Neumann's Principle

#Group Theory #Symmetry #Crystals

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Mathematical Methods for Physicists

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Say Hi to Neumann

From Mathematical Crystallography

Neumann's principle states that the symmetry of any physical property of a crystal must include the symmetry of the crystal itself.

In a nutshell:

Crystal Symmetry
$\Rightarrow$ **Property Symmetry**

Figure: This is Franz Ernst Neumann. (P.S. I do NOT know Group Theory.)

Why Should We Care?

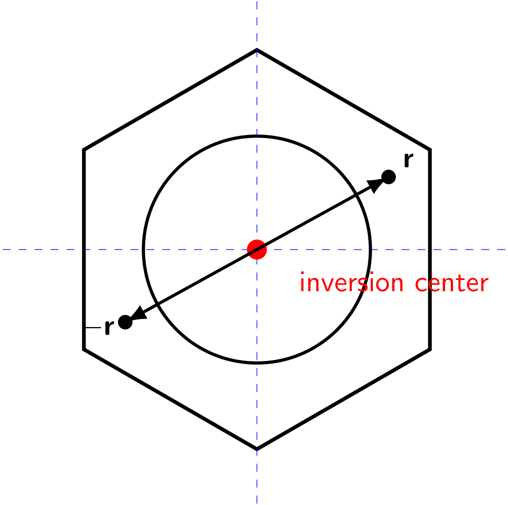
Why does:

- Quartz generate voltage when squeezed?
- BBO double the frequency of laser light?
- Silicon do neither?

Main Message

Symmetry alone can tell us whether these effects are allowed.

Centrosymmetric Crystal



A crystal is **centrosymmetric** if

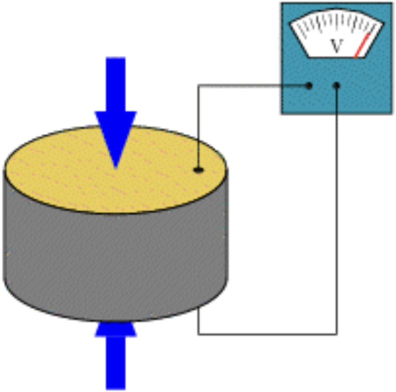
$$\mathbf{r} \xrightarrow{\mathcal{I}} -\mathbf{r}.$$

Here, $\mathcal{I}$ is the **inversion operator**.
For every atom at $\mathbf{r}$, there is an equivalent atom at $-\mathbf{r}$.

Physical Meaning

The crystal looks exactly the same after inversion.

What is Piezoelectricity?



Applied stress σ

Piezoelectricity is the generation of an electric polarization when a crystal is mechanically stressed.

Compression shifts positive and negative charge centers, producing a measurable voltage.

$$P_i = d_{ijk}\,\sigma_{jk}$$

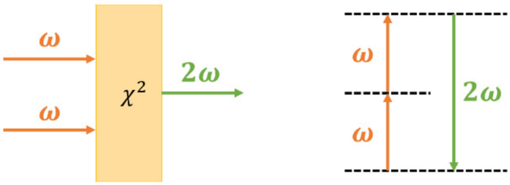
where:

- P_i: polarization
- σ_{jk}: applied stress
- d_{ijk}: piezoelectric tensor

Our goal: show that in centrosymmetric crystals,

$$d_{ijk} = 0.$$

What is Second Harmonic Generation?



Two photons at ω combine to generate one photon at 2ω.

Second Harmonic Generation (SHG) is a nonlinear optical process in which two photons of frequency ω combine to generate one photon of frequency 2ω.

The induced polarization is

$$P_i^{(2)} = \varepsilon_0 \chi_{ijk}^{(2)} E_j E_k.$$

where:

- E_j: electric field
- $\chi_{ijk}^{(2)}$: second-order susceptibility tensor

In centrosymmetric crystals,

$$\chi_{ijk}^{(2)} = 0,$$

The Mathematical Idea: Group Representations

Inversion forms a group with two elements:

$$Z_2 \cong \{E, \mathcal{I}\}, \qquad E : \mathbf{r} \to \mathbf{r}, \qquad \mathcal{I} : \mathbf{r} \to -\mathbf{r}, \qquad \mathcal{I}^2 = E$$

Its two one-dimensional representations are:

$$+1 \quad (\text{even}), \qquad -1 \quad (\text{odd}).$$

- Even: unchanged under inversion
- Odd: changes sign under inversion

Parity Under Inversion

Quantity	Transformation	Parity
$\mathbf{P}$	$\mathbf{P} \to -\mathbf{P}$	odd
$\mathbf{E}$	$\mathbf{E} \to -\mathbf{E}$	odd
σ_{jk}	$\sigma_{jk} \to \sigma_{jk}$	even

Important Point

Polar vectors such as **P** and **E** change sign under inversion, but stress is even.

