Scattering from Crystals.

How can one determine the structure of a crystalline material? One of the common methods, originally implemented in 1912 involves scattering of X-rays from the crystal. Similar schemes are available for scattering of particles such as electrons + neutrons.

Conceptually, the simplest scheme involves bombarding the crystal with monochromatic radiation, i.e., X-rays with one wavelength traveling in a particular direction.

The quantities which can be measured are:

i) the wavelength (or frequency) of the incoming X-rays

ii) the outgoing X-rays.

iii) the angle between the scattered beam and the incoming beam, $2\theta$.

By varying the direction + wavelength of the incoming X-rays and measuring the above, one can hopefully infer something about the lattice structure (is it cubic, fcc, etc., ...) and the lattice spacing.
General framework for describing scattering

Without considering the physical details about the interaction of X-rays with charged particles in the crystal and each other or the interaction between different scattered X-rays, we can set up a general scheme for describing scattering.

Recall that a monochromatic wave travelling in the \( \hat{\mathbf{r}} \) direction is described by specifying a wavenumber

\[
k = \frac{2\pi}{\lambda}
\]

and a corresponding wavefunction whose complex representation is:

\[
\Psi(\mathbf{r}, t) = A e^{i(k \cdot \mathbf{r} - \omega t)}
\]

\( \omega = vk \).

and it is convenient to use a vector wavenumber:

\[
\mathbf{k} = \frac{2\pi}{\lambda} \hat{\mathbf{r}}.
\]

This includes all the information about the wavelength and direction. Thus one can represent the wave by:

\[
\Psi(\mathbf{r}, t) = A e^{i(k \cdot \mathbf{r} - \omega t)}
\]

**Example:** Plane wave in the \( \hat{x} \) direction:

\[
\Psi(x,y,z,t) = A e^{i(kx - \omega t)}
\]

and the real part gives:

\[
A \cos (kx - \omega t)
\]
We will need two vectors to describe the scattering process:

\( \mathbf{k}_o \) - describes incoming wave

\( \mathbf{k} \) - describes scattered wave.

In what follows, we will only consider situations where the magnitudes of these are identical. This is called **elastic scattering** since the momentum of these waves is \( \mathbf{p}_o = \hbar \mathbf{k}_o \) and \( \mathbf{p} = \hbar \mathbf{k} \) and if the magnitude of the momentum is constant, then the energy will also be constant.

**Example:** Consider Bragg scattering off crystal planes.

Then note the two vectors in the diagram above. Can we use these to describe the planes? How is \( \Theta \) related to them? First.

Clearly, \( 2\Theta \) is the angle between the planes.
But we can also see that

\[
\hat{s} = \hat{k} - \hat{k}_0
\]

is normal to the scattering planes. In all circumstances, this is called the scattering vector. In general, we will see that the scattering vector is normal to a crystal plane.

The scattering vector has magnitude,

\[
S = \sqrt{\hat{s} \cdot \hat{s}}
\]

But

\[
\hat{s} \cdot \hat{s} = \hat{k} \cdot \hat{k} + \hat{k}_0 \cdot \hat{k}_0 - 2 \hat{k} \cdot \hat{k}_0
\]

\[
= k^2 + k_0^2 - 2k_k_0 \cos \theta
\]

For elastic scattering \( k_0 = k \) and thus

\[
\hat{s} \cdot \hat{s} = 2k^2 - 2k^2 \cos \theta
\]

\[
= 2k_0^2 \left( 1 - \cos \theta \right) = 2k_0^2 \left( 2 \sin^2 \theta \right)
\]

\[
= 4k_0^2 \sin^2 \theta
\]

\[\Rightarrow \]

\[
S = 2k_0 \sin \theta
\]

Note that \( \theta \) ranges from 0 to \( \pi \). Since \( 2\theta \) ranges from 0 to \( 2\pi \)
Physical description of scattering

The general task will be to:

Relate scattering vectors $\mathbf{s}'$ to the crystal structure. In particular, we will need to relate these to the crystal lattice vectors.

The basic physical mechanism behind scattering involves interactions between electromagnetic (or particle) waves and charged particles. In a crystal lattice this means the scattering of electromagnetic waves off electrons.

To understand this requires several steps:

1) describing scattering of X-rays off one electron.

2) describing scattering of X-rays off a distribution of charge (or electrons) such as is found in one atom.

3) describing the scattering of X-rays off a regular lattice of atoms as is found in a crystal.

These require, in order

1) scattering length of an electron $\rightarrow F_e$

2) atomic scattering factor (for one atom) $\rightarrow F_a$.

3) lattice scattering factor (for lattice) and the crystal scattering factor (for a lattice with basis) $\rightarrow F_S$ and $F_F$

In general these each depend on the scattering angle $\theta$ and $F_S$ and $F_F$ also depend on the lattice structure. Then the intensity of the scattered wave is related to the amplitude of the scattered wave:

$$A_{sc} = SF_aF_e$$

with

$$I = |A_{sc}|^2$$
Of these, the lattice structure factors depend purely on the arrangement of atoms and not on what occupy the lattice sites. We expect that this will best reflect the crystal structure.

How will we calculate these? The basic picture is that an incoming X-ray or EM wave is absorbed by the electron, which then radiates at the same frequency in all directions:

Clearly the scattering length will be calculated by considerations of electromagnetic radiation.

However, the atomic form factor and the lattice and crystal factors can be calculated from more general considerations of interference of waves. So, for example for an atom with two outer shell electrons:

Calculating this will require a detailed knowledge of the atomic structure and the distribution of electronic charge within the atom. The key idea is that interference will occur between the multiple scattered waves.
The crystal structure factor \( F \) will depend on the arrangement of atoms at each site. To simplify the discussion, we shall assume that there is only one, in which case \( |F| \gg 1 \) and can be ignored. The elementary lattice structure factor will depend on the lattice arrangement and interference between scattered waves off the lattice sites.