Symmetry and Properties of Crystals (MSE638)
Symmetry operations in 2D and planar lattices

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Three one step symmetry operations in 2D.

Translation: \((x, y) \xrightarrow{T} (x + ma, y + nb)\), where \(T = (1a, 2b)\).

Reflection: \((x, y) \xrightarrow{m} (-x, y)\).

Rotation: \((x, y) \xrightarrow{A_2} (-x, -y)\).

Translation – a vector (having magnitude and direction but no unique origin).

*Only* reflection changes the chirality – left handed motif becomes right handed and vice versa.

Question: how many 1 step operations are there in 1D and 3D?

1D: Translation and reflection

3D: Translation, reflection, rotation, inversion
Multiply \([1 \ 2]^T\) with any \(2 \times 2\) matrix: transform the vector

Case 1:

\[
\begin{bmatrix}
1 & 1 \\
0 & -1
\end{bmatrix}
\begin{bmatrix}
1 \\
2
\end{bmatrix}
= 
\begin{bmatrix}
3 \\
-2
\end{bmatrix}
\]

Case 2:

\[
\begin{bmatrix}
-4 & 1 \\
0 & -1
\end{bmatrix}
\begin{bmatrix}
1 \\
2
\end{bmatrix}
= 
\begin{bmatrix}
-2 \\
-2
\end{bmatrix}
\]

Case 3:

\[
\begin{bmatrix}
0 & -1 \\
1 & 0
\end{bmatrix}
\begin{bmatrix}
1 \\
2
\end{bmatrix}
= 
\begin{bmatrix}
-2 \\
1
\end{bmatrix}
\]

Case 4:

\[
\begin{bmatrix}
-1 & 0 \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
1 \\
2
\end{bmatrix}
= 
\begin{bmatrix}
-1 \\
2
\end{bmatrix}
\]

We are mainly interested in rotation and reflection matrices
Rotation matrix

- In 2D, $z$-axis is the rotation axis
- Rotation does not change length
- $x' = r \cos(\theta + \alpha) = x \cos \alpha - y \sin \alpha$, $y' = x \sin \alpha + y \cos \alpha$
- Matrix equation:
  \[
  \begin{bmatrix}
  \cos \alpha & -\sin \alpha \\
  \sin \alpha & \cos \alpha 
  \end{bmatrix}
  \begin{bmatrix}
  x \\
  y 
  \end{bmatrix}
  =
  \begin{bmatrix}
  x' \\
  y'
  \end{bmatrix}
  \]
- Rotation matrix in 2D (counter clockwise rotation):
  \[
  R(\alpha) = \begin{bmatrix}
  \cos \alpha & -\sin \alpha \\
  \sin \alpha & \cos \alpha 
  \end{bmatrix}
  \]
- Note that $\det[R] = 1$
**Reflection matrix**

- Reflection about a line $y = px$; reflection does not change length
- $x' = r \cos(2\alpha - \theta) = x \cos 2\alpha + y \sin 2\alpha$, $y' = x \sin 2\alpha - y \cos 2\alpha$
- Matrix equation:

\[
\begin{bmatrix}
\cos 2\alpha & \sin 2\alpha \\
\sin 2\alpha & -\cos 2\alpha
\end{bmatrix}
\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x' \\ y' \end{bmatrix}
\]

- Reflection matrix:

\[
m(\alpha) = \begin{bmatrix}
\cos 2\alpha & \sin 2\alpha \\
\sin 2\alpha & -\cos 2\alpha
\end{bmatrix}
\]

- $\alpha = \arctan(p)$ if $p \geq 0$ and $\alpha = \arctan(|p|) + \frac{\pi}{2}$ if $p < 0$
- Note that $\det[m] = -1$
Properties of rotation and reflection matrix

- Both $R$ and $m$ are orthogonal matrix (rotation/reflection does not change length)

- Matrix $A$ is orthogonal if $A$ preserves the length of vectors: $A\mathbf{v} \cdot A\mathbf{v} = \mathbf{v} \cdot \mathbf{v}$ (check this for $R$ and $m$)

- $A$ also preserves angles: $A\mathbf{u} \cdot A\mathbf{v} = \mathbf{u} \cdot \mathbf{v}$

- Note that $R^{-1}(\alpha) = R(-\alpha) = R^T(\alpha)$

- General property of orthogonal matrix: $A^{-1} = A^T \Rightarrow AA^T = 1$

- Check this for $R$ and $m$:

  $$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad A^{-1} = \frac{1}{\text{det}[A]} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}, \quad A^T = a_{ji} = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

- Reflection matrix is a symmetric matrix also: $m = m^T$

- A Reflection is it’s own inverse: $m = m^{-1}$
Adding two translations

Can the second translation be parallel to $T_1$?

