Point Lattices: Bravais Lattices

Bravais lattices are point lattices that are classified topologically according to the symmetry properties under rotation and reflection, without regard to the absolute length of the unit vectors.

A more intuitive definition:
At every point in a Bravais lattice the “world” looks the same.

1D: Only one Bravais Lattice

-2a  -a   0    a    2a    3a
Wigner-Sietz Cell

1. Choose one point as the origin and draw lines from the origin to each of the other lattice points.
2. Bisect each of the drawn lines with planes normal to the line.
3. Mark the space about the origin bounded by the first set of planes that are encountered. The bounded space is the Wigner-Sietz unit cell.

1D Periodic Crystal Structures

\[ M(x) = \sum_{m=-\infty}^{\infty} M[K_m] e^{iK_m x} \]

\[ M(q) = 2\pi \sum_{m=-\infty}^{\infty} M[K_m] \delta(q - K_m) \]

\[ M[K_m] = \frac{1}{a} \int_{0}^{a} M(x) e^{-iK_m x} dx \]
Reciprocal Lattice Vectors

1. The Fourier transform in q-space is also a lattice.
2. This lattice is called the **reciprocal lattice**.
3. The lattice constant is \(2 \pi / a\).
4. The **Reciprocal Lattice Vectors** are
   \[ K_m = m \frac{2\pi}{a} \quad \text{where} \quad m = 0, \pm 1, \pm 2 \]

Atomic Form Factors & Geometrical Structure Factors

Different Atoms (1) and (2)

\[
M_a(x) = \left( f^{(1)}_a(K_m) e^{-iK_m d_1} + f^{(2)}_a(K_m) e^{-iK_m d_2} \right)
\]

Same atoms at \(d_1\) and \(d_2\)

\[
M_a(K_m) = \frac{f_a(K_m)}{S(K_m)} \left[ e^{iK_m d_1} + e^{iK_m d_2} \right]
\]
2D & 3D Crystal Structures

\[ R_i = n_1a_1 + n_2a_2 + n_3a_3 \]

A. Orthogonal Primitive Lattices Vectors

Then choose primitive lattice vectors along the \( x, y \) and \( z \) axes

\[ R_i = n_1a_1 \hat{x} + n_2a_2 \hat{y} + n_3a_3 \hat{z} \]

The 3D sampling function is

\[ S_p(r) = \sum_{i=-\infty}^{+\infty} \delta^3(r - R_i) \]

Fourier Transform of Sampling Function

\[
S_p(q) = \iiint \left( \sum_{i=-\infty}^{+\infty} \delta^3(r - R_i) \right) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r
\]

\[
= \iiint \sum_{n_1} \sum_{n_2} \sum_{n_3} \delta(x - n_1a_1)\delta(y - n_2a_2)\delta(z - n_3a_3) \cdot e^{-iqa_1x}e^{-iqa_2y}e^{-iqa_3z} dxdydz
\]

\[
= \left( \int_{-\infty}^{\infty} \delta(x - n_1a_1) e^{-iqa_1x} dx \right) \left( \int_{-\infty}^{\infty} \delta(y - n_2a_2) e^{-iqa_2y} dy \right) \left( \int_{-\infty}^{\infty} \delta(z - n_3a_3) e^{-iqa_3z} dz \right)
\]

This is a product of three independent 1D sampling functions
Reciprocal Lattice

Therefore,

\[ s_p(q) = \frac{(2\pi)^3}{a_1 \cdot (a_2 \times a_3)} \sum_{i=-\infty}^{+\infty} \delta(q - K_i) \]

The reciprocal lattice vectors are

\[ K = m_1 \frac{2\pi}{a_1} \hat{x} + m_2 \frac{2\pi}{a_2} \hat{y} + m_3 \frac{2\pi}{a_3} \hat{z} \]

with primitive lattice vectors

\[ b_1 = \frac{2\pi}{a_1} \hat{x}, \quad b_2 = \frac{2\pi}{a_2} \hat{y}, \quad b_3 = \frac{2\pi}{a_3} \hat{z} \]

3D Periodic Functions

A periodic function

\[ M(r) = M(r + R_i) \]

can be written as a convolution

\[ M(r) = M_P(r) \otimes S_P(r) \]

when \( M_P(r) = \begin{cases} M(r) & r \text{ confined to a primitive unit cell} \\ 0 & \text{otherwise} \end{cases} \)

and

\[ S_P(r) = \sum_{i=-\infty}^{\infty} \delta^3(r - R_i) \]
Reciprocal Space Representation

The convolution in real space becomes a product in reciprocal space

\[ M(q) = M_p(q) S_p(q) \]

since \( S(k) \) is a series of delta functions at the reciprocal lattice vectors, \( M_p(k) \) only needs to be evaluated at reciprocal lattice vectors:

\[
M_p(K) = \int_{-\infty}^{\infty} M_p(r) e^{-iK \cdot r} d^3r = \int_{PC} M(r) e^{-iK \cdot r} d^3r.
\]

Here PC mean to integrate over one primitive cell, such as the Wigner-Seitz cell.

