

Chapter 2: Wave Diffraction and the Reciprocal Lattice

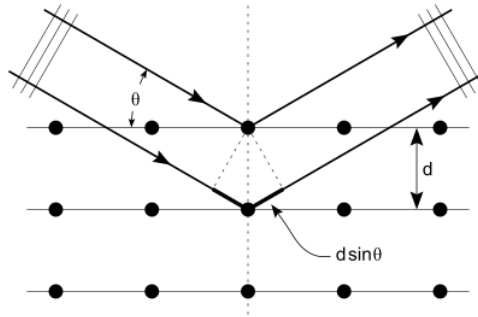


Figure 0.1: Bragg's Law

Scattering and Bragg's Law When two beams of same phase meet, they constructively interfere. When they are out of phase, they destructively interfere. The location of constructive interference, or path difference, is shown by the bold lines in Figure 0.1. The path difference is

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

known as Bragg's Law which is only valid for $\lambda \leq 2d$. In reality each lattice plane will reflect about $10^{-3} \sim 10^{-5}$ of the incident beam. Thus only about $10^3 \sim 10^5$ planes contribute to the diffraction. The periodicity of the lattice leads to a periodic observable...

aside: The electron wavefunction is not observable— ψ is a complex number, but the electron density, $\psi^*\psi$, is observable. Read about the quantized Hall effect (Queen:) and Superconductivity (King).

$$\psi(x + T) = \psi(x)e^{i\theta}n(x + T) = n(x)$$

Fourier Transform The discrete Fourier transform is useful for periodic functions.

$$\begin{aligned} n(x) &= \sum_{P \geq 0} \left[C_P \cos\left(\frac{2\pi}{a}x\right) + S_P \sin\left(\frac{2\pi}{a}x\right) \right] \\ &= \sum_P n_P e^{i\frac{2\pi}{a}Px} \end{aligned}$$

or in vector notation

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}$$

Since $n(x)$ is real, there is a symmetry of the complex conjugate

$$n_p = n_{-p}^*$$

Inverse Fourier Transform

$$n_p = \frac{1}{a} \int_0^a n(x) e^{-i\frac{2\pi}{a}Px} dx$$

and in vector notation

$$n_{\mathbf{G}} = \frac{1}{V} \int_{cell} n(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} dV$$

Reciprocal Space Vectors The basis vectors of the reciprocal lattice are

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

where the denominator is the volume of the unit cell (parallelepiped) $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = V_c$. Taking the dot product of a primitive vector with a reciprocal lattice vector gives

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

where the Kronecker delta tells us that the dot product is either 2π or 0. With this we can write the \mathbf{G} vector as a linear combination of the reciprocal lattice vectors

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

we can also show that

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

which means that this is invariant under translations.

Scattering amplitude

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

where $|\mathbf{k}| = |\mathbf{k}'|$. In vector notation

$$\begin{aligned} F &= \int d\mathbf{r} \sum_{\mathbf{G}} n_G e^{i(\mathbf{G} - \mathbf{r}') \cdot \mathbf{r}} e^{-i\Delta\mathbf{k} \cdot \mathbf{r}} \\ &= \sum_{\mathbf{G}} n_G \int d\mathbf{r} e^{i(\mathbf{G} - \Delta\mathbf{k}) \cdot \mathbf{r}} \end{aligned}$$

where $\Delta\mathbf{k} = -(\mathbf{k} - \mathbf{k}')$. When $\mathbf{G} = \Delta\mathbf{k}$ we can rewrite to

$$\mathbf{k} + \Delta\mathbf{k} = \mathbf{k}'$$

in absolute value

$$|\mathbf{k} + \Delta\mathbf{k}| = |\mathbf{k}'| \rightarrow |\mathbf{k} + \Delta\mathbf{k}| = |\mathbf{k}| \rightarrow |\mathbf{k} + \mathbf{G}| = |\mathbf{k}|$$

and

$$(\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}) = \mathbf{k} \cdot \mathbf{k} \rightarrow 2\mathbf{k} \cdot \mathbf{G} + \mathbf{G}^2 = 0$$

For the 1D crystal $G = 2\pi/a$. Since $\mathbf{k} \cdot \mathbf{G} = 2\pi/\lambda G \sin \theta$ and $2\mathbf{k} \cdot \mathbf{G} = \mathbf{G}^2$ We get

$$\begin{aligned} 2 \cdot \frac{2\pi}{\lambda} G \sin \theta &= \mathbf{G}^2 \\ \rightarrow \frac{4\pi}{\lambda} \sin \theta &= G \end{aligned}$$

since $G = 2\pi/a$ we get Bragg's Law

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

For the SC the reciprocal lattice is SC, but for BCC, the reciprocal lattice is different...

Chapter 2: cont'd

Wigner-Seitz primitive cell: How to create the most symmetric primitive cell.

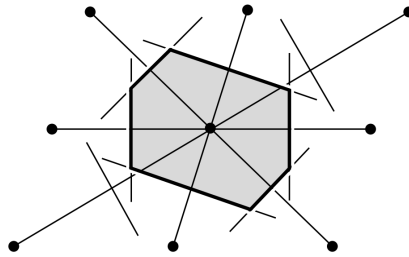


Figure 0.2: Wigner-Seitz Primitive Cell

Steps: Connect a given lattice point to all nearby lattice points. Bisect all lines. The area enclosed by the bisectors is the Wigner-Seitz primitive cell as shown in Figure 0.2.

Reciprocal Lattice of SC The lattice vectors (primitive translation vectors) are

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = a\hat{\mathbf{z}}$$

the reciprocal lattice vectors using the formula from last lecture are

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_c} = \frac{2\pi}{a} \hat{\mathbf{x}}, \quad \mathbf{b}_2 = \frac{2\pi}{a} \hat{\mathbf{y}}, \quad \mathbf{b}_3 = \frac{2\pi}{a} \hat{\mathbf{z}}$$

Reciprocal Lattice of BCC The lattice vectors are

$$\mathbf{a}_1 = \frac{a}{2}(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}})$$

and the reciprocal lattice vectors are

$$\mathbf{b}_1 = \frac{2\pi}{a}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{b}_2 = \frac{2\pi}{a}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \quad \mathbf{b}_3 = \frac{2\pi}{a}(\hat{\mathbf{x}} + \hat{\mathbf{y}})$$

Reciprocal Lattice of FCC The lattice vectors are

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{z}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}})$$

which is the same as the reciprocal space of BCC. Thus, the reciprocal lattice of FCC is BCC!

Brillouin Zone The first Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice.