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## **University of Bath**

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Inconsistencies of the complete sets of electromechanical

constants of relaxor-ferroelectric single crystals

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Complete sets of elastic, dielectric, and piezoelectric constants of relaxor-ferroelectric single

crystals of  $(1 - x)Pb(A_{1/3}Nb_{2/3})O_3 - xPbTiO_3$  (A = Mg or Zn) and  $Pb(In_{1/2}Nb_{1/2})O_3$  -

Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub> – PbTiO<sub>3</sub> are analyzed to demonstrate violations of the interrelations between

particular groups of electromechanical constants and the resulting influence of the inconsistent

properties on the thermodynamic stability and electromechanical coupling in single crystals. The

possibilities of refinement and correction of inconsistent constants are discussed and presented

for specific examples of relaxor-ferroelectric single crystals.

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1

# I. INTRODUCTION

Single crystals (SCs) of relaxor-ferroelectric solid solutions<sup>1</sup> with the perovskite-type structure and compositions near the morphotropic phase boundary exhibit outstanding piezoelectric performance and electromechanical coupling in comparison with conventional ferroelectric ceramics. The ferroelectric-relaxor SCs, such as  $(1 - x)Pb(Mg_{1/3}Nb_{2/3})O_3 - xPbTiO_3$  (PMN-xPT) and  $(1 - x)PbTiO_3$  $x)Pb(Zn_{1/3}Nb_{2/3})O_3 - xPbTiO_3$  (PZN-xPT), are of interest for piezoelectric transducer, actuator, sensor, hydrophone, and solid-state electronic applications<sup>2</sup> as well as a piezo-active components of advanced composites<sup>3</sup>. For these applications and for modeling SC transducers, it is important to have reliable information on the physical properties of the aforementioned and related SCs. Complete sets of elastic, dielectric, and piezoelectric (i.e., electromechanical) constants are usually determined<sup>4-6</sup> for specific SC sample geometries and using the recognized experimental methods. Among the complete sets of constants, of particular interest for many applications are the elastic compliances  $s_{ab}^{E}$  at electric field E = const, piezoelectric coefficients  $d_{ij}$ , and dielectric permittivities  $\varepsilon_{pp}^T$  at mechanical stress T= const. Other important complete sets are the elastic moduli  $c_{ab}^{E}$  at electric field E= const, piezoelectric coefficients  $e_{ij}$ , and dielectric permittivities  $\varepsilon_{mm}^{S}$  at mechanical strain S = const. These electromechanical constants from the complete sets are related via the following constitutive equations<sup>7</sup> of an electroelastic medium:

$$S_p = s_{pq}^E T_q + d_{fp} E_f \text{ and } D_k = d_{kl} T_l + \varepsilon_{kr}^T E_r$$
(1)

or

$$T_p = c_{pq}^E S_q - e_{fp} E_f \text{ and } D_k = e_{kl} S_l + \varepsilon_{kr}^s E_r,$$
 (2)

where  $D_k$  is electric displacement. There are also two pairs of the constitutive equations<sup>7</sup> for the additional piezoelectric coefficients,  $g_{ij}$  and  $h_{ij}$ :

$$S_p = s_{pq}^D T_q + g_{fp} D_f \text{ and } E_k = -g_{kl} T_l + \beta_{kr}^T D_r,$$
 (3)

and

$$T_p = c_{pq}^D S_q - h_{fp} D_f \text{ and } E_k = -h_{kl} S_l + \beta_{kr}^s D_r,$$
 (4)

where  $\beta_{kr}^T$  is dielectric impermeability at T = const and  $\beta_{kr}^S$  is dielectric impermeability at S = const. The piezoelectric coefficients from Eqs. (1) – (4) are interrelated as follows:

$$d_{fp} = \varepsilon_{fk}^{T} g_{kp} = e_{fq} s_{qp}^{E}, e_{fp} = \varepsilon_{fk}^{S} h_{kp} = d_{fq} c_{qp}^{E}, g_{fp} = \beta_{fk}^{T} d_{kp} = h_{fq} s_{qp}^{D}, \text{ and } h_{fp} = \beta_{fk}^{S} e_{kp} = g_{fq} c_{qp}^{D}.$$
(5)

