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propSym: a tool to establish relationships between property constants for material property tensors of any order

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The properties of crystalline materials can be described mathematically by tensors whose components are generally known as property constants. Tabulations of these constants in terms of the independent components are well known for common material properties (*e.g.* elasticity, piezoelectricity *etc.*) aptly described by tensors of lower rank (*e.g.* ranks 2–4). General relationships between constants of higher rank are often unknown and sometimes reported incorrectly. A computer program is developed here to calculate the property constant relationships of a property of any order, represented by a tensor of any rank and point group. Tensors up to rank 12, *e.g.* the tensor of sixth-order elastic constants $c_{ijklmnpqrs}$, can be calculated on a standard computer, while ranks higher than 12 are best handled on a supercomputer. Output is provided in either full index form or a reduced index form, *e.g.* the Voigt index notation common to elasticity. As higher-order tensors are often associated with nonlinear material responses, the program provides an accessible means to investigate the important constants involved in nonlinear material modeling. The routine has been used to discover several incorrect relationships reported in the literature.

1. Introduction

The properties of crystalline materials are inherently linked to their crystal structure and symmetry. By virtue of Neumann's principle (Neumann, 1885), and later confirmed by Curie (1894) for paramagnetic materials, the constitutive behavior relating physical properties stemming from, for example, stored-energy functions carries the crystalline symmetry. It is vital to understand how crystal symmetry influences physical properties throughout the physical sciences. Thus, understanding these structure–property linkages has a rich history and continues to be an active area of research, especially as researchers explore new ways to integrate material behavior into engineered devices, *e.g.* leveraging nonlinear properties.

The relationships between crystalline structure and nonlinear properties are less well known compared with strictly linear constitutive behavior. In part, this results from mathematical challenges associated with material properties described by tensors of non-trivial rank, which carry increasing numbers of components. Also, in many cases of coupled physical phenomena, such as piezoelectric materials exposed to an external bias field, the resulting constitutive equations require a combination of tensors of various high-order ranks. Imposing crystal symmetry on such coupled constitutive equations is challenging and requires accurate relationships between the dependent constants to cast the

governing equations into their simplest analytical form involving only the independent constants for the particular point group of interest. Several researchers have calculated and tabulated interdependencies between tensor components or constants, and tables of this type are spread throughout the topical literature. Examples of such tables can be found in several references (Fumi, 1951; Brugger, 1965; Krishnamurty & Gopalakrishnamurty, 1968; Bechmann & Hearmon, 1969; Chung & Li, 1974; Brendel, 1979; Fumi & Ripamonti, 1980*a*,*b*, 1983; Thurston, 1974; Weis & Gaylord, 1985; Cho & Yamanouchi, 1987; Newnham, 2005; Yang, 2018; Lüthi, 2007; Kholkin *et al.*, 2008; Shimizu *et al.*, 2009; Tichý *et al.*, 2010; Clayton, 2011; de Jong *et al.*, 2015; Zhang *et al.*, 2019, 2020). In our own experience, the disparate tabulations of property relationships have presented a significant hurdle to our targeted focus of modeling the nonlinear behavior of piezoelectric materials under both mechanical loading and external bias. Thus, this work is an attempt to offer a simple-to-use computational routine to calculate symmetry relations for any particular property of crystalline materials that is describable by polar tensors of various rank. In doing so, this work is expected to provide a unified resource accessible to researchers across the physical sciences.

This article is organized as follows. In Section 2, we provide the theoretical background needed to impose crystal and physical symmetry restrictions on specific property tensors in order to calculate the relationships between independent and dependent components. Building from Section 2, the computational routine is described in detail in Section 3, including instructions for the required input and examples of expected output. As a demonstration of the routine, Section 4 provides tabulations of property relationships for specific property tensors that appear in the nonlinear stored-energy function (Tiersten, 1975) commonly used to derive constitutive relations of electroelastic materials. To the best of our knowledge, tables giving the relationships between the independent and dependent components of the third odd and first even electrostatic tensors are given explicitly for the first time. Additionally, we provide a table with the numbers of independent and dependent constants for each of the tensors found in the nonlinear stored-energy function for electroelastic materials (Tiersten, 1975).

2. Theory

The approach used in the present computational routine is categorized as an indirect method, which requires imposing both crystal and physical symmetry on the tensors being used to describe a certain property. Here, physical symmetry refers to the symmetry in the tensor components resulting from consideration of cause-and-effect relationships, *i.e.* constitutive behavior. To apply physical symmetry, the user must input the physical symmetry present in the tensor brought about by cause-and-effect relationships. We illustrate an example of this in Section 3.2 by making use of physical symmetry stemming from a stored-energy function (Tiersten, 1975) for electroelastic materials. Direct methods deal only with imposing crystal symmetry conditions on the tensor, which is done through the application of generator matrices or symmetry elements of particular point groups. Both indirect and direct methods have a deep history in solid-state physics, and the interested reader is directed to Fumi & Ripamonti (1980*a*) for additional background and context to these methods. In either method, the end result is typically a system of equations to be solved for the dependent and independent components. The theory outlined in this section describes the general procedure to generate such a system of equations by imposing crystal symmetry and physical symmetry on a property tensor, as seen in Sections 2.1 and 2.2, respectively.

