# Reciprocal Lattice

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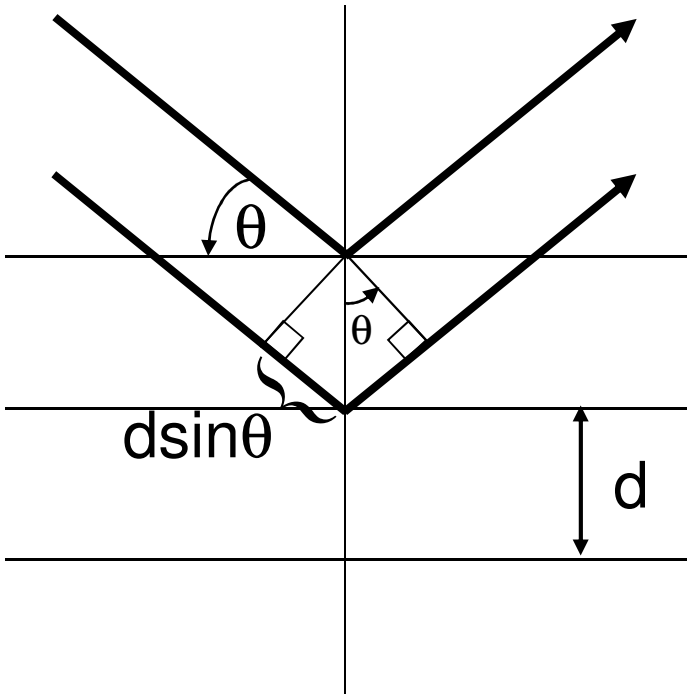
Issues that are addressed in this chapter include:

- Bragg law
- Scattered wave amplitude
- Brillouin Zones
- Fourier analysis of the basis

# 1 Bragg Law

W. L. Bragg presented a simple explanation of the diffracted beams from a crystal based on a specular reflection from planes of atoms.




The difference in the paths traversed by the two beams shown in the figure is:

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

Listed below are some additional notes on the Bragg reflection:

- Although the reflection from each plane is specular, only for certain values of $\theta$ will the reflections from all planes add up in phase to give a strong reflected beam.
- Each plane reflects only $10^{-3}$ to $10^{-5}$ of the incident radiation, i.e. it is not a perfect reflector. Hence, $10^{3}$ to $10^{5}$ planes contribute to the formation of the Bragg-reflected beam in a perfect crystal.
- The composition of the basis determines the relative intensity of the various orders of diffraction.

# 2 Scattered Wave Amplitude

## ❑ Reciprocal Lattice Vectors

The electronic number density is a periodic function in space with a period equal to the lattice translation vector **T**, i.e.

$$n(\mathbf{r}+\mathbf{T}) = n(\mathbf{r})$$

This means that one can use a Fourier series expansion to represent in 1D n(x) as

$$n(x) = n_0 + \sum_{p>0}\left[C_p \cos(2\pi px/a) + S_p \sin(2\pi px/a)\right] = \sum_p n_p e^{i2\pi px/a}$$

where:

$$n_p = \frac{1}{a}\int_0^a dx n(x) e^{-i2\pi px/a}$$

In 3D, we have

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \rightarrow n_{\mathbf{G}} = \frac{1}{V_c} \int_0^a dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}}$$

The set of **reciprocal lattice vectors** that lead to electron density invariant under lattice translations is found from the condition:

$$n(\mathbf{r}+\mathbf{T}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{T})} = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{T}} = n(\mathbf{r}) \quad when \;\; e^{i\mathbf{G}\cdot\mathbf{T}} = 1$$

The reciprocal lattice vectors that satisfy the above requirement are of the form

$$\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3$$

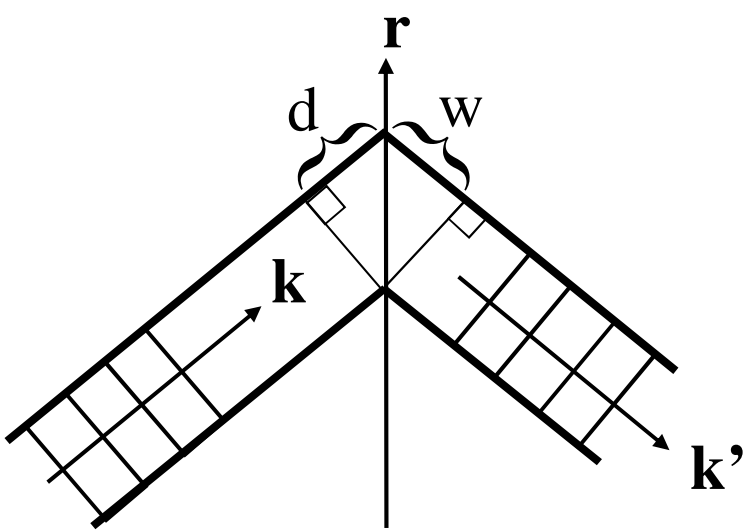
where $v_1$, $v_2$ and $v_3$ are integers and

