• Real crystals

By attaching a basis containing one or more atoms or molecules, to each lattice point, we can construct a real crystal.

Silicon: fcc lattice with lattice constant 5.431 Å

Diamond, Germanium, and α-Sn

Related: Zinc blende structure which is also fcc but has two different atoms in each basis.

What are the lattice vectors of the fcc structure?

\[ \mathbf{a}_1 = \frac{a}{2} (\hat{1} + \hat{2}), \quad \mathbf{a}_2 = \frac{a}{2} (\hat{1} + \hat{3}), \quad a_3 = \frac{a}{2} (\hat{1} + \hat{3}) \]
- What is the volume of the primitive unit cell for fcc lattice?

1. Count the number of atoms in the fcc: 8 corners have \( \frac{1}{8} \) atom each, 6 faces have \( \frac{1}{2} \) atom each so total 4.

2. Volume of fcc cell is \( a^3 \), so the primitive unit cell has volume \( a^3/4 \) (1 atom per primitive unit cell).

Another way: \[ V = a_1 \cdot \left( \frac{a_2 \times a_3}{2} \right) \]
\[ = \frac{a^3}{8} \left( \frac{1}{4} + \frac{1}{2} \right) = a^3/4 \]

Volume of a parallelipiped is area of base times height
\[ V = |a_1 \cdot (a_2 \times a_3)| = |a_2 \cdot (a_3 \times a_1)| = |a_3 \cdot (a_1 \times a_2)| \]

Silicon (and Ge) have a basis of two atoms, so there are 8 atoms per fcc cell and 2 per unit cell, or \( 8/a^3 \) atoms per unit volume.

Crystal lattices have repeating planes of atoms. These parallel,
equally spaced planes are usually represented by Miller indices, which are given by 3 integers in parentheses \((h kn)\).

Miller indices are obtained by:

1. Find the intercept of the atomic plane with the axes formed by the lattice vectors \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \).

2. Take the reciprocal of the intercepts and reduce to the smallest integers that have the same ratio as the original set.

3. If an intercept is negative, place a bar above the corresponding number.

Example: the 6 faces of a cubic unit cell are given by Miller indices \((100), (010), (001), (100), (001), \) and \((00\bar{1})\). All equivalent planes can be denoted by \( \bar{3}100\bar{3} \),
Similarly, a direction in a crystal can be given by a set of indices \([h k l n]\). A family of equivalent directions can be grouped together as \([h k l n]\).

**Note:** the \((h k n l)\) plane is perpendicular to the \([h k l n]\) direction.

- **Reciprocal lattice**

A periodic function in time can be represented by a Fourier series

\[
f(t) = \sum_{n=-\infty}^{\infty} \left[ a_n \sin \left( \frac{2\pi n t}{T} \right) + b_n \cos \left( \frac{2\pi n t}{T} \right) \right] = \sum_{n=-\infty}^{\infty} \left( a_n e^{i2\pi nt/T} + b_n e^{-i2\pi nt/T} \right)
\]

where the complex angular frequency is \(\omega = 2\pi n / T\) and \(T\) is the period \(f(t + T) = f(t)\).

The same can be done with functions in real space: if \(f(x) = f(x + \alpha)\), then

\[
f(x) = \sum_{n=-\infty}^{\infty} \left( a_n e^{i\alpha k_n x} + b_n e^{-i\alpha k_n x} \right)
\]
where the wavevector is \( k_x = 2\pi / a \).

The same applies in 3D if a function \( n(\vec{r}) \) is periodic \( n(\vec{r}) = n(\vec{r} + \vec{G}) \) then we have

\[
n(\vec{r}) = \sum_{\vec{G}} n_\vec{G} e^{i \vec{r} \cdot \vec{G}}
\]

and equivalently

\[
n_{\vec{a}} = \frac{1}{V} \int n(\vec{r}) e^{-i \vec{r} \cdot \vec{G}} \, dV
\]

where \( V \) is the unit cell volume given by the lattice vectors \( \vec{a}_1, \vec{a}_2, \vec{a}_3 \) as \( V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| \).

