Reciprocal Lattice

Basics

Geometric Definition

- The reciprocal lattice is fundamental for all diffraction effects and other processes in a crystal lattice where momentum is transferred.
- The *reciprocal lattice* of any *geometrical point lattice* has a simple geometric definition:
  - It can be constructed by drawing the direct lattice, picking three sets of lattice planes **(h^i, k^i, l^i)** (**i=1,2,3**) that are not coplanar, and by constructing three vectors $g_{h,k,l}$ which are perpendicular to the respective lattice planes and with a length (measured in cm^{-1}) that is given by $|g| = 2\pi/d_{h,k,l}$, with $d_{h,k,l}$=distance between the lattice planes **(h,k,l)**.
  - The three vectors thus obtained, if reduced to the three shortest ones possible (take three lattice planes with largest distance, i.e. lowest values of **(h,k,l)**) define the reciprocal lattice.
- This is, of course, just a complicated way of saying:
  - Take the **(100)**, **(010)**, and the **(001)** planes, and use the vectors perpendicular to those planes with a length given by **2π/*d*** for these **{100}** type planes as the base vectors of the reciprocal lattice.

The Reciprocal Lattice as Fourier Transform of the Regular Lattice

- The reciprocal lattice, however, is best looked at as the **Fourier** **transform** of the regular lattice. We are showing this by constructing the Fourier transform of a real *crystal*.
  - It is easier to look at a real crystal (not just a lattice) because otherwise you have to work with δ-functions.
  - A real crystal has atoms. And atoms contain charge densities $\rho(\mathbf{r})$, or, if we start simple and one-dimensional, $\rho(x)$.
  - Now, $\rho(x)$ must be periodic in *x*-direction with the lattice constant *a*:

$$\rho(x + na) = \rho(x), \qquad n = 0\ \pm1, \pm2, \ldots$$

  - We thus can expand $\rho(x)$ into a Fourier series, i.e.

$$\rho(x) = \sum_n \rho_n \cdot \exp \frac{i \cdot x \cdot n \cdot 2\pi}{a}$$

  - The three-dimensional case, in analogy, can be written as

$$\rho(\underline{r}) = \sum_G \rho_G \cdot \exp(i \cdot \underline{G} \cdot \underline{r})$$

  - The vector $\underline{G}$ so far is just a mathematical construct defining the "inverse" space needed for the Fourier transform.
  - However, since we can always substitute for any $\underline{r}$ a vector $\underline{r} + \underline{T}$ ($\underline{T}$= translation vector of the lattice), or written out, $\underline{r} + n_1 \underline{a}_1 + n_2 \underline{a}_2 + n_3 \underline{a}_3$ with n_i= integers and $\underline{a}_i$= base vectors of the lattice defining the crystal, the product $\underline{r} \cdot \underline{G}$ must not change its value if we substitute $\underline{r}$ with $\underline{r} + n_1 \underline{a}_1 + n_2 \underline{a}_2 + n_3 \underline{a}_3$.
  - This requires that $\underline{G} \cdot \underline{T} = 2\pi \cdot m$ with m= integer.
- This is essentially a definition of the vectors $\underline{G}$ that serve as the Fourier transforms of the vector $\underline{T}$, i.e. the lattice in space. These *reciprocal lattice vectors*, as they are called, can be obtained from the base vectors defining the regular lattice in the following way:
  - If we write $\underline{G}$ in components we obtain

$$\underline{G} = h \cdot \underline{g}_1 + k \cdot \underline{g}_2 + l \cdot \underline{g}_3$$

  - With *h, k, l*= integers.

- The vectors $\underline{g}_1$, $\underline{g}_2$, and $\underline{g}_3$ are then the *unit vectors* of the **reciprocal lattice**. *(yes – they are underlined, you just don't see it with some fonts!)*

If we now form the inner product of $\underline{G} \cdot \underline{T}$, e.g., for simplicity, with $\underline{T} = n_1 \cdot \underline{a}_1$, we obtain

$$(h \cdot \underline{g}_1 + k \cdot \underline{g}_2 + l \cdot \underline{g}_3) \cdot (n_1 \cdot \underline{a}_1) \quad = 2\pi \cdot m$$

- For an arbitrary n_1 this only holds if

$$\underline{g}_1 \cdot \underline{a}_1 = 2\pi$$

$$\underline{g}_2 \cdot \underline{a}_1 = \underline{g}_3 \cdot \underline{a}_1 = 0$$

In general terms, we have

$$\underline{g}_i \cdot \underline{a}_j = 2\pi \cdot \delta_{ij}$$

- With δ_{ij} = **Kronecker** symbol, defined by: δ_{ij}**=0** for ≠ and δ_{ij} **=1** for **i=j**.

The above equation is satisfied with the following definitions for the unit vectors of the reciprocal lattice:

$$\underline{g}_1 = 2\pi \cdot \frac{\underline{a}_2 \times \underline{a}_3}{\underline{a}_1 \cdot \underline{a}_2 \cdot \underline{a}_3}$$

$$\underline{g}_2 = 2\pi \cdot \frac{\underline{a}_3 \times \underline{a}_1}{\underline{a}_1 \cdot \underline{a}_2 \cdot \underline{a}_3}$$

$$\underline{g}_3 = 2\pi \cdot \frac{\underline{a}_1 \times \underline{a}_2}{\underline{a}_1 \cdot \underline{a}_2 \cdot \underline{a}_3}$$