Applications of Group Theory to Cyrstallography

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UCSC

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What is Crystallography

Figure 1: **Quartz Crystal** - Quartz is a simple cystal structure comprised of silicon–oxygen tetrahedral, SiO_4 [2].

Figure 2: **Ice** - Ice has hexagonal Crystal structure built up from H_2O [5].

Crystals in Nature

What is a crystal?

Definition: Crystals are *homogeneous*, *anisotropic*, *solid states* whose *building blocks* are strictly three dimensional and *periodically ordered*.

Crystals:

- Quartz,
- Diamond,
- Ice,
- Snowflake.

Non-cyrstals (Amorphous):

- Plastic,
- Wood,
- Glass,
- Wool.

Divides solid states physics into two categories.

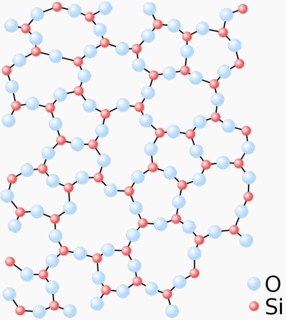


Figure 3: **Chemical Structure of Glass** - The chemical structure of glass is not periodically ordered [4].

Definition: Anisotropy is the directionality of a materials properties.

Possible anistropic properties include:

- Conductivity,
- Magnetization,
- Strength.

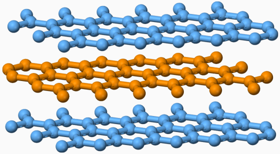
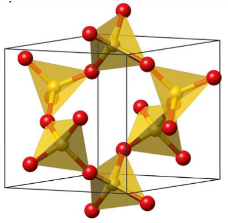


Figure 4: **Graphite** - Graphite's electrical conductivity and strength has anistropic properties [1].

There exists a relationship between the inner structure of a crystal and its outer shape.

(a)



(b)

Figure 5: **Quartz and its Interior Structure** - (a) A macroscopic depiction of quartz crystal [2] next to (b) a depiction of its internal symmetry [3].

Correspondence Principle ii

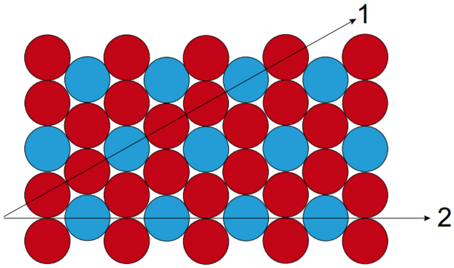


Figure 6: **Anistropy of Integrity** - This crystal has anistropy in structural integrity arising from the inner structure [3].

Basic Mathematical Structure

Crystal Patterns

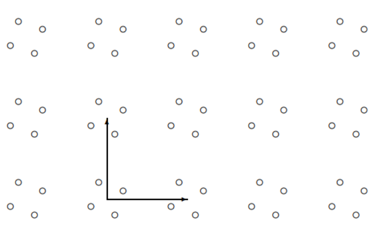


Figure 7: **Crystal Pattern** - A basic crystal pattern in $\mathbb{R}^2$ [6]

Definition: A crystal pattern is a set of points in $\mathbb{R}^n$ where the set translations leaving it invariant from a lattice in $\mathbb{R}^n$.

Definition: An affine mapping on $\mathbb{R}^n$ is a composition of a linear transformation and a translation.

Consider linear transformation, $g \in M_n(\mathbb{R})$, and translation, $t \in \mathbb{R}^n$,

$$t \circ g = \{g|t\}. \tag{1}$$

For $v \in \mathbb{R}^n$,

$$\{g|t\}(v) = gv + t. \tag{2}$$

"Seitz notation"

Consider

$$\mathcal{A}_n := \left\{ \{g|t\} : \mathbb{R}^n \to \mathbb{R}^n | g \in \mathrm{GL}_n(\mathbb{R}), t \in \mathbb{R} \right\}. \tag{3}$$

- Identity element: $\forall \{g|t\} \in \mathcal{A}_n, \quad \{\mathbb{1}|0\} \circ \{g|t\} = \{g|t\} = \{g|t\} \circ \{\mathbb{1}|0\};$
- closure: Consider $v \in \mathbb{R}^n$. Notice $\forall g, h \in \mathrm{GL}_n(\mathbb{R})$ and $\forall t, s \in \mathbb{R}^n$, we have

$$\begin{aligned} \{g|t\} \circ \{h|s\}(v) &= \{g|t\}(hv + s) = g(hv + s) + t, \\ &= (gh)v + (gs + t) = \{gh|gs + t\}(v).^{1} \end{aligned} \tag{4}$$

  Notice $gh \in GL_n(\mathbb{R}$ and $gs + t \in \mathbb{R}^n$, thus $\{gh|gs + t\} \in \mathcal{A}_n$;
- inverse: For $\{g|t\}$ consider $\{g^{-1}| - g^{-1}t\}$. As a result of computation 4 we determine $\{g|t\} \circ \{g^{-1}| - g^{-1}t\} = \{\mathbb{1}|0\} = \{g^{-1}| - g^{-1}t\} \circ \{g|t\}$. Thus $\{g^{-1}| - g^{-1}t\} = \{g|t\}^{-1}$!

[1] An immediate consequence of this rule is that $\mathcal{A}_n \cong \mathrm{GL}_n(\mathbb{R}) \ltimes \mathbb{R}^n$.

