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POLARIZATION MATRICES OF LITHIUM NIOBATE

Arthur Ballato
ELECTRONICS TECHNOLOGY AND DEVICES LABORATORY

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In analytical treatments of piezoelectric-acoustic transducers, signal processors, and resonators, the electromechanical transduction mechanism is most often expressed in terms of the elements of the piezoelectric [e] or [d] matrices. molecular interpretations of piezoelectricity, and especially electrooptical applications, usually involve polarization as the preferred variable, and consequently the alternative [a] and [b] matrices are of interest. The elements of these latter sets are calculated for lithium niobate from measured elastopiezodielectric constants taken from the literature. Key words

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INTRODUCTION

Electromechanical transduction taking place via the piezoelectric effect is characterized phenomenologically by constitutive equations that relate the elastic and electric variables. These equations take a variety of forms, depending upon the choice of independent and dependent variables; the choice is normally dictated by the application. For example, piezoelectric resonators in the form of thickness mode plates are most easily treated using the isagric elastic stiffnesses [cE], the piezoelectric stress constants [e], and the dielectric permittivities at constant strain [(eps)S].

Various measurement techniques yield values for the elements of a particular coefficient set more directly than those of another. The coefficients appearing in the different equation sets are, however, interrelated, so that once any one complete set is available, all the other sets of elements may be found. The most accurate and precise experimental results to date have been from plate resonator (resonance) and pulse-echo (transit-time) measurements. From the [cE], [e], and [(eps)S] matrices determined therefrom, those matrices representing material properties expressed in the other alternative forms may be calculated.

Electrooptical applications are becoming increasingly important. So also are treatments of piezoelectric and ferroelectric phenomena from the standpoint of molecular interactions. In both of these cases the constitutive equations using polarization as the independent electrical variable, rather than either electric intensity or displacement, assume greater importance than the sets traditionally used for transducer, signal processing, and resonator applications.

In this report we give the complete sets of linear constitutive equations relating elastic and electric fields. For each equation set the numerical values are computed for lithium niobate, the preeminent electrooptic and acoustooptic material, from the measured [cE], [e], and [(eps)S] values of Smith and Welsh (Ref.1). Coupling to the thermal field is neglected. Rationalized mks units are used throughout.

CONSTITUTIVE EQUATION SETS

Symbols and units for the quantities employed are given in Table 1. In terms of these, six constitutive equation sets are used. Of these, electric intensity, dielectric displacement, and polarization each appear in two sets as an independent variable. The sets are, in compressed matrix notation, as follows. A prime denotes transpose; [I] is the unit matrix.

I. The Piezoelectric Stress Constant Set

$$[T] = [cE] [S] - [e]' [E] \qquad (1)$$
$$[D] = [e] [S] + [(eps)S] [E] \qquad (2)$$

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TABLE 1. SYMBOLS, UNITS, AND DEFINITIONS.

QUANTITY	UNIT	SYMBOL/DEFINITION
Elastic stress	N/m2	[T]
Elastic strain	-----	[S]
Electric intensity	V/m	[E]
Dielectric displacement	C/m2	[D]
Dielectric polarization	C/m2	[P]
Elastic compliance at constant [E], [D], [P]	m2/N	[cE], [cD], [cP]
Elastic stiffness at constant [E], [D], [P]	N/m2	[sE], [sD], [sP]
Dielectric permittivity at constant [T], [S]	F/m	[(eps)T], [(eps)S]
Dielectric constant, relative, at constant [T], [S]	-----	[(Kr)T], [(Kr)S] =[(eps)T]/(eps)o, [(eps)S]/(eps)o
Dielectric impermeability at constant [T], [S]	m/F	[(bet)T], [(bet)S] =[(eps)T] $^{(-1)}$, [(eps)S] $^{(-1)}$
Dielectric impermeability, relative, at constant [T], [S]	-----	[(betr)T], [(betr)S] =[(bet)T]*(eps)o, [(bet)S]*(eps)o =[(Kr)T] $^{(-1)}$, [(Kr)S] $^{(-1)}$
Dielectric susceptibility at constant [T], [S]	F/m	[(chi)T], [(chi)S] =[(Kr)T-I]*(eps)o, [(Kr)S-I]*(eps)o
Dielectric susceptibility, relative, at constant [T], [S]	-----	[(chir)T], [(chir)S] =[(chi)T]/(eps)o, [(chi)S]/(eps)o
Reciprocal dielectric susceptibility at constant [T], [S]	m/F	[(zet)T], [(zet)S] =[(chi)T] $^{(-1)}$, [(chi)S] $^{(-1)}$
Reciprocal dielectric susceptibility, relative, at constant [T], [S]	-----	[(zetr)T], [(zetr)S] =[(zet)T]*(eps)o, [(zet)S]*(eps)o
Piezoelectric stress constant	C/m2	[e]

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TABLE 1. SYMBOLS, UNITS, AND DEFINITIONS. (continued)
==
         QUANTITY   UNIT   SYMBOL/DEFINITION
==

Piezoelectric strain   m/V = C/N   [d]
coefficient

Piezoelectric stress   N/C = V/m   [h]
modulus

Piezoelectric strain   m2/C   [g]
constant

Piezoelectric polarization   V/m = N/C   [a]
modulus

Piezoelectric polarization   m2/C   [b]
constant
==

Note: Square brackets, sic: [ ], denote matrices.

