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Summary of last lecture

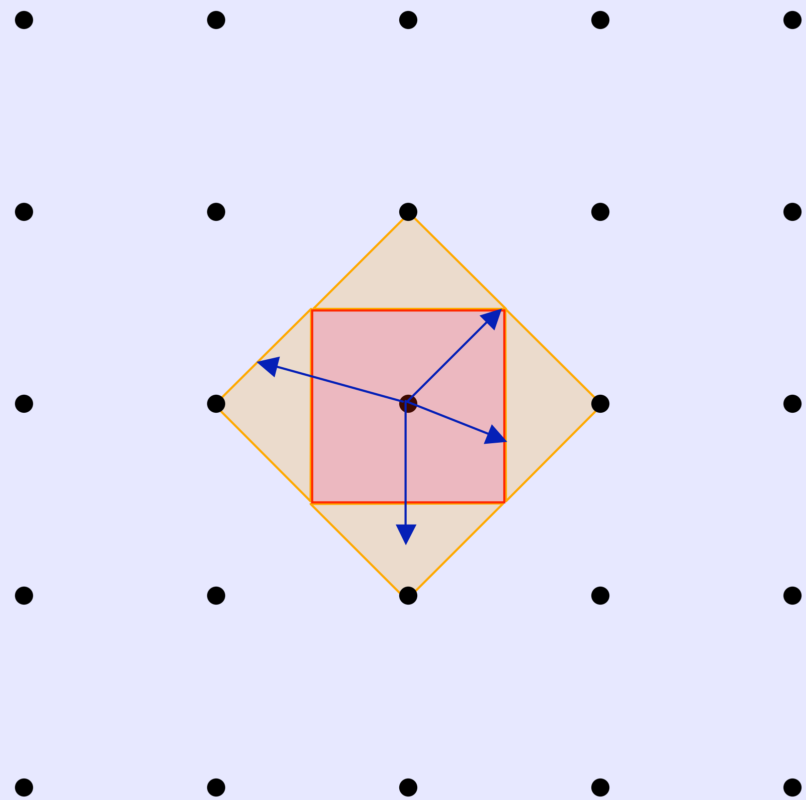
- More about reciprocal lattices:
  - Relationship with diffracting planes (second derivation)
  - Relationship with Bragg condition
  - Brillouin zones

Quiz on last lecture

The lattice shown is the reciprocal lattice of a certain 2D real space lattice.

(a) draw the first and second Brillouin zones

(b) hence state which of the wavevectors shown would *not* give rise to Bragg reflection



Aims of this lecture

- Examples of reciprocal lattices: more cubic Bravais lattices
  - derivation, Miller indices of diffracting planes
- The structure factor

Examples of reciprocal lattices

Simple cubic direct lattice

$$\mathbf{a} = a\mathbf{i}, \quad \mathbf{b} = a\mathbf{j}, \quad \mathbf{c} = a\mathbf{k}$$