If $T_2$ is parallel to $T_1$, it has to be an integer multiple of $T_1$

But then, we are just repeating the old set of lattice points

So, $T_1$ and $T_2$ are non-collinear and forms the 2D lattice

Unit cell: area uniquely associated to one (primitive unit cell) or more (non-primitive unit cell) lattice points

Is the choice of unit cell unique? How to select?

- pick shortest $T_1$ & $T_2$
- pick $T_1$ & $T_2$ such that the unit cell has symmetry of the lattice - do not pick a parallelogram unit cell for a square lattice
Adding translation and rotation

- Translation limits the number of possible rotations in a crystal.
- Rotation axis denoted by $A_\alpha$ or $n$, where $\alpha = \frac{2\pi}{n}$
- Denoted by *n fold* rotation axis
- $\cos \alpha = \frac{1-m}{2}$

<table>
<thead>
<tr>
<th>m</th>
<th>$\cos \alpha$</th>
<th>$\alpha$</th>
<th>n</th>
<th>Geometrical symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$+\frac{1}{2}$</td>
<td>60</td>
<td>6</td>
<td>$\Diamond$</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>90</td>
<td>4</td>
<td>$\Box$</td>
</tr>
<tr>
<td>2</td>
<td>$-\frac{1}{2}$</td>
<td>120</td>
<td>3</td>
<td>$\triangle$</td>
</tr>
<tr>
<td>3</td>
<td>-1</td>
<td>180</td>
<td>2</td>
<td>$\bigcirc$</td>
</tr>
<tr>
<td>-1</td>
<td>$+1$</td>
<td>0/360</td>
<td>1</td>
<td>$\cdot$</td>
</tr>
</tbody>
</table>
List of symmetry operations in 2D and notation

<table>
<thead>
<tr>
<th>Symmetry element</th>
<th>Chirality change</th>
<th>Analytical symbol</th>
<th>Geometrical symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Translation</td>
<td>No</td>
<td>T</td>
<td>→</td>
</tr>
<tr>
<td>Reflection</td>
<td>Yes</td>
<td>m</td>
<td></td>
</tr>
<tr>
<td>6-fold rotation</td>
<td>No</td>
<td>6</td>
<td>◯</td>
</tr>
<tr>
<td>4-fold rotation</td>
<td>No</td>
<td>4</td>
<td>□</td>
</tr>
<tr>
<td>3-fold rotation</td>
<td>No</td>
<td>3</td>
<td>△</td>
</tr>
<tr>
<td>2-fold rotation</td>
<td>No</td>
<td>2</td>
<td>()</td>
</tr>
<tr>
<td>1-fold rotation</td>
<td>No</td>
<td>1</td>
<td>.</td>
</tr>
</tbody>
</table>

Next: combine translation \((T)\) to each of the symmetry elements \((m, 2, 3, 4, 6)\) and derive the 2D lattices
2D lattices

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Translations</th>
<th>$a_1 \angle a_2$</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oblique</td>
<td>$a_1 \neq a_2$</td>
<td>$\alpha$</td>
<td>2</td>
</tr>
<tr>
<td>Rectangle</td>
<td>$a_1 \neq a_2$</td>
<td>$90^\circ$</td>
<td>2, m</td>
</tr>
<tr>
<td>Diamond</td>
<td>$a_1 = a_2$</td>
<td>$\alpha$</td>
<td>2, m</td>
</tr>
<tr>
<td>Square</td>
<td>$a_1 = a_2$</td>
<td>$90^\circ$</td>
<td>2, m, 4</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$a_1 = a_2$</td>
<td>$60^\circ, 120^\circ$</td>
<td>2, m, 3, 6</td>
</tr>
</tbody>
</table>

