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1998 J. Phys.: Condens. Matter 10 451

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# Electromechanical constants and their anisotropy in LiNbO<sub>3</sub>-type crystals having 180° inclined domain walls

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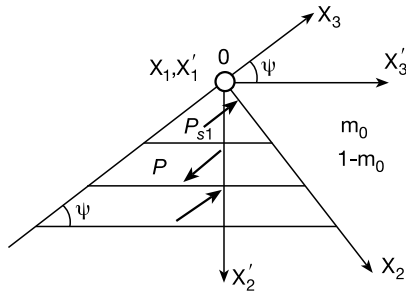
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Received 14 April 1997

**Abstract.** The paper is devoted to the determination of effective electromechanical constants  $d_{ij}^p$ ,  $e_{ij}^p$ ,  $\varepsilon_{kl}^{\sigma,p}$  and  $s_{fg}^{E,p}$  of polydomain LiNbO<sub>3</sub> and LiNb<sub>0.1</sub>Ta<sub>0.9</sub>O<sub>3</sub> crystals at room temperature. 180° domain structures considered here contain inclined plane walls providing a significant anisotropy of piezoelectric constants  $e_{ij}^p$ . The effect of such domain structures is established for the first time and discussed.

## 1. Introduction

Although there are a vast number of experimental data on a structure and properties, lithium niobate (LN, LiNbO<sub>3</sub>) crystals and LN-based solid solutions are still objects important for crystallographic and physical investigations [1–5]. A considerable interest is generated by a variety of domain-structure types which are characteristic of LN as a ferroelectric material (e.g., 180° laminated and cylindrical domains in the *R3c* phase) and as a polysynthetic twin grown under certain conditions (e.g., non-180° domains separated by plane {100} walls in the same phase) [1]. A new type of 180° domain structure containing inclined plane walls is mentioned briefly in [3] and described in detail by authors [4] investigating LN platelike crystals (figure 1).



**Figure 1.** Scheme of the 180° domain structure observed in the *R3c* phase of LiNbO<sub>3</sub> crystals [4]. The domains with the spontaneous polarization vectors  $P_{s1}$  (volume concentration  $m_0$ ) and  $P_{s2}$  (volume concentration  $1 - m_0$ ) are separated by the plane domain walls with Miller indices  $(0hl)$  with respect to the  $OX_i$  axes of a cubic unit cell. For the room temperature, the ratio  $h/l \approx 3/2$  is assumed.

Our previous works allowed us to give a quantitative description of the role of the noncollinear domains in forming the large anisotropy of piezoelectric moduli  $d_{ij}^p$  in two

cases, i.e. for the crystals having the non-180° domains mentioned above (LN and LiTaO<sub>3</sub> [5]) or having the S-type domain structure (KNbO<sub>3</sub> [6]) in low-symmetry phases†. The present paper is devoted to a propagation of methods [5, 6] to the LN-type crystals which may have the new type of 180° domain structure shown in figure 1. A problem of averaging the physical constants of ferroelectric and related crystalline materials with the 180° domain structure [7–9] should be solved for the case of the mentioned new domain structure by taking into consideration the system of the inclined domain walls described by (0 $\bar{h}l$ ) indices in a rectangular ( $X_1X_2X_3$ ) coordinate system.

## 2. Results and discussion

The LN and LiNb<sub>0.1</sub>Ta<sub>0.9</sub>O<sub>3</sub> (LNT) crystals are chosen for our calculations and comparative analysis. In our opinion, due to a symmetry analogy between them, the LNT crystal can also contain such a type of inclined 180° walls. Our calculations are based on initial physical constants measured on single-domain LN [2, 10] and LNT [11] crystals at room temperature. It should be noted that the angle of domain-wall orientation  $\psi$  (figure 1) evaluated by using formulae of twinning [12] is  $\psi \approx 33^\circ$  for LN and practically coincides with the angle  $\psi$  for LNT, in spite of a difference between the corresponding electromechanical single-domain constants of these two crystals. This concerns, for example, the piezoelectric moduli  $d_{ij}$  and the piezoelectric constants  $e_{ij}$  (including the difference in  $e_{31}$  signs), their anisotropy (primarily  $|d_{33}/d_{31}|$  or  $|e_{33}/e_{31}|$  ratios) as well as the anisotropy of dielectric permittivities  $\varepsilon_{ii}^\sigma$  of the stress-free single-domain LN and LNT crystals.