2.1. Imposition of crystal symmetry

Recall that a tensor $\mathbf{P}$ of rank n defined using a basis in one coordinate system can be transformed into the tensor $\mathbf{P}'$ belonging to an alternative coordinate system by applying orthogonal transformation matrices $\mathbf{R}$ to each component of $\mathbf{P}$,

$$P'_{ijk\ldots n} = R_{i\alpha}R_{j\beta}R_{k\gamma}\ldots R_{n\eta}P_{\alpha\beta\gamma\ldots\eta}, \tag{1}$$

where $\mathbf{R}$ is the rotation matrix. For tensors defined on the rotation group SO(3), the matrices $\mathbf{R}$ are rotation matrices. The set of transformation matrices that reproduce the symmetry inherent in a crystal belonging to a particular point group are known as generator matrices for that point group (Newnham, 2005). The number of generator matrices depends on the number of symmetry elements needed to reproduce the crystal symmetry of a particular point group. If $\mathbf{R}^{(1)}$, $\mathbf{R}^{(2)}$, $\mathbf{R}^{(3)}, \ldots,$ $\mathbf{R}^{(N)}$ comprise the minimum set of N generator matrices for a particular point group, then application of any one of the generator matrices in equation (1) must leave each tensor component invariant or unchanged. Thus, the prime notation is no longer needed when applying any of the generator matrices, *e.g.* $P_{ijk\ldots n} = R^{(1)}_{i\alpha}R^{(1)}_{j\beta}R^{(1)}_{k\gamma}\ldots R^{(1)}_{n\eta}P_{\alpha\beta\gamma\ldots\eta}$. As an example, consider the generator matrices $\mathbf{R}^{(1)}$ and $\mathbf{R}^{(2)}$ for point group *mm2* found from Tables 1 and 2 for the symmetry elements $m \perp Z_1$ and $m \perp Z_2$, respectively. Now consider the second-rank tensor $\boldsymbol{\chi}$, which transforms as $\chi_{ij} = R_{i\alpha}R_{j\beta}\chi_{\alpha\beta}$. Application of $\mathbf{R}^{(1)}$ leads to the system of equations

$$\mathbf{R}^{(1)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow \begin{cases} \chi_{11} = \chi_{11}, \\ \chi_{12} = -\chi_{12} \rightarrow \chi_{12} = 0, \\ \chi_{13} = -\chi_{13} \rightarrow \chi_{13} = 0, \\ \chi_{21} = -\chi_{21} = 0 \rightarrow \chi_{21} = 0, \\ \chi_{22} = \chi_{22}, \\ \chi_{23} = \chi_{23}, \\ \chi_{31} = -\chi_{31} \rightarrow \chi_{31} = 0, \\ \chi_{32} = \chi_{32}, \\ \chi_{33} = \chi_{33}. \end{cases} \tag{2}$$

Application of $\mathbf{R}^{(2)}$ adds further dependent relationships between the tensor components,

Table 1
Minimum symmetry elements and case numbering convention (used in the computational routine described in Section 3) corresponding to each point group (Vainshtein, 1995; Newnham, 2005).

The isotropic case or spherical symmetry (Curie group $\infty\infty m$) is also included for comparison.

Case number	Point group	Minimum symmetry elements
1	1	1
2	$\bar{1}$	$\bar{1}$
3	2	$2 \parallel Z_2$
4	m	$m \perp Z_2$
5	$2/m$	$2 \parallel Z_2, m \perp Z_2$
6	222	$2 \parallel Z_1, 2 \parallel Z_2$
7	$mm2$	$m \perp Z_1, m \perp Z_2$
8	mmm	$m \perp Z_1, m \perp Z_2, m \perp Z_3$
9	4	$4 \parallel Z_3$
10	$\bar{4}$	$\bar{4} \parallel Z_3$
11	$4/m$	$4 \parallel Z_3, m \perp Z_3$
12	422	$4 \parallel Z_3, 2 \parallel Z_1$
13	$4mm$	$4 \parallel Z_3, m \perp Z_1$
14	$\bar{4}2m$	$\bar{4} \parallel Z_3, 2 \parallel Z_1$
15	$4/mmm$	$4 \parallel Z_3, m \perp Z_3, m \perp Z_1$
16	3	$3 \parallel Z_3$
17	$\bar{3}$	$\bar{3} \parallel Z_3$
18	32	$3 \parallel Z_3, 2 \parallel Z_1$
19	$3m$	$3 \parallel Z_3, m \perp Z_1$
20	$\bar{3}m$	$\bar{3} \parallel Z_3, m \perp Z_1$
21	6	$6 \parallel Z_3$
22	$\bar{6}$	$\bar{6} \parallel Z_3$
23	$6/m$	$6 \parallel Z_3, m \perp Z_3$
24	622	$6 \parallel Z_3, 2 \parallel Z_1$
25	$6mm$	$6 \parallel Z_3, m \perp Z_1$
26	$\bar{6}m2$	$\bar{6} \parallel Z_3, m \perp Z_1$
27	$6/mmm$	$6 \parallel Z_3, m \perp Z_3, m \perp Z_1$
28	23	$2 \parallel Z_3, 3 \parallel [111]$
29	$m\bar{3}$	$m \perp Z_1, \bar{3} \parallel [111]$
30	432	$4 \parallel Z_3, 3 \parallel [111]$
31	$\bar{4}3m$	$\bar{4} \parallel Z_3, 3 \parallel [111]$
32	$m\bar{3}m$	$4 \parallel Z_3, \bar{3} \parallel [111], m \perp [1\bar{1}0]$
33	$\infty\infty m$	$\infty \parallel Z_3, \infty \parallel Z_1, m \perp Z_1$

