction of the radius vector that coincides with the direction of acoustic waves propagation;
- 2. determine three speeds of acoustic waves as eigenvalues of the Green–Christoffel's equation (5);
- 3. determine the direction of each acoustic wave polarization by substituting the obtained values from the velocities in the Green– Christophe's equation (5);

4. determine the electromechanical coupling coefficient with (6) to study its spatial distribution by substituting three values of the radius vector component ($\alpha_{r1} = \sin(\theta) \cos(\phi)$, $\alpha_{r2} = \sin(\theta) \sin(\phi)$, $\alpha_{r3} = \cos(\theta)$, where ϕ and θ are spherical coordinates) and the components of acoustic wave polarization obtained in the previous step.

3. The results for constructing the indicative surfaces of electromechanical coupling coefficients

The indicative surfaces for the coefficients of electromechanical coupling in $\text{Li}_2\text{B}_4\text{O}_7$ crystals for different acoustic polarizations were constructed using piezoelectric stress constants [10–13], elastic constants [10–12, 14], density [10, 15, 22] and dielectric constants [10–13, 15, 16]. Maximum values have been defined for all indicative surfaces.

Note that by constructing different indicative surfaces of electromechanical coupling for which we change only the values of density (2433 kg/m³ [10], 2439 kg/m³ [15], 2440 kg/m³ [22]), the maximum values of such surfaces do not change within significant digits. Therefore, hereinafter we present the results for the electromechanical coupling for the density equal to 2433 kg/m³ [10].

All the necessary parameters to determine the coefficient of electromechanical coupling are given in [10]. On the basis of these parameters, the indicative surfaces of the electromechanical coupling are constructed and the maximum value of these surfaces was determined. Table I presents the maximum values of some indicative surfaces, where the directions of propagation of acoustic waves are specified for the given coefficients k_{33} , k_{15} , k_{31} .

TABLE I

The maximum values of some indicative surfaces and the coefficients k_{33} , k_{15} , k_{31} in Li₂B₄O₇ crystals (based on parameters from [10]).

	k	θ	ϕ		
Parameters used $C_{km}^1 \varepsilon(10 \text{ kHz})$					
q = 1	0.274	24.84	0		
q = 2	0.178	90	0		
q = 3	0.363	0	0		
$k_{33} = 0.368; k_{15} = 0.178; k_{31} = 0.057$					
Parameters used $C_{km}^1 \varepsilon(100 \text{ kHz})$					
q = 1	0.277	25.02	0		
q = 2	0.182	90	0		
q = 3	0.368	0	0		
$k_{33} = 0.368; k_{15} = 0.182; k_{31} = 0.057$					
Parameters used $C_{km}^2 \ \varepsilon(100 \text{ kHz})$					
q = 1	0.277	25.02	0		
q = 2	0.182	90	0		
q = 3	0.368	0	0		
$k_{33} = 0.368; k_{15} = 0.182; k_{31} = 0.055$					



Fig. 1. The surfaces for coefficients of electromechanical: for q = 1 (a); q = 2 (a); q = 3 (c).

In [10], elastic coefficients are different, namely $C_{11} = 12.67 \times 10^{10} \text{ N/m}^2$; $C_{12} = 0.89 \times 10^{10} \text{ N/m}^2$; $C_{13} = 3.2 \times 10^{10} \text{ N/m}^2$; $C_{33} = 5.47 \times 10^{10} \text{ N/m}^2$; $C_{44} = 5.75 \times 10^{10} \text{ N/m}^2$; $C_{66} = 4.82 \times 10^{10} \text{ N/m}^2$ (the indicative surfaces are determined using these coefficients, they are marked by C_{km}^1 in Table I) and $C_{11} = 13.537 \times 10^{10} \text{ N/m}^2$; $C_{12} = 0.109 \times 10^{10} \text{ N/m}^2$; $C_{13} = 3.186 \times 10^{10} \text{ N/m}^2$; $C_{33} = 5.48 \times 10^{10} \text{ N/m}^2$; $C_{44} = 5.739 \times 10^{10} \text{ N/m}^2$; $C_{66} = 4.738 \times 10^{10} \text{ N/m}^2$ (marked as C_{km}^2), dielectric constants are $\varepsilon_{11} = 7.46$; $\varepsilon_{33} = 9.97$ at 100 kHz (marked as $\varepsilon(100 \text{ kHz})$) and $\varepsilon_{11} = 7.81$; $\varepsilon_{33} = 10.25$ at 10 kHz (marked as $\varepsilon(10 \text{ kHz})$), piezoelectric constants: $e_{311} = 0.19 \text{ C/m}^2$, $e_{113} = 0.36 \text{ C/m}^2$, $e_{333} = 0.87 \text{ C/m}^2$.

