

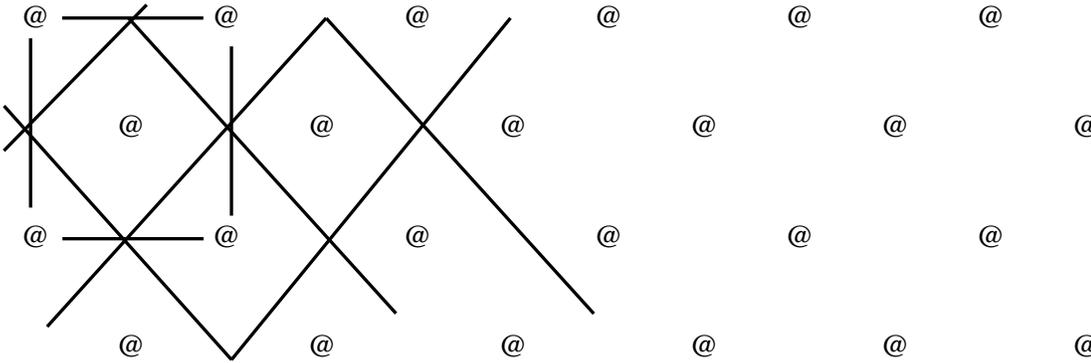
# Diffraction continued: Brilluoin Zone

## 1. Brilluoin zone

### a) Wigner-Seitz cell

a1) Definition: **The Wigner-Seitz cell is a cell that is bounded by perpendicular bisectors of the distances between adjacent lattice points.**

In a 2-D plane, these would like lines enclosing an area around each lattice point – see below. In 3-D, these would look like planes enclosing a volume surrounding each lattice point, and these volumes would completely fill the space with no empty regions.



a2) The **reciprocal lattice** is a **lattice of "points" in k-space** (that is, instead of regular position space (x,y,z) we use axes (k<sub>x</sub>, k<sub>y</sub>, and k<sub>z</sub>). More generally, we use axes (**b**<sub>1</sub>, **b**<sub>2</sub>, **b**<sub>3</sub>) where the **b**<sub>i</sub>'s are defined such that **G • T = N2π** (where N is an integer) and

$$\mathbf{T} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3, \quad \mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3,$$

where **a**<sub>i</sub> are the primitive lattice vectors, u<sub>i</sub> are integers, and

where **b**<sub>1</sub> ≡ 2π(**a**<sub>2</sub> × **a**<sub>3</sub>) / [**a**<sub>1</sub> • (**a**<sub>2</sub> × **a**<sub>3</sub>)], etc., and v<sub>i</sub> are also integers. [≡ means defined to be]

(*Homework problem 8 asks you to find the reciprocal lattice vectors for a bcc lattice.*)

b) Definition: **The first Brilluoin zone is the Wigner-Seitz cell in the reciprocal lattice.** The Brilluoin zone concept will be used throughout the course, not just in this section.

c) First use of the Brilluoin zone: getting a picture of the Bragg diffraction condition:

From:  $\Delta \mathbf{k} = \mathbf{G}$ , we get  $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ , and  $k'^2 = k^2 + 2\mathbf{k} \cdot \mathbf{G} + G^2$ ;

and for elastic collisions (k'=k) we get:  $G^2 = 2\mathbf{k} \cdot \mathbf{G}$ ;

dividing by 4:  $(\frac{1}{2}\mathbf{G})^2 = \mathbf{k} \cdot \frac{1}{2}\mathbf{G}$ ;

this statement says that **the component of k in the G direction must have a value of ½G**; a picture of this would be that any **k** vector that touches the edges of the Wigner-Seitz cell in the reciprocal lattice (first Brilluoin zone) would satisfy this condition.

This Bragg Diffraction condition is such that at a certain direction, only a certain wavelength will diffract, and a certain wavelength will diffract only in a certain direction.

## 2. Fourier Analysis of the Basis:

### a) Structure Factor:

The amplitude of the scattered x-rays in any direction should depend on the electron density at each point in the volume and upon the phases of the scattered waves from each point. Let's call this dependence, A, where A is proportional to the amplitude of the scattered x-rays, so that we have:

$$A = \int_{\text{all space}} n(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r} - i\mathbf{k}' \cdot \mathbf{r}) dV, \\ \text{(x-rays scatter off electrons).}$$

Since the electron density,  $n(\mathbf{r})$ , is periodic we can express it in a Fourier series:  $n(\mathbf{r}) = [\sum n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})]$  so we get:

$$A = \int_{\text{all space}} [\sum n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})] \exp(-i\Delta\mathbf{k} \cdot \mathbf{r}) dV \\ \text{(this = 0 unless } \Delta\mathbf{k} = \mathbf{G} : \text{ Bragg condition).}$$

Since the electron density is a repeating function over space, we can break the integral over all space into N integrals over one cell (with  $\Delta\mathbf{k} = \mathbf{G}$ ):

$A_{\mathbf{G}} = N \int_{\text{one cell}} n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) dV = N S_{\mathbf{G}}$  where N is the number of atoms and  $S_{\mathbf{G}}$  is called the **structure factor**:

$$S_{\mathbf{G}} = \int_{\text{one cell}} n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) dV$$

### b) Atomic Form Factor:

We can break the electron density of the cell up into the sum of the electron densities of the atoms in the cell (with the vector  $\mathbf{r}_j$  being the position of the jth atom in the cell):

$$n(\mathbf{r}) = \sum_j n_j(\mathbf{r} - \mathbf{r}_j); \text{ we can also define } \boldsymbol{\rho} = \mathbf{r} - \mathbf{r}_j, \text{ and } \mathbf{r} = \boldsymbol{\rho} + \mathbf{r}_j, \text{ so}$$

$$S_{\mathbf{G}} = \sum_j \int n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G} \cdot [\boldsymbol{\rho} + \mathbf{r}_j]) dV$$

$$S_{\mathbf{G}} = \sum_j \exp(-i\mathbf{G} \cdot \mathbf{r}_j) \int n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G} \cdot \boldsymbol{\rho}) dV = \sum_j \exp(-i\mathbf{G} \cdot \mathbf{r}_j) f_j$$

$$\text{where } f_j = \int n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G} \cdot \boldsymbol{\rho}) dV$$

is called the **atomic form factor**.

The structure factor is related to the amplitude of the wave, and so it need not be real. The intensity of the reflected wave, which is real, depends on the amplitude squared, or  $S_{\mathbf{G}} S_{\mathbf{G}}^*$  where  $S_{\mathbf{G}}^*$  is the complex conjugate of  $S_{\mathbf{G}}$ . [Recall what the complex conjugate is: given  $c$  is complex, and  $a$  and  $b$  are real, then if  $c = (a+ib)$ , then by definition of complex conjugate  $c^* = (a-ib)$ ; and so  $cc^* = a^2 + b^2$  which is real.]