

1. **Glide and screw axes**

- a) The hcp lattice contains a screw axis in the c direction. Describe the Cartesian coordinates of a point through which this axis can pass, so that the lattice remains invariant under translation along c by $c/2$ followed by rotation through 60 degrees.
- b) The hcp also has a glide plane parallel to a plane containing both the a and c axes. Describe where this plane may be located, so that translation along $c/2$ followed by reflection about the plane leaves the lattice invariant.

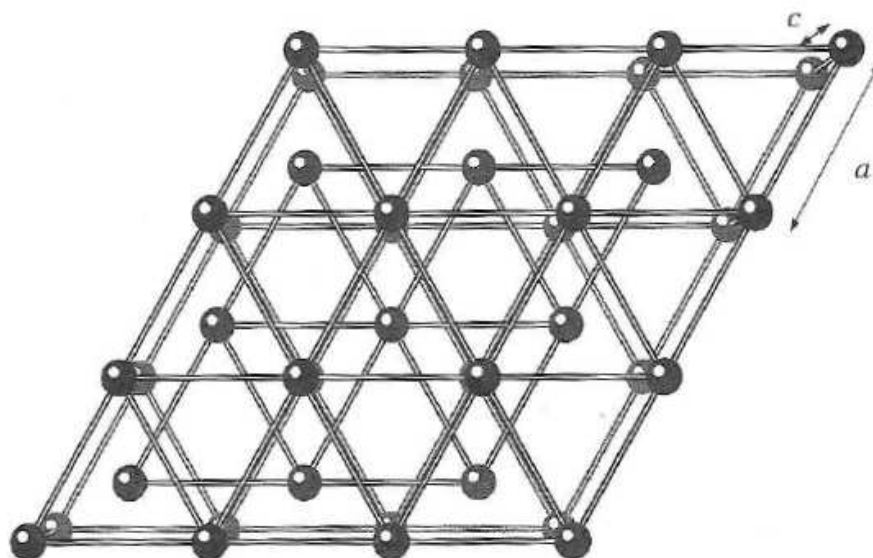


Figure 2.19. Top view of an hcp lattice.

2. **Reciprocal lattice**

Let \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 be the primitive vectors of a Bravais lattice, and \mathbf{b}_1 , \mathbf{b}_2 , and \mathbf{b}_3 the primitive vectors of the corresponding reciprocal lattice.

- a) Using the construction

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \quad (+c.p.),$$

show that the reciprocal lattice of the fcc lattice is bcc with lattice spacing $4\pi/a$, and vice versa.

- b) Find the reciprocal lattice vectors of smallest magnitude for simple cubic, fcc, and bcc lattices, and write down their Miller indices. Show that these correspond to planes in the direct lattice whose distance is $d = 2\pi/K$.

3. Hcp extinctions

- a) Prove that the reciprocal lattice of a hexagonal lattice

$$\mathbf{a}_1 = (a, 0, 0), \quad \mathbf{a}_2 = \left(\frac{a}{2}, \frac{a\sqrt{3}}{2}, 0\right), \quad \mathbf{a}_3 = (0, 0, c)$$

is another hexagonal lattice rotated at 30 degrees with respect to the original one, and find primitive vectors for the reciprocal lattice.

- b) The hcp lattice is built upon the hexagonal, with the basis

$$\mathbf{v}_1 = (0, 0, 0), \quad \mathbf{v}_2 = \left(\frac{a}{2}, \frac{a}{2\sqrt{3}}, \frac{c}{2}\right).$$

Show that the structure factor induced by the basis is

$$F_{\vec{q}} = \left| 1 + e^{i\frac{\pi}{3}[2(n_1+n_2)+3n_3]} \right|^2.$$

- c) Describe all the cases in which scattering from the hcp lattice vanishes because of an extinction.

4. Bragg peaks

Bragg's model for reflection of X-rays from a solid was based on the view that the solid was constructed out of a series of parallel planes. The rays bounced off the planes so that angle of incidence θ equaled the angle of reflection, and diffraction peaks occurred when radiation from successive planes added constructively.

- a) Show that in general the condition for a scattering peak can be written as

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

where d is the distance between lattice planes, θ is the Bragg scattering angle, λ is the wavelength, and l is an integer.

- b) Show that the condition follows from the conditions derived for a Bragg peak, $\vec{q} \equiv \vec{k}_0 - \vec{k} = \vec{K}$.

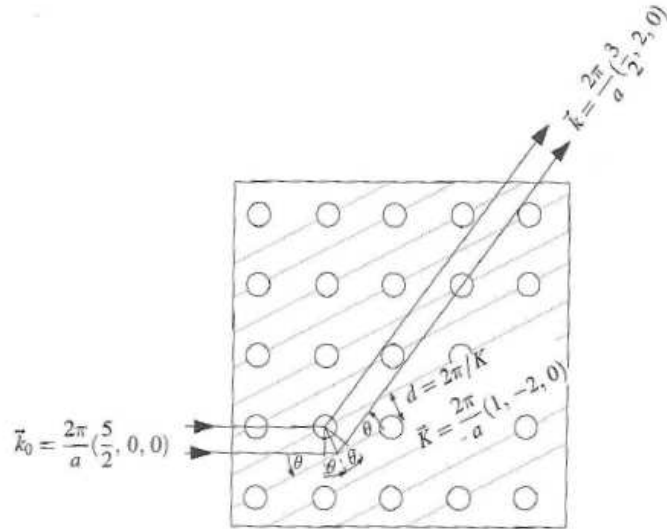


Figure 3.2. Illustration of Bragg scattering at angle $\theta = 26.56^\circ$ from the (21) planes of a square lattice. The magnitudes of \vec{k}_0 , \vec{k} , and \vec{K} are determined using Eqs. (3.38) and (3.39).