II. The Piezoelectric Strain Coefficient Set

$$[S] = [sE] [T] + [d]' [E] \qquad (3)$$
$$[D] = [d] [T] + [(eps)T] [E] \qquad (4)$$

III. The Piezoelectric Stress Modulus Set

$$[T] = [cD] [S] - [h]' [D] \qquad (5)$$
$$[E] = -[h] [S] + [(bet)S] [D] \qquad (6)$$

IV. The Piezoelectric Strain Constant Set

$$[S] = [sD] [T] + [g]' [D] \qquad (7)$$
$$[E] = -[g] [T] + [(bet)T] [D] \qquad (8)$$

V. The Piezoelectric Polarization Modulus Set

$$[T] = [cP] [S] - [a]' [P] \qquad (9)$$
$$[E] = -[a] [S] + [(zet)S] [P] \qquad (10)$$

VI. The Piezoelectric Polarization Constant Set

$$[S] = [sP] [T] + [b]' [P] \qquad (11)$$
$$[E] = -[b] [T] + [(zet)T] [P] \qquad (12)$$

The electric variables are connected by the relation

$$[D] = (eps)o * [E] + [P] \qquad (13)$$

where (eps)o is the permittivity of free space, defined by

$$(eps)o * (mu)o * (c) * (c) = 1 ; \qquad (14)$$

(mu)o is the permeability of free space, equal, by definition, to $4\ PI * 10^{(-7)}$, and (c) is the velocity of light in vacuo and, also by definition, is equal exactly to 2.99792458×10^{8} m/s.

From (13) the expressions for the remaining electric variables associated, respectively, with the six equation sets (1) to (12) may be found:

$$[P] = [e] [S] + [(chi)S] [E] \qquad (15)$$

$$[P] = [d] [T] + [(chi)T] [E] \qquad (16)$$

$$[P] = (eps)o * [h] [S] + [I - (eps)o * (bet)S] [D] \qquad (17)$$

$$[P] = (eps)o * [g] [T] + [I - (eps)o * (bet)T] [D] \qquad (18)$$

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$$[D] \; = \; -(eps)o \; * \; [\;a] \; [S] \; + \; [I \; + \; (eps)o \; * \; (zet)S] \; [P] \qquad (19)$$

$$[D] \; = \; -(eps)o \; * \; [\;b] \; [T] \; + \; [I \; + \; (eps)o \; * \; (zet)T] \; [P] \qquad (20)$$

RELATIONS AMONG MATERIAL CONSTANTS

The material constants are interrelated by the following formulas:

$$[cX] \; [sX] \; = \; [(eps)Y] \; [(bet)Y] \; = \; [I] \qquad (21)$$

$$[(chi)Y] \; [(zet)Y] \; = \; [(\;Kr)Y \; - \; (chir)Y] \; = \; [I] \qquad (22)$$

In (21) and (22), X = E, D, or P and Y = T or S.

$$[cD] \; - \; [cE] \; = \; [h]' \; [e] \; = \; [e]' \; [h]$$

$$= \; [h]' \; [(eps)S] \; [h] \; = \; [e]' \; [(bet)S] \; [e]$$

$$= \; [a]' \; [e \; - \; h \; * \; (eps)o] \; = \; [e \; - \; h \; * \; (eps)o]' \; [a] \qquad (23)$$

$$[cP] \; - \; [cD] \; = \; [h]' \; [a] \; * \; (eps)o \; = \; [a]' \; [h] \; * \; (eps)o$$

$$= \; [h]' \; [(eps)S] \; [(zet)S] \; [h] \; * \; (eps)o$$

$$= \; [a]' \; [(bet)S] \; [(chi)S] \; [a] \; * \; (eps)o$$

$$= \; [a \; - \; h]' \; [e] \; = \; [e]' \; [a \; - \; h] \qquad (24)$$

$$[cP] \; - \; [cE] \; = \; [a]' \; [e] \; = \; [e]' \; [a]$$

$$= \; [a]' \; [(chi)S] \; [a] \; = \; [e]' \; [(zet)S] \; [e]$$

$$= \; [h]' \; [e \; + \; a \; * \; (eps)o] \; = \; [e \; + \; a \; * \; (eps)o]' \; [h] \qquad (25)$$

$$[sE] \; - \; [sD] \; = \; [d]' \; [g] \; = \; [g]' \; [d]$$

$$= \; [d]' \; [(bet)t] \; [d] \; = \; [g]' \; [(eps)t] \; [q]$$

$$= \; [b]' \; [d \; - \; g \; * \; (eps)o] \; = \; [d \; - \; g \; * \; (eps)o]' \; [b] \qquad (26)$$

$$[sD] \; - \; [sP] \; = \; [b]' \; [g] \; * \; (eps)o \; = \; [g]' \; [b] \; * \; (eps)o$$

$$= \; [g]' \; [(eps)T] \; [(zet)T] \; [g] \; * \; (eps)o$$

$$= \; [b]' \; [(bet)T] \; [(chi)T] \; [b] \; * \; (eps)o$$

$$= \; [b \; - \; g]' \; [d] \; = \; [d]' \; [b \; - \; g] \qquad (27)$$

$$[sE] \; - \; [sP] \; = \; [b]' \; [d] \; = \; [d]' \; [b]$$

$$= \; [b]' \; [(chi)T] \; [b] \; = \; [d]' \; [(zet)T] \; [d]$$

$$= \; [g]' \; [d \; + \; b \; * \; (eps)o] \; = \; [d \; + \; b \; * \; (eps)o]' \; [g] \qquad (28)$$