Therefore, \( M(q) \) is crystal structure in q-space

\[
M(q) = \sum_i \frac{(2\pi)^3}{a_1 \cdot (a_2 \times a_3)} M_p(K_i) \delta^3(q - K_i)
\]

Generalized Fourier Transform

\[
M(r) = \int_{-\infty}^{\infty} M(q) e^{iq \cdot r} \frac{d^3q}{(2\pi)^3}
= \int_{-\infty}^{\infty} \sum_i \frac{(2\pi)^3}{a_1 \cdot (a_2 \times a_3)} M_p(K_i) \delta^3(q - K_i) e^{iq \cdot r} \frac{d^3q}{(2\pi)^3}
= \sum_i \frac{1}{a_1 \cdot (a_2 \times a_3)} M_p(K_i) e^{iK_i \cdot r}
\]

Therefore this is a generalized Fourier Transform in 2D and 3D

\[
M(r) = \sum_i M[K_i] e^{iK_i \cdot r}
\]

with

\[
M[K_i] = \frac{1}{a_1 \cdot (a_2 \times a_3)} \int_{PC} M(r) e^{-iK_i \cdot r} d^3r
\]
Form factors and Structure Factors

\[ M(q) = M_p(q)S_p(q) \]

\( M_p(q) \) is the FT of atoms in one primitive cell. Let each atom \( j \) of an \( n \) atom basis have a density function \( f_{a}^{(j)}(r) \) and be located a position \( d_j \). The Fourier components that are needed for \( M_p \) are

\[ M_p(K) = \sum_{j=1}^{n} f_{a}^{(j)}(K)e^{-iK \cdot d_j} \]

where the atomic form factor is \( f_{a}^{(j)}(K) \).

If the basis consist of all the same type of atoms then,

\[ M_p(K) = f_p(K) \sum_{j=1}^{n} e^{-iK \cdot d_j} \]

Atomic form factor

Geometrical Structure Factor

Oblique Primitive Lattice Vectors

\[ a_1 \cdot a_2 \neq 0 \]
**Periodic functions with oblique lattice vectors**

Periodic function

\[ M(r) = M(r + R_i) \]

\[ M(r) = \int_{-\infty}^{\infty} M(q) e^{i\mathbf{q} \cdot \mathbf{r}} \frac{d^3 q}{(2\pi)^3} \]

\[ M(r + R_i) = \int_{-\infty}^{\infty} M(q) e^{i\mathbf{q} \cdot (r + R_i)} \frac{d^3 q}{(2\pi)^3} \]

\[ = \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot \mathbf{R}_i} M(q) e^{i\mathbf{q} \cdot \mathbf{r}} \frac{d^3 q}{(2\pi)^3}. \]

Therefore need to find a set \( \{K_j\} \) of all possible vectors \( q \) such that

\[ e^{iK_j \cdot R_i} = 1 \quad \Rightarrow \quad K_j \cdot R_i = 2\pi (\text{integer}) \]

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**Reciprocal Lattice Vectors for Oblique vectors**

Let

\[ \mathbf{R}_i = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \]

And assume that \( \{K_j\} \) also forms a lattice with primitive vectors \( b_k \)

\[ \mathbf{K}_j = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3 \]

Then to have \( \mathbf{K}_j \cdot \mathbf{R}_i = 2\pi (\text{integer}) \) we need \( a_i \cdot b_j = 2\pi \delta_{i,j} \)

By construction, the primitive reciprocal lattice vectors are

\[ b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} \quad b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot (a_2 \times a_3)} \quad b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot (a_2 \times a_3)} \]
**Sampling function for oblique vectors**

Write all vectors in real space in terms of the \(a_i\)'s and write all vectors in reciprocal space in terms of the \(b_j\)'s

\[
\mathbf{r} = \alpha_1 a_1 \hat{a}_1 + \alpha_2 a_2 \hat{a}_2 + \alpha_3 a_3 \hat{a}_3 \\
\mathbf{q} = \gamma_1 b_1 \hat{b}_1 + \gamma_2 b_2 \hat{b}_2 + \gamma_3 b_3 \hat{b}_3
\]

Then the dot product is simply

\[
\mathbf{q} \cdot \mathbf{r} = 2\pi (\gamma_1 \alpha_1 + \gamma_2 \alpha_2 + \gamma_3 \alpha_3)
\]

And as proven in the notes, even for the oblique vectors,

\[
S_p(r) = \sum_{i=-\infty}^{\infty} \delta^3(r - R_i) \quad \leftrightarrow \quad S_p(q) = \frac{(2\pi)^3}{a_1 \cdot (a_2 \times a_3)} \sum_i \delta^3(q - K_i)
\]

---

**Rectangular Lattice**

The primitive lattice vectors are orthogonal in this case.

\[
\mathbf{a}_1 = a_1 \mathbf{i}_x \quad \mathbf{a}_2 = a_2 \mathbf{i}_y \quad \mathbf{a}_3 = a_3 \mathbf{i}_z
\]

