# 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

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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

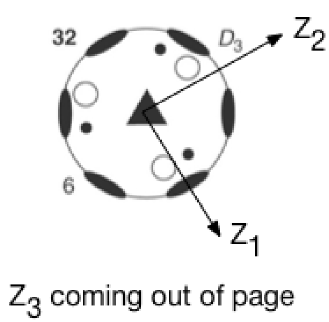


Figure 1: The 32 point group

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 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

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

## 3 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,

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

Hence, our piezoelectric matrix is now simplified to:

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

## 4 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:

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

Hence, the mapping is given as:

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

## 4.1 Constraints on $d_{13}$

Let us start with some "simple" ones first.

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

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

## 4.2 Constraints on $d_{35}$

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

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

## 4.3 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, $d_{36} = d_{312} + d_{321} = 0$

## 4.4 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:

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

## 4.5 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 relation derived for $d_{11}$ and $d_{12}$, we get:

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

# 5 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:

1. Convert from Voigt to tensor notation
2. Determine the mapping of axes for the symmetry operations.
3. Apply mapping to tensor elements and Neumann's Principle.
4. Determine equalities and elements with value 0.