

Can we do something about reducing the number of components?

Use:

"A physical property measured along two different directions must be equal if these two directions are crystallographically equivalent."

Example:

Let  $J(x, y, z)$  &  $J'(x', y', z')$

represent the same quantity.

$$\begin{pmatrix} J_1' \\ J_2' \\ J_3' \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix}$$

Unitary matrix

$$A^{-1} = A^T$$

e.g., for centrosymmetry,  $A = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ .

for rotation about principal axis  $A = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$ .

Electric field is transformed in same way;  $\Rightarrow \begin{pmatrix} E_1' \\ E_2' \\ E_3' \end{pmatrix} = A \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}$

$$\text{or, } E_i' = a_{ij} E_j.$$

Then we can calculate  $\sigma'$  tensor defined by  $J' = \sigma' E'$ .

$$\Rightarrow \begin{pmatrix} \sigma_{11}' & \sigma_{12}' & \sigma_{13}' \\ \sigma_{21}' & \sigma_{22}' & \sigma_{23}' \\ \sigma_{31}' & \sigma_{32}' & \sigma_{33}' \end{pmatrix} = A \sigma A^{-1} = A \sigma A^T.$$

$$\text{or, } \boxed{\sigma_{ij}' = a_{ik} a_{jl} \sigma_{kl}} \quad \text{--- (vii)}$$

Example: When the crystal has a 2-fold axis along the z-axis, the electrical conductivity should have same tensorial form in terms of transformation

$$\underbrace{\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{T_2}$$

$$\text{i.e., } \sigma' = T_2 \sigma T_2^{-1}$$

$$\Rightarrow \sigma_{31} = \sigma_{13} = \sigma_{32} = \sigma_{23} = 0.$$

(Note  $\varphi = \frac{2\pi}{2}$ ).

"After little algebra"