- Hexagonal lattice is also known as a triangular lattice
- You may find more names in the literature
- Example: centered rectangular lattice—same as diamond lattice
- Example: honeycomb lattice (famous for graphene)—this is a hexagonal lattice with two point basis
- Example: Kagome lattice—this is a hexagonal lattice with three point basis
Honeycomb and Kagome lattice
# 2D unit cells

<table>
<thead>
<tr>
<th>Unit cell</th>
<th>Translations</th>
<th>$a_1 \angle a_2$</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oblique (P)</td>
<td>$a_1 \neq a_2$</td>
<td>$\alpha$</td>
<td>2</td>
</tr>
<tr>
<td>Rectangle (P)</td>
<td>$a_1 \neq a_2$</td>
<td>$90^\circ$</td>
<td>2, m</td>
</tr>
<tr>
<td>Diamond (P)</td>
<td>$a_1 = a_2$</td>
<td>$\alpha$</td>
<td>2, m</td>
</tr>
<tr>
<td>Centered rectangle (NP)</td>
<td>$a_1 \neq a_2$</td>
<td>$90^\circ$</td>
<td>2, m</td>
</tr>
<tr>
<td>Square (P)</td>
<td>$a_1 = a_2$</td>
<td>$90^\circ$</td>
<td>2, m, 4</td>
</tr>
<tr>
<td>Hexagonal (P)</td>
<td>$a_1 = a_2$</td>
<td>$60^\circ, 120^\circ$</td>
<td>2, m, 3, 6</td>
</tr>
</tbody>
</table>

- P = Primitive (one lattice point per unit cell).
- NP = Non-primitive (multiple lattice points per unit cell).
- Lattice translation vectors: sensible choice of unit cell for a given lattice.
- But there is no unique unit cell for a given lattice - one draw an oblique unit cell in a square lattice.
- Symmetry of lattice does not depend on symmetry of unit cell !!
- Symmetry of unit cell $\leq$ symmetry of lattice.
Wigner-Seitz cell — a special primitive cell.

Area enclosing the space closer to a particular lattice point than any other is defined as the WS cell of that particular lattice point.

How to draw — join neighbors of a lattice point by lines and draw perpendicular bisectors of those lines.
Corresponding to $\vec{a}_1$ and $\vec{a}_2$ (real space lattice translation vectors), there exist a pair of vectors $\vec{b}_1$ and $\vec{b}_2$ such that $\vec{a}_i \cdot \vec{b}_j = \delta_{ij}$.

Using $\vec{b}_1$ and $\vec{b}_2$ as two translation vectors, we can construct a lattice, known as the reciprocal space lattice.

Dimension of $\vec{b}_i$ is 1/length and it’s magnitude is inversely proportional to $\vec{a}_i$.

Wigner-Seitz cell in reciprocal space: known as first Brillouin zone.

Useful for studies of diffraction, solid state physics etc.
Real and reciprocal lattice in 2D

- Real lattice vectors \( \vec{a_1} \) and \( \vec{a_2} \)
- Reciprocal lattice vectors \( \vec{b_1} \) and \( \vec{b_2} \)
- Satisfies: \( \vec{a_i} \cdot \vec{b_j} = \delta_{ij} \)
- Wigner-Seitz cell and first Brillouin zone – rotated by 90° w.r.t. each other
Experimental observation of real lattice

STM image of graphene (Nature Materials volume 10, pages 443449 (2011))
Experimental observation of reciprocal lattice

Electron diffraction pattern of graphene (PNAS)
Directions and Intercepts in real space lattice

- In crystallography, directions and intercepts are measured with respect to the lattice translation vectors (not necessarily same as Cartesian).
- However, lattice translation vectors represented in Cartesian system.
- Direction – represented by vectors in \( \vec{a}_1 \) and \( \vec{a}_2 \) basis.
- Intercepts – represented w.r.t. \( \vec{a}_1 - \vec{a}_2 \) coordinate system.
- Example: hexagonal lattice – \( \vec{a}_1 = (a, 0), \vec{a}_2 = \left( -\frac{a}{2}, \frac{\sqrt{3}a}{2} \right) \).