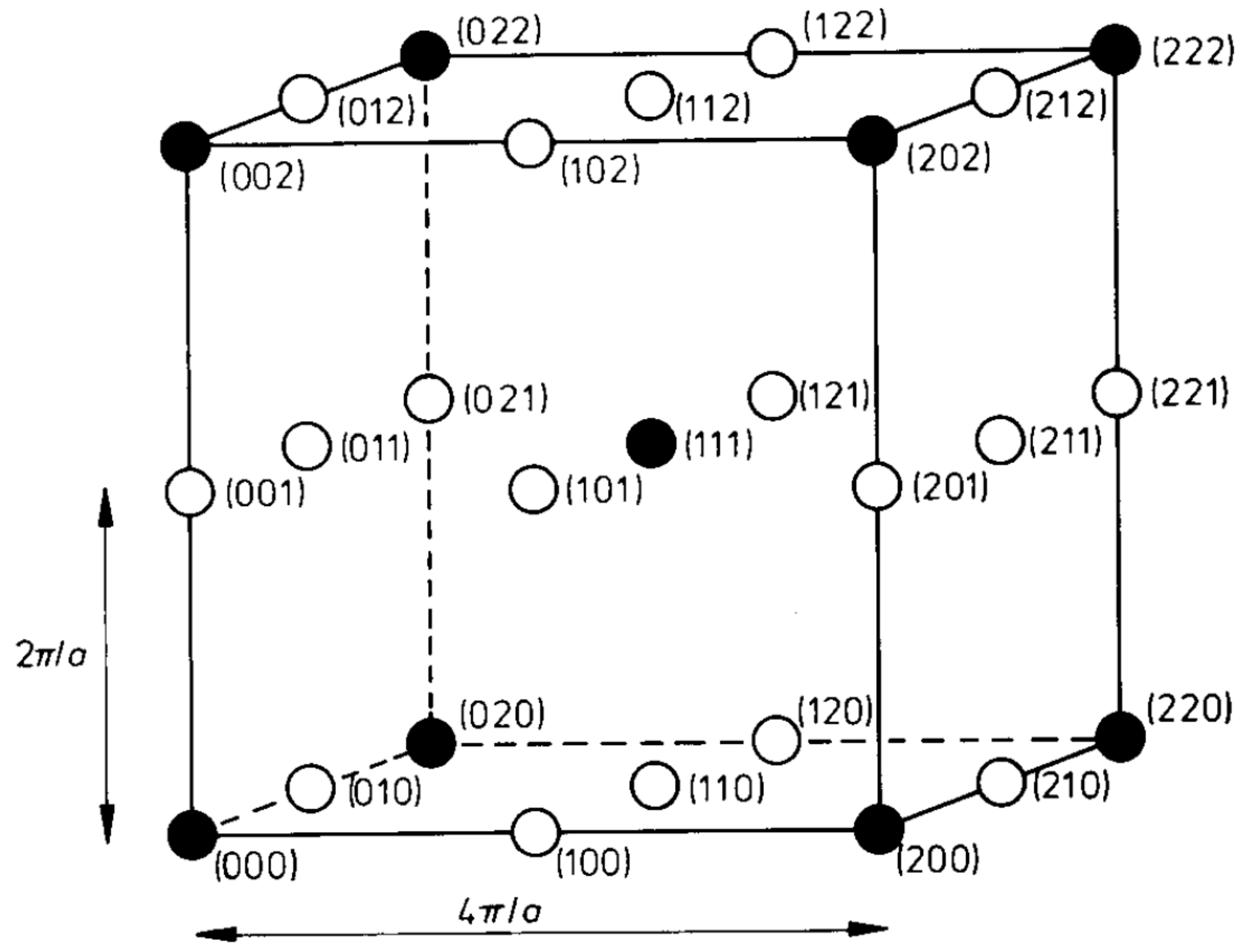
Hence $$\mathbf{a}^* = 2\pi \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a}.(\mathbf{b} \times \mathbf{c})}$$

Similarly $$\mathbf{b}^* = \frac{2\pi}{a}\mathbf{j}, \mathbf{c}^* = \frac{2\pi}{a}\mathbf{k}$$

The reciprocal lattice is also simple cubic, with side 2π/a

Examples of reciprocal lattices

$$\mathbf{G}_{hk\ell} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^*$$



Examples of reciprocal lattices

Face-centred cubic direct lattice

$$\mathbf{a} = \frac{a}{2}(\mathbf{j}+\mathbf{k}), \quad \mathbf{b} = \frac{a}{2}(\mathbf{k}+\mathbf{i}), \quad \mathbf{c} = \frac{a}{2}(\mathbf{i}+\mathbf{j})$$

