NANO106 Handout 11 - Piezoelectric coefficients for the 32 point group

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1 Introduction

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.

2 The 32 point group

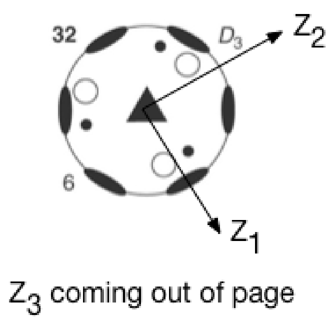

Figure 1: The 32 point group

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.

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:

$$\begin{aligned} X_1' &= X_1 \\ X_2' &= -X_2 \\ X_3' &= -X_3 \end{aligned}$$

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:

$$\begin{aligned} & X_1'X_1'X_1' = X_1X_1X_1 \\ \implies & d_{111}' = d_{111} = d_{111} \text{ (Neumanm's Principle)} \end{aligned}$$

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:

$$\begin{aligned} & X_2'X_1'X_1' = (-X_2)X_1X_1 \\ \implies & d_{211}' = -d_{211} = d_{211} \text{ (Neumanm's Principle)} \\ \implies & d_{211} = 0 \end{aligned}$$

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,

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

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 "simple" ones first.

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

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

5.2 Constraints on d_{35}

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

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

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:

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

d_{312} transforms as (just swapping indices above):

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

Combining the two, we find that:

$$
\begin{aligned}
d_{312} = d_{321} &= 0 \\
d_{36} &= 0
\end{aligned}
$$

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 relation derived for d_{11} and $d12$, 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:

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