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$$[(zet)S] - [(zet)T] = [b] [a]' = [a] [b]'$$
$$= [b] [cP] [b]' = [a] [sP] [a]' \qquad (29)$$
$$[(chi)T] - [(chi)S] = [(eps)T] - [(eps)S]$$
$$= [e] [d]' = [d] [e]'$$
$$= [d] [cE] [d]' = [e] [sE] [e]' \qquad (30)$$
$$[(bet)S] - [(bet)T] = [h] [g]' = [g] [h]'$$
$$= [g] [cD] [g]' = [h] [sD] [h]' \qquad (31)$$
$$[e] = [d] [cE] = [(eps)S] [h] = [(chi)S] [a] \qquad (32)$$
$$[d] = [e] [sE] = [(eps)T] [g] = [(chi)T] [b] \qquad (33)$$
$$[h] = [g] [cD] = [(bet)S] [e] = [(chi)S] [(bet)S] [a]$$
$$= [I - (bet)S * (eps)o] [a] \qquad (34)$$
$$[g] = [h] [sD] = [(bet)T] [d] = [(chi)T] [(bet)T] [b]$$
$$= [I - (bet)T * (eps)o] [b] \qquad (35)$$
$$[a] = [b] [cP] = [(zet)S] [e] = [(eps)S] [(zet)S] [h]$$
$$= [I + (zet)S * (eps)o] [h] \qquad (36)$$
$$[b] = [a] [sP] = [(zet)T] [d] = [(eps)T] [(zet)T] [g]$$
$$= [I + (zet)T * (eps)o] [g] \qquad (37)$$

Some alternative relations are the following:

$$[a - h] = [(zet)S] [h] * (eps)o$$
$$= [(bet)S] [a] * (eps)o \qquad (38)$$
$$[b - g] = [(zet)T] [g] * (eps)o$$
$$= [(bet)T] [b] * (eps)o \qquad (39)$$
$$[e + a * (eps)o] = [(eps)S] [a] \qquad (40)$$
$$[d + b * (eps)o] = [(eps)T] [b] \qquad (41)$$
$$[e - h * (eps)o] = [(chi)S] [h] \qquad (42)$$
$$[d - g * (eps)o] = [(chi)T] [g] \qquad (43)$$

Equations (21) to (43) result from equating like dependent variables pairs selected from equations (1) to (12) and (15) to (20).

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Each pair yields one equation in three variables, one mechanical and two electrical, or vice versa. Two other equations exist, again from (1) to (12) and (15) to (20), that contain the same three variables found in each paired equation. One of these auxiliary equations is used to eliminate one of the two variables of the same kind; the result is one equation in two variables, one electrical and one mechanical. These are now independent variables, so the coefficients must vanish; two relations between the material coefficients result. As an example, (3) and (7) both have [S] as dependent variable. Equating them produces one relation in [T], [E], and [D]; one of the electrical variables must be eliminated. This is done by using either (4) or (8); each contains the same three variables. If (8) is used to eliminate [E], one obtains [sE - d' g - sD] [T] = [d' (bet)T - g'] [D]. Therefore, [sE] - [sD] = [d]' [g] and [g] = [(bet)T] [d]. Use of (4) instead of (8) leads to the equations [sE] - [sD] = [g]' [d] and [d] = [(eps)T] [g]. There are 36 pairs, six each equating [S] and [T], and eight each equating [E], [D], and [P]. The 72 relations contain many redundancies. Relations between the elastic, piezoelectric, and dielectric constants are shown schematically in Tables 2 and 3.

CALCULATION SEQUENCE

Using as input [cE], [e], and [(eps)S], one may compute the remaining quantities in a variety of ways. The following sequence is typical:

$$[sE] = [cE]^{(-1)} \tag{44}$$

$$[(bet)S] = [(eps)S]^{(-1)} \tag{45}$$

$$[d] = [e] [sE] \tag{46}$$

$$[h] = [(bet)S] [e] \tag{47}$$

$$[(eps)T] - [(eps)S] = [e] [d]' \tag{48}$$

$$[(eps)T] = [(eps)S] + [e] [d]' \tag{49}$$

$$[(bet)T] = [(eps)T]^{(-1)} \tag{50}$$

$$[cD] - [cE] = [e]' [h] \tag{51}$$

$$[cD] = [cE] + [e]' [h] \tag{52}$$

$$[g] = [(bet)T] [d] \tag{53}$$

$$[sE] - [sD] = [d]' [g] \tag{54}$$

$$[sD] = [sE] - [d]' [g] \tag{55}$$

$$[(betr)S] = [(bet)S] * (eps)o \tag{56}$$

$$[(zetr)S] = [(betr)S] (I - (betr)S]^{(-1)} \tag{57}$$

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TABLE 2. RELATIONS AMONG MATERIAL CONSTANTS.

$$[d] \xrightarrow{\Delta s^{EP}} [b]$$

$$[d] \xrightarrow{\Delta s^{ED}} [g] \xrightarrow{\frac{\Delta s^{DP}}{\varepsilon_0}} [b]$$

$$[d] \xrightarrow[\Delta \varepsilon = \Delta X]{} [e]$$

$$[g] \xrightarrow{\Delta \beta} [h]$$

$$[e] \xrightarrow{\Delta c^{DE}} [h] \xrightarrow{\frac{\Delta c^{PD}}{\varepsilon_0}} [a]$$

