NANO106 Handout 11 - Piezoelectric coefficients for the 32 point group

Shyue Ping Ong
University of California, San Diego
9500 Gilman Drive, Mail Code 0448, La Jolla, CA 92093-0448

May 15, 2015

In this handout, we will go through the full exercise of deriving the form of the piezoelectric matrix for the 32 point group, which is fairly complex.

1 The 32 point group

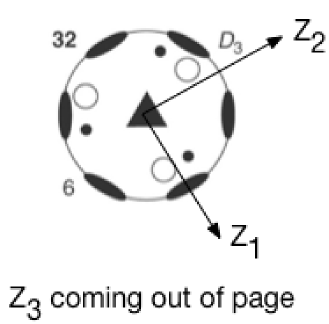

Figure 1: The 32 point group

The IEEE standard setting for the 32 point group is given above. The 3-fold rotation is oriented parallel to Z_3 and one of the 2-fold rotations is oriented parallel to Z_1.

2 General procedure for deriving symmetry restrictions

The general procedure for deriving symmetry restrictions in tensors is given below.

1. Convert from Voigt to tensor notation if necessary. This is only required if you are working with higher-order tensors that utilizes the Voigt matrix form.

2. Determine the mapping of axes for the symmetry operations of the point group.
3. Apply mapping to tensor elements and Neumann's Principle.
4. Determine equalities and elements with value 0.

3 Piezoelectric matrix and tensor

The piezoelectric matrix has the following Voigt form:

$$\begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{pmatrix}$$

If we explicitly write out all the elements in terms of the tensor elements, we have:

$$\begin{pmatrix} d_{111} & d_{122} & d_{133} & d_{123}+d_{132} & d_{113}+d_{131} & d_{112}+d_{121} \\ d_{211} & d_{222} & d_{233} & d_{223}+d_{232} & d_{213}+d_{231} & d_{212}+d_{221} \\ d_{311} & d_{322} & d_{333} & d_{323}+d_{332} & d_{313}+d_{331} & d_{312}+d_{321} \end{pmatrix}$$

4 Symmetry constraints of the 2-fold rotation about Z_1

Let us start with the simpler symmetry operation of the 2-fold rotation about Z_1. The relationship between the rotated axes and the original axes is given as:

$$X_1' = X_1$$
$$X_2' = -X_2$$
$$X_3' = -X_3$$

Let us consider the implications of this mapping on a few tensor elements.
For d_{11}, we have $d_{11} \to d_{111}$ (Voigt to tensor). d_{111} transforms as:

$$X_1'X_1'X_1' = X_1X_1X_1$$
$$\implies d_{111}' = d_{111} = d_{111} \text{ (Neumann's Principle)}$$

Hence, there are no restrictions on d_{11}.
For d_{21}, we have $d_{21} \to d_{211}$ (Voigt to tensor). d_{211} transforms as:

$$X_2'X_1'X_1' = (-X_2)X_1X_1$$
$$\implies d_{211}' = -d_{211} = d_{211} \text{ (Neumann's Principle)}$$
$$\implies d_{211} = 0$$

Hence, $d_{21} = 0$. From this result, we can infer that all tensor elements that have an odd number of indices 2 and 3 will be constrained to be 0 by the 2-fold rotation (because of the negation of the X_2 and X_3). Hence,

$$d_{113} = d_{131} = d_{112} = d_{121} = d_{211} = d_{222} = d_{233} = d_{223} = d_{232} = d_{311} = d_{322} = d_{333} = d_{323} = d_{332} = 0$$
$$\implies d_{15} = d_{16} = d_{21} = d_{22} = d_{23} = d_{24} = d_{31} = d_{32} = d_{33} = d_{34} = 0 \text{ (after conversion to Voigt form)}$$

Hence, our piezoelectric matrix is now simplified to:

$$\begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{25} & d_{26} \\ 0 & 0 & 0 & 0 & d_{35} & d_{36} \end{pmatrix}$$

5 Symmetry constraints of the 3-fold rotation about Z_3

For the 3-fold rotation about Z_3, the relationship between the rotated axes and the original axes is given as:

$$\begin{pmatrix} \mathbf{e_1'} \\ \mathbf{e_2'} \\ \mathbf{e_3'} \end{pmatrix} = \begin{pmatrix} \cos 120° & -\sin 120° & 0 \\ \sin 120° & \cos 120° & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{e_1} \\ \mathbf{e_2} \\ \mathbf{e_3} \end{pmatrix}$$

Hence, the mapping is given as:

$$\begin{aligned} X_1' &= -\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2 \\ X_2' &= \frac{\sqrt{3}}{2}X_1 - \frac{1}{2}X_2 \\ X_3' &= X_3 \end{aligned}$$

5.1 Constraints on d_{13}

Let us start with some of the simpler relationships first.