The primitive reciprocal lattice vectors are also define a rectangular lattice, but rescaled inversely.

\[
\mathbf{b}_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} \quad \mathbf{b}_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot (a_2 \times a_3)} \quad \mathbf{b}_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot (a_2 \times a_3)}
\]

\[
\mathbf{b}_1 = \frac{2\pi}{a_1} \mathbf{i}_x \quad \mathbf{b}_2 = \frac{2\pi}{a_2} \mathbf{i}_y \quad \mathbf{b}_3 = \frac{2\pi}{a_3} \mathbf{i}_z
\]
Real & Reciprocal lattices in 2 D

- Two lattices associated with crystal lattice
- \( b_1 \) perpendicular to \( a_2 \), \( b_2 \) perpendicular to \( a_1 \)
- Wigner-Seitz Cell of Reciprocal lattice called the "First Brillouin Zone" or just "Brillouin Zone"

BCC ↔ FCC

BCC in real space
\[
\begin{align*}
a_1 &= \frac{a}{2} (i_y + i_z - i_x) \\
a_2 &= \frac{a}{2} (i_z + i_x - i_y) \\
a_3 &= \frac{a}{2} (i_x + i_y - i_z)
\end{align*}
\]
has an FCC reciprocal lattice with
\[
\begin{align*}
b_1 &= \frac{2\pi}{a} (i_y + i_z) \\
b_2 &= \frac{2\pi}{a} (i_z + i_x) \\
b_3 &= \frac{2\pi}{a} (i_x + i_y)
\end{align*}
\]

FCC in real space
\[
\begin{align*}
a_1 &= \frac{a}{2} (i_y + i_z) \\
a_2 &= \frac{a}{2} (i_z + i_x) \\
a_3 &= \frac{a}{2} (i_x + i_y)
\end{align*}
\]
has a BCC reciprocal lattice with
\[
\begin{align*}
b_1 &= \frac{2\pi}{a} (i_y + i_z - i_x) \\
b_2 &= \frac{2\pi}{a} (i_z + i_x - i_y) \\
b_3 &= \frac{2\pi}{a} (i_x + i_y - i_z)
\end{align*}
\]
Face Centered - Body Centered Cubic
Reciprocal to one another

Reciprocal lattice is
Face Centered Cubic

Primitive vectors and the
conventional cell of base lattice

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Face Centered Cubic

Wigner-Seitz Cell for
Face Centered Cubic Lattice

Brillouin Zone =
Wigner-Seitz Cell for
Reciprocal Lattice
X-Ray Diffraction

Plane wave $e^{i\mathbf{k} \cdot \mathbf{r}}$

Observation point $\mathbf{r}'$

Outgoing spherical wave

scattering point $\mathbf{r}$

The total amplitude of the wave arriving at $\mathbf{r}'$ from all the $\mathbf{r}$ points in the sample located with density $n(\mathbf{r})$ is

$$\Phi(\mathbf{r}') = \int_{\text{sample}} e^{i\mathbf{k} \cdot \mathbf{r}} n(\mathbf{r}) \phi(\mathbf{r} - \mathbf{r}') \, d^3\mathbf{r}$$
Scattering in the Far-field

In the far-field region, |r' - r| >> L and we can use the approximation

\[ |r' - r| \approx |r' - r_o| \]

so that

\[ \Phi(r') \approx \frac{A e^{i k' \cdot r'}}{|k' \cdot (r_o - r')|} \int_{\text{all space}} n(r) e^{-i(k-k') \cdot r} d^3r \]

Because the density is a periodic function,

\[ n(r) = \sum_{\ell} \tilde{n} \delta_{\ell,0} = \sum_{\ell} n[K_\ell] e^{i K_\ell \cdot r} \]

So that

\[ \Phi(r') = \frac{A e^{i k' \cdot r_o}}{|k' \cdot (r_o - r')|} \sum_{\ell} n[K_\ell] \delta^3(k' - k + K_\ell) \]

Therefore, the amplitude is zero unless \( k' = k - K_\ell \).

The Bragg Condition

Squaring the condition \( k' = k - K_\ell \) gives

\[ |k'|^2 = |k|^2 - 2k \cdot K_\ell + |K_\ell|^2 \]

X-ray diffraction is elastic, it does not change the magnitude of the wave vector, so that |k| = |k'|, which gives the Bragg Condition

\[ k \cdot \widehat{K_\ell} = \frac{1}{2} |K_\ell| \]

unit vector
Bragg Condition

This sweeps out a plane at the perpendicular bisector of $K$. These are the same planes that define the Wigner-Sietz cell construction, and for this reciprocal space define the First Brillouin zone.

\[ k \cdot \hat{K}_\ell = \frac{1}{2} |K_\ell| \]

\[ k \sin \theta = \frac{\pi m}{a} \]

Or

\[ \sin \theta = \frac{n\lambda}{2a} \]