Matrices of the effective piezoelectric moduli  $d_{ij}^p$ , piezoelectric constants  $e_{ij}^p$ , dielectric permittivities  $\varepsilon_{ij}^{\sigma,p}$ , and elastic compliances  $s_{fg}^{E,p}$  of the polydomain crystals may be written in the ( $X_1X_2X_3$ ) coordinate system as

$$\begin{aligned} \|d_{ij}^p\| &= \begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^p & d_{16}^p \\ d_{21}^p & d_{22}^p & d_{23}^p & d_{24}^p & 0 & 0 \\ d_{31}^p & d_{32}^p & d_{33}^p & d_{34}^p & 0 & 0 \end{pmatrix} \\ \|e_{ij}^p\| &= \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15}^p & e_{16}^p \\ e_{21}^p & e_{22}^p & e_{23}^p & e_{24}^p & 0 & 0 \\ e_{31}^p & e_{32}^p & e_{33}^p & e_{34}^p & 0 & 0 \end{pmatrix} \\ \|\varepsilon_{ij}^{\sigma,p}\| &= \begin{pmatrix} \varepsilon_{11}^{\sigma,p} & 0 & 0 \\ 0 & \varepsilon_{22}^{\sigma,p} & \varepsilon_{23}^{\sigma,p} \\ 0 & \varepsilon_{23}^{\sigma,p} & \varepsilon_{33}^{\sigma,p} \end{pmatrix} \text{ and } \|s_{fg}^{E,p}\| = \begin{pmatrix} s_{11}^{E,p} & s_{12}^{E,p} & s_{13}^{E,p} & s_{14}^{E,p} & 0 & 0 \\ s_{12}^{E,p} & s_{22}^{E,p} & s_{23}^{E,p} & s_{24}^{E,p} & 0 & 0 \\ s_{13}^{E,p} & s_{23}^{E,p} & s_{33}^{E,p} & s_{34}^{E,p} & 0 & 0 \\ s_{14}^{E,p} & s_{24}^{E,p} & s_{34}^{E,p} & s_{44}^{E,p} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{55}^{E,p} & s_{56}^{E,p} \\ 0 & 0 & 0 & 0 & s_{56}^{E,p} & s_{66}^{E,p} \end{pmatrix}. \end{aligned}$$

All the matrix forms correspond to the point group  $m$ , and in the polydomain crystal the mirror plane  $m \perp OX_1$ . All the non-zero elements of the  $\|d_{ij}^p\|$  and  $\|e_{ij}^p\|$  matrices become zero at the domain volume concentration  $m_0 = 0.5$  that is interpreted by a lack of the piezoelectric activity in the crystal having the equal volume concentrations of the domains with the spontaneous polarization vectors  $\mathbf{P}_{s1}$  and  $\mathbf{P}_{s2} = -\mathbf{P}_{s1}$  (see figure 1). All the non-zero elements of the four matrices written above coincide with the corresponding elements  $d_{ij}$ ,  $e_{ij}$ ,  $\varepsilon_{kl}^\sigma$  and  $s_{fg}^E$  of the single-domain crystals [10] for  $m_0 = 1$ . A comparative analysis of the  $\|s_{fg}^{E,p}\|$  matrix forms on the basis of conceptions [13] leads to a determination of the point group  $2/m$  for the equal domain volume concentrations ( $m_0 = 0.5$ ) only and of

† Hereafter we use an upper index  $p$  to mark any constants of the polydomain crystal.

the point group  $3m$  [1, 2, 10] in the case of the single-domain crystal ( $m_0 = 1$ ). It should be noted that the mutual orientation of the coordinate axes  $OX_i$  and vectors  $P_{si}$  (figure 1) provides the  $\|s_{fg}^{E,p}\|$  matrix forms if we assume  $2\|OX_1$ . However such an arrangement differs from the usual one [13] for the crystallographic axes in accordance with the point group  $2/m$ .

