POLARIZATION MATRICES OF LITHIUM NIOBATE

Arthur Ballato
ELECTRONICS TECHNOLOGY AND DEVICES LABORATORY

April 1989

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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.

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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 isagic elastic stiffnesses \([cE]\), the piezoelectric stress constants \([e]\), and the dielectric permittivities at constant strain \([(\varepsilon)S]\).

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 \([(\varepsilon)S]\) 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 \([(\varepsilon)S]\) 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

\[
[T] = [cE] [S] - [e]' [E] \tag{1}
\]

\[
[D] = [e] [S] + [(\varepsilon)S] [E] \tag{2}
\]
<table>
<thead>
<tr>
<th>QUANTITY</th>
<th>UNIT</th>
<th>SYMBOL/DEFINITION</th>
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<tbody>
<tr>
<td>Elastic stress</td>
<td>N/m²</td>
<td>[T]</td>
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<tr>
<td>Elastic strain</td>
<td>-----</td>
<td>[S]</td>
</tr>
<tr>
<td>Electric intensity</td>
<td>V/m</td>
<td>[E]</td>
</tr>
<tr>
<td>Dielectric displacement</td>
<td>C/m²</td>
<td>[D]</td>
</tr>
<tr>
<td>Dielectric polarization</td>
<td>C/m²</td>
<td>[P]</td>
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<tr>
<td>Elastic compliance at constant</td>
<td>m²/N</td>
<td>[cE], [cD], [cP]</td>
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<tr>
<td>constant [E], [D], [P]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Elastic stiffness at constant</td>
<td>N/m²</td>
<td>[sE], [sD], [sP]</td>
</tr>
<tr>
<td>constant [E], [D], [P]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dielectric permittivity at constant</td>
<td>F/m</td>
<td>[(eps)T], [(eps)S]</td>
</tr>
<tr>
<td>[T], [S]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dielectric constant, relative, at</td>
<td>-----</td>
<td>[(Kr)T], [(Kr)S]</td>
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<tr>
<td>constant [T], [S]</td>
<td></td>
<td>=[(eps)T]/(eps)₀,</td>
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<td></td>
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<td>[(eps)S]/(eps)₀</td>
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<tr>
<td>Dielectric impermeability at constant</td>
<td>m/F</td>
<td>[(bet)T], [(bet)S]</td>
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<tr>
<td>[T], [S]</td>
<td></td>
<td>=<a href="-1">(eps)T</a>,</td>
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<td></td>
<td></td>
<td><a href="-1">(eps)S</a>'</td>
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<tr>
<td>Dielectric impermeability, relative,</td>
<td>-----</td>
<td>[(betr)T], [(betr)S]</td>
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<tr>
<td>at constant [T], [S]</td>
<td></td>
<td>=[(bet)T]*[(eps)₀,</td>
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<tr>
<td></td>
<td></td>
<td><a href="-1">(Kr)S</a>'</td>
</tr>
<tr>
<td>Dielectric susceptibility at constant</td>
<td>F/m</td>
<td>[(chi)T], [(chi)S]</td>
</tr>
<tr>
<td>[T], [S]</td>
<td></td>
<td>=[(Kr)T-I]*[(eps)₀,</td>
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<tr>
<td></td>
<td></td>
<td>[(Kr)S-I]*[(eps)₀</td>
</tr>
<tr>
<td>Dielectric susceptibility, relative,</td>
<td>-----</td>
<td>[(chir)T], [(chir)S]</td>
</tr>
<tr>
<td>at constant [T], [S]</td>
<td></td>
<td>=[(chi)T]/[(eps)₀,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[(chi)S]/[(eps)₀</td>
</tr>
<tr>
<td>Reciprocal dielectric susceptibility</td>
<td>m/F</td>
<td>[(zet)T], [(zet)S]</td>
</tr>
<tr>
<td>at constant [T], [S]</td>
<td></td>
<td>=<a href="-1">(chi)T</a>,</td>
</tr>
<tr>
<td></td>
<td></td>
<td><a href="-1">(chi)S</a>'</td>
</tr>
<tr>
<td>Reciprocal dielectric susceptibility</td>
<td>-----</td>
<td>[(zet)T], [(zet)S]</td>
</tr>
<tr>
<td>relative, at constant [T], [S]</td>
<td></td>
<td>=[(zet)T]*[(eps)₀,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[(zet)S]*[(eps)₀</td>
</tr>
<tr>
<td>Piezoelectric stress constant</td>
<td>C/m²</td>
<td>[e]</td>
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TABLE 1. SYMBOLS, UNITS, AND DEFINITIONS. (continued)

<table>
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<tr>
<th>QUANTITY</th>
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<tr>
<td>Piezoelectric strain coefficient</td>
<td>m/V = C/N</td>
<td>[d]</td>
</tr>
<tr>
<td>Piezoelectric stress modulus</td>
<td>N/C = V/m</td>
<td>[h]</td>
</tr>
<tr>
<td>Piezoelectric strain constant</td>
<td>m²/C</td>
<td>[g]</td>
</tr>
<tr>
<td>Piezoelectric polarization modulus</td>
<td>V/m = N/C</td>
<td>[a]</td>
</tr>
<tr>
<td>Piezoelectric polarization constant</td>
<td>m²/C</td>
<td>[b]</td>
</tr>
</tbody>
</table>