$$[e] \xrightarrow{\Delta c^{PE}} [a]$$

$$[b] \xrightarrow{\Delta \xi} [a]$$

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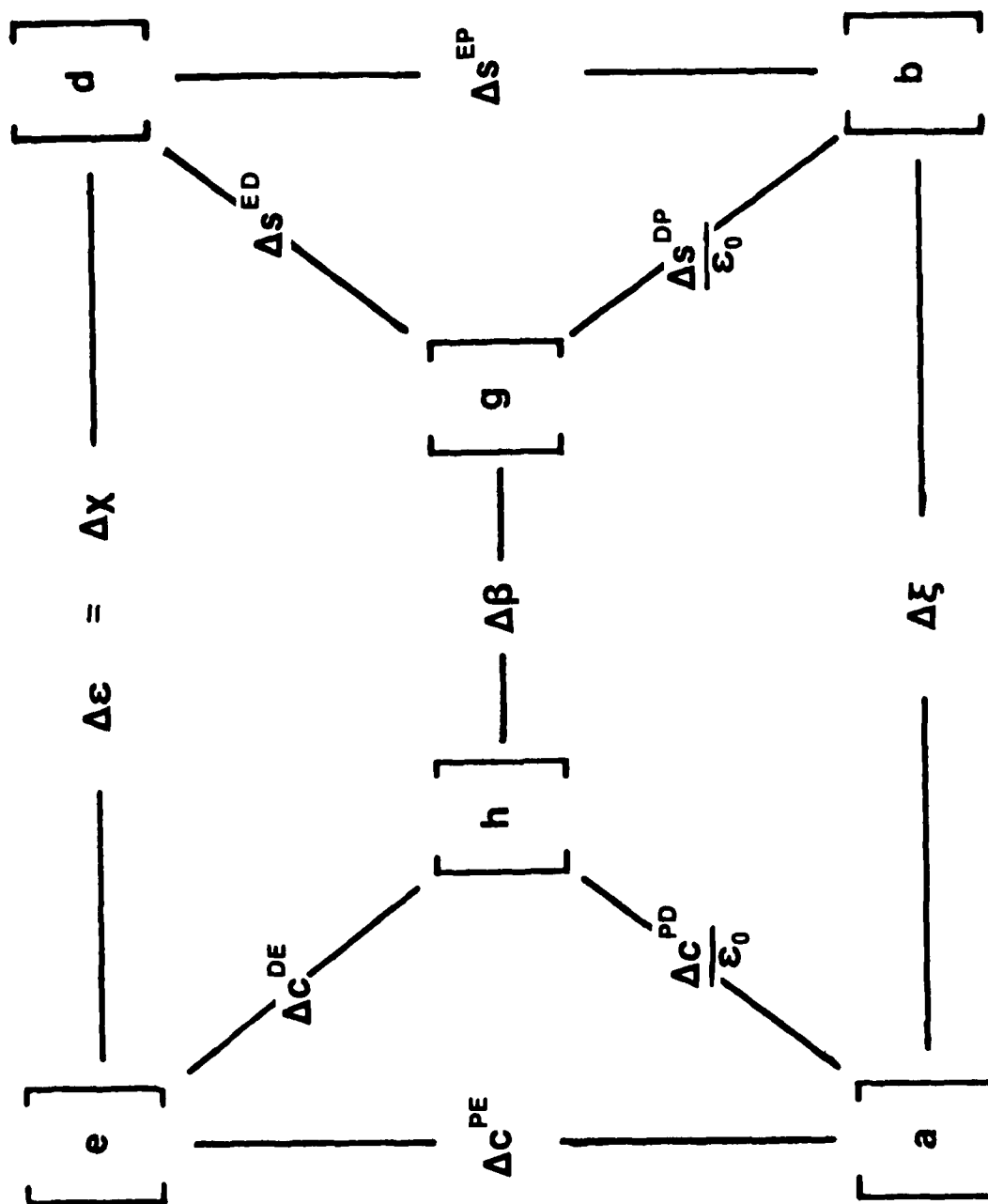
TABLE 3. FURTHER RELATIONS AMONG MATERIAL CONSTANTS.
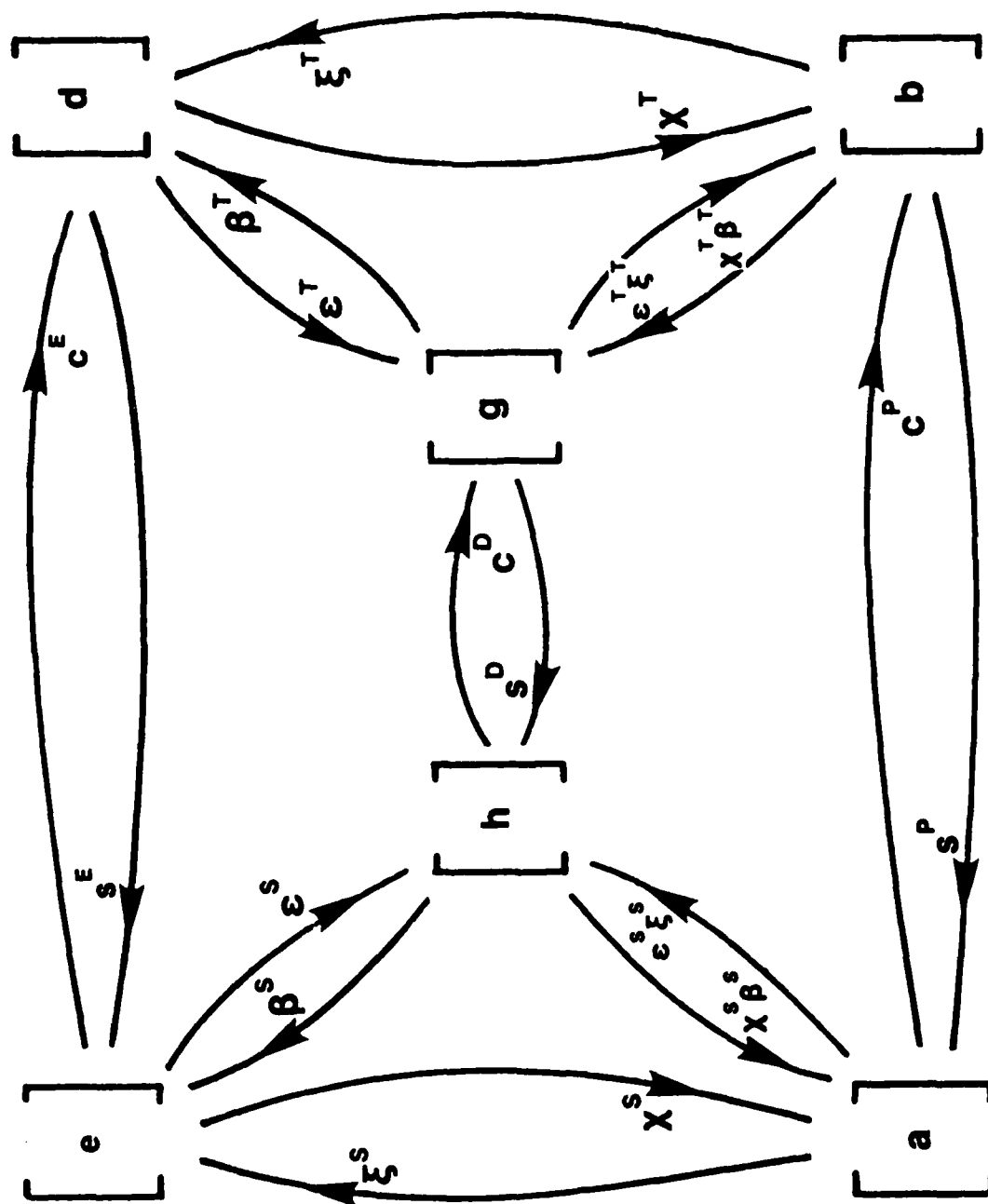
$$[(zet)S] = [(zetr)] / (eps)o \tag{58}$$