Results of our calculations are shown in tables 1 and 2. The  $d_{ij}^p(m_0)$  dependences for the fixed  $ij$  indices are analogous and characterized by relations  $|d_{21}^p/d_{23}^p| \approx |d_{22}^p/d_{23}^p|$ ,  $|d_{33}^p/d_{31}^p| \approx |d_{33}^p/d_{32}^p|$  for both the crystals. Within the concentration range of  $0.8 \leq m_0 \leq 0.9$  an unusual relation  $|d_{22}^p/d_{23}^p| \gg |d_{33}^p/d_{31}^p|$  is reached. A feature of these crystals and, undoubtedly, their single-domain constants consists in a slight change in the anisotropy  $|d_{33}^p/d_{31}^p|$  at the transition from the single-domain ( $m_0 = 1$ ) to the polydomain ( $m_0 \approx 0.5$ ) crystal: e.g., there are

$$|d_{33}/d_{31}| = 6.0 \quad |d_{33}^p/d_{31}^p|_{m_0 \rightarrow 0.5} \approx 4.5 \text{ and } |d_{33}^p/d_{32}^p|_{m_0 \rightarrow 0.5} \approx 8.9$$

in LN as well as

$$|d_{33}/d_{31}| = 3.5 \quad |d_{33}^p/d_{31}^p|_{m_0 \rightarrow 0.5} \approx 3.3 \text{ and } |d_{33}^p/d_{32}^p|_{m_0 \rightarrow 0.5} \approx 3.7$$

in LNT.

The concentration behaviour of the piezoelectric constants  $e_{ij}^p(m_0)$  is more diverse. One can single out a few important trends. A nonmonotonic function with alternating signs

$$e_{23}^p(m_0) = d_{21}^p c_{13}^{E,p} + d_{22}^p c_{23}^{E,p} + d_{23}^p c_{33}^{E,p} + d_{24}^p c_{34}^{E,p}$$

pertaining to the polydomain LN crystal (see table 1), is caused by a realization of conditions

$$|d_{21}^p| c_{13}^{E,p} \approx d_{22}^p c_{23}^{E,p} \quad |d_{23}^p| < d_{24}^p \quad c_{33}^{E,p} > c_{34}^{E,p}$$

for  $m_0 = \text{constant}$  where  $c_{fg}^{E,p}$  are elastic moduli of the polydomain crystal. Slight deviations of the  $e_{23}^p$  values from the zero value are accounted for by competition and different signs of the items  $d_{ij}^p c_{fg}^{E,p}$  determining the  $e_{23}^p(m_0)$  function. Its behaviour differs from that of the  $e_{23}^p(m_0)$  function determined for the LNT crystal (see table 2) where, for example, a single-domain constant  $e_{31} < 0$  [11] and ratios between some single-domain elastic compliances  $s_{fg}^E$  differ from  $e_{31} > 0$  and the corresponding compliance ratios characteristic of the LN crystal [2, 10], respectively.

