

Solid State Physics - A Summary

1 Crystallography

Structure: array of atoms, specified by a basis, plus lattice;

Basis: Group of atoms, which is repeated;

Lattice: Pattern of repeats;

Primitive unit cell: Cell with 1 lattice site only, and smallest area;

Bravais Lattice: Fill all space, and environment of all lattice sites identical;

Packing fraction: Fraction of space filled by touching spheres;

Coordination number: Number of nearest neighbours.

There are **5 2D Bravais lattices**: *square, rectangular, triangular, rhombic & oblique*.

There are **14 3D Bravais lattices**: we only consider a few *sc, bcc, fcc*.

Examples:

sc: Polonium

bcc: Li, Na, Fe

fcc: Sr, Ag, Cu

1.1 Miller Indices

Denoted (h, k, l) . To find the indices of a plane:

Get planes intercepts with axes. Reciprocate (putting 'bars' over negative intercepts). Multiply up, to integers.

We often refer to some structure, from the basis of some crystal:

Diamond: fcc lattice, with basis $(0, 0, 0), (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. Visualise this: at each fcc lattice site, put a C atom there, and one at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ relative to that site.

1.2 X-ray Diffraction

Probe crystals with λ of the order inter-site spacing.

We could use *thermal neutrons*, but very expensive to produce, but do scatter only once (which is good: easy to interpret data).

We can also use *electrons*, but results are very hard to interpret, because multiple scattering: use for surface investigations.

1.2.1 Braggs Law

An X-ray is incident, at angle θ to *plane*, which are spaced by d . Constructive interference if:

$$2d \sin \theta = n\lambda \tag{1.1}$$

For a plane with Miller indices h, k, l ; they are spaced by:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (1.2)$$

If a is the lattice spacing.

Intensity is higher for lower Miller indices: more atoms on planes.
We get Bragg reflections for $\sin \theta < 1$. That is, for:

$$\frac{n\lambda}{2a} \sqrt{h^2 + k^2 + l^2} < 1 \quad (1.3)$$

Indexing of lines:

$$\frac{\sin \theta_2}{\sin \theta_1} = \frac{\sqrt{h_2^2 + k_2^2 + l_2^2}}{\sqrt{h_1^2 + k_1^2 + l_1^2}} \quad (1.4)$$

For reflections at θ_1, θ_2 .

1.3 Reciprocal Lattice

If \mathbf{a}_i are the real space lattice basis vectors, and if \mathbf{b}_i are the reciprocal lattice basis vectors, then, we have the relations:

$$\mathbf{R} = n_i \mathbf{a}_i \quad \mathbf{G} = m_i \mathbf{b}_i \quad \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij} \quad e^{i\mathbf{R} \cdot \mathbf{G}} = 1 \quad (1.5)$$

We find \mathbf{b}_i via:

$$V \equiv \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) \quad \mathbf{b}_1 = \frac{2\pi}{V} (\mathbf{a}_2 \times \mathbf{a}_3) \quad (1.6)$$

Cycle through indices to get other \mathbf{b}_i 's.

The spacing of planes, with Miller indices h, k, l ; is given by:

$$d = \frac{2\pi}{|\mathbf{G}|} \quad \mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \quad (1.7)$$

If a wave \mathbf{k} is incident to a plane, and \mathbf{k}' comes out; if *elastic scattering* then:

$$\mathbf{k} - \mathbf{k}' = \mathbf{G} \quad (1.8)$$

Thus, strong reflection for waves which differ by a reciprocal lattice vector (way to derive Bragg's law).

1.3.1 Ewald Construction

Consider a circle, over lattice sites. Then strong reflection only if circle cuts a lattice site. Thus, low probability.

Laue Method: Vary the incident wavelength. Then, all lattice sites within the circle get picked up. We basically fire white X-rays at a single crystal, and observe the diffraction pattern. We see spots, and they have the same symmetry as the lattice.

Powder Method: Fire mono-chromatic X-rays through a hole in a cylinder of film. In the centre is a rod of specimen. Lines are seen in the film.

1.3.2 Effect of a Basis

The *structure factor* gives the amplitude of waves, from reflection:

$$S(\mathbf{G}) = \sum_{j=1}^N f_j(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}_j} \quad (1.9)$$

For N basis vectors. Ignore the *atomic form factor*, f for mono-atomic lattices. It is related to the density of electrons.

Intensity of reflected wave: multiply by $|S|^2$