\( \vec{G} \) is the reciprocal space lattice vector composed from lattice vectors in reciprocal space as

\[
\vec{G} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3
\]

where \( m_1, m_2, m_3 \) are integers.

What are reciprocal space lattice vectors \( \vec{b}_1, \vec{b}_2, \text{ and } \vec{b}_3 \)?
We require that \( \phi(\vec{r}) = n(\vec{r} + \vec{R}) \) is periodic, with \( \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \).

\[
\phi(\vec{r} + \vec{R}) = \sum_{n} n e^{i(\vec{R} \cdot \vec{r} + \vec{R} \cdot \vec{a})} = \sum_{n} n e^{i\vec{R} \cdot \vec{r}}
\]

Therefore we need \( \vec{R} \cdot \vec{a} = 2\pi \) so \( \vec{R} \cdot \vec{a} = 2\pi \).

\[
2\pi = (n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3) \cdot (m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3)
\]

Make life simple, require that \( a_i \cdot b_j = 2\pi \delta_{ij} \) where \( \delta_{ij} \) is the Kronecker delta (\( \delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i \neq j \end{cases} \)).

Then \( a_i \cdot b_i = 2\pi \) so let

\[
b_i = 2\pi \frac{(\vec{a}_2 \times \vec{a}_3)}{|V|} \quad \text{where} \quad V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| \quad \text{so that}
\]

\[
a_i \cdot b_i = 2\pi \frac{2\pi a_i \cdot (\vec{a}_2 \times \vec{a}_3)}{a_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi 
\]

\[
b_2 = 2\pi \frac{(\vec{a}_2 \times \vec{a}_1)}{|V|} \quad \text{and} \quad b_3 = 2\pi \frac{(\vec{a}_1 \times \vec{a}_2)}{|V|}
\]
What is the reciprocal lattice of the fcc lattice?

\[ \vec{a}_1 = \frac{a}{2} (\hat{1} + \hat{2}), \quad \vec{a}_2 = \frac{a}{2} (\hat{2} + \hat{3}), \quad \vec{a}_3 = \frac{a}{2} (\hat{3} + \hat{1}) \]

\[ \vec{b}_1 = \frac{2\pi}{a} (\hat{1} + \hat{2} - \hat{3}), \quad \vec{b}_2 = \frac{2\pi}{a} (\hat{2} - \hat{1} + \hat{3}), \quad \vec{b}_3 = \frac{2\pi}{a} (\hat{3} + \hat{1} - \hat{2}) \]

This is the bcc lattice in reciprocal space, with a lattice constant \( \frac{2\pi}{a} \).

Ex: Reciprocal lattice of the SC (simple cubic) lattice:

\[ \vec{a}_1 = a \hat{x}, \quad \vec{a}_2 = a \hat{y}, \quad \vec{a}_3 = a \hat{z} \]

\[ \mathbf{V} = \vec{a}_1 \times (\vec{a}_2 \times \vec{a}_3) = a^3 \hat{x} \times (\hat{y} \times \hat{z}) = a^3 \]

\[ \vec{b}_1 = \frac{2\pi}{\sqrt{3}} (\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a} \times a^2 \left( \frac{\hat{y}}{a} \times \frac{\hat{z}}{a} \right) = \frac{2\pi}{a} \hat{x} \]

\[ \vec{b}_2 = \frac{2\pi}{a} (\hat{x} \times \hat{z}) = \frac{2\pi}{a} \hat{y} \]

\[ \vec{b}_3 = \frac{2\pi}{a} (\hat{x} \times \hat{y}) = \frac{2\pi}{a} \hat{z} \]

The reciprocal lattice of the SC lattice is again a SC lattice with a lattice constant \( \frac{2\pi}{a} \).