The character of the  $e_{31}^p(m_0)$  and  $e_{32}^p(m_0)$  functions for both the crystals (compare data given in tables 1 and 2) is associated with two following factors. The first factor is the  $\text{sgn } e_{31}$  difference mentioned above. The second factor stems from a balance of the items  $d_{ij}^p c_{fg}^{E,p}$  given in expressions

$$e_{31}^p(m_0) = d_{31}^p c_{11}^{E,p} + d_{32}^p c_{12}^{E,p} + d_{33}^p c_{13}^{E,p} + d_{34}^p c_{14}^{E,p}$$

$$e_{32}^p(m_0) = d_{31}^p c_{12}^{E,p} + d_{32}^p c_{22}^{E,p} + d_{33}^p c_{23}^{E,p} + d_{34}^p c_{24}^{E,p}$$

and from conditions

$$d_{31}^p c_{11}^{E,p} + d_{32}^p c_{12}^{E,p} < d_{33}^p c_{13}^{E,p} + d_{34}^p c_{14}^{E,p}$$

$$d_{31}^p c_{12}^{E,p} + d_{32}^p c_{22}^{E,p} < d_{33}^p c_{23}^{E,p} + d_{34}^p c_{24}^{E,p}$$

realized for LNT at  $0.5 < m_0 < 1$ . The relatively small  $e_{23}^p$ ,  $e_{31}^p$  and  $e_{32}^p$  values favour the large anisotropy of  $e_{ij}^p$  that is realized appreciably particularly in the LN crystal. According to our evaluations, for  $0.5 < m_0 < 1$

$$|e_{21}^p| \approx e_{22}^p \gg |e_{23}^p| \quad (1)$$

**Table 1.** Effective electromechanical constants calculated for polydomain LiNbO<sub>3</sub> crystals in a wide domain volume concentration range of  $0.5 < m_0 \leq 1$  at 25 °C.

	$d_{15}^p$	$d_{16}^p$	$d_{21}^p$	$d_{22}^p$	$d_{23}^p$	$d_{24}^p$	$d_{31}^p$	$d_{32}^p$
	(10 <sup>-12</sup> C N <sup>-1</sup> )							
$m_0 - 0.5$								
$1.0 \times 10^{-6}$	$1.36 \times 10^{-4}$	$-8.40 \times 10^{-5}$	$-3.15 \times 10^{-5}$	$3.21 \times 10^{-5}$	$-1.89 \times 10^{-6}$	$1.03 \times 10^{-4}$	$-2.69 \times 10^{-4}$	$-1.36 \times 10^{-6}$
0.10	13.6	-8.40	-3.18	3.24	-0.184	10.4	-0.267	-0.138
0.20	27.2	-16.8	-6.56	6.67	-0.331	20.0	-0.521	-0.288
0.30	40.8	-25.2	-10.4	10.5	-0.397	33.9	-0.746	-0.466
0.40	60.3	-33.6	-15.0	15.1	-0.321	48.8	-0.914	-0.693
0.49	66.6	-41.2	-20.3	20.3	$-4.71 \times 10^{-2}$	65.8	-0.998	-0.967
0.50	68.0	-42.0	-21.0	21.0	0	68.0	-1.00	-1.00
	$d_{33}^p$	$d_{34}^p$	$e_{15}^p$	$e_{16}^p$	$e_{21}^p$	$e_{22}^p$	$e_{23}^p$	$e_{24}^p$
	(10 <sup>-12</sup> C N <sup>-1</sup> )							
$m_0 - 0.5$								
$1.0 \times 10^{-6}$	$1.21 \times 10^{-5}$	$2.18 \times 10^{-6}$	$7.39 \times 10^{-6}$	$-5.07 \times 10^{-6}$	$-6.85 \times 10^{-6}$	$6.46 \times 10^{-6}$	$1.43 \times 10^{-7}$	$-1.10 \times 10^{-5}$
0.10	1.21	0.211	0.739	-0.507	-0.665	0.632	$8.25 \times 10^{-3}$	0.998
0.20	2.42	0.381	1.48	-1.01	-1.26	1.21	$-5.52 \times 10^{-4}$	1.65
0.30	3.62	0.457	2.22	-1.52	-1.82	1.67	$-3.43 \times 10^{-2}$	2.42
0.40	4.82	0.370	3.31	-1.97	-2.26	2.07	$-6.28 \times 10^{-3}$	3.13
0.49	5.88	$5.61 \times 10^{-2}$	3.62	-2.48	-2.51	2.50	$-3.09 \times 10^{-4}$	3.66
0.50	6.00	0	3.70	-2.54	-2.54	2.54	0	3.70

