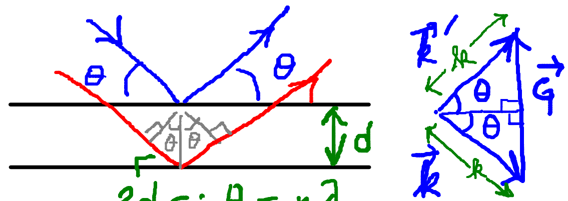
Lecture 05

Tuesday, January 24, 2012

The relation between $\Delta\vec{k} = \vec{G}$ and $2d\sin\theta = n\lambda$

$\Delta\vec{k} = \vec{G}$ is the one to remember, and is much deeper in content. Using this, the familiar $2d\sin\theta = n\lambda$ can be *derived*.

The derivation depends critically on homework 2. So, it is worth summarizing the result of that homework problem.



$2d\sin\theta = n\lambda$
(constructive interference)

This situation is noted in the above diagram, where $\vec{G} \perp$ planes. Let us apply $\Delta\vec{k} = \vec{G} = \vec{G}_n$. Thus, $|\Delta\vec{k}| = |\vec{G}_n| = n2\pi/d$. On the other hand, from the above triangle, $|\Delta\vec{k}| = 2k\sin\theta = \frac{4\pi}{\lambda}\sin\theta$. Equating these two expressions for $|\Delta\vec{k}|$, we get $2d\sin\theta = n\lambda$.

For a set of lattice planes (h,k,l), reciprocal vectors $\vec{G}_n = n(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$, with non-zero integer n, and only they, are perpendicular to those planes, with $d = 2\pi/|\vec{G}_{n=\pm 1}|$.

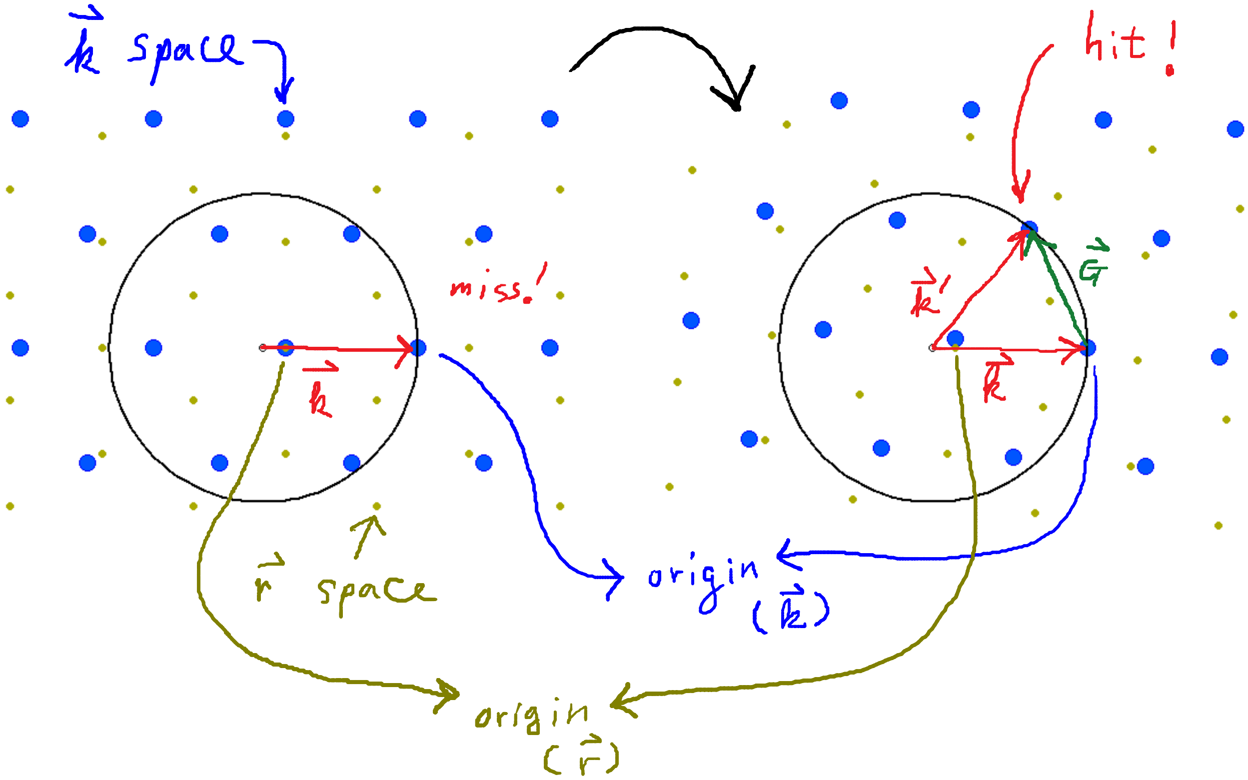
A 1-to-1 correspondence between
(h,k,l) plane $\Leftrightarrow \vec{G} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