Note: Square brackets, sic: [ ], denote matrices.
II. The Piezoelectric Strain Coefficient Set

\[ [S] = [sE] [T] + [d]' [E] \]  
\[ [D] = [d] [T] + [(\epsilon)T] [E] \]  

III. The Piezoelectric Stress Modulus Set

\[ [T] = [cD] [S] - [h]' [D] \]  
\[ [E] = -[ h] [S] + [(\eta)S] [D] \]  

IV. The Piezoelectric Strain Constant Set

\[ [S] = [sD] [T] + [g]' [D] \]  
\[ [E] = -[ g] [T] + [(\eta)T] [D] \]  

V. The Piezoelectric Polarization Modulus Set

\[ [T] = [cP] [S] - [a]' [P] \]  
\[ [E] = -[ a] [S] + [(\gamma)S] [P] \]  

VI. The Piezoelectric Polarization Constant Set

\[ [S] = [sP] [T] + [b]' [P] \]  
\[ [E] = -[ b] [T] + [(\gamma)T] [P] \]  

The electric variables are connected by the relation

\[ [D] = (\epsilon) \ast [E] + [P] \]  

where \((\epsilon)\) is the permittivity of free space, defined by

\[ (\epsilon) \ast (\mu) \ast (c) \ast (c) = 1 \]  

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

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

\[ [P] = [ e] [S] + [(\chi)S] [E] \]  
\[ [P] = [ d] [T] + [(\chi)T] [E] \] 
\[ [P] = (\epsilon) \ast [ h] [S] + [I - (\epsilon) \ast (\eta)S] [D] \] 
\[ [P] = (\epsilon) \ast [ g] [T] + [I - (\epsilon) \ast (\eta)T] [D] \]
\[ [D] = -(\varepsilon_0) [a] [S] + [I + (\varepsilon_0) (\zeta_S)] [P] \quad (19) \]
\[ [D] = -(\varepsilon_0) [b] [T] + [I + (\varepsilon_0) (\zeta_T)] [P] \quad (20) \]

**RELATIONS AMONG MATERIAL CONSTANTS**

The material constants are interrelated by the following formulas:

\[ [(\chi_X) [s_X] = [(\pi_X) [(\beta_X) = [I] \quad (21) \]
\[ [(\chi_Y) [(\zeta_Y) = [(\chi_T) - (\chi_S)] = [I] \quad (22) \]

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

\[ [c_D] - [c_E] = [h]' [e] = [e]' [h] \]
\[ = [h]' [(\pi_S) [h] = [e]' [(\beta_S) [e] \]
\[ = [a]' [e - h * (\varepsilon_0)] = [e - h * (\varepsilon_0)]' [a] \quad (23) \]

\[ [c_P] - [c_D] = [h]' [a] * (\varepsilon_0) = [a]' [h] * (\varepsilon_0) \]
\[ = [h]' [(\pi_S) [(\zeta_S) [h] * (\varepsilon_0) \]
\[ = [a]' [(\beta_S) [(\chi_S) [a] * (\varepsilon_0) \]
\[ = [a - h]' [e] = [e]' [a - h] \quad (24) \]

\[ [c_P] - [c_E] = [a]' [e] = [e]' [a] \]
\[ = [a]' [(\chi_S) [a] = [e]' [(\zeta_S) [e] \]
\[ = [h]' [e + a * (\varepsilon_0)] = [e + a * (\varepsilon_0)]' [h] \quad (25) \]

\[ [s_E] - [s_D] = [d]' [g] = [g]' [d] \]
\[ = [d]' [(\beta_T) [d] = [g]' [(\pi_T) [g] \]
\[ = [b]' [d - g * (\varepsilon_0)] = [d - g * (\varepsilon_0)]' [b] \quad (26) \]

\[ [s_D] - [s_P] = [b]' [g] * (\varepsilon_0) = [g]' [b] * (\varepsilon_0) \]
\[ = [g]' [(\pi_T) [(\zeta_T) [g] * (\varepsilon_0) \]
\[ = [b]' [(\beta_T) [(\chi_T) [b] * (\varepsilon_0) \]
\[ = [b - g]' [d] = [d]' [b - g] \quad (27) \]

\[ [s_E] - [s_P] = [b]' [d] = [d]' [b] \]
\[ = [b]' [(\chi_T) [b] = [d]' [(\zeta_T) [d] \]
\[ = [g]' [d + b * (\varepsilon_0)] = [d + b * (\varepsilon_0)]' [g] \quad (28) \]
\[(\zeta)S\] - \[(\zeta)T\] = \[b\] \[a]\' = \[a\] \[b]\'  \hspace{1cm} (29)

\[(\chi)T\] - \[(\chi)S\] = \[(\epsilon)T\] - \[(\epsilon)S\]
\hspace{1cm} = \[e\] \[d]\' = \[d\] \[e]\'  \hspace{1cm} (30)

\[(\beta)S\] - \[(\beta)T\] = \[h\] \[g]\' = \[g\] \[h]\'
\hspace{1cm} = \[g\] \[cD\] \[g]\' = \[h\] \[sD\] \[h]\'  \hspace{1cm} (31)