$$[(betr)T] = [(bet)T] * (eps)o \tag{59}$$

$$[(zetr)T] = [(betrT] [I - (betr)T]^{(-1)} \tag{60}$$

$$[(zet)T = [(zetr)T] / (eps)o \tag{61}$$

$$[(chi)S] = [(zet)S]^{(-1)} \tag{62}$$

$$[(chi)T] = [(zet)T]^{(-1)} \tag{63}$$

$$[a] = [(zet)S] [e] \tag{64}$$

$$[b] = [(zet)T] [d] \tag{65}$$

$$[cP] - [cE] = [e]' [a] \tag{66}$$

$$[cP] = [cE] + [e]' [a] \tag{67}$$

$$[cP] - [cD] = [a]' [h] * (eps)o \tag{68}$$

$$[sE] - [sP] = [d]' [b] \tag{69}$$

$$[sP] = [sE] - [d]' [b] \tag{70}$$

$$[sD] - [sP] = [g]' [b] * (eps)o \tag{71}$$

$$[(bet)S] - [(bet)T] = [h] [g]' \tag{72}$$

$$[(chi)T] - [(chi)S] = [(eps)T] - [(eps)S] \tag{73}$$

$$[(zet)S] - [(zet)T] = [a] [b]' \tag{74}$$

A number of these relations are used as checks. For example,
[(bet)S] and [(bet)T] are known from (45) and (50), but the differ-
ence is recomputed in (72).

EXPLICIT FORMULAS FOR POINT GROUP 3m

Elastic:

The 6x6 elastic constant portions of Tables 4 and 5 partition into
4x4 and 2x2 submatrices. The 4x4 elastic stiffness and compliance
submatrices are interrelated by formulas (75) to (93), taken from
Cady (Ref. 2):

$$A = s33 * (s11 + s12) - 2 * s13 * s13 \tag{75}$$

$$B = s44 * (s11 - s12) - 2 * s14 * s14 \tag{76}$$

$$2 * c11 = s33 / A + s44 / B \tag{77}$$

$$2 * c12 = s33 / A - s44 / B \tag{78}$$

TABLE 4. ELASTOPIEZODIELECTRIC MATRICES FOR POINT GROUP 3m: THE [e], [h], AND [a] SETS.

==

11	12	13	14	00	00	]	00	-22	31	
12	11	13	-14	00	00	]	00	22	31	cE] e'
13	13	33	00	00	00	]	00	00	33	----]----- e](eps)S
14	-14	00	44	00	00	]	00	15	00	
00	00	00	00	44	14	]	15	00	00	cD] h' ----]-----
00	00	00	00	14	66	]	-22	00	00	h](bet)S
00	00	00	00	15	-22	]	11	00	00	
-22	22	00	15	00	00	]	00	11	00	cP] a' ----]-----
31	31	33	00	00	00	]	00	00	33	a](zet)S

$$66 = (11 - 12) / 2$$

==

Matrix entries show only subscripts.

TABLE 5. ELASTOPIEZODIELECTRIC MATRICES FOR POINT GROUP 3m: THE [d], [g], AND [b] SETS.

==

11	12	13	14	00	00	]	00	-22	31	
12	11	13	-14	00	00	]	00	22	31	sE] d' ----]------
13	13	33	00	00	00	]	00	00	33	d](eps)T
14	-14	00	44	00	00	]	00	15	00	
00	00	00	00	44	14*2	]	15	00	00	sD] g' ----]------
00	00	00	00	14*2	66	]	-22*2	00	00	g](bet)T
00	00	00	00	15	-22*2	]	11	00	00	
-22	22	00	15	00	00	]	00	11	00	sP] b' ----]------
31	31	33	00	00	00	]	00	00	33	b](zet)T

$$66 = (11 - 12) * 2$$

==

Matrix elements show only subscripts.