$$\mathbf{R}^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow \begin{cases} \chi_{11} = \chi_{11}, \\ \chi_{12} = -\chi_{12} \rightarrow \chi_{12} = 0, \\ \chi_{13} = \chi_{13}, \\ \chi_{21} = -\chi_{21} \rightarrow \chi_{21} = 0, \\ \chi_{22} = \chi_{22}, \\ \chi_{23} = -\chi_{23} \rightarrow \chi_{23} = 0, \\ \chi_{31} = \chi_{31}, \\ \chi_{32} = -\chi_{32} \rightarrow \chi_{32} = 0, \\ \chi_{33} = \chi_{33}. \end{cases} \quad (3)$$

Combining equations (2) and (3) leads to the result of χ_{11}, χ_{22} and χ_{33} being three independent constants and all others being zero. At this point, this example demonstrates the relations between tensor components after invoking crystal symmetry. The following section considers additional reduction and relations found from imposing physical symmetry (cause–effect relationships).

2.2. Imposition of physical symmetry

Here, physical symmetry is referred to as symmetry on tensor components resulting from cause and effect, *i.e.* constitutive relations. Physical symmetry, together with crystal symmetry as described in Section 2.1, results in the minimum set of relationships amongst tensor components or property constants. Consider the simple canonical case of a linear elastic solid having the stored (strain) energy function

$$U = \tfrac{1}{2} c_{2ijkl} E_{ij} E_{kl}, \quad (4)$$

where c_{2ijkl} is the tensor of second-order elastic constants and **E** is the strain tensor. As repeated indices imply summation over the values 1, 2 and 3, it is apparent that the pairs of indices (ij) and (kl) can be swapped, *i.e.* $c_{2ijkl} = c_{2klij}$. This is referred to as a major symmetry and reduces the number of independent constants to 36 in the most general case (prior to invoking crystal symmetry). Furthermore, the strain tensor **E** is symmetric. Thus, it is easily seen that $c_{2ijkl} = c_{2ijlk} = c_{2jikl} = c_{2jilk}$, which are referred to as minor symmetries and reduce the number of constants from 36 to 21. Often, constitutive relations are nothing more than approximate models of the actual behavior of physical systems and usually built on assumptions. Additional assumptions can be included to reduce the number of independent components further. For example, the elastic Cauchy relations stem from c_{2ijkl} being completely symmetric (any two indices can be interchanged), which reduces the number of independent constants to 15. It is noted that the vast majority of crystalline materials do not meet the criteria for the Cauchy relations to hold (Hehl & Itin, 2002; Haussühl, 1967).

Most often, the tensor of second-order elastic constants c_{2ijkl} of a linear elastic material invokes the physical symmetry conditions present resulting from equation (4) and symmetric **E**. Thus, without crystal symmetry conditions applied, c_{2ijkl} consists of 21 independent constants with no dependencies between them. This is also the case for materials belonging to the triclinic class (point groups 1 or $\bar{1}$). Invoking crystalline symmetry as described in Section 2.1 reduces the number of independent constants and introduces dependencies. For example, considering again the *mm*2 point group, upon solving the system of equations resulting from expanding $c_{2ijkl} = R^{(\mathrm{I})}_{i\alpha} R^{(\mathrm{I})}_{j\beta} R^{(\mathrm{I})}_{k\gamma} R^{(\mathrm{I})}_{l\delta} c_{2\alpha\beta\gamma\delta}$ and $c_{2ijkl} = R^{(\mathrm{II})}_{i\alpha} R^{(\mathrm{II})}_{j\beta} R^{(\mathrm{II})}_{k\gamma} R^{(\mathrm{II})}_{l\delta} c_{2\alpha\beta\gamma\delta}$, one finds the result of $c_{11}, c_{12}, c_{13}, c_{22}, c_{23}, c_{33}, c_{44}, c_{55}$ and c_{66} as the nine independent and non-zero second-order elastic constants for materials belonging to point group *mm*2, or to the orthorhombic class more generally.

The computational routine presented in Section 3 is based on solving the system of equations obtained once physical and crystal symmetry are both imposed on the tensor of interest as described in this section.

3. Computational routine, *propSym*

The computational routine *propSym* was inspired by the program developed by Brendel (1979), which calculated and tabulated the relationships between the fourth-order elastic constants, which are components of the eighth-rank elastic modulus tensor $c_{4ijklmnpq}$. Rather than focusing on a single tensor property as done previously, the goal here is to allow the user to generate similar tabulations for a tensor of their

Table 2
Generator matrices corresponding to the minimum symmetry elements seen in Table 1 (Vainshtein, 1995; Newnham, 2005).