Table 1. (Continued)

$m_0 - 0.5$	$e_{31}^p$	$e_{32}^p$	$e_{33}^p$	$e_{34}^p$	$\epsilon_{11}^{\sigma,p}/\epsilon_0$	$\epsilon_{22}^{\sigma,p}/\epsilon_0$	$\epsilon_{23}^{\sigma,p}/\epsilon_0$	$\epsilon_{33}^{\sigma,p}/\epsilon_0$
	(C m <sup>-2</sup> )							
$1.0 \times 10^{-6}$	$2.26 \times 10^{-7}$	$5.34 \times 10^{-7}$	$2.79 \times 10^{-6}$	$2.98 \times 10^{-7}$	43.6	59.3	2.74	29.7
0.10	$2.40 \times 10^{-2}$	$5.25 \times 10^{-2}$	$2.79 \times 10^{-2}$	$2.58 \times 10^{-2}$	45.2	60.1	2.69	29.7
0.20	$5.44 \times 10^{-2}$	0.102	0.558	$3.97 \times 10^{-2}$	50.1	62.5	2.52	29.7
0.30	$9.21 \times 10^{-2}$	0.140	0.828	$4.07 \times 10^{-2}$	58.2	66.8	2.21	29.8
0.40	0.141	0.172	1.08	$2.76 \times 10^{-2}$	69.5	73.6	1.73	29.9
0.49	0.189	0.190	1.27	$2.85 \times 10^{-3}$	82.4	82.7	1.08	30.0
0.50	0.191	0.191	1.28	0	84.0	84.0	1.00	30.0

$m_0 - 0.5$	$s_{11}^{E,p}$	$s_{12}^{E,p}$	$s_{13}^{E,p}$	$s_{14}^{E,p}$	$s_{22}^{E,p}$	$s_{23}^{E,p}$	$s_{24}^{E,p}$	$s_{33}^{E,p}$	$s_{34}^{E,p}$	$s_{44}^{E,p}$
	(10 <sup>-12</sup> Pa <sup>-1</sup> )									
$1.0 \times 10^{-6}$	5.23	-0.495	-1.37	0.702	5.10	-1.39	-0.369	4.75	-0.273	9.99
0.10	5.25	-0.511	-1.37	0.648	5.12	-1.39	-0.319	4.75	-0.263	11.1
0.20	5.30	-0.560	-1.38	0.482	5.15	-1.39	-0.163	4.75	-0.233	12.6
0.30	5.40	-0.650	-1.40	0.183	5.41	-1.41	-0.119	4.78	-0.179	14.0
0.40	5.55	-0.792	-1.43	-0.291	5.55	-1.43	0.564	4.86	-0.0927	15.0
0.49	5.75	-0.983	-1.46	-0.932	5.75	-1.47	1.01	4.99	-0.0236	16.8
0.50	5.78	-1.01	-1.47	-1.02	5.78	-1.47	1.02	5.02	0	17.0

(1) All the calculated matrix elements belong to principal axes of the polydomain crystal sample.  
 (2) The elastic compliances (in 10<sup>-12</sup> Pa<sup>-1</sup>)  $s_{55}^{E,p} = s_{55}^E = 17.0$ ,  $s_{56}^{E,p} = s_{56}^E = -2.04$  and  $s_{66}^{E,p} = s_{66}^E = 13.6$  are constant for any concentrations  $m_0$ .

