

2.1.2 Diffraction of Electron Waves

Note: It is too tiresome to underline all vectors, and we will simply stop doing it except if it is absolutely necessary.

The Reciprocal Lattice

Electron waves like all waves experience diffraction effects in periodic structures like crystals. This is best described in the **reciprocal lattice** of the crystal in question. There are several ways to construct a **reciprocal** lattice from a **space** lattice.

- Remember that a **lattice** – in contrast to a **crystal** – is a **mathematical construct**. A lattice becomes a crystal by putting a set of atoms – the **base** of the crystal – at every lattice point.
- There are **14** different kinds of lattices – the **Bravais lattices** – with different symmetries that are sufficient to describe the lattice of any crystal.
- If you are unsure about this topic, refer to the appropriate chapter in "[Introduction to Materials Science I](#)" (in German) or in "[Defects](#)" (in English)

Lets look at three definitions of the reciprocal lattice, which are – of course – all equivalent but at different levels of abstraction. This is [elaborated in the link](#).

- The reciprocal lattice is the **Fourier** transform of the space lattice.
- The reciprocal lattice with an elementary cell (**EC**) as defined by the base vectors $\mathbf{b}_{1,2,3}$ is obtained from the space lattice as defined by its base vectors $\mathbf{a}_{1,2,3}$ by the equations

$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_x \times (\mathbf{a}_y \cdot \mathbf{a}_z)}$	$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_x \times (\mathbf{a}_y \cdot \mathbf{a}_z)}$	$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_x \times (\mathbf{a}_y \cdot \mathbf{a}_z)}$
$\mathbf{a}_x \times (\mathbf{a}_y \cdot \mathbf{a}_z) = \text{volume } V \text{ of EC}$		

- The base vectors of the reciprocal lattice can be constructed by drawing vectors perpendicular to the three **{100}** planes of the space lattice and taking their length as $2\pi/d_{hkl}$ with d_{hkl} = spacing between the **lattice** planes with **Miller indices** $\{hkl\}$.
- You will, of course, never confuse the spacing between lattice planes with the spacing between crystal planes, i.e. sheets of atoms, which may be something different.*

Bragg Condition

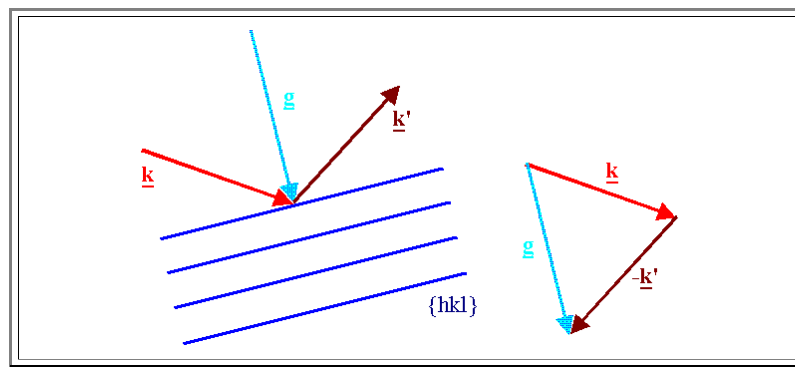
If a wave impinges on a crystal – and it doesn't matter if it is an electromagnetic wave, e.g. **X-rays**, or an electron, or neutron "wave" – it will be reflected at a particular set of lattice planes **{hkl}** characterized by its reciprocal lattice vector **g** *only* if the so-called **Bragg condition** is met.

- Let the wave vector of the incoming wave be \mathbf{k} , the wave vector of the reflected wave is \mathbf{k}' . The Bragg condition correlates the three vectors involved – \mathbf{k} , \mathbf{k}' , and \mathbf{g} – in the **simplest possible form**:

$$\mathbf{k} - \mathbf{k}' = \mathbf{g}$$

- There is no simpler relation correlating three vectors – mother nature again makes life as easy as possible for us!