$1, \bar{1}$	$2 \parallel Z_1$	$2 \parallel Z_2$	$2 \parallel Z_3$
$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$m \perp Z_1$	$m \perp Z_2$	$m \perp Z_3$	$m \perp [1\bar{1}0]$
$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$3 \parallel Z_3$	$\bar{3} \parallel Z_3$	$3 \parallel [111]$	$\bar{3} \parallel [111]$
$\begin{pmatrix} -1/2 & 3^{1/2}/2 & 0 \\ -3^{1/2}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -3^{1/2}/2 & 0 \\ 3^{1/2}/2 & 1/2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$
$4 \parallel Z_3$	$\bar{4} \parallel Z_3$	$6 \parallel Z_3$	$\bar{6} \parallel Z_3$
$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & 3^{1/2}/2 & 0 \\ -3^{1/2}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -3^{1/2}/2 & 0 \\ 3^{1/2}/2 & -1/2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

Table 3
Reduced index convention for full symmetry (any interchange of indices) between 2, 3 or 4 indices, *e.g.* $\chi_{1ij} \rightarrow \chi_{1i}$, $\chi_{2ijk} \rightarrow \chi_{2i}$, $\chi_{3ijkl} \rightarrow \chi_{3i}$.

Full index			Reduced index
11	111	1111	1
22	222	2222	2
33	333	3333	3
23	223	2223	4
13	113	1113	5
12	112	1112	6
	233	2233	7
	133	1133	8
	122	1122	9
	123	2333	10
		1333	11
		1222	12
		1123	13
		2213	14
		3312	15

choosing of arbitrary rank and symmetry (interchange of indices). In this way, the developed method has much broader application than the previous calculations and routines found in the topical literature. An overview of the logic used to generate the required system of equations and for subsequent solving is given in Section 3.1. The execution of *propSym* based on MATLAB command-line input is given in Section 3.2, along with an example of the expected outputs. Lastly, Section 3.3 lists execution times and discusses MATLAB version restrictions.

3.1. Overview of the code

The backbone of the routine is based on the theory described in Section 2. Here, the general computational steps to obtain the independent and dependent relationships between tensor components are highlighted. Note that the following description provides the essence of the routine and omits some of the fine details, to avoid being overly cumbersome and confusing.

propSym begins once the user inputs the point group and lists the indices that can be interchanged based on physical symmetry conditions. Conventions for user input and expected output are described in Section 3.2. Then, the N_g generator matrices for that point group from Table 2 are retrieved from the function `inputSym`, which calls the primary function `getComps`. In `getComps`, a `For` loop iterates through all possible 3^N combinations of index values, where N is the rank of the tensor or the number of indices that appear; *e.g.* c_{2ijkl} has four indices present and thus $N = 4$ and the `For` loop iterates over $3^4 = 81$ possible combinations of index values. Within the `For` loop, MATLAB's native function `ind2sum` maps each possible 3^N index combination to a single index, which circumvents the need for N nested `For` loops. Each index combination is stored in a $3^N \times N$ cell array `indR`, which describes all possible indices that are called during the expansion of the right-hand side of equation (1). For each index combination, the function `tensor` is called, which receives a list of minor and major symmetries and outputs a string representing the reduced index form for that particular component. Upon each iteration, the output of `tensor` is stored as a 3^N cell array `cs`. The reduced index form follows the convention seen in Table 3 and is a generalization of the Voigt index form popularized by Nye (1957, 1985).

Application of the reduced index form is dictated by the physical symmetry input by the user and greatly speeds up the execution of the routine if applied. The current version of `tensor` applies the reduced index form only up to four indices. Once the initial `For` loop completes, only the N_c unique elements in `cs` are retained, and these are stored in an $N_c \times 1$ vector **cm**. The vector **cm** is then concatenated N_g times to form a vector **C** of size $(N_g \times N_c) \times 1$. The entries of **C** form the left-hand side of the system of equations to be solved, *e.g.* the left-hand side seen in equations (2) and (3). At this point, another `For` loop is initiated that iterates from 1 to $N_g \times N_c$ or the length of the vector **C**. At each iteration, the inner product involving generator matrices seen in equation (1) is expanded over repeated indices. During the expansion, the function `tensor` is applied to each tensor component to give a reduced index form. At this point, the generated system of equations is cast into a matrix form of size $N_c \times N_g \times N_c$ and solved using Gaussian elimination. The resultant matrix coming from this Gaussian elimination is multiplied by the

unique terms in the vector **cm**. At this point, all of the dependent relationships between constants have been formed and the remainder of the code acts to reproduce these relationships in a sensible manner in preparation for being displayed as output.