The complete sets of room-temperature electromechanical constants of PMN–*x*PT, PZN–*x*PT, and Pb(In<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub>–Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>–PbTiO<sub>3</sub> (PIN–PMN–PT) SCs have been experimentally determined in both the single-domain and polydomain states and reported in a series of papers (see, e.g., Refs. 4–6). These complete sets refer to fixed poling directions, often to [001], [110] or [111] of the perovskite unit cell. Good agreement, or *good consistency*, between the different sets of electromechanical constants related to the same SC [see Eqs. (1) – (5)] is observed for data on the [001]-poled samples of PMN–0.30PT<sup>8</sup> and PIN–PMN–PT<sup>9</sup>. In these cases, any deviations of constants from conditions (5) are less than 5 %.<sup>10</sup> However, in some cases we have observed issues concerned with an

inconsistency<sup>11</sup> of the electromechanical constants and related parameters of SCs. In the context of this paper, an 'inconsistency' is expressed as a 5 % or greater disagreement between the values of electromechanical constants from the related complete sets. Examples of inconsistency include the transition from elastic compliances  $s_{ab}^E$  to elastic moduli  $c_{ab}^E$ , from the piezoelectric coefficients  $e_{kp}$  to the piezoelectric coefficients  $h_{fp}$  [see Eqs. (5)], etc. An inconsistency can also represent a violation of conditions for the thermodynamic stability<sup>7</sup> of SCs.

The aim of this paper is to demonstrate examples of the inconsistencies for relaxor-ferroelectric SCs and to discuss the possibilities of the refinement of particular electromechanical constants of these materials.

# II. EXAMPLES OF INCONSISTENCY AND REFINEMENT

## A. PZN-xPT

The complete sets of electromechanical constants of PZN–(0.06–0.07)PT SCs in the single-domain<sup>12</sup> and polydomain<sup>13</sup> states are characterized by a particular inconsistency. In case of the single-domain SC, this inconsistency is concerned with interrelations between different electromechanical constants, mainly, between the piezoelectric coefficients from Eqs. (5). Below we consider some quantitative interrelations between the constants listed in Table I.

Taking into account the link between the piezoelectric coefficients  $h_{fp}$  and  $e_{kp}$  from Eqs. (5), the equality  $\|\beta^S\| = \|\epsilon^S\|^{-1}$ , and the 3m symmetry of the single-domain PZN-(0.06-0.07)PT SC<sup>12</sup> at room temperature, we obtain

$$h_{22} = e_{22} / \varepsilon_{22}^s > 0.$$
 (6)

However, Table I contains  $h_{22} < 0$  and  $e_{22} > 0$ . Such a discrepancy can stem from an erroneous sign of dielectric permittivity  $\varepsilon_{22}^S$  at the frequency of measuements, <sup>12</sup> but our evaluation suggests that  $h_{22}$  from condition (6) would be 8.3 times more than  $|h_{22}|$  from Table I. Using the relation  $h_{33} = e_{33}/\varepsilon_{33}^S$ , we obtain  $h_{33} = 25.1 \cdot 10^8 \text{ V/m}$ , and the difference between this value and  $h_{33}$  from Table I is about 8.7 %. The evaluation of  $h_{31}$  and  $h_{15}$  from formulas  $h_{31} = e_{31}/\varepsilon_{33}^S$  and  $h_{15} = e_{15}/\varepsilon_{11}^S$  leads to  $h_{31} = -9.17 \cdot 10^8 \text{ V/m}$  and  $h_{15} = 8.48 \cdot 10^8 \text{ V/m}$ . Both of these values are in disagreement with the  $h_{31}$  and  $h_{15}$  values from Table I, where  $h_{31} = -5.9$  and  $h_{15} = 19.7$  (in  $10^8 \text{ V/m}$ ).