\[e\] = \[d\] \[cE\] = \[(\epsilon)S\] \[h\] = \[(\chi)S\] \[a\]  \hspace{1cm} (32)

\[d\] = \[e\] \[sE\] = \[(\epsilon)T\] \[g\] = \[(\chi)T\] \[b\]  \hspace{1cm} (33)

\[h\] = \[g\] \[cD\] = \[(\beta)S\] \[e\] = \[(\chi)S\] \[(\beta)S\] \[a\]
\hspace{1cm} = \[I - (\beta)S \ast (\epsilon)o\] \[a\]  \hspace{1cm} (34)

\[g\] = \[h\] \[sD\] = \[(\beta)T\] \[d\] = \[(\chi)T\] \[(\beta)T\] \[b\]
\hspace{1cm} = \[I - (\beta)T \ast (\epsilon)o\] \[b\]  \hspace{1cm} (35)

\[a\] = \[b\] \[cP\] = \[(\zeta)S\] \[e\] = \[(\epsilon)S\] \[(\zeta)S\] \[h\]
\hspace{1cm} = \[I + (\zeta)S \ast (\epsilon)o\] \[h\]  \hspace{1cm} (36)

\[b\] = \[a\] \[sP\] = \[(\zeta)T\] \[d\] = \[(\epsilon)T\] \[(\zeta)T\] \[g\]
\hspace{1cm} = \[I + (\zeta)T \ast (\epsilon)o\] \[g\]  \hspace{1cm} (37)

Some alternative relations are the following:

\[a - h\] = \[(\zeta)S\] \[h\] \ast (\epsilon)o
\hspace{1cm} = \[(\beta)S\] \[a]\ast (\epsilon)o  \hspace{1cm} (38)

\[b - g\] = \[(\zeta)T\] \[g]\ast (\epsilon)o
\hspace{1cm} = \[(\beta)T\] \[b]\ast (\epsilon)o  \hspace{1cm} (39)

\[e + a \ast (\epsilon)o\] = \[(\epsilon)S\] \[a\]  \hspace{1cm} (40)

\[d + b \ast (\epsilon)o\] = \[(\epsilon)T\] \[b\]  \hspace{1cm} (41)

\[e - h \ast (\epsilon)o\] = \[(\chi)S\] \[h\]  \hspace{1cm} (42)

\[d - g \ast (\epsilon)o\] = \[(\chi)T\] \[g\]  \hspace{1cm} (43)

Equations (21) to (43) result from equating like dependent variables pairs selected from equations (1) to (12) and (15) to (20).
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 \([\text{sE} - d' g - sD] [T] = [d' (\text{bet}) T - g'] [D]\). Therefore, \([\text{sE}] - [\text{sD}] = [d]' [g] \) and \([g] = [(\text{bet}) T] [d]\). Use of (4) instead of (8) leads to the equations \([\text{sE}] - [\text{sD}] = [g]' [d] \) and \([d] = [(\text{eps}) T] [g]\). 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 \([\text{cE}], [\text{e}], \) and \([(\text{eps}) S]\), one may compute the remaining quantities in a variety of ways. The following sequence is typical:

\[
\begin{align*}
[\text{sE}] &= [\text{cE}] \quad (-1) \\
[(\text{bet}) S] &= [(\text{eps}) S] \quad (-1) \\
[d] &= [\text{e}] [\text{sE}] \\
[h] &= [(\text{bet}) S] [\text{e}] \\
[(\text{eps}) T] - [(\text{eps}) S] &= [\text{e}] [d]' \\
[(\text{eps}) T] &= [(\text{eps}) S] + [\text{e}] [d]' \\
[(\text{bet}) T] &= [(\text{eps}) T] \quad (-1) \\
[\text{cD}] - [\text{cE}] &= [\text{e}]' [h] \\
[\text{cD}] &= [\text{cE}] + [\text{e}]' [h] \\
[g] &= [(\text{bet}) T] [d] \\
[\text{sE}] - [\text{sD}] &= [d]' [g] \\
[\text{sD}] &= [\text{sE}] - [d]' [g] \\
[(\text{betr}) S] &= [(\text{betr}) S] \ast (\text{eps}) o \\
[(\text{zetr}) S] &= [(\text{betr}) S] (I - (\text{betr}) S) \quad (-1)
\end{align*}
\]
TABLE 2. RELATIONS AMONG MATERIAL CONSTANTS.