3.2. Inputs and expected outputs

To execute the routine, the user is required to input or specify the point group, the rank of the tensor (number of indices present in the tensor), the indices that participate in pair-wise major symmetry, index sets that can interchange elements (minor symmetries), a letter to label the tensor, and whether full index output is desired. As an example, the input

```
Enter the point group case number: 7

Enter the rank of the tensor: 4

Enter the major symmetry indices: [1,2,3,4]

Enter the minor symmetry indices: {[1,2],[3,4]}

Enter the label of the property: c

View full index output (y/n - additional time): n
```

produces the output

```
[Original, Reduced]:
[ c11,              c11]
[ c12,              c12]
[ c13,              c13]
[ c14,                0]
[ c15,                0]
[ c16,                0]
[ c22,              c22]
[ c23,              c23]
[ c24,                0]
[ c25,                0]
[ c26,                0]
[ c33,              c33]
[ c34,                0]
[ c35,                0]
[ c36,                0]
[ c44,              c44]
[ c45,                0]
[ c46,                0]
[ c55,              c55]
[ c56,                0]
[ c66,              c66]

Number of nonzero constants:9
Number of independent constants:9
Would you like to try another case? (y/n):
```

which is the example case for point group *mm*2 discussed in Section 2.2. It gives the relations for the second-order elastic constants for materials belonging to the orthorhombic class (or engineering materials with 'orthotropic' symmetry). Now, consider the exemplified input. The point group is given by the respective case number seen in Table 1. The order of the case numbers is chosen such that point groups belonging to the same Laue group are together. Note that this ordering differs from that used by others, *e.g.* Groth (1895). The rank of the tensor is the number of indices present in the general form. In this example, the elastic modulus tensor c_{2ijkl} consists of $N = 4$ indices (i, j, k, l). The major symmetry list [1, 2, 3, 4] constitutes all of the indices that contribute to a major symmetry. In this case, the major symmetry of c_{2ijkl} gives c_{2klij}, which indicates that each of the first four indices (1, 2, 3, 4) is involved in the major symmetry. The minor symmetry list gives sets of indices that can be interchanged. In this example, $c_{2ijkl} = c_{2jikl} = c_{2ijlk}$ indicates that the first (1) and second (2) indices can be interchanged and the third (3) and fourth (4) indices can be interchanged; thus, the cell input `{[1,2],[3,4]}` is used. The label `c` is evident in the output. Lastly, an option to display full index relationships is made available, which allows the user to save a complete mapping of tensor indices to the independent constants. Additional examples for tensors of various physical symmetries are given in Section 4. If the user selects full matrix output, a symbolic array containing the indices and reduced tensor components is produced. An abbreviated portion of the full matrix output for the current example is

```
The full index output (stored in variable tens) is:
[ 1, 1, 1, 1, c11]
[ 2, 1, 1, 1,   0]
[ 3, 1, 1, 1,   0]
[ 1, 2, 1, 1,   0]
[ 2, 2, 1, 1, c12]
[ 3, 2, 1, 1,   0]
[ 1, 3, 1, 1,   0]
[ 2, 3, 1, 1,   0]
[ 3, 3, 1, 1, c13]
[ 1, 1, 2, 1,   0]
[ 2, 1, 2, 1, c66]
[ 3, 1, 2, 1,   0]
[ 1, 2, 2, 1, c66]...
```

which would display 81 rows if shown in full. The full index output is stored in the variable `fmat` after execution. The user can save `fmat` or transform it into an array to be used directly in models.

3.3. Computational requirements and efficiency of the program

propSym is based on MATLAB in conjunction with the MATLAB *Symbolic Math Toolbox* and was tested on versions R2018b, R2019b and R2020a. To the best of our knowledge, no native MATLAB function is newer than R2006. No compatibility issues were found in a compatibility report generated by executing the command `codeCompatibilityReport`. *propSym* does rely on MATLAB conversion of double-precision numbers back into symbolic form. For example, `sym(1.732050807568877)` returns the symbolic form `3^(1/2)`. The versions and cases tested could all be successfully converted to the appropriate symbolic form. Examples of execution times for point group *mm*2 for the tensors found in equation (5), which is the stored-energy

Table 4
Execution times for electroelastic properties for materials belonging to the *mm*2 point group.

Property	Minor symmetry input	Major symmetry input	Execution times (ss.xx)
χ_{2ij}	`{[1,2]}`	`[ ]`	00.14
χ_{3ijk}	`{[1,2,3]}`	`[ ]`	00.20
χ_{4ijkl}	`{[1,2,3,4]}`	`[ ]`	00.32
e_{ijk}	`{[2,3]}`	`[ ]`	00.29
d_{1ijklm}	`{[2,3],[4,5]}`	`[2:5]`	00.79
$d_{2ijklmnp}$	`{[2,3],[4,5],[6,7]}`	`[2:7]`	03.39
b_{ijkl}	`{[1,2],[3,4]}`	`[ ]`	00.49
$a_{1ijklmn}$	`{[1,2],[3,4],[5,6]}`	`[3:6]`	01.76
d_{3ijklm}	`{[1,2,3],[4,5]}`	`[ ]`	01.08
c_{2ijkl}	`{[1,2],[3,4]}`	`[1:4]`	00.24
$c_{3ijklmn}$	`{[1,2],[3,4],[5,6]}`	`[1:6]`	00.69
$c_{4ijklmnpq}$	`{[1,2],[3,4],[5,6],[7,8]}`	`[1:8]`	02.66

function for electroelastic materials (Tiersten, 1975), are given in Table 4.

As can be seen, most of these cases execute in a matter of seconds. Note that the *mm*2 point group requires a minimum of two generator matrices. The execution time scales approximately linearly for the number of generator matrices, at least up to rank 10. Table 4 describes the necessary inputs and associated execution times for various electroelastic properties. Symmetry results for these properties are discussed in Section 4. The calculations followed from inputting the associated minor symmetry and major symmetry inputs from Table 4 via the MATLAB command window input, as seen in the example highlighted in Section 3.2. For each case, the full index output was not chosen to be generated, only the reduced table outputs.