We have also checked quantitative relations between the piezoelectric coefficients  $h_{fp}$  and  $g_{fq}$  from Eqs. (5). Good agreement between the evaluated and published values of  $h_{33}$  (22.6·10<sup>8</sup> V / m from our evaluation) is observed, but there is a significant difference between the remaining piezoelectric coefficients  $h_{fp}$ . For example, based on our evaluation of  $g_{fq}$  and  $c_{qp}^D$ , the piezoelectric coefficients  $h_{31} = -6.84 \cdot 10^8$  V / m (difference about 16 %) and  $h_{15} = 30.9 \cdot 10^8$  V / m (difference about 57 %) indicate the presence of the inconsistency in the data of Table I.

On checking the link between the piezoelectric coefficients  $e_{fp}$  and  $d_{fq}$  from Eqs. (5), there is good agreement between the evaluated and published<sup>12</sup> values of  $e_{3p}$  (p = 1 and 3); while the difference in the  $e_{15}$  values ( $e_{15} = 29.4$  C / m<sup>2</sup> from our evaluation) is 7.8 %. From the link between the piezoelectric coefficients  $g_{fp}$  and

 $d_{kp}$  [see Eqs. (5)], we obtain  $g_{22} = d_{22} / \varepsilon_{22}^T = -1.32 \cdot 10^{-2} \text{ V} \cdot \text{m} / \text{N} < 0$ , but according to Table I,  $g_{22} = 1.3 \cdot 10^{-2} \text{ V} \cdot \text{m} / \text{N}$ . The remaining values of  $g_{fp}$ , evaluated using  $d_{kp}$ , are in agreement with data shown in Table I.

Next we consider some interrelations that involve electromechanical constants related to the elastic, piezoelectric, and dielectric properties of SCs. As is known for a piezoelectric medium<sup>7</sup>, its elastic moduli  $c_{33}^D$  and  $c_{33}^E$  are linked by an equality  $c_{33}^D - c_{33}^E = e_{33}h_{33}$ . Taking the values of these constants from Table I, we observe a difference between  $c_{33}^D - c_{33}^E$  and  $e_{33}h_{33}$  as large as 6.9 %; while the thickness electromechanical coupling factor  $k_t = [(c_{33}^D - c_{33}^E)/c_{33}^D]^{1/2}$  of 0.392 is in good agreement with the  $k_t$  value from Table I. Additionally,  $k_t$  evaluated using the conventional formula<sup>7</sup>

$$k_t = e_{33} / \left( \varepsilon_{33}^S c_{33}^D \right)^{1/2} \tag{7}$$

equals 0.396 and is consistent with data from Table I.

Of independent interest are evaluations of electromechanical coupling factors<sup>7</sup>

$$k_{ij} = d_{ij} / \left(\varepsilon_{ii}^T s_{jj}^E\right)^{1/2}. \tag{8}$$

Taking the pertinent electromechanical constants from Table I and using Eq. (8), we obtain  $k_{33} = 0.46$ ,  $|k_{31}| = 0.078$ , and  $k_{15} = 0.97$ , which are different to the values in Table I, where  $k_{33} = 0.33$ ,  $|k_{31}| = 0.18$ , and  $k_{15} = 0.73$ . This and the above-given examples of our evaluations suggest that the inconsistency of electromechanical constants<sup>12</sup> of the single-domain PZN–(0.06–0.07)PT SC cannot be avoided at a re-measurement of several constants, and the complete set of the

electromechanical properties is needed to be carefully refined on high-qualitative samples in a relatively stable single-domain state.

Analyzing the complete set of electromechanical constants of the polydomain PZN-(0.06-0.07)PT SCs,<sup>13</sup> we observe an inconsistency at the transition from elastic compliances  $s_{qp}^E$  and piezoelectric coefficients  $d_{fp}$  to  $e_{fq}$  [see Eqs. (5)]. According to our evaluations,  $e_{31} < 0$ ,  $e_{33} < 0$ , and  $|e_{31}| > |e_{33}|$ , i.e., these constants are in obvious disagreement with those from Ref. 13.