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$$c13 = - s13 / A \quad ; \quad c14 = - s14 / B \qquad \text{(79a), (79b)} \qquad (79)$$

$$c33 = (s11 + s12) / A \qquad (80)$$

$$c44 = (s11 - s12) / B \qquad (81)$$

$$c66 = (c11 - c12) / 2 = s44 / (2 * B) \qquad (82)$$

$$K = c33 * (c11 + c12) - 2 * c13 * c13 \qquad (83)$$

$$L = c44 * (c11 - c12) - 2 * c14 * c14 \qquad (84)$$

$$2 * s11 = c33 / K + c44 / L \qquad (85)$$

$$2 * s12 = c33 / K - c44 / L \qquad (86)$$

$$s13 = - c13 / K \quad ; \quad s14 = - c14 / L \qquad \text{(87a), (87b)} \qquad (87)$$

$$s33 = (c11 + c12) / K \qquad (88)$$

$$s44 = (c11 - c12) / L \qquad (89)$$

$$s66 = (s11 - s12) = 2 * c44 / L \qquad (90)$$

$$\det (4x4) [s] = A * B \qquad (91)$$

$$\det (4x4) [c] = K * L \qquad (92)$$

$$A * K = B * L = A * B * K * L = 1 \qquad (93)$$

Formulas (75) to (93) hold for each set of constant electrical conditions: either E, D, or P constant.

$$[cD] - [cE] = [del \ cDE] = [e]' \ [h] = [h]' \ [e] \qquad (23)$$

$$del \ cDE11 = + e22 \ h22 + e31 \ h31 \qquad (94)$$

$$del \ cDE12 = - e22 \ h22 + e31 \ h31 \qquad (95)$$

$$del \ cDE13 = + e31 \ h33 = + h31 \ e33 \qquad (96)$$

$$del \ cDE14 = - e22 \ h15 = - h22 \ e15 \qquad (97)$$

$$del \ cDE33 = + e33 \ h33 \qquad (98)$$

$$del \ cDE44 = + e15 \ h15 \qquad (99)$$

$$del \ cDE66 = + e22 \ h22 \qquad (100)$$

$$[cP] - [cD] = [del \ cPD] = [a]' \ [h] * (eps)o$$
$$= [h]' \ [a] * (eps)o \qquad (24)$$

$$\text{del } cPD11 = (+ a22\ h22 + a31\ h31) * (eps)o \tag{101}$$

$$\text{del } cPD12 = (- a22\ h22 + a31\ h31) * (eps)o \tag{102}$$

$$\text{del } cPD13 = (+ a31\ h33) * (eps)o$$

$$= (+ h31\ a33) * (eps)o \tag{103}$$

$$\text{del } cPD14 = (- a22\ h15) * (eps)o$$

$$= (- h22\ a15) * (eps)o \tag{104}$$

$$\text{del } cPD33 = (+ a33\ h33) * (eps)o \tag{105}$$

$$\text{del } cPD44 = (+ a15\ h15) * (eps)o \tag{106}$$

$$\text{del } cPD66 = (+ a22\ h22) * (eps)o \tag{107}$$

$$[cP] - [cE] = [\text{del } cPE] = [e]'\ [a] = [a]'\ [e] \tag{25}$$

$$\text{del } cPE11 = + e22\ a22 + e31\ a31 \tag{108}$$

$$\text{del } cPE12 = - e22\ a22 + e31\ a31 \tag{109}$$

$$\text{del } cPE13 = + e31\ a33 = + a31\ e33 \tag{110}$$

$$\text{del } cPE14 = - e22\ a15 = - a22\ e15 \tag{111}$$

$$\text{del } cPE33 = + e33\ a33 \tag{112}$$

$$\text{del } cPE44 = + e15\ a15 \tag{113}$$

$$\text{del } cPE66 = + e22\ a22 \tag{114}$$

From the del c13 entries we have the ratios

$$e31\ /\ e33 = h31\ /\ h33 = a31\ /\ a33. \tag{115}$$

From the del c14 entries we have the further ratios

$$e15\ /\ e22 = h15\ /\ h22 = a15\ /\ a22. \tag{116}$$

$$[sE] - [sD] = [\text{del } sED] = [d]'\ [g] = [g]'\ [d] \tag{26}$$

$$\text{del } sED11 = + d22\ g22 + d31\ g31 \tag{117}$$

$$\text{del } sED12 = - d22\ g22 + d31\ g31 \tag{118}$$

$$\text{del } sED13 = + d31\ g33 = + g31\ d33 \tag{119}$$

$$\text{del } sED14 = - d22\ g15 = - g22\ d15 \tag{120}$$

$$\text{del } sED33 = + d33\ g33 \tag{121}$$

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$$\text{del sED44} = + \text{d15 g15} \tag{122}$$

$$\text{del sED66} = + \text{d22 g22} * 4 \tag{123}$$

$$[\text{sD}] - [\text{sP}] = [\text{g}]' \, [\text{b}] * (\text{eps})\text{o}$$

$$= [\text{b}]' \, [\text{g}] * (\text{eps})\text{o} \tag{27}$$

$$\text{del sDP11} = (+ \text{g22 b22} + \text{g31 b31}) * (\text{eps})\text{o} \tag{124}$$

$$\text{del sDP12} = (- \text{g22 b22} + \text{g31 b31}) * (\text{eps})\text{o} \tag{125}$$

$$\text{del sDP13} = (+ \text{g31 b33}) * (\text{eps})\text{o}$$

$$= (+ \text{b31 g33}) * (\text{eps})\text{o} \tag{126}$$

$$\text{del sDP14} = (- \text{g22 b15}) * (\text{eps})\text{o}$$

$$= (- \text{b22 g15}) * (\text{eps})\text{o} \tag{127}$$

$$\text{del sDP33} = (+ \text{g33 b33}) * (\text{eps})\text{o} \tag{128}$$

$$\text{del sDP44} = (+ \text{g15 b15}) * (\text{eps})\text{o} \tag{129}$$

$$\text{del sDP66} = (+ \text{g22 b22}) * 4 * (\text{eps})\text{o} \tag{130}$$

$$[\text{sE}] - [\text{sP}] = [\text{del sEP}] = [\text{b}]' \, [\text{d}] = [\text{d}]' \, [\text{b}] \tag{28}$$

$$\text{del sEP11} = + \text{d22 b22} + \text{d31 b31} \tag{131}$$

$$\text{del sEP12} = - \text{d22 b22} + \text{d31 b31} \tag{132}$$

$$\text{del sEP13} = + \text{d31 b33} = + \text{b31 d33} \tag{133}$$

$$\text{del sEP14} = - \text{d22 b15} = - \text{b22 d15} \tag{134}$$

$$\text{del sEP33} = + \text{d33 b33} \tag{135}$$

$$\text{del sEP44} = + \text{d15 b15} \tag{136}$$

$$\text{del sEP66} = + \text{d22 b22} * 4 \tag{137}$$

From the del s13 entries we have the ratios

$$\text{d31} / \text{d33} = \text{g31} / \text{g33} = \text{b31} / \text{b33.} \tag{138}$$