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}, \;\; i = x, y, z \;\rightarrow\; \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

## ❑ Diffraction Condition

The TEM maps the direct lattice, whereas the diffraction pattern of the lattice is a map of the reciprocal lattice of the crystal. The above statement is clarified with the following theorem:

*The set of reciprocal lattice vectors **G** determines the possible x-ray reflections.*




- The scattering wave amplitude is given by:

$$F = \int dV n(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}$$

$$= \int dV n(\mathbf{r}) e^{-i\Delta\mathbf{k}\cdot\mathbf{r}}$$

- When $\mathbf{G}=\Delta\mathbf{k}$, then $F=V n_{\mathbf{G}}$, i.e. has significant value when the difference in lattice vectors equals the RLV.

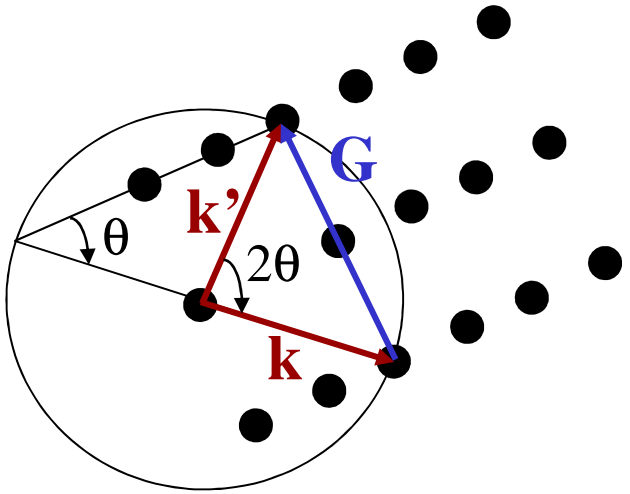
- Let us now elaborate on this condition for the case of elastic scattering:

$$\mathbf{G} = \Delta\mathbf{k} = \mathbf{k}'-\mathbf{k} \rightarrow 2\mathbf{k}\cdot\mathbf{G} + G^2 = 0$$

## ❑ The Laue Equations

The original result that $\Delta\mathbf{k}=\mathbf{G}$ can also be expressed to give the Laue equations, that are obtained by taking the dot product of both $\Delta\mathbf{k}$ and $\mathbf{G}$ with $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$:

$$\Delta\mathbf{k}\cdot\mathbf{a}_i = 2\pi v_i, \quad i = 1,2,3$$

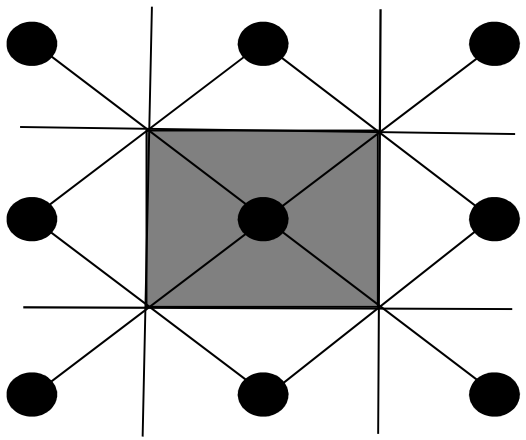



Note that *x*-ray difraction can be used to map all the reciprocal lattice vectors by changing θ.

# 3 Brillouin Zones and Reciprocal Lattice to SC, BCC and FCC lattice

## ❑ Brillouin zones

A Brillouin zone is defined as a Wigner-Seitz primitive cell in the reciprocal lattice and gives geometric interpretation of the diffraction condition.



- The Brillouin construction exhibits all wavevectors k that can be Bragg reflected by the crystal.
- The constructions divide the Fourier space into fragments, out of which the first Brillouin zone is of greatest importance.