Recent work<sup>14</sup> on the performance of the  $[110]^L \times [001]^T$  cuts of the polydomain relaxor-ferroelectric SCs poled along [001] of the perovskite unit cell contains some complete sets of electromechanical constants deduced using the method put forward by Shukla et al. Analyzing these constants, one can observe the inconsistency at the transition from the elastic compliances  $s_{ab}^E$  to elastic moduli  $c_{ab}^E$  and piezoelectric coefficients  $e_{fq}$ . The interrelation between elastic constants<sup>7</sup> is represented in the matrix form as

$$||c^{E}|| = ||s^{E}||^{-1},$$
 (9)

and the piezoelectric coefficients  $e_{fq}$  are evaluated in accordance with Eqs. (5). Data from Table II show that both the elastic and piezoelectric constants of PZN–0.045PT SC<sup>14</sup> are characterized by an inconsistency ( $\delta > 5\%$  in Table II). This can be a result of the influence of the domain structure and defects in SCs on the electromechanical properties, especially as they are measured in non-polar directions and on specific SC cuts.

# B. PIN-PMN-PT

The characteristics of the piezoelectric and dielectric properties of singledomain [001]-poled PIN-PMN-PT SCs near the morphotropic phase boundary, namely the high electromechanical coupling and the stability of the single-domain state<sup>6</sup> may be useful for future piezotechnical and smart-materials applications. However, a comparison of data<sup>6</sup> on the tetragonal single-domain PIN-PMN-PT SC (measured and calculated properties) suggests inconsistencies among the electromechanical constants of the studied composition. Examples of the inconsistency (Table III) concern different kinds of electromechanical constants. Values of X (see the second column in Table III) were calculated using Eqs. (5) and taking into account tetragonal symmetry of the studied PIN-PMN-PT composition. It is important to emphasize the large difference between the calculated values (X) of elastic constants and those reported<sup>6</sup> (see  $X_{tab}$  in Table III). This concerns, for example, the elastic moduli  $c_{ab}^E$  and  $c_{ab}^D$  from the fourth column in Table III. Elastic constants involve expressions<sup>7</sup> suitable for the determination of dielectric and piezoelectric properties, and the influence of inconsistent elastic properties on these properties is also observed in Table III [see, e.g., data on  $\varepsilon_{11}^{S}$  /  $\varepsilon_0$  and  $h_{33}$  calculated using  $c_{qp}^D$  and  $g_{fq}$  in accordance with Eqs. (5)]. At the same time, the low differences between values of X and  $X_{tab}$  (less than 1% in Table III) suggest that the procedure<sup>6</sup> of the determination of electromechanical constants allows one to avoid any inconsistency by careful consideration of measurement data on the studied PIN-PMN-PT SCs.

# C. PMN-xPT

Very recently, examples of the inconsistency among electromechanical constants were analysed<sup>11</sup> for polydomain [011]-poled SCs of PMN–xPT<sup>15</sup> with x =0.28, 0.30, and 0.32. The complete set of electromechanical constants was also measured<sup>16</sup> on [001]-poled domain-engineered PMN-0.28PT samples with macroscopic tetragonal (4mm) symmetry at room temperature. Elastic constants  $c_{ab}^{E}$  and  $s_{ab}^{E}$  from Ref. 16 are consistent as stated using Eq. (9). However, the piezoelectric coefficients  $e_{3j}$  calculated using Eqs. (5) and values of  $c_{ab}^E$  and  $d_{ij}$ from paper  $^{16}$  differ considerably from the piezoelectric coefficients  $e_{ij}$  published in the same paper. <sup>16</sup> For instance, conditions  $e_{33} < 0$  and  $|e_{33}| < |e_{31}|$  are achieved in our calculations based on Eqs. (5), while the piezoelectric coefficients 16 obey inequalities  $e_{33} > 0$  and  $e_{33} > |e_{31}|$ . Electromechanical constants from Ref. 16 are also inconsistent because of an overestimated value of the longitudinal electromechanical coupling factor  $k_{33}$  from Eq. (8). Taking  $d_{33} = 2365$  pC / N,  $\varepsilon_{33}^T$  $\varepsilon_0 = 6833$ , and  $s_{33}^E = 86.46 \cdot 10^{-12} \text{ Pa}^{-1}$  from paper and substituting these values into right part of Eq. (8), we obtain  $k_{33} = 2365 / 2287 > 1$ , that clearly does not have any physical justification. This highlights the potential future problems of using the complete sets of electromechanical constants<sup>16</sup> of the polydomain PMN-0.28PT SC.