From the del s14 entries we have the further ratios

$$\text{d15} / \text{d22} = \text{g15} / \text{g22} = \text{b15} / \text{b22.} \tag{139}$$

Piezoelectric:

$$[\text{d}] = [\text{e}] \, [\text{sE}] \tag{33}$$

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$$d15 = + e15\ sE44 - e22\ sE14 * 2 \tag{140}$$

$$d22 = + e22\ (sE11 - sE12) - e15\ sE14 \tag{141}$$

$$d31 = + e31\ (sE11 + sE12) + e33\ sE13 \tag{142}$$

$$d33 = + e33\ sE33 + e13\ sE13 * 2 \tag{143}$$

$$[h] = [(bet)S]\ [e] \tag{34}$$

$$h15 = (bet)S11\ e15 \tag{144}$$

$$h22 = (bet)S11\ e22 \tag{145}$$

$$h31 = (bet)S33\ e31 \tag{146}$$

$$h33 = (bet)S33\ e33 \tag{147}$$

$$[g] = [(bet)T]\ [d] \tag{35}$$

$$g15 = (bet)T11\ d15 \tag{148}$$

$$g22 = (bet)T11\ d22 \tag{149}$$

$$g31 = (bet)T33\ d31 \tag{150}$$

$$g33 = (bet)T33\ d33 \tag{151}$$

$$[a] = [(zet)S]\ [e] \tag{36}$$

$$a15 = (zet)S11\ e15 \tag{152}$$

$$a22 = (zet)S11\ e22 \tag{153}$$

$$a31 = (zet)S33\ e31 \tag{154}$$

$$a33 = (zet)S33\ e31 \tag{155}$$

$$[b] = [(zet)T]\ [d] \tag{37}$$

$$b15 = (zet)T11\ d15 \tag{156}$$

$$b22 = (zet)T11\ d22 \tag{157}$$

$$b31 = (zet)T33\ d31 \tag{158}$$

$$b33 = (zet)T33\ d33 \tag{159}$$

Dielectric:

$$[(bet)Y] = [(eps)Y]^{(-1)} \tag{21}$$

$$(bet)Y11 = 1\ /\ (eps)Y11 \tag{160}$$

$$(bet)Y33 = 1\ /\ (eps)Y33 \tag{161}$$

15

$$[(zetr)Y] = [(betr)Y] \; [I - (betr)Y]^{(-1)} \tag{162}$$

$$(zet)Y11 = 1 \; / \; ((eps)Y11 - (eps)o) \tag{163}$$

$$(zet)Y33 = 1 \; / \; ((eps)Y33 - (eps)o) \tag{164}$$

$$[(eps)T - (eps)S] = [del \; (eps)] = [e] \; [d]' =$$

$$[(chi)T - (chi)S] = [del \; (chi)] = [d] \; [e]' \tag{30}$$

$$del \; (eps)11 = del \; (chi)11 = \; + e15 \; d15 + e22 \; d22 * 2 \tag{165}$$

$$del \; (eps)33 = del \; (chi)33 = \; + e33 \; d33 + e31 \; d31 * 2 \tag{166}$$

$$[(bet)S - (bet)T] = [h] \; [g]' = [g] \; [h]' \tag{31}$$

$$del \; (bet)11 = + h15 \; g15 + h22 \; g22 * 2 \tag{167}$$

$$del \; (bet)33 = + h33 \; g33 + h31 \; g31 * 2 \tag{168}$$

$$[(zet)S - (zet)T] = [del \; (zet)] = [a] \; [b]' = [b] \; [a]' \tag{169}$$

$$del \; (zet)11 = + a15 \; b15 + a22 \; b22 * 2 \tag{170}$$

$$del \; (zet)33 = + a33 \; b33 + a31 \; b31 * 2 \tag{171}$$

PIEZOELECTRIC CONSTANT DETERMINATIONS

Determinations of the [e], [d], [h], and [g] values for lithium niobate have been made by various investigators. The most consistent of these are shown in Tables 6, 7, 8, and 9 for comparison purposes.

TABLE 6. PIEZOELECTRIC STRESS CONSTANT [e].

e15	e22	e31	e33	T(OC)	Ref
3.7	2.5	0.2	1.3	RT	(3)
3.60	2.52	0.747	1.67	RT	(4)
3.76	2.43	0.23	1.33	25	(1)
3.8	2.5	0.35	1.42	20	(5)
3.83	2.37		1.80	RT	(6)
3.61	2.40	0.28	1.59	RT	(7)

Estimated inaccuracies: e15, e22: 3% ; e31: 60% ; e33: 15%.
Units: C/m^2.

TABLE 7. PIEZOELECTRIC STRAIN COEFFICIENT [d].

d15	d22	d31	d33	T(OC)	Ref
74.0	20.8	−0.863	16.2	20	(8)
68.	21.	−1.	6.	RT	(3)
64.3	20.6	+1.15	6.53	RT	(4)
69.2	20.8	−0.85	6.0	25	(1)
68.9	20.9	+0.003	5.8	20	(5)
65.36	20.29	−1.22	8.27	RT	(7)

Units: $10^{(-12)}$ C/N.