\[
\begin{align*}
\Delta \varepsilon &= \Delta \chi \\
\Delta \beta &= \frac{\Delta s_{EP}}{\varepsilon_0} \\
\Delta \xi &= \frac{\Delta s_{EP}}{\varepsilon_0} \\
\Delta e &= \Delta \varepsilon \\
\Delta \varepsilon_{Ed} &= \Delta \varepsilon_{Ed} \\
\Delta C_{PD} &= \Delta C_{PD} \\
\end{align*}
\]
TABLE 3. FURTHER RELATIONS AMONG MATERIAL CONSTANTS.
\[
(zet)_S = [(zetr)] / (eps) o \\
(betr)_T = [(bet)T] * (eps) o \\
(zetr)_T = [(betrT) [I - (betr)_T]^{-1} \\
(zet)_T = [(zet)rT] / (eps) o \\
(chi)_S = [(zet)_S]^{-1} \\
(chi)_T = [(zet)_T]^{-1} \\
[a] = [(zet)_S] [e] \\
[b] = [(zet)_T] [d] \\
[cP] - [cE] = [e]' [a] \\
[cP] = [cE] + [e]' [a] \\
[cP] - [cD] = [a]' [h] * (eps) o \\
[sE] - [sP] = [d]' [b] \\
[sP] = [sE] - [d]' [b] \\
[sD] - [sP] = [g]' [b] * (eps) o \\
[(bet)_S] - [(bet)_T] = [h] [g]' \\
[(zet)_S] - [(zet)_T] = [a] [b]' \\
\]

A number of these relations are used as checks. For example, \([(bet)_S]\) and \([(bet)_T]\) are known from (45) and (50), but the difference 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):

\[
A = s33 * (s11 + s12) - 2 * s13 * s13 \\
B = s44 * (s11 - s12) - 2 * s14 * s14 \\
2 * c11 = s33 / A + s44 / B \\
2 * c12 = s33 / A - s44 / B \\
\]

10
TABLE 4. ELASTOPIEZODIELECTRIC MATRICES FOR POINT GROUP 3m:
THE [e], [h], AND [a] SETS.

<p>| | | | | | | | | | | |</p>
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</tbody>
</table>

\[66 = (11 - 12) / 2\]

Matrix entries show only subscripts.

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

<p>| | | | | | | | | | | |</p>
<table>
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</tbody>
</table>

\[66 = (11 - 12) * 2\]

Matrix elements show only subscripts.
\[ c_{13} = -\frac{s_{13}}{A} , \quad c_{14} = -\frac{s_{14}}{B} \] (79a), (79b) (79)
\[ c_{33} = \frac{(s_{11} + s_{12})}{A} \] (80)
\[ c_{44} = \frac{(s_{11} - s_{12})}{B} \] (81)
\[ c_{66} = \frac{(c_{11} - c_{12})}{2} = \frac{s_{44}}{(2B)} \] (82)
\[ K = c_{33} \times (c_{11} + c_{12}) - 2 \times c_{13} \times c_{13} \] (83)
\[ L = c_{44} \times (c_{11} - c_{12}) - 2 \times c_{14} \times c_{14} \] (84)
\[ 2 \times s_{11} = c_{33} / K + c_{44} / L \] (85)
\[ 2 \times s_{12} = c_{33} / K - c_{44} / L \] (86)
\[ s_{13} = -c_{13} / K \; ; \; s_{14} = -c_{14} / L \] (87a), (87b) (87)
\[ s_{33} = \frac{(c_{11} + c_{12})}{K} \] (88)
\[ s_{44} = \frac{(c_{11} - c_{12})}{L} \] (89)
\[ s_{66} = \frac{(s_{11} - s_{12})}{2} = \frac{2 \times c_{44}}{L} \] (90)
\[ \text{det} (4\times4) [s] = A \times B \] (91)
\[ \text{det} (4\times4) [c] = K \times L \] (92)
\[ A \times K = B \times L = A \times B \times K \times L = 1 \] (93)

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

\[ [cD] - [cE] = [\text{del} cDE] = [e]' [h] = [h]' [e] \] (23)
\[ \text{del} cDE_{11} = + e_{22} h_{22} + e_{31} h_{31} \] (94)
\[ \text{del} cDE_{12} = - e_{22} h_{22} + e_{31} h_{31} \] (95)
\[ \text{del} cDE_{13} = + e_{31} h_{33} = + h_{31} e_{33} \] (96)
\[ \text{del} cDE_{14} = - e_{22} h_{15} = - h_{22} e_{15} \] (97)
\[ \text{del} cDE_{33} = + e_{33} h_{33} \] (98)
\[ \text{del} cDE_{44} = + e_{15} h_{15} \] (99)
\[ \text{del} cDE_{66} = + e_{22} h_{22} \] (100)

\[ [cP] - [cD] = [\text{del} cPD] = [a]' [h] \times (\text{eps})o \]
\[ = [h]' [a] \times (\text{eps})o \] (24)
\[ \text{del CPD11} = (a22 h22 + a31 h31) \cdot (\text{eps})^{o} \]  
\[ \text{del CPD12} = (-a22 h22 + a31 h31) \cdot (\text{eps})^{o} \]  
\[ \text{del CPD13} = (a31 h33) \cdot (\text{eps})^{o} \]  
\[ = (h31 a33) \cdot (\text{eps})^{o} \]  
\[ \text{del CPD14} = (-a22 h15) \cdot (\text{eps})^{o} \]  
\[ = (-h22 a15) \cdot (\text{eps})^{o} \]  
\[ \text{del CPD33} = (a33 h33) \cdot (\text{eps})^{o} \]  
\[ \text{del CPD44} = (a15 h15) \cdot (\text{eps})^{o} \]  
\[ \text{del CPD66} = (a22 h22) \cdot (\text{eps})^{o} \]  

\[ [CP] - [CE] = [\text{del CPE}] = [e]' [a] = [a]' [e] \]  
\[ \text{del CPE11} = + e22 a22 + e31 a31 \]  
\[ \text{del CPE12} = - e22 a22 + e31 a31 \]  
\[ \text{del CPE13} = + e31 a33 = + a31 e33 \]  
\[ \text{del CPE14} = - e22 a15 = - a22 e15 \]  
\[ \text{del CPE33} = + e33 a33 \]  
\[ \text{del CPE44} = + a15 a15 \]  
\[ \text{del CPE66} = + e22 a22 \]  