These execution times are based on a laptop computer with 128 GB usable memory, a 64 bit Intel Core i7-8850H CPU with a processing rate of 2.60 GHz, and MATLAB R2020a. During execution of the $c_{4ijklmnpq}$ tensor, MATLAB utilizes around 4 GB of memory. The laptop was used to calculate tensors up to 14th rank, *e.g.* the higher-rank elasticity tensors $c_{5ijklmnpqrs}$ (fifth-order elastic constants), $c_{6ijklmnpqrstu}$ (sixth-order elastic constants) and $c_{7ijklmnpsrstuxy}$ (seventh-order elastic constants), which executed in 00:00:23.77, 00:05:27.78 and 01:12:45.00 (hh:mm:ss.xx), respectively. The $c_{7ijklmnpsrstuxy}$ peak memory usage reached 17.5 GB. This suggests that 14th rank tensors, when physical symmetry is applied, are the practical upper limit when utilizing standard desktop or laptop computers. The eighth-rank case is the practical upper limit on a standard computer when no physical symmetry is applied, which executes in 02:20:03.42 (hh:mm:ss.xx).

While the rank 10, 12 and 14 examples were primarily used to evaluate the efficiency of the code, to the best of our knowledge this is the first instance where the components of the tensors $c_{6ijklmnpqrstu}$ and $c_{7ijklmnpsrstuxy}$ have been fully reduced in terms of their independent components. Usage of advanced processing techniques like GPUs and the expanded memory capabilities of super computers would extend the upper limit on tensor rank even further.

4. Results and verification

This work was motivated by trying to find a reduced form of the effective properties of piezoelectric materials in terms of the minimum number of independent tensor components. The effective properties are derived from the thermodynamic potential function given by Tiersten (1975) for electroelastic materials,

$$\begin{aligned} U = {} & \tfrac{1}{2}c_{2ijkl}E_{ij}E_{kl} - e_{ijk}W_iE_{jk} - \tfrac{1}{2}\chi_{2ij}W_iW_j \\ & + \tfrac{1}{6}c_{3ijklmn}E_{ij}E_{kl}E_{mn} + \tfrac{1}{2}d_{1ijklm}W_iE_{jk}E_{lm} \\ & - \tfrac{1}{2}b_{ijkl}W_iW_jE_{kl} - \tfrac{1}{6}\chi_{3ijk}W_iW_jW_k \\ & + \tfrac{1}{24}c_{4ijklmnpq}E_{ij}E_{kl}E_{mn}E_{pq} + \tfrac{1}{6}d_{2ijklmnp}W_iE_{jk}E_{lm}E_{np} \\ & + \tfrac{1}{4}a_{1ijklmn}W_iW_jE_{kl}E_{mn} - \tfrac{1}{6}d_{3ijklm}W_iW_jW_kE_{lm} \\ & - \tfrac{1}{24}\chi_{4ijkl}W_iW_jW_kW_l, \end{aligned} \tag{5}$$

where **W** and **E** describe the electric field and strain, respectively. The property tensors c_{2ijkl}, e_{ijk}, χ_{2ij}, $c_{3ijklmn}$, d_{1ijklm}, b_{ijkl}, χ_{3ijk}, $c_{4ijklmnpq}$, $d_{2ijklmnp}$, $a_{1ijklmn}$, d_{3ijklm} and χ_{4ijkl} are the second-order elastic, piezoelectric, second-order electric permeability, third-order elastic, first odd electroelastic, electrostrictive, third-order electric permeability, fourth-order elastic, second odd electroelastic, first even electroelastic, third odd electroelastic and fourth-order electric permeability, respectively (Tiersten, 1975). The use of the numbering follows from Tiersten's convention. This is needed to differentiate between tensors like d_{1ijklm} and d_{3ijklm}, which have the same number of indices but different symmetries. The property tensors govern the degree to which **W** and **E** influence the stored energy, which clearly includes nonlinear effects and cases that stem from coupling between **W** and **E**.

The computational routine described here can be used to reduce each of these tensors into a minimum number of components. Then, any material property derivable from equation (5) can be described in terms of the minimum number of components. To demonstrate the utility of the routine, we have formed tables for each of the tensors involved in the stored energy. The tables are too lengthy to be reproduced here, but can be viewed at https://sites.psu.edu/kube/spr/ or easily generated using the computational routine. The site http://www.chriskube.com/ contains links to download the MATLAB source code for the computational routine.

