

Lecture 5 – The reciprocal lattice

Reading

Ashcroft & Mermin, Ch. 5, pp. 86 – 93.

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Central concepts

- **Definition of the reciprocal lattice**

The reciprocal lattice is a construction with vast importance for condensed matter physics. Starting with a Bravais lattice, the reciprocal lattice is the set of all wave vectors \mathbf{G} that give plane waves $e^{i\mathbf{G}\cdot\mathbf{r}}$ with the periodicity of the Bravais lattice. If the Bravais lattice is given by points \mathbf{R} , one thus have

$$e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R})} = e^{i\mathbf{G}\cdot\mathbf{r}}$$

The \mathbf{G} -vectors correspond to the reciprocal lattice points.

The reciprocal lattice is also a Bravais lattice.

- **Construction of the reciprocal lattice**

If \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 are the primitive vectors of the direct lattice the reciprocal lattice is described by the corresponding primitive vectors

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

which corresponds to

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

where δ_{ij} is the Kronecker delta.

- **First Brillouin zone**

The *first Brillouin zone* is defined as the Wigner-Seitz cell of the reciprocal lattice.

- **Lattice planes**

A *lattice plane* is any plane given by three Bravais lattice points that are not all aligned. Parallel, equally spaced lattice planes form a *family* of lattice planes. Each family of lattice planes have an associated reciprocal lattice vector that is perpendicular to the planes and that have a length $2\pi/d$ if the plane spacing is d .

- **Miller indices**

The orientation of a family of lattice planes is described by a vector normal to the planes. The shortest reciprocal lattice vector that is normal to the planes gives the *Miller indices* of the plane family: A family of planes associated with a shortest reciprocal lattice vector

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

has Miller indices (h, k, l) .

The intercepts of a lattice plane with the crystal axes are inversely proportional to the Miller indices of the plane.

To simplify nomenclature, one writes negative numbers as \bar{n} instead of $-n$. The commas can then be skipped, to give Miller indices such as $(14\bar{2})$ and (111) .

All symmetry-equivalent families of lattice planes are written with $\{ \}$ instead of $()$. The planes (100) , (010) , and (001) together are thus the $\{100\}$ -planes.

A *direction* $n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ is similarly written with $[]$ as $[n_1n_2n_3]$ and a family of directions $[100]$, $[010]$, $[\bar{1}00]$ etc. is written as $\langle 100 \rangle$.

Distance between planes decrease with increasing Miller indices while the atomic density increases with decreasing Miller indices.

- **Useful facts and relations**

- The reciprocal lattice of a reciprocal lattice is the original, direct lattice.
- The reciprocal lattice of a simple cubic lattice with primitive cell side a is again a simple cubic lattice, but with cell side $2\pi/a$.
- The reciprocal lattice of an *fcc* Bravais lattice with conventional cubic cell side a is a *bcc* lattice with conventional cubic cell side $4\pi/a$.
- The reciprocal lattice of an *bcc* lattice with conventional cell side a is similarly an *fcc* lattice with conventional cell side $4\pi/a$.
- The reciprocal lattice on a *simple hexagonal* Bravais lattice with lattice constants a and c is also a simple hexagonal lattice but with lattice constants $4\pi/\sqrt{3}a$ and $2\pi/c$, and rotated 30° around the c -axis.
- The volume v_g of the reciprocal lattice primitive cell is $v_g = (2\pi)^3/v_c$, where v_c is the volume of the direct lattice primitive cell. The cell volumes can be obtained from the corresponding primitive vectors by taking $v_c = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ and $v_g = \mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)$.
- The reciprocal lattice is the fourier transform of the direct lattice.
- A reciprocal lattice vector $\mathbf{G}(hkl)$ is perpendicular to the plane (hkl) .
- If a function is periodic in the direct lattice, so that $f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R})$ one can write

$$f(\mathbf{r}) = \sum_{\mathbf{G}} a_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}$$

so that the sum is taken only over the reciprocal lattice points.

Ch. 6 – X-ray diffraction

- **Conditions for diffraction**

- For a Bravais lattice, the condition for diffraction is that the change in x-ray wave vector is a reciprocal lattice vector, i.e.,

$$\Delta \mathbf{k} = \mathbf{G}$$

- For a Bravais lattice + basis, the condition is that of a Bravais lattice, but with the additional condition that the *geometrical structure factor* $S_{\mathbf{G}}$ is non-zero, where

$$S_{\mathbf{G}} = \sum_{j=1}^n f_j e^{i\mathbf{G} \cdot \mathbf{d}_j}$$

is a sum over the ions of the basis. Here f_j is the *atomic form factor*, which depends on the charge distribution of the ion j . It can often be approximated by the atomic number Z of the ion.

- **Bragg's law**

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

- **Laue condition**

$$\mathbf{k} \cdot \hat{\mathbf{G}} = \frac{1}{2}G$$

where $\hat{\mathbf{G}}$ is a unit vector along \mathbf{G} .

- **Quadratic expression**

Start with the Laue diffraction condition, which can be written as $G = |\mathbf{G}| = 2|\mathbf{k}| \sin \theta$. Assume a cubic crystal structure with lattice parameter a . Then one can write the relation between Miller indices (hkl) of the Bragg plane and the Bragg angle θ as

$$\sin^2 \theta = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2)$$

Depending on the basis, there will be rules on the (hkl) for diffraction to occur. (Do not confuse the k here being a Miller index with $k = |\mathbf{k}| = 2\pi/\lambda$ being the wave number.) For a *simple cubic* system, all (hkl) give reflections. For a *bcc* lattice, the sum $h + k + l$ should be even. For an *fcc* lattice, all indices should be either even or odd.

To index a structure means to determine (hkl) for all given reflections.

- **Wavelengths**

For x-rays, $\varepsilon = hc/\lambda$ so that

$$\lambda = hc/\varepsilon$$

For electrons, $\varepsilon = \hbar^2 k^2 / 2m$ so that

$$\lambda = h / \sqrt{2m\varepsilon}$$

For neutrons, similarly,

$$\lambda = h / \sqrt{2m_n \varepsilon}$$