## ❑ Reciprocal Lattices to SC, FCC and BCC

| | Direct lattice | Reciprocal lattice | Volume |
|---|---|---|---|
| SC | $\begin{cases}\mathbf{a}_1 = a\mathbf{x} \\ \mathbf{a}_2 = a\mathbf{y} \\ \mathbf{a}_3 = a\mathbf{z}\end{cases}$ | $\begin{cases}\mathbf{b}_1 = (2\pi/a)\mathbf{x} \\ \mathbf{b}_2 = (2\pi/a)\mathbf{y} \\ \mathbf{b}_3 = (2\pi/a)\mathbf{z}\end{cases}$ | $(2\pi/a)^3$ |
| FCC | $\begin{cases}\mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}) \\ \mathbf{a}_2 = \frac{1}{2}a(\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{z}+\mathbf{x})\end{cases}$ | $\begin{cases}\mathbf{b}_1 = \frac{2\pi}{a}(-\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}-\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}-\mathbf{z})\end{cases}$ | $2(2\pi/a)^3$ |
| BCC | $\begin{cases}\mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{a}_2 = \frac{1}{2}a(-\mathbf{x}+\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{x}-\mathbf{y}+\mathbf{z})\end{cases}$ | $\begin{cases}\mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y})\end{cases}$ | $4(2\pi/a)^3$ |

# 4 Fourier Analysis of a Basis

## ❑ Structure and Atomic Form Factors

Recall that the scattering amplitude equals to

$$F = \int_{cell} dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} = NS_G$$

where $\boldsymbol{S_G}$ is the **structure factor** defined as an integral over a single unit cell.

If we write the electron density as a superposition of the electron densities in the cell, taking into account the # of atoms per basis, we have

$$n(\mathbf{r}) = \sum_{j=1}^{s} n_j(\mathbf{r} - \mathbf{r}_j)$$

where *s* is the # of atoms in the unit cell.

Substituting this back gives

$$S_G = \sum_{j=1}^{s} \int_{cell} dV n_j(\mathbf{r}-\mathbf{r}_j) e^{-i\mathbf{G}\cdot\mathbf{r}}$$

$$= \sum_{j=1}^{s} e^{-i\mathbf{G}\cdot\mathbf{r}_j} \int_{cell} dV n_j(\rho) e^{-i\mathbf{G}\cdot\rho} = \sum_{j=1}^{s} e^{-i\mathbf{G}\cdot\mathbf{r}_j} f_j$$

where $f_j$ is the **atomic form factor**. Now if we specify **G** and $\mathbf{r}_j$ as

$$\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3 \quad \text{and} \quad \mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3$$

we get:

$$S_G = \sum_{j=1}^{s} f_j e^{-2\pi i\left(x_j v_1 + y_j v_2 + z_j v_3\right)}$$

Note that $S_G$ can be complex, because the scattering intensity involves the magnitude squared of $S_G$.

The atomic form factor can also be written in the following form for spherically-symmetric electron density

$$f_j = 4\pi \int_0^\infty n_j(r) r^2 \frac{\sin(Gr)}{Gr} dr$$

That means that when $n(r)=Z\delta(r)$, then $f_j=Z$, i.e. $f_j$ is the ratio of radiation amplitude scattered by the electron distribution to that scattered by a localized electron.

- Examples of Structure Factor Calculations

(a) BCC lattice

For a BCC lattice, we have two atoms per init cell located at (000) and (1/2 ½ ½). The structure factor is then:

$$S_G = \left[1 + e^{-\pi i(v_1+v_2+v_3)}\right]_f$$

- The structure factor is maximum $S_G = 2f$ when the sum of the indices is even, i.e. $v_1+v_2+v_3=2n$ .
- The structure factor is $S_G = 0$ when the sum of the indices is odd, i.e. $v_1+v_2+v_3=2n+1$ .

## (b) FCC lattice

For a FCC lattice, we have four atoms per init cell located at (000), (0 ½ ½), (½ 0 ½) and (½ ½ 0). The structure factor is then:

$$S_G = \left[1 + e^{-\pi i(v_1+v_2)} + e^{-\pi i(v_1+v_3)} + e^{-\pi i(v_2+v_3)}\right] f$$

- When all indices are even or odd, then $S_G = 4f$.
- When the indices are partially even and partially odd, then $S_G = 0$.

To summarize, in a FCC lattice, no reflections occur when the indices are partially even and partially odd.