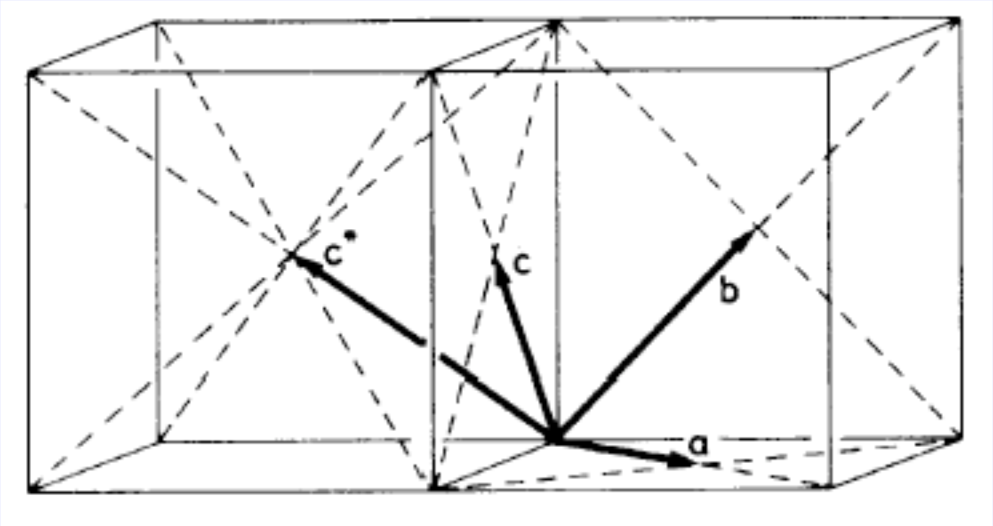
Hence
$$\mathbf{a}^* = \frac{4\pi}{a}\frac{(\mathbf{k}+\mathbf{i})\times(\mathbf{i}+\mathbf{j})}{(\mathbf{j}+\mathbf{k}).((\mathbf{k}+\mathbf{i})\times(\mathbf{i}+\mathbf{j}))}$$

Similarly
$$\mathbf{b}^* = \frac{2\pi}{a}(\mathbf{k}+\mathbf{i}-\mathbf{j}), \quad \mathbf{c}^* = \frac{2\pi}{a}(\mathbf{i}+\mathbf{j}-\mathbf{k})$$

The reciprocal lattice is body-centred cubic, with cube side $4\pi/a$

Examples of reciprocal lattices

Face-centred cubic direct lattice

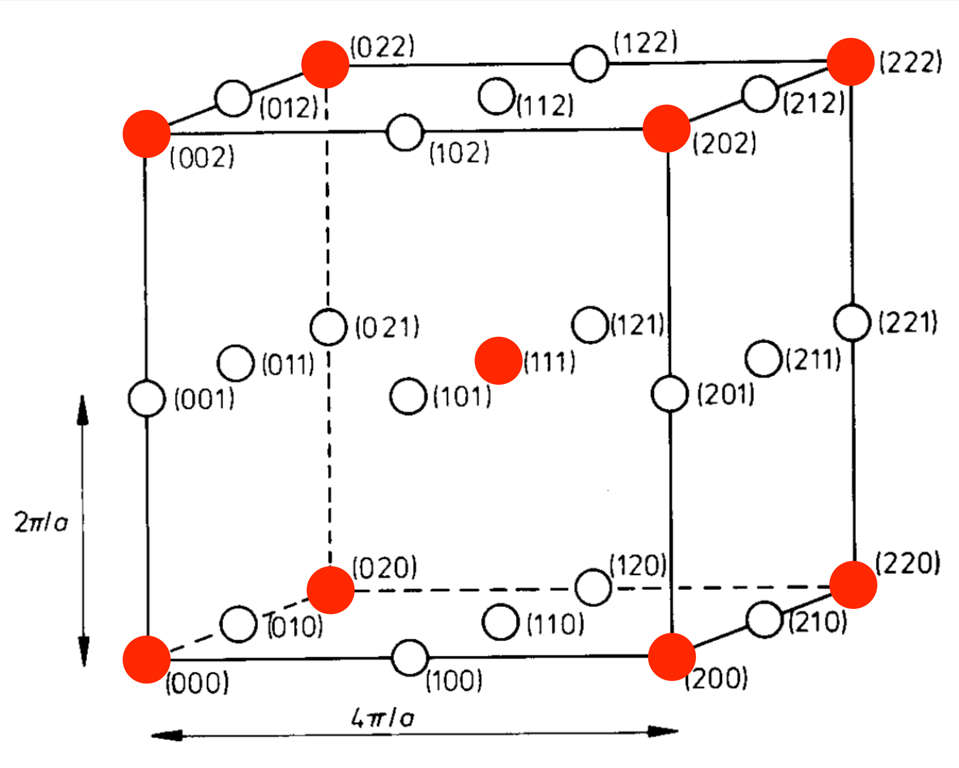


Right-hand cube is the direct lattice, left-hand one shows reciprocal lattice:

c* is perpendicular to both **a** and **b**, so is along the [111] direction

Examples of reciprocal lattices

The allowed reflections for the fcc direct lattice are the highlighted points.



These form the bcc lattice, with cube side $4\pi/a$

and they have h, k, ℓ either all even or all odd.

Examples of reciprocal lattices

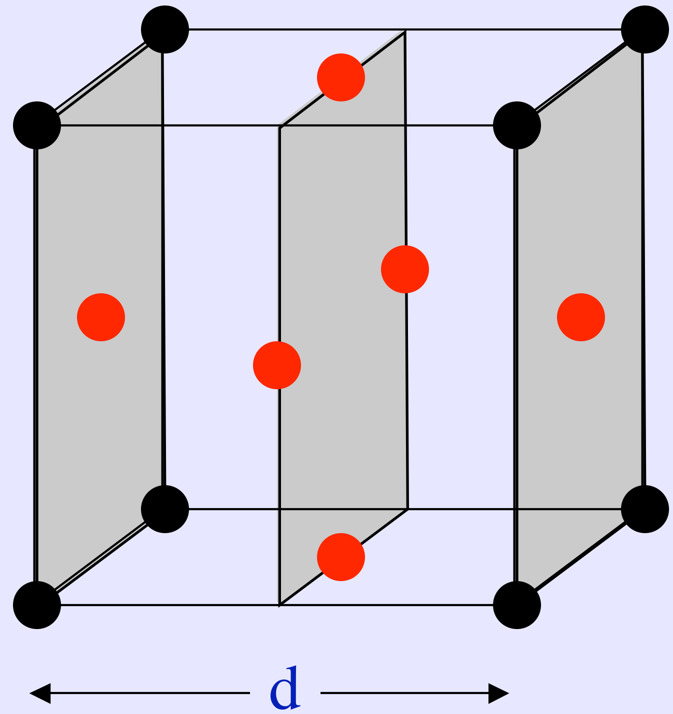
Some sets of planes which gave Bragg reflections in the sc lattice, do not do so for fcc.

WHY??

Examples of reciprocal lattices

e.g. the {100} planes:

First consider the simple cube:



suppose the Bragg condition is satisfied for these planes:

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

→ constructive interference

But for the face-centred cube, we have extra lattice points

These add an extra plane between the two shown

separation between planes has halved → destructive interference

Examples of reciprocal lattices

Body-centred cubic direct lattice

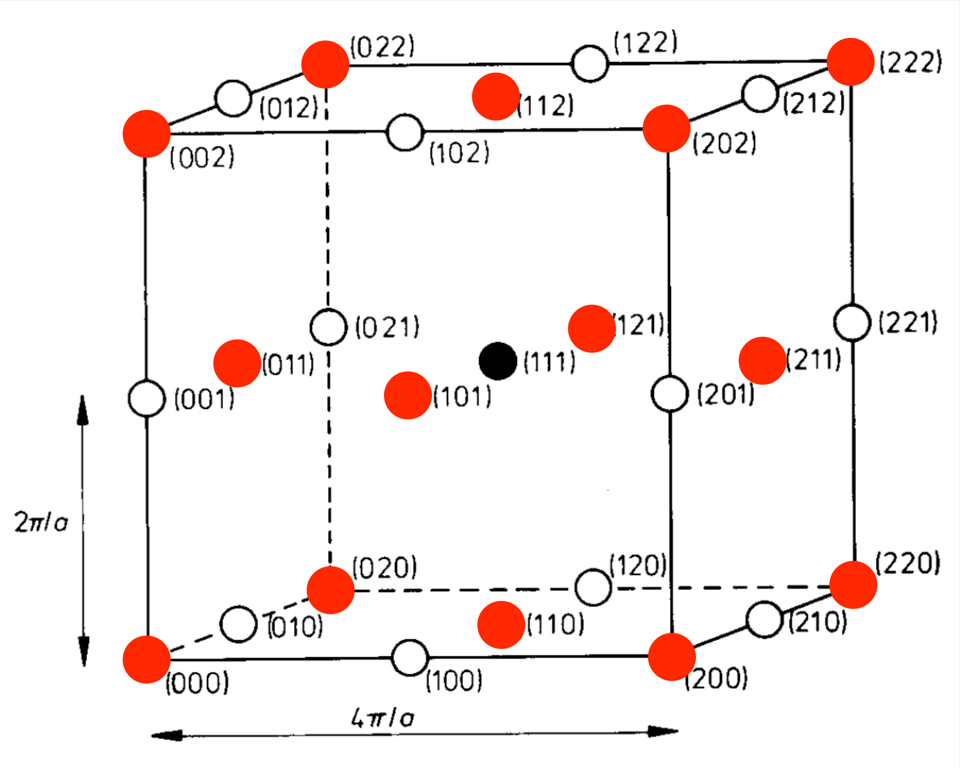
$$\mathbf{a} = \frac{a}{2}(\mathbf{j} + \mathbf{k} - \mathbf{i}), \quad \mathbf{b} = \frac{a}{2}(\mathbf{k} + \mathbf{i} - \mathbf{j}), \quad \mathbf{c} = \frac{a}{2}(\mathbf{i} + \mathbf{j} - \mathbf{k})$$