To the best of our knowledge, the relationships between components of the third odd electroelastic tensor d_{3ijklm} and first even electroelastic tensor $a_{1ijklmn}$ are calculated here for the first time [Thurston (1974) reports d_{3ijklm} but does not reduce the symmetry fully and reports the equivalent symmetry as d_{1ijklm}]. Relationships between components for the first odd electroelastic tensor d_{1ijklm}, sometimes referred to as third-order piezoelectric constants (ε_{ijklm}), have been given recently (Zhang *et al.*, 2019). However, incorrect relationships were observed for the third-order piezoelectric constants. Namely, Zhang and co-workers mistakenly conclude that the third-order piezoelectric constants for point groups $\bar{4}2m$, $\bar{6}2m$, 432 and $\bar{4}3m$ are zero, which disagrees with the present results and those published previously [see Table 1

Table 5
Number of non-zero constants (number of independent constants) for different physical properties from Tiersten's equation throughout all the point groups.

	c_{2ijkl}	e_{ik}	χ_{2ij}	$c_{3ijklmn}$	d_{1ijklm}	b_{ijkl}	χ_{3ijk}	$c_{4ijklmnpq}$	$d_{2ijklmnp}$	$a_{1ijklmn}$	d_{3ijklm}	χ_{4ijkl}
1	21 (21)	18 (18)	6 (6)	56 (56)	63 (63)	36 (36)	10 (10)	126 (126)	168 (168)	126 (126)	60 (60)	15 (15)
$\bar{1}$	21 (21)	0 (0)	6 (6)	56 (56)	0 (0)	36 (36)	0 (0)	126 (126)	0 (0)	126 (126)	0 (0)	15 (15)
2	13 (13)	8 (8)	4 (4)	32 (32)	29 (29)	20 (20)	4 (4)	70 (70)	80 (80)	68 (68)	28 (28)	9 (9)
m	13 (13)	10 (10)	4 (4)	32 (32)	34 (34)	20 (20)	6 (6)	70 (70)	88 (88)	68 (68)	32 (32)	9 (9)
2/*m*	13 (13)	0 (0)	4 (4)	32 (32)	0 (0)	20 (20)	0 (0)	70 (70)	0 (0)	68 (68)	0 (0)	9 (9)
222	9 (9)	3 (3)	3 (3)	20 (20)	12 (12)	12 (12)	1 (1)	42 (42)	36 (36)	39 (39)	12 (12)	6 (6)
*mm*2	9 (9)	5 (5)	3 (3)	20 (20)	17 (17)	12 (12)	3 (3)	42 (42)	44 (44)	39 (39)	16 (16)	6 (6)
mmm	9 (9)	0 (0)	3 (3)	20 (20)	0 (0)	12 (12)	0 (0)	42 (42)	0 (0)	39 (39)	0 (0)	6 (6)
4	11 (7)	7 (4)	3 (2)	28 (16)	27 (15)	18 (10)	3 (2)	64 (36)	76 (40)	63 (34)	26 (14)	8 (5)
$\bar{4}$	11 (7)	7 (4)	3 (2)	28 (16)	26 (14)	18 (10)	3 (2)	64 (36)	76 (40)	63 (34)	26 (14)	8 (5)
4/*m*	11 (7)	0 (0)	3 (2)	28 (16)	0 (0)	18 (10)	0 (0)	64 (36)	0 (0)	63 (34)	0 (0)	8 (5)
422	9 (6)	2 (1)	3 (2)	20 (12)	10 (5)	12 (7)	0 (0)	42 (25)	32 (16)	39 (22)	10 (5)	6 (4)
4*mm*	9 (6)	5 (3)	3 (2)	20 (12)	17 (10)	12 (7)	3 (2)	42 (25)	44 (24)	39 (22)	16 (9)	6 (4)
$\bar{4}$2*m*	9 (6)	3 (2)	3 (2)	20 (12)	12 (7)	12 (7)	1 (1)	42 (25)	36 (20)	39 (22)	12 (7)	6 (4)
4/*mmm*	9 (6)	0 (0)	3 (2)	20 (12)	0 (0)	12 (7)	0 (0)	42 (25)	0 (0)	39 (22)	0 (0)	6 (4)
3	15 (7)	13 (6)	3 (2)	50 (20)	55 (21)	30 (12)	7 (4)	118 (42)	160 (56)	117 (42)	54 (20)	10 (5)
$\bar{3}$	15 (7)	0 (0)	3 (2)	50 (20)	0 (0)	30 (12)	0 (0)	118 (42)	0 (0)	117 (42)	0 (0)	10 (5)
32	12 (6)	5 (2)	3 (2)	31 (14)	23 (8)	18 (8)	2 (1)	69 (28)	74 (24)	66 (26)	24 (8)	8 (4)
3*m*	12 (6)	8 (4)	3 (2)	31 (14)	32 (13)	18 (8)	5 (3)	69 (28)	86 (32)	66 (26)	30 (12)	8 (4)
$\bar{3}$*m*	12 (6)	0 (0)	3 (2)	31 (14)	0 (0)	18 (8)	0 (0)	69 (28)	0 (0)	66 (26)	0 (0)	8 (4)
6	9 (5)	7 (4)	3 (2)	28 (12)	25 (11)	18 (8)	3 (2)	64 (24)	76 (28)	63 (24)	26 (10)	6 (3)
$\bar{6}$	9 (5)	6 (2)	3 (2)	28 (12)	30 (10)	18 (8)	4 (2)	64 (24)	84 (28)	63 (24)	28 (10)	6 (3)
6/*m*	9 (5)	0 (0)	3 (2)	28 (12)	0 (0)	18 (8)	0 (0)	64 (24)	0 (0)	63 (24)	0 (0)	6 (3)
622	9 (5)	2 (1)	3 (2)	20 (10)	8 (3)	12 (6)	0 (0)	42 (19)	32 (10)	39 (17)	10 (3)	6 (3)
6*mm*	9 (5)	5 (3)	3 (2)	20 (10)	17 (8)	12 (6)	3 (2)	42 (19)	44 (18)	39 (17)	16 (7)	6 (3)
$\bar{6}$*m*2	9 (5)	3 (1)	3 (2)	20 (10)	15 (5)	12 (6)	2 (1)	42 (19)	42 (14)	39 (17)	14 (5)	6 (3)
6/*mmm*	9 (5)	0 (0)	3 (2)	20 (10)	0 (0)	12 (6)	0 (0)	42 (19)	0 (0)	39 (17)	0 (0)	6 (3)
23	9 (3)	3 (1)	3 (1)	20 (8)	12 (4)	12 (4)	1 (1)	42 (14)	36 (12)	39 (13)	12 (4)	6 (2)
432	9 (3)	0 (0)	3 (1)	20 (6)	6 (1)	12 (3)	0 (0)	42 (11)	24 (4)	39 (9)	6 (1)	6 (2)
$m\bar{3}$	9 (3)	0 (0)	3 (1)	20 (8)	0 (0)	12 (4)	0 (0)	42 (14)	0 (0)	39 (13)	0 (0)	6 (2)
$\bar{4}$3*m*	9 (3)	3 (1)	3 (1)	20 (6)	12 (3)	12 (3)	1 (1)	42 (11)	36 (8)	39 (9)	12 (3)	6 (2)
$m\bar{3}m$	9 (3)	0 (0)	3 (1)	20 (6)	0 (0)	12 (3)	0 (0)	42 (11)	0 (0)	39 (9)	0 (0)	6 (2)
$\infty\infty m$	9 (2)	0 (0)	3 (1)	20 (3)	0 (0)	12 (2)	0 (0)	42 (4)	0 (0)	39 (4)	0 (0)	6 (1)

