

1. A plane wave $A \exp \{i(\mathbf{k}_0 \cdot \mathbf{r} - \omega t)\}$ is incident upon a regular lattice having identical atoms situated at points \mathbf{r}_n relative to the origin O. Consider the interaction of the wave with a particular atom leading to an elastically scattered wave which reaches a detector D, distant $r_D \gg 2\pi/k_0$ from O. Show that the total scattered amplitude S reaching D from all atoms may be written as

$$S = fA e^{i\mathbf{k} \cdot \mathbf{r}_D} \sum_n e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r}_n},$$

where fA is the scattered wave amplitude from a single atom and \mathbf{k} is the scattered wavevector (assumed the same for all atoms).

Let \mathbf{a} , \mathbf{b} , \mathbf{c} be the unit cell vectors of the lattice. A general reciprocal lattice vector takes the form

$$\mathbf{R} = s\mathbf{A} + t\mathbf{B} + u\mathbf{C},$$

where $\mathbf{A} \cdot \mathbf{a} = 2\pi$, $\mathbf{A} \cdot \mathbf{b} = \mathbf{A} \cdot \mathbf{c} = 0$, $\mathbf{B} \cdot \mathbf{b} = 2\pi$, $\mathbf{B} \cdot \mathbf{a} = \mathbf{B} \cdot \mathbf{c} = 0$, $\mathbf{C} \cdot \mathbf{c} = 2\pi$, $\mathbf{C} \cdot \mathbf{a} = \mathbf{C} \cdot \mathbf{b} = 0$ and s , t , and u are integers. Show that, for atom locations

$$\mathbf{r}_n = \alpha\mathbf{a} + \beta\mathbf{b} + \gamma\mathbf{c},$$

where α , β , γ are integers, diffraction maxima will be observed at D when $\mathbf{k}_0 - \mathbf{k}$ is a reciprocal lattice vector.

Define a *Brillouin zone* and demonstrate that all wavevectors which start from the origin and satisfy the condition for a maximum will terminate on a Brillouin zone boundary.

A two-dimensional crystal contains a single type of atom. The atomic spacing is a along one axis of the unit cell, b along the second axis, and the angle between the axes is α . Find the reciprocal lattice for this crystal and draw a labelled diagram showing the first Brillouin zone.