Notation matter

(hkl)	Miller indices for lattice <u>planes</u>; think $h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$
{hkl}	Symmetry equivalent lattice planes For example, in a cubic lattice $\{100\}$ means the collection of $(100), (\bar{1}00), (010), (0\bar{1}0), (001), (00\bar{1})$.
[hkl]	The <u>direction</u> parallel to $h\vec{a} + k\vec{b} + l\vec{c}$

Ewald sphere

rotate sample



A nice graphical representation of $\Delta\vec{k} = \vec{G}$.

- Put the end point of $\vec{k}$ at one of the reciprocal lattice points.
- Draw a sphere around the starting point of $\vec{k}$.
- If any other reciprocal lattice point is on the sphere, then that point defines $\vec{k}'$ such that $\Delta\vec{k} = \vec{G}$.
- Why sphere? Since $|\vec{k}| = |\vec{k}'|$, i.e. an elastic scattering.

Shows that the diffraction condition, while not easy to meet, is met.
So a diffraction experiment is characterized by flat background with some well defined peaks as the experimental geometry is changed (e.g. in a "θ-2θ" scan). See figures in text.

A peak in a diffraction experiment is indexed as (hkl), the Miller indices corresponding to $\vec{G}$.

$\boxed{\text{Scattering amplitude, form factor, structure factor and notations}}$

As we discussed already, the scattering amplitude f is generally defined as

$$\psi = \exp(i\vec{k}\cdot\vec{r}) + \frac{f}{r}\exp(ikr)$$

Note that the dimension of f is length. Often, however, we will define a dimensionless quantity: atomic form factor or basis structure factor, as we will discuss now are examples. They are related to f. In defining these dimensionless quantities, a typical length scale is divided out. In the case of (the normal) X-ray scattering, that length scale is the well-known Thomson scattering length $= r_c\sqrt{\frac{1+\cos^2 2\theta}{2}}$ where $r_c = \frac{e^2}{mc^2}$ is the classical radius of the electron.

Unfortunately, there is a notation issue here. Atomic form factor is also written as f! As in the textbook! In this note, however, we will use $\tilde{f}$ for the structure factor, reserving f for the scattering amplitude.

Lastly, the textbook uses the word "scattering amplitude" to mean not f but f divided by a certain distance. Kittel uses F for that scattering amplitude. We do not need to be too concerned with it. It suffices to know that our f is proportional to his F.

Atomic form factor

Recall that $f = f_b L$, with $f_b \propto \int d\vec{r} V_b(\vec{r}) e^{-i\Delta\vec{k}\cdot\vec{r}}$, and $L = \sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}}$.

- f_b is identical for each lattice point.
- Thus, it suffices to consider the basis assigned to $\vec{R} = 0$ when we consider f_b.

Now, assume that there are s atoms in the basis at positions $\vec{r}_j$. Then,

$$\begin{aligned} f_b &\propto \sum_j \int d\vec{r} V_j(\vec{r} - \vec{r}_j) e^{-i\Delta\vec{k}\cdot\vec{r}} \\ &= \sum_j e^{-i\Delta\vec{k}\cdot\vec{r}_j} \int d\vec{r} V_j(\vec{r} - \vec{r}_j) e^{-i\Delta\vec{k}\cdot(\vec{r}-\vec{r}_j)} \\ &= \sum_j e^{-i\Delta\vec{k}\cdot\vec{r}_j} \int d\vec{s} V_j(\vec{s}) e^{-i\Delta\vec{k}\cdot\vec{s}} \end{aligned}$$