From the del c13 entries we have the ratios
\[ \frac{e31}{e33} = \frac{h31}{h33} = \frac{a31}{a33}. \]  
From the del c14 entries we have the further ratios
\[ \frac{e15}{e22} = \frac{h15}{h22} = \frac{a15}{a22}. \]  

\[ [SE] - [SD] = [\text{del SED}] = [d]' [g] = [g]' [d] \]  
\[ \text{del SED11} = + d22 g22 + d31 g31 \]  
\[ \text{del SED12} = - d22 g22 + d31 g31 \]  
\[ \text{del SED13} = + d31 g33 = + g31 d33 \]  
\[ \text{del SED14} = - d22 g15 = - g22 d15 \]  
\[ \text{del SED33} = + d33 g33 \]
\[ \text{del sED44} = + d_{15} g_{15} \] (122)

\[ \text{del sED66} = + d_{22} g_{22} \times 4 \] (123)

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

\[ = [b]' [g] \times (\text{eps})o \] (27)

\[ \text{del sDP11} = ( + g_{22} b_{22} + g_{31} b_{31} ) \times (\text{eps})o \] (124)

\[ \text{del sDP12} = ( - g_{22} b_{22} + g_{31} b_{31} ) \times (\text{eps})o \] (125)

\[ \text{del sDP13} = ( + g_{31} b_{33} ) \times (\text{eps})o \]

\[ = ( + b_{31} g_{33} ) \times (\text{eps})o \] (126)

\[ \text{del sDP14} = ( - g_{22} b_{15} ) \times (\text{eps})o \]

\[ = ( - b_{22} g_{15} ) \times (\text{eps})o \] (127)

\[ \text{del sDP33} = ( + g_{33} b_{33} ) \times (\text{eps})o \] (128)

\[ \text{del sDP44} = ( + g_{15} b_{15} ) \times (\text{eps})o \] (129)

\[ \text{del sDP66} = ( + g_{22} b_{22} ) \times 4 \times (\text{eps})o \] (130)

\[ [sE] - [sP] = (\text{del sEP}) = [b]' [d] = [d]' [b] \] (28)

\[ \text{del sEP11} = + d_{22} b_{22} + d_{31} b_{31} \] (131)

\[ \text{del sEP12} = - d_{22} b_{22} + d_{31} b_{31} \] (132)

\[ \text{del sEP13} = + d_{31} b_{33} = + b_{31} d_{33} \] (133)

\[ \text{del sEP14} = - d_{22} b_{15} = - b_{22} d_{15} \] (134)

\[ \text{del sEP33} = + d_{33} b_{33} \] (135)

\[ \text{del sEP44} = + d_{15} b_{15} \] (136)

\[ \text{del sEP66} = + d_{22} b_{22} \times 4 \] (137)

From the del s13 entries we have the ratios

\[ d_{31} / d_{33} = g_{31} / g_{33} = b_{31} / b_{33}. \] (138)

From the del s14 entries we have the further ratios

\[ d_{15} / d_{22} = g_{15} / g_{22} = b_{15} / b_{22}. \] (139)

Piezoelectric:

\[ [d] = [e] [sE] \] (33)
\[ d_{15} = + e_{15} \, sE_{44} - e_{22} \, sE_{14} \times 2 \]  
(140)
\[ d_{22} = + e_{22} \, (sE_{11} - sE_{12}) - e_{15} \, sE_{14} \]  
(141)
\[ d_{31} = + e_{31} \, (sE_{11} + sE_{12}) + e_{33} \, sE_{13} \]  
(142)
\[ d_{33} = + e_{33} \, sE_{33} + e_{13} \, sE_{13} \times 2 \]  
(143)

\[ [h] = [(\text{bet})S] \, [e] \]  
(34)
\[ h_{15} = (\text{bet})S_{11} \, e_{15} \]  
(144)
\[ h_{22} = (\text{bet})S_{11} \, e_{22} \]  
(145)
\[ h_{31} = (\text{bet})S_{33} \, e_{31} \]  
(146)
\[ h_{33} = (\text{bet})S_{33} \, e_{33} \]  
(147)

\[ [g] = [(\text{bet})T] \, [d] \]  
(35)
\[ g_{15} = (\text{bet})T_{11} \, d_{15} \]  
(148)
\[ g_{22} = (\text{bet})T_{11} \, d_{22} \]  
(149)
\[ g_{31} = (\text{bet})T_{33} \, d_{31} \]  
(150)
\[ g_{33} = (\text{bet})T_{33} \, d_{33} \]  
(151)

\[ [a] = [(\text{zet})S] \, [e] \]  
(36)
\[ a_{15} = (\text{zet})S_{11} \, e_{15} \]  
(152)
\[ a_{22} = (\text{zet})S_{11} \, e_{22} \]  
(153)
\[ a_{31} = (\text{zet})S_{33} \, e_{31} \]  
(154)
\[ a_{33} = (\text{zet})S_{33} \, e_{31} \]  
(155)

\[ [b] = [(\text{zet})T] \, [d] \]  
(37)
\[ b_{15} = (\text{zet})T_{11} \, d_{15} \]  
(156)
\[ b_{22} = (\text{zet})T_{11} \, d_{22} \]  
(157)
\[ b_{31} = (\text{zet})T_{33} \, d_{31} \]  
(158)
\[ b_{33} = (\text{zet})T_{33} \, d_{33} \]  
(159)