**Table 2.** Effective electromechanical constants calculated for polydomain  $\text{LiNb}_{0.1}\text{Ta}_{0.9}\text{O}_3$  crystals in a wide domain volume concentration range of  $0.5 < m_0 \leq 1$  at  $25^\circ\text{C}$ .

	$d_{15}^p$	$d_{16}^p$	$d_{21}^p$	$d_{22}^p$	$d_{23}^p$	$d_{24}^p$	$d_{31}^p$	$d_{32}^p$
$m_0 - 0.5$	( $10^{-12} \text{ C N}^{-1}$ )							
$1.0 \times 10^{-6}$	$5.51 \times 10^{-5}$	$-4.74 \times 10^{-5}$	$-2.08 \times 10^{-5}$	$2.15 \times 10^{-5}$	$-1.11 \times 10^{-6}$	$4.92 \times 10^{-5}$	$-4.91 \times 10^{-6}$	$-4.37 \times 10^{-6}$
0.10	5.51	-4.74	-2.09	2.16	-0.107	4.08	-0.490	-0.437
0.20	11.0	-9.48	-4.25	4.36	-0.189	10.0	-0.973	-0.880
0.30	16.5	-14.2	-6.54	6.67	-0.220	15.4	-1.44	-1.33
0.40	22.0	-19.0	-9.04	9.13	-0.170	21.1	-1.89	-1.81
0.49	27.0	-23.2	-11.6	11.6	$-2.37 \times 10^{-2}$	26.9	-2.26	-2.25
0.50	27.5	-23.7	-11.8	11.8	0	27.5	-2.30	-2.30
	$d_{33}^p$	$d_{34}^p$	$e_{15}^p$	$e_{16}^p$	$e_{21}^p$	$e_{22}^p$	$e_{23}^p$	$e_{24}^p$
$m_0 - 0.5$	( $10^{-12} \text{ C N}^{-1}$ )							
$1.0 \times 10^{-6}$	$1.62 \times 10^{-5}$	$8.66 \times 10^{-6}$	$5.28 \times 10^{-6}$	$-4.48 \times 10^{-6}$	$-5.63 \times 10^{-6}$	$4.16 \times 10^{-6}$	$-1.10 \times 10^{-7}$	$7.62 \times 10^{-6}$
0.10	1.62	3.61	0.528	-0.447	-0.537	0.419	$-9.18 \times 10^{-2}$	0.633
0.20	3.24	5.83	1.06	-0.896	-1.05	0.857	-0.160	1.26
0.30	4.85	2.45	1.58	-1.34	-1.52	1.28	-0.195	1.84
0.40	6.46	1.35	2.11	-1.79	-1.92	1.75	-0.169	2.33
0.49	7.89	0.702	2.59	-2.19	-2.20	2.20	$-1.05 \times 10^{-2}$	2.61
0.50	8.05	0	2.64	-2.24	-2.24	2.24	0	2.64

Table 2. (Continued)

$m_0 - 0.5$	$(\text{C m}^{-2})$						$\epsilon_{11}^{\sigma,p}/\epsilon_0$	$\epsilon_{22}^{\sigma,p}/\epsilon_0$	$\epsilon_{33}^{\sigma,p}/\epsilon_0$
	$e_{31}^p$	$e_{32}^p$	$e_{33}^p$	$e_{34}^p$	$e_{11}^p$	$e_{22}^p$			
$1.0 \times 10^{-6}$	$-4.74 \times 10^{-7}$	$-2.26 \times 10^{-7}$	$3.30 \times 10^{-6}$	$1.14 \times 10^{-6}$	39.2	32.7	20.7	17.5	
0.10	-0.119	$-5.01 \times 10^{-2}$	0.252	0.515	39.7	33.4	19.9	18.6	
0.20	-0.157	$-6.31 \times 10^{-2}$	0.562	0.680	41.4	35.7	17.7	21.9	
0.30	$-9.13 \times 10^{-2}$	$-4.15 \times 10^{-2}$	0.949	0.258	44.2	39.6	13.9	27.5	
0.40	$-5.41 \times 10^{-2}$	$-2.75 \times 10^{-2}$	1.35	0.119	48.1	45.3	8.39	35.7	
0.49	$-1.94 \times 10^{-2}$	$-1.44 \times 10^{-2}$	1.76	$-6.49 \times 10^{-2}$	52.6	52.2	1.85	45.6	
0.50	$-1.00 \times 10^{-2}$	$-1.00 \times 10^{-2}$	1.78	0	53.1	53.1	1.00	46.8	