An important example of the inconsistency is revealed after a careful analysis of experimental data<sup>4</sup> on [001]-poled PMN-0.38PT SCs. According to results,<sup>4</sup> this

SC has tetragonal symmetry at room temperature, however, no specifics on domain structure (single-domain, near single-domain, polydomain, etc.) is provided. Our comments on the electromechanical constants from Ref. 4 are given as follows. First, elastic moduli of PMN–0.38PT SC (see  $c_{11}^E$ ,  $c_{12}^E$ , and  $c_{13}^E$  from Table IV and  $c_{33}^E$  from footnote b after Table IV) do not obey the condition for the thermodynamic stability<sup>17</sup>

$$(c_{11}^E + c_{12}^E)c_{33}^E > 2(c_{13}^E)^2.$$
 (10)

Second, a transition from  $||s^E||$  to  $||c^E||$  in accordance with Eq. (9) enables us to obtain  $c_{33}^E = 14.89 \cdot 10^{10}$  Pa instead of  $c_{33}^E = 9.92 \cdot 10^{10}$  Pa. The set of refined elastic moduli  $c_{ab}^E$  from Table IV obeys inequality (10) and other related conditions<sup>7,17</sup> for stability. Based on this set of refined data, one can confirm full agreement between the piezoelectric coefficients  $e_{3j}$  calculated using Eqs. (5) and those determined in Ref. 4. Correctness of values<sup>4</sup> of the piezoelectric coefficients  $d_{3j}$  and  $e_{3j}$  is also confirmed when checking a link between dielectric permittivities<sup>7</sup>

$$\varepsilon_{pp}^{T} - \varepsilon_{pp}^{S} = d_{pj}e_{pj}. \tag{11}$$

It is also observed that a value of  $d_{15}e_{15}$  from Eq. (11) at p=1 does not correspond to the difference  $\varepsilon_{11}^T - \varepsilon_{11}^S$  that is calculated from data published in paper.<sup>4</sup>

Third, our calculation of the electromechanical coupling factor  $k_{33}$  [see Eq. (8)] using  $d_{33}$ ,  $\varepsilon_{33}^T$ , and  $s_{33}^E$  from experimental data<sup>4</sup> leads to  $k_{33} = 0.802$  that is less than  $k_{33}$  from Ref. 4. The value of the thickness electromechanical coupling factor

 $k_t$  from Eq. (7) is evaluated taking into account  $e_{33}$ ,  $\mathcal{E}_{33}^S$  from Eq. (11), and a relation  $^7$   $c_{33}^D = c_{33}^E + e_{33}h_{33}$ . This  $k_t$  value becomes 14.7% less than the  $k_t$  value from paper (see Table IV). The main reason for such a difference is associated with the refined (larger) elastic modulus  $c_{33}^E$  and its influence on  $c_{33}^D$  and, therefore, on  $k_t$  from Eq. (7).