**Dielectric:**

\[ [(\text{bet})Y] = [(\text{eps})Y]^{-1} \]  
(21)
\[ (\text{bet})Y_{11} = 1 / (\text{eps})Y_{11} \]  
(160)
\[ (\text{bet})Y_{33} = 1 / (\text{eps})Y_{33} \]  
(161)
\[ [(zetr)Y] = [(betr)Y] \left[ I - (betr)Y \right]^{-1} \]  
\[ (zet)Y11 = 1 / ((eps)Y11 - (eps)o) \]  
\[ (zet)Y33 = 1 / ((eps)Y33 - (eps)o) \]  

\[ ((eps)T - (eps)S) = [\text{del (eps)}] = [e] [d]' = \]  
\[ ((chi)T - (chi)S) = [\text{del (chi)}] = [d] [e]' \]  
\[ \text{del (eps)11} = \text{del (chi)11} = + e15 d15 + e22 d22 \times 2 \]  
\[ \text{del (eps)33} = \text{del (chi)33} = + e33 d33 + e31 d31 \times 2 \]  
\[ ((bet)S - (bet)T) = [h] [g]' = [g] [h]' \]  
\[ \text{del (bet)11} = + h15 g15 + h22 g22 \times 2 \]  
\[ \text{del (bet)33} = + h33 g33 + h31 g31 \times 2 \]  
\[ ((zet)S - (zet)T) = [\text{del (zet)}] = [a] [b]' = [b] [a]' \]  
\[ \text{del (zet)11} = + a15 b15 + a22 b22 \times 2 \]  
\[ \text{del (zet)33} = + a33 b33 + a31 b31 \times 2 \]
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 \([e]\).

<table>
<thead>
<tr>
<th>(e_{15})</th>
<th>(e_{22})</th>
<th>(e_{31})</th>
<th>(e_{33})</th>
<th>(T(OC))</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.7</td>
<td>2.5</td>
<td>0.2</td>
<td>1.3</td>
<td>RT</td>
<td>(3)</td>
</tr>
<tr>
<td>3.60</td>
<td>2.52</td>
<td>0.747</td>
<td>1.67</td>
<td>RT</td>
<td>(4)</td>
</tr>
<tr>
<td>3.76</td>
<td>2.43</td>
<td>0.23</td>
<td>1.33</td>
<td>25</td>
<td>(1)</td>
</tr>
<tr>
<td>3.8</td>
<td>2.5</td>
<td>0.35</td>
<td>1.42</td>
<td>20</td>
<td>(5)</td>
</tr>
<tr>
<td>3.83</td>
<td>2.37</td>
<td></td>
<td>1.80</td>
<td>RT</td>
<td>(6)</td>
</tr>
<tr>
<td>3.61</td>
<td>2.40</td>
<td>0.28</td>
<td>1.59</td>
<td>RT</td>
<td>(7)</td>
</tr>
</tbody>
</table>

Estimated inaccuracies: \(e_{15}, e_{22}: 3\%; e_{31}: 60\%; e_{33}: 15\%.

Units: \(\text{C/m}^2\).

### TABLE 7. PIEZOELECTRIC STRAIN COEFFICIENT \([d]\).

<table>
<thead>
<tr>
<th>(d_{15})</th>
<th>(d_{22})</th>
<th>(d_{31})</th>
<th>(d_{33})</th>
<th>(T(OC))</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>74.0</td>
<td>20.8</td>
<td>-0.863</td>
<td>16.2</td>
<td>20</td>
<td>(8)</td>
</tr>
<tr>
<td>68.</td>
<td>21.</td>
<td>-1.</td>
<td>6</td>
<td>RT</td>
<td>(3)</td>
</tr>
<tr>
<td>64.3</td>
<td>20.6</td>
<td>+1.15</td>
<td>6.53</td>
<td>RT</td>
<td>(4)</td>
</tr>
<tr>
<td>69.2</td>
<td>20.8</td>
<td>-0.85</td>
<td>6.0</td>
<td>25</td>
<td>(1)</td>
</tr>
<tr>
<td>68.9</td>
<td>20.9</td>
<td>+0.003</td>
<td>5.8</td>
<td>20</td>
<td>(5)</td>
</tr>
<tr>
<td>65.36</td>
<td>20.29</td>
<td>-1.22</td>
<td>8.27</td>
<td>RT</td>
<td>(7)</td>
</tr>
</tbody>
</table>

