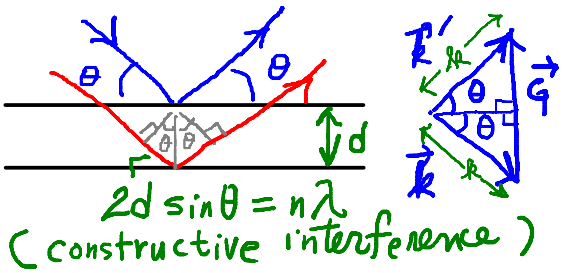
# Lecture 05

Tuesday, January 18, 2011
10:00 AM

**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 2.5 (extra credit). So, it is worth summarizing the result of that homework problem.




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 $2d\sin\theta = n\lambda$.

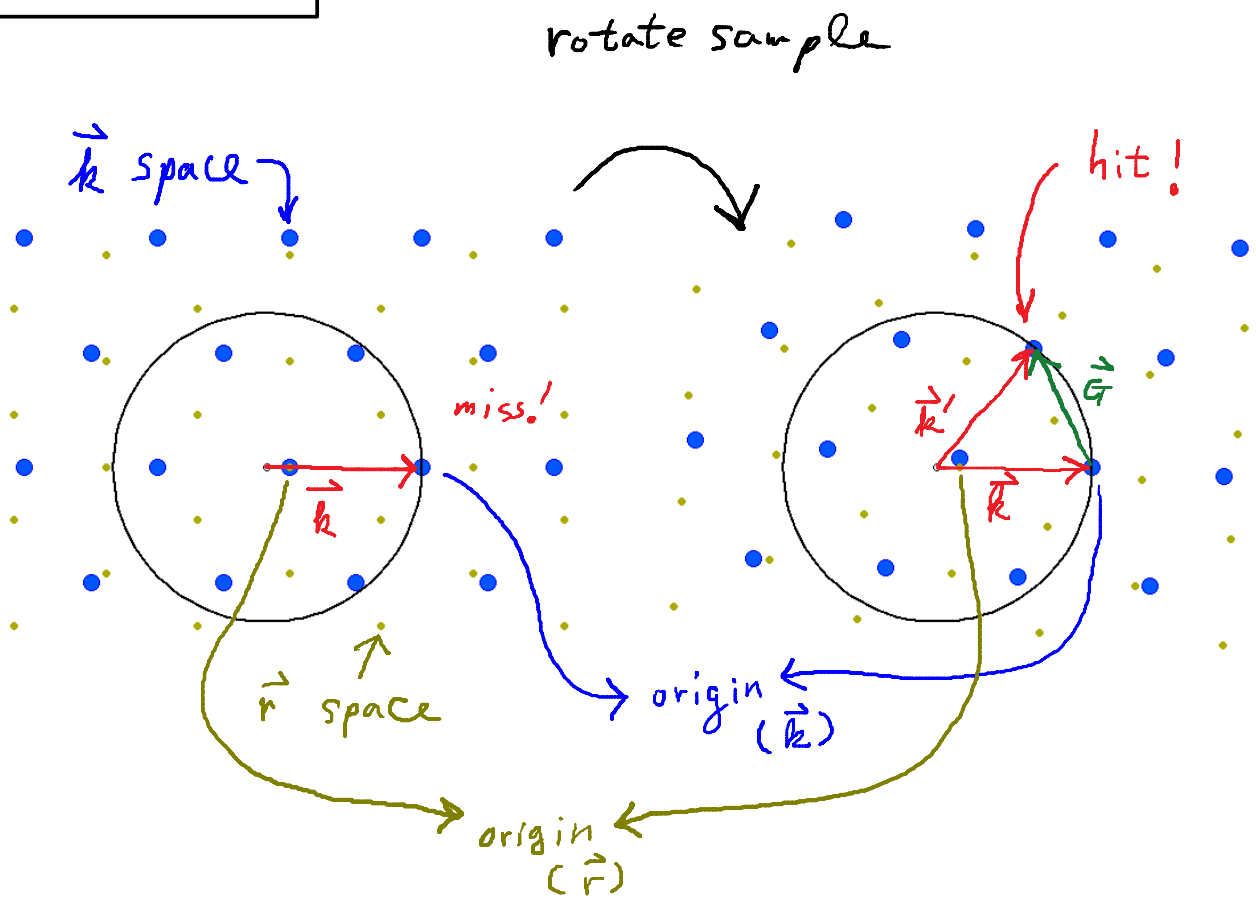
For a set of lattice planes $(h,k,l)$, reciprocal vectors $\vec{G}_n = n(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$, with non-zero integer $n$, and only they, are perpendicular to those planes, with $d = 2\pi/|\vec{G}_{n=\pm1}|$.

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 planes; think $h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$ |
| {hkl} | Symmetry equivalent lattice planes<br>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 direction parallel to $h\vec{a} + k\vec{b} + l\vec{c}$ |

## Ewald sphere




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 "$\theta$-$2\theta$" scan). See figures in text.

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

## 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,

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

This motivates the following definition of the atomic form factor, $f_j \propto \int d\vec{r} V_j(\vec{r}) e^{-i\Delta\vec{k}\cdot\vec{r}}$. 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, the simple approximation for the **atomic form factor** is

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

electron number density

Note that, here, the atomic form factor is defined so that, if the exponential factor was absent, then $f_j =$ 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 $f_j$.

Importantly, notice that $f_j$ 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) $f_j$ 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) $f_j \propto Z$, the atomic number (when the probing beam is electron or photon).

Structure factor

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

$\vec{r}_j$: 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 normalization constant 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 $f_j$'s are nearly identical.

## Born - von Karman boundary condition

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In solid state physics, we often use the **Born - von Karman boundary condition**, which is often called **periodic boundary condition**. Consider a crystal with lattice points, $\vec{R} = \sum_i n_i \vec{a}_i$, with $n_i = 0, \ldots, N_i - 1$. That is, this crystal has $\Pi_i N_i$ bases.

Born - von Karman boundary condition

$$n_i = n_i \ \% \ N_i$$

where $a \ \% \ b$ = remainder of $a/b$.

Under the Born - von Karman boundary condition, a one dimensional crystal can be viewed as a circle, a two dimensional crystal as a torus, and a three dimensional crystal as a hyper torus.

Born - von Karman (BvK) boundary condition will be used throughout this course [as in the next topics that we will discuss below].

- Why use BvK? The math becomes very nice.
- Is it absolutely necessary? No. Sometimes it may even be harmful (see below).
- When is it OK to use? For a large crystal size and for the bulk property. I.e. for the majority of topics in a course like this.
- When should you not use this or at least re-examine this boundary condition? For surface, interface, or nano-scale physics.