TABLE 8. PIEZOELECTRIC STRESS MODULUS [h].

h15	h22	h31	h33	T(OC)	Ref
9.5	6.4	0.8	5.1	RT	(3)
9.04	6.33	3.07	6.86	RT	(4)
9.59	6.20	0.93	5.38	25	(1)
9.2	6.1	1.3	5.87	20	(5)
9.16	6.09	1.2	6.88	RT	(7)

Units: $10^{(9)}$ N/C

TABLE 9.   PIEZOELECTRIC STRAIN CONSTANT [g].

==

g15	g22	g31	g33	T(OC)	Ref
91.	28.	-4.	23.	RT	(3)
87.7	28.1	+4.79	24.4	RT	(4)
91.8	27.6	-3.3	23.6	25	(1)
92.5	28.1	+0.01	23.5	20	(5)
89.5	27.8	-4.87	33.0	RT	(7)

Units: $10^{(-3)}$ m2/C.

==

INPUT VALUES FOR LI NB 03

The values measured by Smith and Welsh (Ref. 1) using the pulse-echo (transit-time) technique are as follows:

TABLE 10.   ISAGRIC ELASTIC STIFFNESSES.

==

cE11	cE12	cE13	cE14	cE33	cE44	cE66
203.0	57.4*	75.2	8.5	242.4	59.5	72.8

Units: $10^{(9)}$ N/m2.

==

* The value of 57.3 appearing in Ref. (1) has been changed so
  that the relation c66 = (c11 - c12)/2 holds; c11 and c66 are
  directly measured and hence are more accurately known than
  c12.

TABLE 11.   PIEZOELECTRIC STRESS CONSTANTS.

==

e15	e22	e31	e33
3.76	2.43	0.23	1.33

Units: C/m2.

==

TABLE 12.   DIELECTRIC PERMITTIVITIES AT CONSTANT STRAIN.
===
(eps)S11   (eps)S33
===

   392.   247.

Units: $10^{(-12)}$ F/m.
===

OUTPUT VALUES FOR LI NB 03

The input values from Tables 10, 11, and 12 were used to compute
the remaining elastic, piezoelectric, and dielectric quantities for
lithium niobate in the manner discussed in prior sections of this
report.   The results are given in Tables 13 to 20.

TABLE 13.   ELASTIC STIFFNESSES.
===
	cE	cD	cP	del cDE	del cPE	del cPD
11	203.0	218.3	218.6	15.3	15.6	0.356
12	57.4 *	42.6	42.2	-14.8	-15.2	-0.340
13	75.2	76.4	76.5	1.24	1.28	0.0460
14	8.5	-14.8	-15.3	-23.3	-23.8	-0.539
33	242.4	249.6	249.8	7.16	7.43	0.266
44	59.5	95.6	96.4	36.1	36.9	0.833
66	72.8	87.9	88.2	15.1	15.4	0.348

Units: $10^{(9)}$ N/m2.
===
* The value of 57.3 appearing in Ref. (1) has been changed so
  that the relation c66 = (c11 - c12)/2 holds; c11 and c66 are
  directly measured and hence are more accurately known than
  c12.

TABLE 14.   ELASTIC COMPLIANCES.
===
	sE	sD	sP	del sED	del sEP	del sDP
11	5.83	5.26	5.25	0.574	0.580	0.00690
12	-1.15	-0.585	-0.579	0.568	-0.575	-0.00690
13	-1.45	-1.43	-1.43	0.0202	-0.0209	-0.000727
14	-0.998	0.905	0.928	1.90	-1.93	-0.0227
33	5.03	4.88	4.88	0.142	0.147	0.00512
44	17.09	10.74	10.67	6.35	6.42	0.0756
66	13.97	11.69	11.66	2.28	2.31	0.0272

Units: $10^{(-12)}$ m2/N.
===

TABLE 15.   PIEZOELECTRIC [e], [h], AND [a] VALUES.
==
                    e   h   a
==

15   3.76   9.59   9.81
22   2.43   6.20   6.34
31   0.23   0.931   0.966
33   1.33   5.38   5.58

Units: e: C/m2; h and a: $10^{(9)}$ V/m.
==

TABLE 16.   PIEZOELECTRIC [d], [g], AND [b] VALUES.
==
                    d   g   b
==

15   69.1   91.8   92.9
22   20.7   27.5   27.9
31   -0.854   -3.36   -3.48
33   6.02   23.6   24.5

Units: d: $10^{(-12)}$ m/V; g and b: $10^{(-3)}$ m2/C.
==

TABLE 17.   DIELECTRIC (eps) VALUES.
==
                 (eps)S   (eps)T   del (eps)TS
==

11   392.0   752.6   360.6
33   247.0   254.6   7.61

Units: $10^{(-12)}$ F/m.
==
del (eps)TS = del (chi)TS

TABLE 18.   DIELECTRIC (chi) VALUES.
==
                 (chi)S   (chi)T   del (chi)TS
==

11   383.1   743.7   360.6
33   238.1   245.8   7.61

Units: $10^{(-12)}$ F/m.
==
del (chi)TS = del (eps)TS

TABLE 19. DIELECTRIC (bet) VALUES.

	(bet)S	(bet)T	del (bet)TS
11	2.551	1.329	-1.222
33	4.049	3.928	-0.121

Units: $10^{(9)}$ m/F.

TABLE 20. DIELECTRIC (zet) VALUES.

	(zet)S	(zet)T	del (zet)TS
11	2.610	1.345	-1.265
33	4.199	4.069	-0.130

Units: $10^{(9)}$ m/F.

CONCLUSIONS

This report provides formulas interrelating the coefficients that appear in the several alternative sets of constitutive equations involving the elastic, piezoelectric, and dielectric properties of crystals. These are then specialized for crystals of class 3m; using measured values reported for lithium niobate, numerical values of the elements of the polarization matrices are calculated.

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