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

### TABLE 8. PIEZOELECTRIC STRESS MODULUS \([h]\).

<table>
<thead>
<tr>
<th>(h_{15})</th>
<th>(h_{22})</th>
<th>(h_{31})</th>
<th>(h_{33})</th>
<th>(T(OC))</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.5</td>
<td>6.4</td>
<td>0.8</td>
<td>5.1</td>
<td>RT</td>
<td>(3)</td>
</tr>
<tr>
<td>9.04</td>
<td>6.33</td>
<td>3.07</td>
<td>6.86</td>
<td>RT</td>
<td>(4)</td>
</tr>
<tr>
<td>9.59</td>
<td>6.20</td>
<td>0.93</td>
<td>5.38</td>
<td>25</td>
<td>(1)</td>
</tr>
<tr>
<td>9.2</td>
<td>6.1</td>
<td>1.3</td>
<td>5.87</td>
<td>20</td>
<td>(5)</td>
</tr>
<tr>
<td>9.16</td>
<td>6.09</td>
<td>1.2</td>
<td>6.88</td>
<td>RT</td>
<td>(7)</td>
</tr>
</tbody>
</table>

Units: \(10^9 \text{N/C}\)
TABLE 9. PIEZOELECTRIC STRAIN CONSTANT $[g]$.  

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

Units: $10^{-3}$ m$^2$/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.

<table>
<thead>
<tr>
<th>cE11</th>
<th>cE12</th>
<th>cE13</th>
<th>cE14</th>
<th>cE33</th>
<th>cE44</th>
<th>cE66</th>
</tr>
</thead>
<tbody>
<tr>
<td>203.0</td>
<td>57.4</td>
<td>75.2</td>
<td>8.5</td>
<td>242.4</td>
<td>59.5</td>
<td>72.8</td>
</tr>
</tbody>
</table>

Units: $10^9$ N/m$^2$.

* The value of 57.3 appearing in Ref. (1) has been changed so that the relation $c_{66} = (c_{11} - c_{12})/2$ holds; $c_{11}$ and $c_{66}$ are directly measured and hence are more accurately known than $c_{12}$.

TABLE 11. PIEZOELECTRIC STRESS CONSTANTS.

<table>
<thead>
<tr>
<th>e15</th>
<th>e22</th>
<th>e31</th>
<th>e33</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.76</td>
<td>2.43</td>
<td>0.23</td>
<td>1.33</td>
</tr>
</tbody>
</table>

Units: C/m$^2$.
TABLE 12. DIELECTRIC PERMITTIVITIES AT CONSTANT STRAIN.

<table>
<thead>
<tr>
<th>(eps)S11</th>
<th>(eps)S33</th>
</tr>
</thead>
<tbody>
<tr>
<td>392.</td>
<td>247.</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>cE</th>
<th>cD</th>
<th>cP</th>
<th>del cDE</th>
<th>del cPE</th>
<th>del cPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>203.0</td>
<td>218.3</td>
<td>218.6</td>
<td>15.3</td>
<td>15.6</td>
</tr>
<tr>
<td>12</td>
<td>57.4</td>
<td>42.6</td>
<td>42.2</td>
<td>-14.8</td>
<td>-15.2</td>
</tr>
<tr>
<td>13</td>
<td>75.2</td>
<td>76.4</td>
<td>76.5</td>
<td>1.24</td>
<td>1.28</td>
</tr>
<tr>
<td>14</td>
<td>8.5</td>
<td>-14.8</td>
<td>-15.3</td>
<td>-23.3</td>
<td>-23.8</td>
</tr>
<tr>
<td>33</td>
<td>242.4</td>
<td>249.6</td>
<td>249.8</td>
<td>7.16</td>
<td>7.43</td>
</tr>
<tr>
<td>44</td>
<td>59.5</td>
<td>95.6</td>
<td>96.4</td>
<td>36.1</td>
<td>36.9</td>
</tr>
<tr>
<td>66</td>
<td>72.8</td>
<td>87.9</td>
<td>88.2</td>
<td>15.1</td>
<td>15.4</td>
</tr>
</tbody>
</table>

Units: \(10^9\) N/m².

* The value of 57.3 appearing in Ref. (1) has been changed so that the relation \(c_{66} = (c_{11} - c_{12})/2\) holds; \(c_{11}\) and \(c_{66}\) are directly measured and hence are more accurately known than \(c_{12}\).

TABLE 14. ELASTIC COMPLIANCES.

<table>
<thead>
<tr>
<th>sE</th>
<th>sD</th>
<th>sP</th>
<th>del sED</th>
<th>del sEP</th>
<th>del sDP</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>5.83</td>
<td>5.26</td>
<td>5.25</td>
<td>0.574</td>
<td>0.580</td>
</tr>
<tr>
<td>12</td>
<td>-1.15</td>
<td>-0.585</td>
<td>-0.579</td>
<td>0.568</td>
<td>-0.575</td>
</tr>
<tr>
<td>13</td>
<td>-1.45</td>
<td>-1.43</td>
<td>-1.43</td>
<td>0.0202</td>
<td>-0.0209</td>
</tr>
<tr>
<td>14</td>
<td>-0.298</td>
<td>0.905</td>
<td>0.928</td>
<td>1.90</td>
<td>-1.93</td>
</tr>
<tr>
<td>33</td>
<td>5.03</td>
<td>4.88</td>
<td>4.88</td>
<td>0.142</td>
<td>0.147</td>
</tr>
<tr>
<td>44</td>
<td>17.09</td>
<td>10.74</td>
<td>10.67</td>
<td>6.35</td>
<td>6.42</td>
</tr>
<tr>
<td>66</td>
<td>13.97</td>
<td>11.69</td>
<td>11.66</td>
<td>2.28</td>
<td>2.31</td>
</tr>
</tbody>
</table>

Units: \(10^{-12}\) m²/N.
### TABLE 15. PIEZOELECTRIC \([e], [h], \) AND \([a]\) VALUES.