Hence $\mathbf{a}^* = \frac{2\pi}{a}(\mathbf{j} + \mathbf{k}), \quad \mathbf{b}^* = \frac{2\pi}{a}(\mathbf{k} + \mathbf{i}), \quad \mathbf{c}^* = \frac{2\pi}{a}(\mathbf{i} + \mathbf{j})$

The reciprocal lattice is face-centred cubic, with cube side 4π/a

Examples of reciprocal lattices

Again we can identify these points on the reciprocal lattice cube:



These all have $h + k + \ell =$ even

5. Structure factor

The expression $$A \propto \sum_{\mathbf{R}} \exp(i\Delta\mathbf{k}.\mathbf{R})$$

assumes that one point-like atom is positioned at each lattice point.

- Atoms are not points
- Basis may be more than one atom

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$$A \propto \sum_{\mathbf{R}} \exp(i\Delta\mathbf{k}.\mathbf{R})$$

5. Structure factor

Atoms are not points

Wave scattered from one side of atom, not quite in phase with wave scattered from other side.

Following exactly the argument that gave us the scattered amplitude for a blob, this means that we should multiply A by a factor:

$$f = \int n(\mathbf{r})\exp(-i\mathbf{G}.\mathbf{r})dV$$ Atomic Form Factor

- integral is over the volume of the atom
- n(**r**) is the density of ‘stuff’ in the atom doing the scattering:
  - x-rays ‘see’ the atom’s electrons n(**r**) would be the electron density (~ charge density).

$$A \propto \sum_{\mathbf{R}} \exp(i\Delta\mathbf{k}.\mathbf{R})$$

5. Structure factor

Basis of more than one atom

– so not all atoms are at lattice points

So for each term in the sum for A above, there actually needs to be as many terms as there are atoms in the basis

Multiply A by a sum over atoms in the basis:

$$S_{\mathbf{G}} = \sum_{j} f_j \exp\left(-i\mathbf{G}.\mathbf{r}_j\right) \quad \text{Structure Factor}$$

- $\mathbf{r}_j$ is the position of the j-th atom in the basis relative to the lattice point
- f_j is the atomic form factor of the j-th atom

5. Structure factor

Basis of more than one atom

For the reflection involving the $(hk\ell)$ planes,

$$\mathbf{G}_{hk\ell} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^*$$

So if we let the j-th atom in the basis have fractional coordinates (u_j, v_j, w_j), so that $\mathbf{r}_j = u_j\mathbf{a} + v_j\mathbf{b} + w_j\mathbf{c}$ then

$$S(hk\ell) = \sum_j f_j \exp\left(-i2\pi\left(hu_j + kv_j + \ell w_j\right)\right)$$

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Summary of this lecture

- Examples of reciprocal lattices: more cubic Bravais lattices
  - derivation, Miller indices of diffracting planes
  - how to distinguish crystal types from scattering angles
- The structure factor