Consider

$$G := \{\{g|t\} \in \mathcal{A}_n | g \text{ is an } \textit{isometry}\} . \tag{5}$$

Definition: An isometry is a transformation that preserves distances.

Definition: A space group is a group of isometries which leave a crystal pattern invariant.

Lemma: A linear map g is an isometry if and only if g is orthagonal, that is $g^T = g^{-1}$.

The Euclidean group is thus

$$\varepsilon_n := \left\{\{g|t\} \in \mathcal{A}_n | g^T = g^{-1}\right\} \tag{6}$$

Consider mapping from a space group $\Pi : G \to \mathrm{GL}(n)$ given by

$$\Pi : \{g|t\} \mapsto g \tag{7}$$

We define

- The translation group, $T := \ker \Pi = \{\{\mathbb{1}|t\} \in G\}$ (normal in $\mathcal{A}_n$), and
- The point group, $P := \Pi(G) \cong G/T$.

Example: $\mathbb{Z}^2$

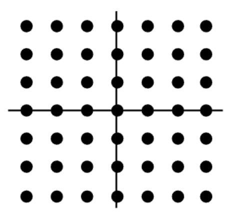


Figure 8: **Integer Lattice** - Visual depiction of the set $\mathbb{Z}^2$ [7].

Definition: A lattice in $\mathbb{R}^n$ is a set L defined as

$$L := \left\{ \sum_{i \leq n} x_i v_i \middle| x_i \in \mathbb{Z}, v_i \in B \right\} \tag{8}$$

with respect to a basis $B = \{v_i\}_{i \leq n}$ of $\mathbb{R}^n$. The set B is called the basis lattice.

Let G be a space group with translation group $T = \ker \Pi$. The translation lattice of G is then

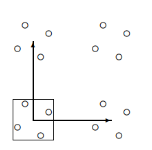
$$L = \left\{ v \in \mathbb{R}^n | \{\mathbb{1}|v\} \in T \right\}. \tag{9}$$

Unit Cell

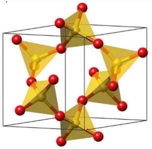
Definition: Let $L \subset \mathbb{R}^n$ be a lattice with basis $B = \{v_i\}_{i \leq n}$. The unit cell is the set, C, defined as

$$C := \left\{ \sum_{i \leq n} x_i v_i \,\middle|\, x_i \in [0,1), v_i \in B \right\}. \tag{10}$$

"Fundamental Domain"



(a)



(b)

Figure 9: **Unit Cells** - (a) The unit cell for the crystal pattern in figure 7 [6] and the unit cell for quartz from figure 5 [3].

The unit cell also fully describes stoichiometry of a crystal.

Notation: The space group element $\{g|t\}(v)$ can be described by an augmented matrix

$$\{g|t\}(v) \mapsto \left(\begin{array}{c|c} \begin{pmatrix} g_{11} & g_{12} & \dots & g_{1n} \\ g_{21} & \ddots & & \\ \vdots & & & \\ g_{n1} & & & g_{nn} \end{pmatrix} & \begin{pmatrix} t_1 \\ \vdots \\ t_n \end{pmatrix} \\ \hline 0 \quad \dots \quad 0 & 1 \end{array}\right) \begin{pmatrix} v_1 \\ \vdots \\ v_n \\ \hline 1 \end{pmatrix}$$
$$= \begin{pmatrix} g & \vec{t} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{v} \\ 1 \end{pmatrix} = \begin{pmatrix} g\vec{v} \\ 0 \end{pmatrix} + \begin{pmatrix} \vec{t} \\ 1 \end{pmatrix} = \begin{pmatrix} g\vec{v} + \vec{t} \\ 1 \end{pmatrix} \tag{11}$$

Example: The Space Group $G = p2gg$ ii

Consider basis

$$S = \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 1/2 \\ 0 & -1 & 1/2 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 1/2 \\ 0 & 1 & 1/2 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}. \tag{12}$$

We want to determine the orbit of a “molecule” at point $x = (0.2,\ 0.15)$. Let $G = \langle S \rangle$. An equivalent notion to the unit cell is the Dirichlet cell,

$$C = \left\{ w \in \mathbb{R}^n \middle| \, |w| \leq |w - v|, \forall v \in L \right\}. \tag{13}$$

Recall from equation 9, the vector latice, L, is given by

$$L = \{v \in \mathbb{R}^2 | \{\mathbb{1}|v\} \in \textbf{ker}\,\Pi\}, \text{ where } \textbf{ker}\,\Pi := \{\{g|t\} \in G\} | \{g|t\} \mapsto \mathbb{1}\} \tag{14}$$

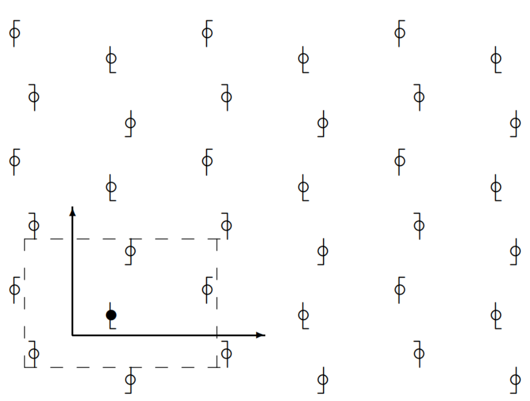


Figure 10: **Crystal patter** *p2gg* - Crystal pattern generated by the orbit of $x = (0.2, 0.15)$ under the space group generated by S in equation 12. The unit cell is in the dashed lines [6].

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