NaCl (rock salt) structure

- FCC
- 2-ion basis
- \((000, \frac{1}{2}00)\)
- 4 formula units in a unit cell.

CsCl Structure

- SC
- 2-ion basis
- \((000, \frac{1}{2} \frac{1}{2} \frac{1}{2})\)
- 1 formula unit in a unit cell.

HCP Structure

- A layer
- B layer
- C layer
- \((111)\)
- FCC

Hexagonal Close-Packed Structure (Be, Mg, Ti)

- Lattice: HCP
- Basis: 2 atoms \((000, \frac{2}{3} \frac{1}{3} \frac{1}{3})\)
- PF = 0.74
(D) Diamond Structure (C, Si, Ge)

Lattice: FCC
Basis: 2 carbon atoms (000, \(\frac{1}{4} \frac{1}{4} \frac{1}{4}\)), 4 basis units (8 atoms) in a unit cell. PF = 0.34

Diamonds Aren't Forever

Alchemy for diamonds? A flash of laser light can briefly put a few atomic layers of graphite (which is considered a form of coal) into a form closer to diamond, according to experiments. A future technology may be able to permanently convert precisely selected regions of a graphite thin film into diamond, perhaps for use in nanoscale circuits.

A flash of light can temporarily alter the structure of graphite. A team reporting in the 15 August Physical Review Letters Daniel reported for a brief moment at low-exposure to light changes the chemical bonding in graphite to a form reminiscent of diamond. Future improvements may allow a complete conversion to diamond. This research could lead to new nanoscale techniques wherein a laser builds structures of diamond and graphite on a surface of a carbon thin film.
Chapter 2. Wave Diffraction and Reciprocal Lattice

What do we need to study crystal structures?

A probe that can “see” or “feel” the crystal lattice structures, i.e., a probe with a size comparable to that of the lattice unit cells, 2 – 5 Å.

-- Diffraction of X-ray photons, neutrons, electrons.

de Broglie wavelength:
\[ \lambda = \frac{h}{p} = \frac{h}{(mv)} = \frac{h}{(2mE)^{1/2}} \]

X-ray diffraction setup

-- Scanning probe microscopes
1. Diffraction of Waves by Crystals

(A) Diffraction techniques

(a) X-ray: $\lambda \sim 0.01 \, \text{Å} - 100 \, \text{Å}$

Electromagnetic radiation spectrum

<table>
<thead>
<tr>
<th>$10^{-16}$</th>
<th>$10^{-14}$</th>
<th>$10^{-12}$</th>
<th>$10^{-10}$</th>
<th>$10^{-8}$</th>
<th>$10^{-6}$</th>
<th>$10^{-4}$</th>
<th>$10^{-2}$</th>
<th>$10^{0}$</th>
<th>$10^{2}$</th>
<th>$10^{4}$</th>
<th>$10^{6}$</th>
<th>$10^{8}$</th>
<th>$10^{10}$</th>
<th>$10^{12}$</th>
<th>$10^{14}$</th>
<th>$10^{16}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma$</td>
<td>X</td>
<td>UV</td>
<td>IR</td>
<td>Microwave</td>
<td>FM</td>
<td>AM</td>
<td>Radio waves</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Synchrotron radiation

Spectrum of x-ray from synchrotron radiation

Diffraction re-visited

X-ray diffraction by crystals can be treated from two different (but equivalent) views:

- Bragg’s view: the lattice is a stack of planes, where Bragg reflection (refraction) occurs.
- von Laue’s view: the lattice is a periodic array of atoms.
(b) Electron beam
\[ \lambda = \frac{h}{p} = \frac{h}{(m_e v)} = \frac{h}{(2m_e E)^{1/2}} \]
For \( \lambda = 1 \text{ Å}, E \sim 150 \text{ eV} \quad (v \sim 7 \times 10^6 \text{ m/s})

(c) Neutron beam
\[ \lambda = \frac{h}{(2m_n E)^{1/2}}, \]
For \( \lambda = 1 \text{ Å}, v \sim 4 \times 10^3 \text{ m/s}, \quad E \sim 0.08 \text{ eV} \).

Neutrons do not interact with electrons, therefore, they are scattered entirely by nuclei (x-ray is scattered entirely by electrons).

Neutrons are more useful than x-rays for determining the crystal structures of solids containing light elements.

(B) The Bragg Law
For the two light rays to have constructive interference, the path difference must be an integer multiple of the wavelength, i.e.,
\[ \Delta l = n\lambda \]
If the spacing between adjacent planes is \( d \), then
\[ \Delta l = 2d \sin \theta \]

The conditions for constructive interference (bright spot) is:
\[ 2d \sin \theta = n\lambda \quad \text{for } \lambda \leq 2d \]
(Bragg law)

Bragg diffraction
-- Specular (mirror like) reflection from crystal planes.
-- No reflection if \( \lambda > 2d \)
-- For \( \lambda < 2d \), reflection only at certain angles

Sir William Henry Bragg (1862-1942),
William Lawrence Bragg (1890-1971)
The values of $\lambda$ and $\theta$ yield the distances between crystal planes, $d$, which is used to deduce the structure.

**Low index planes**
- High atom density
- Large spacing

**High index planes**
- Low atom density
- Smaller spacing

- The lattice structure determines the position of the lines.
- The basis determines the relative intensity.

### 2. Scattered Wave Amplitude

**(A) Fourier Analysis**

Any periodic function, $f(t) = f(t+T)$, can be expressed as an infinite sum of *sines* and *cosines* with frequencies $n/T$.

$$f(t) = a_0 + \sum_{n=1}^{\infty} a_n \cos \left( \frac{2\pi n t}{T} \right) + \sum_{n=1}^{\infty} b_n \sin \left( \frac{2\pi n t}{T} \right) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi n t/T}$$

For real functions, $c_n^* = c_n$.
The same approach can be used to a periodic function of space.

For a Bravais lattice, a local physical property (e.g., electron density) can be expressed as:

\[ n(r + T) = n(r), \]

where \( T = u_1a_1 + u_2a_2 + u_3a_3 \)

\( u_i \rightarrow \) integers

In 1-dimension, \( n(x+a) = n(x) \)

Direct lattice (Real space)
\[ x \Rightarrow \text{direct lattice vector} \]

Fourier Transform
\[ n(x) = \sum_p n_p e^{i2\pi px/a} \equiv \sum_p n_p e^{iGx} \]

where \( n^*_{-p} = n_p \)

The allowed values of \( G=2\pi p/a \) also form a periodic 1-d array.