For d_{13}, we have $d_{13} \to d_{133}$ (Voigt to tensor). d_{133} transforms as:

$$\begin{aligned} X_1'X_3'X_3' &= (-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2)X_3X_3 \\ &= -\frac{1}{2}X_1X_3X_3 - \frac{\sqrt{3}}{2}X_2X_3X_3 \\ \implies d_{133}' &= -\frac{1}{2}d_{133} - \frac{\sqrt{3}}{2}d_{233} \\ \implies d_{133}' &= -\frac{1}{2}d_{133} \text{ (d_{233} was shown to be zero earlier)} \\ \implies -\frac{1}{2}d_{133} &= d_{133} \text{ (Neumann's Principle)} \\ \implies d_{133} &= 0 \\ \implies d_{13} &= 0 \end{aligned}$$

5.2 Constraints on d_{35}

For d_{35}, we have $d_{35} \to d_{313} + d_{331}$ (Voigt to tensor). d_{313} transforms as:

$$\begin{aligned}
X_3'X_1'X_3' &= X_3(-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2)X_3 \\
&= -\frac{1}{2}X_3X_1X_3 - \frac{\sqrt{3}}{2}X_3X_2X_3 \\
\implies d'_{313} &= -\frac{1}{2}d_{313} - \frac{\sqrt{3}}{2}d_{323} \\
\implies d'_{313} &= -\frac{1}{2}d_{313} \text{ (d_{323} was shown to be zero earlier)} = d_{313} \\
\implies d_{313} &= 0 \\
\text{Similarly, } d_{331} &= 0 \\
\implies d_{35} &= 0
\end{aligned}$$

5.3 Constraints on d_{36}

For d_{36}, we have $d_{36} \to d_{312} + d_{321}$ (Voigt to tensor). d_{312} transforms as:

$$\begin{aligned}
X_3'X_1'X_2' &= X_3(-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2)(\frac{\sqrt{3}}{2}X_1 - \frac{1}{2}X_2) \\
&= -\frac{\sqrt{3}}{4}X_3X_1X_1 + \frac{1}{4}X_3X_1X_2 - \frac{3}{4}X_3X_2X_1 + \frac{\sqrt{3}}{4}X_3X_2X_2 \\
\implies d'_{312} &= -\frac{\sqrt{3}}{4}d_{311} + \frac{1}{4}d_{312} - \frac{3}{4}d_{321} + \frac{\sqrt{3}}{4}d_{322}
\end{aligned}$$

Zeroing out the elements we have determined earlier and applying Neumann's Principle, we have

$$\begin{aligned}
d'_{312} &= \frac{1}{4}d_{312} - \frac{3}{4}d_{321} = d_{312} \\
\implies d_{312} &= -d_{321}
\end{aligned}$$

Hence, $d_{36} = d_{312} + d_{321} = 0$

5.4 Constraints on d_{14} and d_{25}

For d_{25}, we have $d_{25} \to d_{213} + d_{231}$ (Voigt to tensor). d_{213} transforms as:

$$
\begin{aligned}
X_2'X_1'X_3' &= (\frac{\sqrt{3}}{2}X_1 - \frac{1}{2}X_2)(-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2)X_3 \\
&= -\frac{\sqrt{3}}{4}X_1X_1X_3 - \frac{3}{4}X_1X_2X_3 + \frac{1}{4}X_2X_1X_3 + \frac{\sqrt{3}}{4}X_2X_2X_3 \\
\implies d_{213}' &= -\frac{\sqrt{3}}{4}d_{113} - \frac{3}{4}d_{123} + \frac{1}{4}d_{213} + \frac{\sqrt{3}}{4}d_{223} \\
\implies d_{213}' &= -\frac{3}{4}d_{123} + \frac{1}{4}d_{213} = d_{213} \\
\implies -d_{123} &= d_{213} \\
\implies d_{25} &= -d_{14}
\end{aligned}
$$