\[ \vec{R} = h\vec{a}_1 + k\vec{a}_2 \]

- \([hk]\) direction: \( \vec{R} = h\vec{a}_1 + k\vec{a}_2 \)
- \((hk)\) intercept: fractional coordinates \( \left( \frac{a_1}{h}, \frac{a_2}{k} \right) \)
- In general, \([hk]\) is not perpendicular to \((hk)\) intercept
- Square lattice: \([hk]\) is perpendicular to \((hk)\) intercept
- Spacing between \((hk)\) intercept: \( d_{hk} = \frac{a}{\sqrt{h^2+k^2}} \) (square lattice only)
Reciprocal space lattice

- \( (hk) \) direction, \( \vec{G}_{hk} = h\vec{b}_1 + k\vec{b}_2 \)
- Looks like \( (hk) \) direction in reciprocal lattice is perpendicular to the \( (hk) \) intercept in the real lattice (prove it)
- Perpendicular distance of the intercept from the origin: \( d_{hk} = \frac{1}{|\vec{G}_{hk}|} \)
- Reciprocal lattice points represent orientation and spacing of intercepts (2D) or planes (3D) in real lattice
- Reciprocal lattice: alternate geometrical construction of real lattice
- Using \( \vec{G}_{hk} \), one can find interplanar distance (in real space)
- Using \( \vec{G}_{hk} \), one can find angle between planes (in real space)
Reciprocal lattice: important applications

- $\vec{a}_i \cdot \vec{b}_j = \delta_{ij}$: easy to solve for the components of $\vec{b}$ in 2D
- General definition: $\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$, $\vec{b}_2 = \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$, $\vec{b}_3 = \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$
- In case of 2D, $\vec{a}_3 = a_3 \hat{z}$
- Reciprocal of $(\vec{b}_1, \vec{b}_2)$ is $(\vec{a}_1, \vec{a}_2)$
- $\vec{R} = u\vec{a}_1 + v\vec{a}_2$ can be written as $\vec{R} = \sum_j (\vec{R} \cdot \vec{b}_j) \vec{a}_j$
- Compare it with Cartesian coordinate system !!
- $\exp[2\pi i \vec{G} \cdot (\vec{r} + \vec{R})] = \exp[2\pi i \vec{G} \cdot \vec{r}]$
- Any function $u(\vec{r})$, having the periodicity of the lattice can be written as: $u(\vec{r}) = \sum_\vec{G} C(\vec{G}) \exp(2\pi i \vec{G} \cdot \vec{r})$
- Solid state physics (Bloch theorem): eigenfunction of an electron in a crystal (periodic potential) expressed as $\psi(\vec{r}) = u(\vec{r}) \exp(\vec{k} \cdot \vec{r})$, where $u(\vec{r})$ has the periodicity of the lattice
- Observed peaks in a diffraction pattern (structure factor calculation): $F_{hkl} = \sum_{j=1}^{N} f_{\vec{r}_j} \exp(2\pi i \vec{G}_{hkl} \cdot \vec{r}_j)$
Translation restricts the possible rotational symmetries in a crystal – only 2, 3, 4 and 6-fold rotation axes possible.

There exist five plane lattices in 2D – oblique, primitive rectangle, diamond or centered rectangle, square and hexagonal.

No unique unit cell for a given lattice - most sensible choice is the cell formed by lattice translation vectors $\vec{a}_1$ and $\vec{a}_2$.

Symmetry of unit cell $\leq$ symmetry of lattice.

In crystallography, directions and intercepts are measured with respect to the lattice translation vectors.

However, lattice translation (both real and reciprocal) vectors represented in Cartesian system.

$\vec{G}_{hk}$ is perpendicular to the $(h,k)$ intercept in the real lattice.

Perpendicular distance of the intercept from the origin: $d_{hk} = \frac{1}{|\vec{G}_{hk}|}$.

Reciprocal lattice points represent orientation and spacing of intercepts in real lattice.

Reciprocal lattice: alternate geometrical construction of real lattice.