For example, Fig. 1 shows the indicative surface of the coefficient of electromechanical coupling, the maximum values of which are presented in Table I (case $C_{km}^1 \varepsilon(100 \text{ kHz})$). The case q = 1 is presented in Fig. 1 in two different foreshortenings.

TABLE	Ħ

The maximum values of some indicative surfaces and the coefficients k_{33} , k_{15} , k_{31} in Li₂B₄O₇ crystals (based on parameters from [10–15]).

	k	θ	ϕ			
Parameters used: e_{jn} [13], C_{km} [10], ε_{ii} [13]						
$\underline{q=1}$	0.301	23.4	0			
q = 2	0.180	90	0			
q = 3	0.425	0	0			
$k_{33} = 0.42$	25; $k_{15} = 0.180$; $k_{31} = 0.079$				
Paramete	Parameters used: e_{jn} [12], C_{km} [14], ε_{ii} [15]					
q = 1	<u>0.253</u>	20.34	0			
$\overline{q=2}$	0.211	90	0			
q = 3	0.385	0	0			
$k_{33} = 0.385; k_{15} = 0.211; k_{31} = 0.087$						
Parameters used: e_{jn} [12], C_{km} [11], ε_{ii} [10]						
q = 1	0.269	24.3	0			
$\underline{q=2}$	0.240	90	0			
q = 3	0.392	0	0			
$k_{33} = 0.392; k_{15} = 0.240; k_{31} = 0.086$						
Parameters used: e_{jn} [10], C_{km} [12], ε_{ii} [15]						
q = 1	0.269	24.12	0			
q=2	0.162	90	0			
$\underline{q=3}$	0.363	0	0			
$k_{33} = 0.363; k_{15} = 0.162; k_{31} = 0.055$						
Parameters used: e_{jn} [12], C_{km} [11], ε_{ii} [13]						
q = 1	0.283	22.86	0			
q = 2	0.221	90	0			
$\underline{q} = 3$	0.426	0	0			
$k_{00} = 0.426; k_{12} = 0.221; k_{01} = 0.005$						

 $k_{33} = 0.426; k_{15} = 0.221; k_{31} = 0.095$

Although the two decimals numbers are important for the electromagnetic coupling coefficient, we have presented three numbers in Table I as well as for the results presented below. This allowed a better comparison of the results based on the components used from different sources. If we limit ourselves to only two numbers in Table I, then these coefficients coincide.

For the slow transverse acoustic waves (q = 1), the maximum values of indicative surfaces of electromechanical coupling coefficient are in the range from 0.25 to 0.3 (extreme cases, as shown in Table II) on the plane X_1X_3 , while the angle of deviation from the X_3 axis is in the range from 20.34 to 25.38 (see Table II). The parameters, which are used for calculation of the indicative surfaces are following: piezoelectric stress constants as e_{jn} , elastic constants as C_{km} and dielectric constants as ε_{ii} (see Table II).

For the fast transverse acoustic waves (q = 1), the maximum values of indicative surfaces of electromechanical coupling are observed along the axis X_1 and coincides with k_{15} , and the values are from 0.16 to 0.24 see Table II. For the longitudinal polarization (q = 1), the maximum values of the indicative surfaces of electromechanical coupling from 0.36 to 0.42, are in the direction of the X_3 axis and coincides with k_{33} (see Table II).

Analyzing the obtained results, we can see that the maximum values for the longitudinal acoustic wave correspond to k_{33} . The maximum value for the transverse wave when q = 2 coincides with k_{15} .

4. Conclusion

The indicative surfaces for coefficients of electromechanical coupling in $\text{Li}_2\text{B}_4\text{O}_7$ crystals have been obtained for the first time. On the basis of parameters from different articles, the directions of efficient use of $\text{Li}_2\text{B}_4\text{O}_7$ crystal for acoustic devices have been determined. These surfaces were constructed using piezoelectric stress constants, elastic constants, density and dielectric constants.

For the transverse polarization, the maximum coefficient of electrical communication is from 0.16 to 0.3, and for the longitudinal polarization from 0.36 to 0.42, depending on the referenced articles. The maximum coefficient of electrical communication for the longitudinal polarization is along the direction of the X_3 axis.

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