$m_0 - 0.5$	$(10^{-12} \text{ Pa}^{-1})$									
	$s_{11}^{E,p}$	$s_{12}^{E,p}$	$s_{13}^{E,p}$	$s_{14}^{E,p}$	$s_{22}^{E,p}$	$s_{23}^{E,p}$	$s_{24}^{E,p}$	$s_{33}^{E,p}$	$s_{34}^{E,p}$	$s_{44}^{E,p}$
$1.0 \times 10^{-6}$	4.59	-0.349	-1.18	0.681	4.22	-1.21	0.0823	4.94	0.352	9.99
0.10	4.60	-0.357	-1.19	0.660	4.30	-1.21	0.0804	4.93	0.343	7.01
0.20	4.64	-0.380	-1.20	0.596	4.35	-1.22	0.0312	4.92	0.309	8.46
0.30	4.69	-0.421	-1.22	0.486	4.57	-1.24	-0.0263	4.87	0.245	8.77
0.40	4.77	-0.481	-1.25	0.325	4.67	-1.26	-0.0704	4.70	0.179	9.40
0.49	4.86	-0.555	-1.29	0.128	4.85	-1.29	-0.126	4.49	0.0119	10.5
0.50	4.87	-0.564	-1.29	0.127	4.87	-1.29	-0.127	4.52	0	10.7

(1) All the calculated matrix elements belong to principal axes of the polydomain crystal sample.  
 (2) The elastic compliances (in  $10^{-12} \text{ Pa}^{-1}$ )  $s_{55}^{E,p} = s_{55}^E = 10.7$ ,  $s_{56}^{E,p} = s_{56}^E = 0.255$  and  $s_{66}^{E,p} = s_{66}^E = 10.9$  are constant for any concentrations  $m_0$ .



(compare data from table 1) that is considerably associated with items  $d_{21}^p c_{11}^{E,p}$  and  $d_{22}^p c_{22}^{E,p} \approx |d_{21}^p| c_{11}^{E,p}$  giving marked contributions to the  $e_{21}^p$  and  $e_{22}^p$  values of the polydomain LN crystal.

Equation (1) may be well compared with a known condition

$$d_{33}^* \gg |d_{31}^*| = |d_{32}^*| \quad (2)$$

for the piezoelectric moduli  $d_{ij}^*$  of highly anisotropic ferroelectric PbTiO<sub>3</sub>-based ceramics [14] polarized along the OX<sub>3</sub> axis. In spite of symmetry differences between the polydomain crystal [1–4, 12] and the polarized ceramics [14], large piezoelectric anisotropy is reached in the polydomain LN and LNT crystals (see  $d_{ij}^p$  from tables 1 and 2) and in the PbTiO<sub>3</sub>-based ceramics (even up to  $|d_{33}^*/d_{31}^*| \rightarrow \infty$  [15]). The ratio  $|d_{33}^*/d_{31}^*|$  of the single-domain crystal constants is equal to 6.0 and 5.5 in LN [10] and PbTiO<sub>3</sub> [14], respectively. Nevertheless the ways for reaching the piezoelectric anisotropy in accordance with equations (1) and (2) are different and associated with a difference in structural elements responsible for this effect, e.g., domains or grains (single domain or polydomain depending on circumstances), their shape, orientations, etc.