Tensor Transformation Under Inversion

Under inversion, spatial coordinates transform as

$$\mathbf{r} \to -\mathbf{r}.$$

For a rank-n tensor, the components transform as

$$T'_{i_1 i_2 \cdots i_n} = \sum_{j_1, j_2, \cdots, j_n} R_{i_1 j_1} R_{i_2 j_2} \cdots R_{i_n j_n} T_{j_1 j_2 \cdots j_n}.$$

For inversion:

$$R_{ij} = -\delta_{ij}.$$

Therefore, every index picks up a factor of -1.
For a rank-3 tensor:

$$T'_{ijk} = (-1)^3 T_{ijk} = -T_{ijk}.$$

Neumann's Principle Consequence

If the crystal is centrosymmetric, inversion leaves the crystal unchanged.

By Neumann's Principle, the physical tensor must also remain invariant:

$$T'_{ijk} = T_{ijk}.$$

But for a rank-3 polar tensor under inversion:

$$T'_{ijk} = -T_{ijk}.$$

Therefore:

$$T_{ijk} = -T_{ijk} \quad \Rightarrow \quad \boxed{T_{ijk} = 0}.$$

Application 1: Piezoelectricity

Piezoelectricity is described by

$$P_i = d_{ijk}\sigma_{jk}.$$

Here, d_{ijk} is a rank-3 tensor.

For a centrosymmetric crystal:

$$d_{ijk} = 0.$$

$$\boxed{P_i = d_{ijk}\sigma_{jk} = 0}$$

Conclusion: Centrosymmetric crystals are not piezoelectric.

Why Neumann's Principle Is Powerful

Direct physical reasoning:

$$P_i = d_{ijk}\sigma_{jk}$$

Under inversion,

$$P_i \to -P_i, \qquad \sigma_{jk} \to \sigma_{jk}.$$

For a centrosymmetric crystal, the response must be unchanged:

$$P_i = -P_i \Rightarrow P_i = 0.$$

Neumann's Principle:

$$d'_{ijk} = R_{ia}R_{jb}R_{kc}d_{abc}.$$

For inversion, $R = -I$, so

$$d'_{ijk} = (-1)^3 d_{ijk} = -d_{ijk}.$$

But symmetry requires $d'_{ijk} = d_{ijk}$, hence

$$d_{ijk} = 0.$$

Neumann's Principle turns physical intuition into a general tensor-selection rule.

The Direct Approach: Very complex

To prove whether piezoelectricity is allowed, one could try to analyze the microscopic displacement of charges under stress.

$$P_i = \frac{1}{V} \sum_{\alpha} q_\alpha u_{\alpha i}$$

The displacement depends on the elastic deformation of the lattice:

$$u_{\alpha i} = u_{\alpha i}(\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12})$$

So,

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

This approach depends on microscopic structure and many tensor components.
(Of course, a lot of calculation)

Application 2: Second Harmonic Generation

Second harmonic generation is described by

$$P_i(2\omega) = \epsilon_0 \chi^{(2)}_{ijk} E_j(\omega) E_k(\omega).$$

Here, $\chi^{(2)}_{ijk}$ is also a rank-3 tensor.

For a centrosymmetric crystal:

$$\chi^{(2)}_{ijk} = 0.$$

$$\boxed{P_i(2\omega) = 0}$$

Conclusion: Centrosymmetric crystals cannot exhibit bulk electric-dipole SHG.

A Single Symmetry Test Predicts Material Functionality

Centrosymmetric?

Yes	No
$\Rightarrow$ No Piezoelectricity	$\Rightarrow$ Piezoelectricity Possible
$\Rightarrow$ No SHG	$\Rightarrow$ SHG Possible

Crystal symmetry alone predicts material functionality.

Real Materials

Material	Centrosymmetric?	Piezoelectric?	SHG?
Quartz	No	Yes	Yes
BBO	No	Possible	Yes
Silicon	Yes	No	No

Experimental observations agree exactly with the symmetry prediction.

Neumann's Principle is not just a mathematical argument – it correctly predicts the behavior of real materials.

Summary

1. Inversion symmetry corresponds to the group Z_2.
2. Polar vectors are odd under inversion.
3. A rank-3 polar tensor changes sign under inversion.
4. In a centrosymmetric crystal, Neumann's Principle requires invariance.
5. Therefore:
    - No piezoelectricity
    - No bulk electric-dipole SHG

Thank You!

Q&A

The bear is **not** centrosymmetric. $\rightarrow$

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