Electromechanical constants were also found<sup>14</sup> for the  $[110]^{L} \times [001]^{T}$  cut of the polydomain PMN-0.28PT SC poled along [001]. It seems probable that elastic compliance  $s_{13}^{E}$  equals  $-37.8^{\circ}10^{-12} \text{ Pa}^{-1}$  instead of  $37.8^{\circ}10^{-12} \text{ Pa}^{-1}$  from Ref. 14. Our subsequent checking the interrelations between elastic and piezoelectric constants enables us to conclude that the largest differences between the elastic moduli evaluated using Eq. (9) and those from paper<sup>14</sup> are attained for  $c_{11}^E$  (about 12 %) and  $c_{33}^{E}$  (about 7.4 %). Along with these differences, the considerable discrepancy is revealed when comparing the values of the piezoelectric coefficients  $e_{3i}$ . Our evaluation based on Eqs. (5) would lead to  $e_{31} = -17.7$  and  $e_{33} = 8.22$  (in C / m<sup>2</sup>), while the published <sup>14</sup> values are  $e_{31} = -4.7$  and  $e_{33} = 20.5$  (in C / m<sup>2</sup>). In contrast to this, a difference between the  $e_{15}$  values determined in the same way is only about 0.2 %. Such discrepancies may stimulate careful experimental determination of the elastic and piezoelectric properties of the polydomain PMN-0.28PT SC14 at various orientations of its main crystallographic axes.

# III. CONCLUSIONS

This paper reports a few examples of the inconsistency in the complete sets of room-temperature electromechanical constants of advanced relaxor-ferroelectric SCs. The inconsistent constants violate relations (5), (7) - (9), and (11) for the piezoelectric medium and condition (10) for thermodynamic stability of SCs. Moreover, the inconsistency can lead to an overestimation of the electromechanical coupling factors. The inconsistency reported in this paper is accounted for by different reasons (measurement conditions, accuracy of measurement, quantitative treatment of measured data, 10,11 etc.) and can be corrected in several cases. Our results of correction (Tables II – IV) suggest that the difference between the inconsistent and consistent values can reach a few tens of a percent which can be significant in transducer design and modeling of transducer behavior. In particular, it concerns the electromechanical constants of the single-domain PZN-(0.06-0.07)PT12 and PIN-PMN-PT6 SCs, and further careful measurements of their properties are desirable. The further refinement of data 12-14,16 is also needed for PMN-0.28PT SCs. As for PMN-0.38PT SC, the corrected of electromechanical constants (Table IV) can be suitable for further studies, design purposes and prediction of effective parameters. Of independent interest are conditions for stability of the single-domain state in PIN-PMN-PT, PZN-(0.06-0.07)PT, and PMN-0.38PT SCs. It is believed that this problem may be considered, and inconsistencies will be avoided in experimental studies and piezotechnical applications in the future.

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the accuracy of the calculation of the complete set of material coefficients depends on material variability and measuring accuracy. In our study we assume that the consistency takes place as electromechanical constants from Eqs. (1) - (4) obey constitutive formulas for the piezoelectric medium (see Ref. 7) with an accuracy to 5 %.

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TABLE I. Elastic compliances  $s_{ab}^E$  (in  $10^{-12}$  Pa<sup>-1</sup>), elastic moduli  $c_{ab}^E$  and  $c_{ab}^D$  (in  $10^{10}$  Pa), piezoelectric coefficients  $d_{ij}$  (in pC / N),  $e_{ij}$  (in C / m<sup>2</sup>),  $g_{ij}$  (in  $10^{-2}$  V·m / N), and  $h_{ij}$  (in  $10^8$  V / m), relative dielectric permittivities  $\varepsilon_{pp}^S/\varepsilon_0$  and  $\varepsilon_{pp}^T/\varepsilon_0$ , and electromechanical coupling factors  $k_{ij}$  and  $k_t$  of single-domain PZN–(0.06–0.07)PT SC<sup>12</sup>