As for sets of other electromechanical constants from tables 1 and 2, the two following examples of the considerable anisotropy should be singled out. The anisotropy of the dielectric permittivities  $\varepsilon_{11}^{\sigma,p}/\varepsilon_{33}^{\sigma,p}$  of the LN and LNT polydomain crystals show their contrasting behaviour: it decreases from 2.8 to 1.5 when decreasing  $m_0$  from 1 to 0.5 in LN, but it increases from 1.1 to 2.2 in the same case in LNT. The anisotropy  $\varepsilon_{22}^{\sigma,p}/\varepsilon_{33}^{\sigma,p}$  has similar features; however it is varied within narrower ranges in both the crystals. Perhaps the  $\varepsilon_{11}^{\sigma,p}/\varepsilon_{33}^{\sigma,p}$  values calculated here influence reaching significant anisotropy of the piezoelectric moduli  $d_{ij}^p$ , but not very distinctly in comparison with PbTiO<sub>3</sub>-based ferroelectrics [14] where the 90° domain structure of grains [15] plays an important role too. A more detailed consideration of the concentration behaviour of the whole sets of the  $s_{fg}^{E,p}(m_0)$  and  $\varepsilon_{ij}^{\sigma,p}(m_0)$  functions in the LN-based polydomain crystals should be a subject of an independent research work.

### 3. Conclusions

In this paper we have studied the features of the electromechanical properties and found the significant piezoelectric anisotropy of the LN and LNT crystals with the unusual 180° domain structure. These features belong to the evaluated  $e_{ij}^p$  constants first of all and to the evaluated  $d_{ij}^p$  constants to a lesser degree: their anisotropy can reach values being more or even significantly more than the same anisotropy in the corresponding single-domain crystals. The analysis carried out in the present work may be a good stimulus for an experimental investigation of similar effects in single- and polycrystalline LN-type compounds with the purpose of applying them in technical devices.

### References

- [1] Kouz'minov Yu S 1987 *The Electrooptic and Nonlinear-Optic Lithium Niobate Crystal* (Moscow: Nauka) (in Russian)
- [2] Smolensky G A, Bokov V A, Isupov V A, Krainik N N, Pasyukov R Ye, Sokolov A I and Yushkin N K 1985 *Physics of Ferroelectric Phenomena* (Leningrad: Nauka) (in Russian)
- [3] Aleksandrovski A L, Naumova I I and Tarasenko V V 1993 *Ferroelectrics* **141** 147
- [4] Chartier J, Moustapha A A, Le Bihan R and Aleksandrovski A L 1996 *Int. Symp. on Ferroic Domains and Mesoscopic Structures, ISFD4 (Vienna, 1996)* p 71
- [5] Topolov V Yu and Turik A V 1994 *Tech. Phys. Lett.* **20** 610

- [6] Topolov V Yu 1995 *J. Phys.: Condens. Matter* **7** 7405
- [7] Turik A V and Bondarenko E I 1974 *Fiz. Tverd. Tela* **16** 1240 (in Russian)
- [8] Turik A V and Bondarenko E I 1974 *Ferroelectrics* **7** 303
- [9] Turik A V, Shevchenko N B and Chernobabov A I 1978 *Fiz. Tverd. Tela* **20** 2860 (in Russian)
- [10] Smith T R and Welsh F S 1974 *J. Appl. Phys.* **42** 2219
- [11] Wang H and Wang M 1986 *J. Crystal Growth* **79** 527
- [12] Deshmukh K G and Singh K 1972 *J. Phys. D: Appl. Phys.* **5** 1680
- [13] Nye J F 1985 *Physical Properties of Crystals* 2nd edn (Oxford: Clarendon)
- [14] Topolov V Yu, Turik A V and Chernobabov A I 1994 *Crystallogr. Rep.* **39** 805
- [15] Turik A V and Topolov V Yu 1997 *J. Phys. D: Appl. Phys.* **30** 1541