This Bragg condition is easily visualized:



- If, and only if the three vectors involved form a **closed triangle**, is the Bragg condition met. If the Bragg condition is **not** met, the incoming wave just moves through the lattice and emerges on the other side of the crystal (neglecting absorption).

So far we assumed implicitly that the diffraction (or, in more general terms, the **scattering**) of the incoming wave is **elastic**, i.e. the magnitude of \mathbf{k}' is identical to that of \mathbf{k} , i.e. $|\mathbf{k}| = |\mathbf{k}'|$ – which means that the diffracted wave has the same momentum, wavelength and especially energy as the incoming wave.

- This is not necessarily implied by Bragg's law – the equation $\mathbf{k} - \mathbf{k}' = \mathbf{g}$ can also be met if \mathbf{k}' differs from \mathbf{k} by a reciprocal lattice vector; i.e. if scattering with a change of energy takes place. This will become important later.

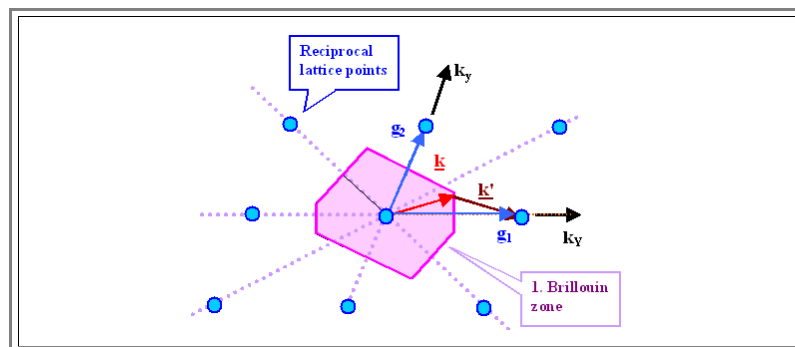
Brillouin Zones

In X-ray analysis of crystals we often deal with an (idealized) situation where **one** well-defined plane wave with fixed wavelength impinges on a crystal, and the question is which set of lattice planes will reflect the **one** incoming beam.

- This question can be answered most easily in a qualitative way by a geometric construction called the **Ewald construction** which can be found in the "[Introduction to Materials Science II](#)" Hyperscript.

However, if we consider the diffraction effects occurring to the free electrons contained in the crystal, we are looking at a (quasi) continuum of wave vectors: We have all possible directions and many wavelengths.

- The question is now a bit different: We want to know which **particular** wave vectors out of **many** (an infinite set, in fact) meet the Bragg condition for a given crystal lattice plane.
- This question can be answered most easily and semi-quantitatively by a geometric construction called the **Brillouin construction**. Let's look at it in a simplified two-dimensional form.



- If we construct **Wigner–Seitz cells** in the **reciprocal lattice** as shown by the pink lines, all wave vectors ending on the Wigner–Seitz cell walls will meet the Bragg condition for the set of lattice planes represented by the cell wall.

The Wigner–Seitz cells form a **nested system of polyhedra** which can be numbered according to size. These cells are called **Brillouin zones (BZ)**; the smallest one is called the **1. BZ**, the next smallest one the **2. BZ**, and so on.

- All wave vectors that end on a **BZ** wall will fulfill the Bragg condition and thus are diffracted. Of course, the origin must be at the center of that **BZ**.
- Wave vectors completely in the interior of the **1. BZ**, or in between any two **BZs**, will **never** get diffracted; they move pretty much as if the potential would be constant, i.e. they behave very close to the solutions of the free electron gas.

Of course, if we talk about diffraction in a crystal, we assumed implicitly that the potential is no longer constant, but **periodic** with the crystal.

- The statement above is thus not trivial, but a first important conclusion from diffraction geometry alone: We have good reasons (albeit no ironclad justification) to believe that the free electron gas model is a **decent approximation** for electrons with wave vectors **not** ending on (or close to) a Brillouin zone edge of the crystal in question.
- We thus only have to consider what happens to the electrons with wave vectors on or close to a **BZ** edge. In which properties do they differ from electrons of the free electron gas model?

Questions

Quick Questions to 2.1.2