<table>
<thead>
<tr>
<th></th>
<th>(e)</th>
<th>(h)</th>
<th>(a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>3.76</td>
<td>9.59</td>
<td>9.81</td>
</tr>
<tr>
<td>22</td>
<td>2.43</td>
<td>6.20</td>
<td>6.34</td>
</tr>
<tr>
<td>31</td>
<td>0.23</td>
<td>0.931</td>
<td>0.966</td>
</tr>
<tr>
<td>33</td>
<td>1.33</td>
<td>5.38</td>
<td>5.58</td>
</tr>
</tbody>
</table>

Units: \(e\): \(C/m^2\); \(h\) and \(a\): \(10^9 V/m\).

### TABLE 16. PIEZOELECTRIC \([d], [g], \) AND \([b]\) VALUES.

<table>
<thead>
<tr>
<th></th>
<th>(d)</th>
<th>(g)</th>
<th>(b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>69.1</td>
<td>91.8</td>
<td>92.9</td>
</tr>
<tr>
<td>22</td>
<td>20.7</td>
<td>27.5</td>
<td>27.9</td>
</tr>
<tr>
<td>31</td>
<td>-0.854</td>
<td>-3.36</td>
<td>-3.48</td>
</tr>
<tr>
<td>33</td>
<td>6.02</td>
<td>23.6</td>
<td>24.5</td>
</tr>
</tbody>
</table>

Units: \(d\): \(10^{-12} m/V\); \(g\) and \(b\): \(10^{-3} m^2/C\).

### TABLE 17. DIELECTRIC \((\text{eps})\) VALUES.

<table>
<thead>
<tr>
<th></th>
<th>((\text{eps})S)</th>
<th>((\text{eps})T)</th>
<th>(\text{del (eps)TS})</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>392.0</td>
<td>752.6</td>
<td>360.6</td>
</tr>
<tr>
<td>33</td>
<td>247.0</td>
<td>254.6</td>
<td>7.61</td>
</tr>
</tbody>
</table>

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

\(\text{del (eps)TS} = \text{del (chi)TS}\)

### TABLE 18. DIELECTRIC \((\text{chi})\) VALUES.

<table>
<thead>
<tr>
<th></th>
<th>((\text{chi})S)</th>
<th>((\text{chi})T)</th>
<th>(\text{del (chi)TS})</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>383.1</td>
<td>743.7</td>
<td>360.6</td>
</tr>
<tr>
<td>33</td>
<td>238.1</td>
<td>245.8</td>
<td>7.61</td>
</tr>
</tbody>
</table>

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

\(\text{del (chi)TS} = \text{del (eps)TS}\)
TABLE 19. DIELECTRIC (bet) VALUES.

<table>
<thead>
<tr>
<th></th>
<th>(bet)S</th>
<th>(bet)T</th>
<th>del (bet)TS</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>2.551</td>
<td>1.329</td>
<td>-1.222</td>
</tr>
<tr>
<td>33</td>
<td>4.049</td>
<td>3.928</td>
<td>-0.121</td>
</tr>
</tbody>
</table>

Units: $10^9$ m/F.

TABLE 20. DIELECTRIC (zet) VALUES.

<table>
<thead>
<tr>
<th></th>
<th>(zet)S</th>
<th>(zet)T</th>
<th>del (zet)TS</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>2.610</td>
<td>1.345</td>
<td>-1.265</td>
</tr>
<tr>
<td>33</td>
<td>4.199</td>
<td>4.069</td>
<td>-0.130</td>
</tr>
</tbody>
</table>

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.

REFERENCES


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<tr>
<th>Code</th>
<th>Name and Position</th>
<th>Address</th>
<th>Phone</th>
</tr>
</thead>
<tbody>
<tr>
<td>205</td>
<td>Director</td>
<td>Naval Research Laboratory&lt;br&gt;ATTN: CODE 2627&lt;br&gt;Washington, DC 20375-5000</td>
<td>603</td>
</tr>
<tr>
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<td>Cdr, PM JTfusion</td>
<td>1500 Planning Research Drive&lt;br&gt;McLean, VA 22102</td>
<td>607</td>
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<td>524</td>
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<tr>
<td>564</td>
<td>Dir, US Army Signals Warfare Ctr&lt;br&gt;ATTN: AMSEL-SW-OS&lt;br&gt;Vint Hill Farms Station&lt;br&gt;Warrenton, VA 22186-5100</td>
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</tr>
</tbody>
</table>