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 enviroment of all lattice sites identical;
Packing fraction: Fraction of space filled by touching spheres;
Coordination number: Number of nearest neighbours.

There are **5 2D Bravias lattices**: *square, rectangular, triangular, rhomic & oblique.*
There are **14 3D Bravias 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:

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

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:

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

Indexing of lines:

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

For reflections at θ_1, θ_2.

1.3 Reciprocal Lattice

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

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

We find $\boldsymbol{b}_i$ via:

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

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

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

$$d = \frac{2\pi}{|\boldsymbol{G}|} \qquad \boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3 \tag{1.7}$$

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

$$\boldsymbol{k} - \boldsymbol{k}' = \boldsymbol{G} \tag{1.8}$$

Thus, strong reflection for waves which differ by a reciprocal lattice vector (way to derive Braggs 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:

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

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 $|S|^2$