$S_{11}^E$	$S_{12}^E$	$S_{13}^E$	$S_{14}^E$	$s_{33}^E$	$S_{44}^E$	$S_{66}^E$	$c_{11}^E$	$c_{12}^E$
32.8	-28.5	-1.2	100.1	6.5	390.4	122.6	18.0	8.0
$c_{13}^E$	$c_{14}^E$	$c_{33}^E$	$c_{44}^E$	$c_{66}^{\it E}$	$c_{11}^{D}$	$c_{12}^D$	$c_{13}^D$	$c_{14}^D$
4.8	-2.6	17.1	1.6	5.0	19.4	8.0	6.4	-2.2
$c_{33}^D$	$c_{44}^D$	$c_{66}^{D}$	$d_{15}$	$d_{22}$	$d_{31}$	$d_{33}$	$e_{15}$	$e_{22}$
20.2	4.0	5.7	6000	-1280	-35	93	31.7	30.9
$e_{31}$	$e_{33}$	<i>g</i> <sub>15</sub>	822	<b>8</b> 31	<b>8</b> 33	$h_{15}$	$h_{22}$	$h_{31}$
-4.6	12.6	6.3	1.3	-0.6	1.5	19.7	-1.0	-5.9
h <sub>33</sub>	$\mathcal{E}_{11}^{S}/\mathcal{E}_{0}$	$\mathcal{E}_{33}^{S}/\mathcal{E}_{0}$	$\mathcal{E}_{11}^T / \mathcal{E}_0$	$\mathcal{E}_{33}^T/\mathcal{E}_0$	<i>k</i> <sub>15</sub>	k <sub>31</sub>	k <sub>33</sub>	$k_t$
23.1	4222	567	11000	700	0.73	0.18	0.33	0.39

TABLE II. Elastic moduli  $c_{ab}^{E}$  (in  $10^{10}$  Pa)<sup>a</sup> and piezoelectric coefficients  $e_{ij}$  (in C / m<sup>2</sup>)<sup>b</sup> of [001]-poled  $[110]^{L} \times [001]^{T}$  cuts of polydomain PZN–0.045PT SC

Value of <i>X</i> (current evaluation)	Value of $X_{tab}$ from Ref. 14	$\delta =  (X - X_{tab}) / X_{tab} ,$ %
15.7	17.0	6.4
3.05	4.35	30
8.85	10.1	12
9.29	10.5	12
6.41	6.4	< 1
0.452	0.45	< 1
-4.79	-3.7	< 1
14.0	15.0	6.3
8.97	8.9	< 1
	(current evaluation)  15.7  3.05  8.85  9.29  6.41  0.452  -4.79  14.0	(current evaluation) $X_{tab}$ from Ref. 1415.717.03.054.358.8510.19.2910.56.416.40.4520.45-4.79-3.714.015.0

<sup>&</sup>lt;sup>a</sup> Evaluated using Eq. (9)

<sup>&</sup>lt;sup>b</sup> Evaluated using Eqs. (5)

TABLE III. Published ( $X_{tab}$ ) and refined (X) values of electromechanical constants determined for [001]-poled PIN–PMN–PT SCs