This motivates the following definition of the atomic form factor, $\tilde{f}_j \propto \int d\vec{r} V_j(\vec{r}) e^{-i\Delta\vec{k}\cdot\vec{r}}$. Note that the theory described so far is for an electron/neutron diffraction. For light scattering, the details of the interaction $(-\frac{m}{2\pi\hbar^2} V_j(\vec{r}))$ will be different while the phase factor $(e^{-i\Delta\vec{k}\cdot\vec{r}})$ will remain the same. In the case of X-ray scattering by electron charge, a simple approximation for the **atomic form factor** is

electron number

atomic form factor is

$$\boxed{\tilde{f}_j = \int d\vec{r}\, n_j(\vec{r})\, e^{-i\Delta\vec{k}\cdot\vec{r}}}$$

electron number density

Note that, here, the atomic form factor is defined so that, if the exponential factor was absent, then $\tilde{f}_j =$ number of electrons. I.e., the scattering amplitude of the distribution of electrons is divided by the [Thomson] scattering amplitude by a point electron to obtain $\tilde{f}_j$.

Importantly, notice that $\tilde{f}_j$ represents, properly, a completely atomic property, dependent only on the potential or the electron density of atom j in the coordinate system where that atom is at the origin.
Generally, (1) $\tilde{f}_j$ decreases at large $\Delta\vec{k}$, unless $V_j(\vec{r})$ or $n_j(\vec{r})$ is a delta function, which is the reason why "high order" diffraction spots, e.g. (997), are weaker than "low order" spots such as (110) or (100) etc, and (2) $\tilde{f}_j \propto Z$, the atomic number (when the probing beam is electron or photon).

Structure factor

$$\boxed{S_{\vec{G}} = \sum_{j=1}^{s} \tilde{f}_j e^{-i\vec{G}\cdot\vec{r}_j}}$$

$\vec{r}_j$: positions of atom j of the basis ($j = 1\ \ldots\ s$) corresponding to $\vec{R} = 0$.

Thus, the **structure factor**, $S_{\vec{G}}$, is basically the quantity f_b but up to a multiplicative length scale factor that is applied in the definition of the atomic form factor (see above).

The structure factor is especially interesting to consider when there is more than one atom per basis and atoms in the basis have (nearly) identical atomic form factors. For instance, bcc with one atom basis = sc (conventional unit cell) + two atom basis. By calculating the structure factor for these two atoms, it is easy to prove that the reciprocal lattice of bcc = fcc, and vice versa. Also, see Figure 17 of Kittel, which shows that the consideration of the structure factor is quite useful when $\tilde{f}_j$'s are nearly identical.

Note on the view points

In this lecture note, a very specific example of the electron diffraction as explained by the Born approximation within the non-relativistic Schrödinger equation has been used.

In the lecture itself, a slightly more general, and more formal, view point was used to point out the *general structure* of the diffraction theory, while this particular view presented in this lecture note was not discussed. The two views are complimentary. Either view leads to the general understanding of the scattering amplitude, the structure factor and the atomic form factor. Here is a summary of the key results from the lecture itself. It should be noted that these key results are repetitive with respective to what has been discussed in this lecture note (and the last one).

From a formal view (https://griffin.ucsc.edu/forum/question/68/heart-of-diffraction-a-simple-challenge), it is easily seen that the following hierarchy of equations follow.

$$f = \sum_{j=1}^{N_{atom}} f_j(\Delta\vec{k})\, e^{-i\Delta\vec{k}\cdot\vec{r}_j}$$

$$f_b = \sum_{j=1}^{s} f_j(\Delta\vec{k})\, e^{-i\Delta\vec{k}\cdot\vec{r}_j}$$

$$f = \sum_{j=1}^{N} f_b(\Delta\vec{k})\, e^{-i\Delta\vec{k}\cdot\vec{R}_j} = f_b(\Delta\vec{k}) \sum_{j=1}^{N} e^{-i\Delta\vec{k}\cdot\vec{R}_j}$$

where f is the total scattering amplitude, f_j is the scattering amplitude from atom at j, s is the number of atoms in a basis, N_{atom} is the number of atoms in the crystal, and N is the number of bases in the crystal. As mentioned above, f_j is $\tilde{f}_j$ up to a multiplicative length factor and f_b is $S_{\vec{G}}$ up to a multiplicative length factor.