5.5 Constraints on d_{11}, d_{12} and d_{26}

For d_{11}, we have $d_{11} \to d_{111}$ (Voigt to tensor). d_{111} transforms as:

$$
\begin{aligned}
X_1'X_1'X_1' &= (-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2)(-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2)(-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2) \\
&= -\frac{1}{8}X_1X_1X_1 - \frac{\sqrt{3}}{8}X_1X_1X_2 \\
&- \frac{\sqrt{3}}{8}X_1X_2X_1 - \frac{3}{8}X_1X_2X_2 \\
&- \frac{\sqrt{3}}{8}X_2X_1X_1 - \frac{3}{8}X_2X_1X_2 \\
&- \frac{3}{8}X_2X_2X_1 - \frac{3\sqrt{3}}{8}X_2X_2X_2 \\
\implies d_{111}' &= -\frac{1}{8}d_{111} - \frac{\sqrt{3}}{8}d_{112} - \frac{\sqrt{3}}{8}d_{121} - \frac{3}{8}d_{122} - \frac{\sqrt{3}}{8}d_{211} - \frac{3}{8}d_{212} - \frac{3}{8}d_{221} - \frac{3\sqrt{3}}{8}d_{222} \\
&= -\frac{1}{8}d_{111} - \frac{3}{8}d_{122} - \frac{3}{8}d_{212} - \frac{3}{8}d_{221} \text{ (some of the tensor elements are already 0)}
\end{aligned}
$$

In matrix form, we have:

$$
\begin{aligned}
d_{11}' = -\frac{1}{8}d_{11} - \frac{3}{8}d_{12} - \frac{3}{8}d_{26} &= d_{11} \\
\implies 3d_{11} + d_{12} + d_{26} &= 0
\end{aligned}
$$

For d_{12}, we have $d_{12} \to d_{122}$ (Voigt to tensor). d_{122} transforms as:

$$
\begin{aligned}
X_1'X_2'X_2' &= (-\frac{1}{2}X_1 - \frac{\sqrt{3}}{2}X_2)(\frac{\sqrt{3}}{2}X_1 - \frac{1}{2}X_2)(\frac{\sqrt{3}}{2}X_1 - \frac{1}{2}X_2) \\
&= -\frac{3}{8}X_1X_1X_1 + \frac{\sqrt{3}}{8}X_1X_1X_2 \\
&+ \frac{\sqrt{3}}{8}X_1X_2X_1 - \frac{1}{8}X_1X_2X_2 \\
&- \frac{3\sqrt{3}}{8}X_2X_1X_1 + \frac{3}{8}X_2X_1X_2 \\
&+ \frac{3}{8}X_2X_2X_1 - \frac{\sqrt{3}}{8}X_2X_2X_2 \\
\implies d_{122}' &= -\frac{3}{8}d_{111} + \frac{\sqrt{3}}{8}d_{112} + \frac{\sqrt{3}}{8}d_{121} - \frac{1}{8}d_{122} - \frac{3\sqrt{3}}{8}d_{211} + \frac{3}{8}d_{212} + \frac{3}{8}d_{221} - \frac{\sqrt{3}}{8}d_{222} \\
&= -\frac{3}{8}d_{111} - \frac{1}{8}d_{122} + \frac{3}{8}d_{212} + \frac{3}{8}d_{221} \text{ (some of the tensor elements are already 0)}
\end{aligned}
$$

In matrix form, we have:

$$
\begin{aligned}
d_{12}' = -\frac{3}{8}d_{11} - \frac{1}{8}d_{12} + \frac{3}{8}d_{26} = d_{12} \\
\implies d_{11} + 3d_{12} - d_{26} = 0
\end{aligned}
$$

Combining the relations derived for d_{11} and d_{12}, we get:

$$
\begin{aligned}
4d_{11} + 4d_{12} = 0 \\
\implies d_{12} = -d_{11} \text{ and } d_{26} = -2d_{11}
\end{aligned}
$$

6 Conclusion

Incorporating all the symmetry restrictions, we finally get the simplified form of the piezo-electric matrix as follows:

$$
\begin{pmatrix}
d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\
0 & 0 & 0 & 0 & -d_{14} & -2d_{11} \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

In general, this is a more involved process than usual because the trigonal 3-fold rotation does not align with orthogonal axes. For 4-fold symmetry, the process is considerably simpler. But it is useful to go through this, which illustrates all the key steps of deriving symmetry restrictions.