Electromechanical constant <i>X</i> to be evaluated using data from Ref. 6 and formulas from Ref. 7	Value of <i>X</i> (current evaluation)	Value of $X_{tab}$ from Ref. 6	$\delta =  (X - X_{tab}) / X_{tab} ,$ %
$c_{11}^{E}$ (in 10 <sup>10</sup> Pa) using $s_{ab}^{E}$	15.1	20.6	27
$c_{12}^{E}$ (in $10^{10}$ Pa) using $s_{ab}^{E}$	10.2	15.5	34
$c_{13}^E$ (in $10^{10}$ Pa) using $s_{ab}^E$	8.7	12.5	30
$c_{33}^{E}$ (in $10^{10}$ Pa) using $s_{ab}^{E}$	8.5	12.5	32
$c_{44}^E$ (in $10^{10}$ Pa) using $s_{ab}^E$	1.8	1.8	0
$c_{66}^E$ (in $10^{10}$ Pa) using $s_{ab}^E$	4.0	4.5	11
$c_{11}^{D}$ (in $10^{10}$ Pa) using $s_{ab}^{D}$	14.6	21.3	31
$c_{12}^{D}$ (in $10^{10}$ Pa) using $s_{ab}^{D}$	9.4	16.3	42
$c_{13}^{D}$ (in $10^{10}$ Pa) using $s_{ab}^{D}$	5.0	10.9	54
$c_{33}^{D}$ (in $10^{10}$ Pa) using $s_{ab}^{D}$	10.3	19.4	47
$c_{44}^D$ (in $10^{10}$ Pa) using $s_{ab}^D$	6.6	6.8	2.9
$c_{66}^{D}$ (in $10^{10}$ Pa) using $s_{ab}^{D}$	4.0	4.5	11
$e_{31}$ (in C / m <sup>2</sup> ) using $s_{ab}^{E}$ and $d_{ij}$	-4.1	-4.2	2.4
$e_{33}$ (in C / m <sup>2</sup> ) using $s_{ab}^{E}$ and $d_{ij}$	10.1	9.5	6.3
$e_{15}$ (in C / m <sup>2</sup> ) using $s_{ab}^{E}$ and $d_{ij}$	42.7	46.4	8.0
$\mathcal{E}_{11}^{S}/\mathcal{E}_{0}$ using $\mathcal{E}_{pp}^{T}$ , $s_{ab}^{E}$ , and $d_{ij}$	3650	4800	24
$\mathcal{E}_{33}^{S}/\mathcal{E}_{0}$ using $\mathcal{E}_{pp}^{T}$ , $s_{ab}^{E}$ , and $d_{ij}$	300	310	3.2
$h_{31}$ (in $10^8$ N/C) using $c_{ab}^D$ and $g_{ij}$	-17.5	-16.5	6.1
$h_{33}$ (in $10^8$ N/C) using $c_{ab}^D$ and $g_{ij}$	61.8	34.9	77
$h_{15}$ (in $10^8$ N/C) using $C_{ab}^D$ and $g_{ij}$	11.2	10.8	3.7
$h_{31}$ (in $10^8$ N / C) using $e_{ij}$ and $\mathcal{E}_{pp}^S$	-15.3	-16.5	7.3
$h_{33}$ (in $10^8$ N/C) using $e_{ij}$ and $\mathcal{E}_{pp}^S$	34.6	34.9	0.9
$h_{15}$ (in $10^8$ N / C) using $e_{ij}$ and $\varepsilon_{pp}^S$	10.9	10.8	0.9

TABLE IV. Refined electromechanical constants of [001]-poled PMN-0.38PT SC. Elastic moduli  $c_{ab}^E$  and  $c_{33}^D$  are in  $10^{10}\,\mathrm{Pa}$ 

$c_{11}^{\it E}$	$c_{12}^E$	$c_{13}^E$	$c_{33}^{E}$	$c_{44}^E$	$c_{66}^{\it E}$	$c_{33}^D$
21.25 <sup>a</sup>	14.33 <sup>a</sup>	13.51 <sup>a</sup>	14.89 <sup>b</sup>	5.56 <sup>a</sup>	6.95 <sup>a</sup>	20.72 <sup>c</sup>
$\mathcal{E}_{11}^{S}/\mathcal{E}_{0}$	$\mathcal{E}_{33}^{S}/\mathcal{E}_{0}$	$\mathcal{E}_{11}^T / \mathcal{E}_0$	$\mathcal{E}_{33}^T / \mathcal{E}_0$	$ k_{31} $	k <sub>33</sub>	$k_t$
3395 <sup>d</sup>	255 <sup>a</sup>	4301 <sup>a</sup>	734 <sup>a</sup>	0.446 <sup>a</sup>	0.802 <sup>e</sup>	$0.530^{\rm f}$

<sup>&</sup>lt;sup>a</sup> Data from Ref. 4

<sup>&</sup>lt;sup>b</sup> Instead of  $c_{33}^E = 9.92 \cdot 10^{10}$  Pa from Ref. 4

<sup>&</sup>lt;sup>c</sup> Instead of  $c_{33}^D = 15.74 \cdot 10^{12}$  Pa from Ref. 4

<sup>&</sup>lt;sup>d</sup> Instead of  $\mathcal{E}_{11}^S / \mathcal{E}_0 = 2171$  from Ref. 4

<sup>&</sup>lt;sup>e</sup> Instead of  $k_{33} = 0.846$  from Ref. 4

f Instead of  $k_t = 0.608$  from Ref. 4