of Nelson & Lax (1971) and Table 16.5 of Thurston (1974)]. This result is seen in Table 5, which gives the number of independent tensor components for each of the tensors considered. Results such as Table 5 allow one easily to see the complexity of particular tensors, their anisotropic behavior and whether physical phenomena display certain behavior.

Validation of the computational results was based on comparison with other reports in the literature (Brugger, 1965; Brendel, 1979; Thurston, 1974; Newnham, 2005; Tichý *et al.*, 2010; Clayton, 2011; de Jong *et al.*, 2015; Yang, 2018; Zhang *et al.*, 2019), in addition to the output of our independently developed Python code *PyMTensor*. The *PyMTensor* code utilizes much of the same logic to generate the required system of equations as presented here and can also be applied for tensors of any rank and point group. Results from the current code and *PyMTensor* were corroborated for all of the components in the tensors considered in the electroelastic stored energy [equation (5)]. The first cross checks with the literature were with the work of Brendel (1979) for the fourth-order elastic constants and Brugger (1965) for the third-order elastic constants. All relationships established by the present code, *PyMTensor*, Brendel (1979) and Brugger (1965) agree.

Once the *propSym* output had been verified, *propSym* was used to discover several incorrect values reported in the literature. For example, for the first-order piezoelectric tensor e_{ijk}, agreement is observed amongst the computational routines of Newnham (2005), Clayton (2011) and Tichý *et al.* (2010) for the 27 point groups: 1, $\bar{1}$, 2, *m*, 2/*m*, 222, *mm*2, *mmm*, $\bar{4}$2*m*, 4/*m*, 4*mm*, 4/*mmm*, 3, $\bar{3}$, 32, 3*m*, $\bar{3}$*m*, $\bar{6}$, 6/*m*, 6*mm*, 6/*mmm*, $\bar{6}$*m*2, 23, 432, $m\bar{3}$, $\bar{4}$3*m* and $m\bar{3}m$. However, discrepancies exist amongst the others. For example, mutual agreement is not found for the $\bar{4}$ point group; the component e_{15} is noted as $-e_{15}$ by Newnham (2005) and is not present in the tables of Clayton (2011), but is given by Tichý *et al.* (2010) and de Jong *et al.* (2015) and in the present results. Also for the point group $\bar{4}$, the e_{33} component is reported as non-zero by Tichý *et al.* (2010), but zero by Newnham (2005), Clayton (2011) and de Jong *et al.* (2015) and in the present results. Similarly, for the point groups 4 and 6, Clayton (2011) considers the components e_{15}, e_{31} and e_{33} to be zero, which is not the case for Newnham (2005), Tichý *et al.* (2010) and the present results. Some published tables do not recognize 622 (Clayton, 2011; de Jong *et al.*, 2015) and 422 (Clayton, 2011) as point groups exhibiting piezoelectricity, while the present results indicate they do exhibit piezoeletricity, in agreement with Newnham (2005) and Tichý *et al.* (2010).

At the beginning of this study, it was expected that typographical errors and disagreements could be present for tabulations involving higher-rank tensors. However, the disagreements involving the leading-order piezoelectric constants e_{ijk} were surprising. These observed discrepancies served as further motivation to develop and offer the

computational routine presented here, which allows the user to input their own tensor of interest of arbitrary rank.

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