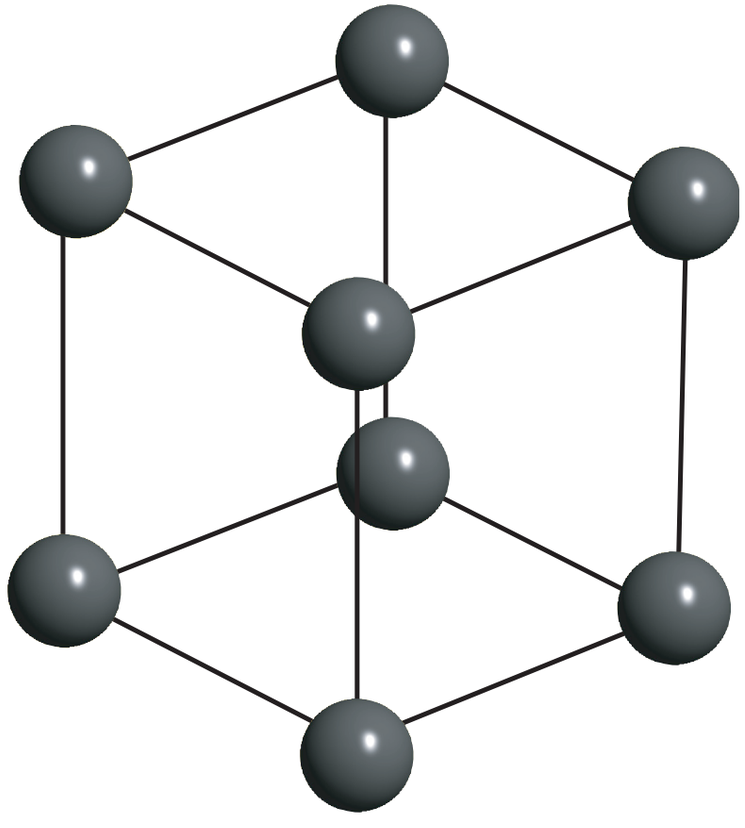
Condensed Matter Physics

- Dr. Baris Emre

Real crystal structures

- What structure do the solids have? Can we predict it?
- Consider inert elements (spheres). This could be anything with no directional bonding (noble gases, simple and noble metals).
- Just put the spheres together in order to fill all space. This should have the lowest energy.
- A simple cubic structure?



Simple cubic

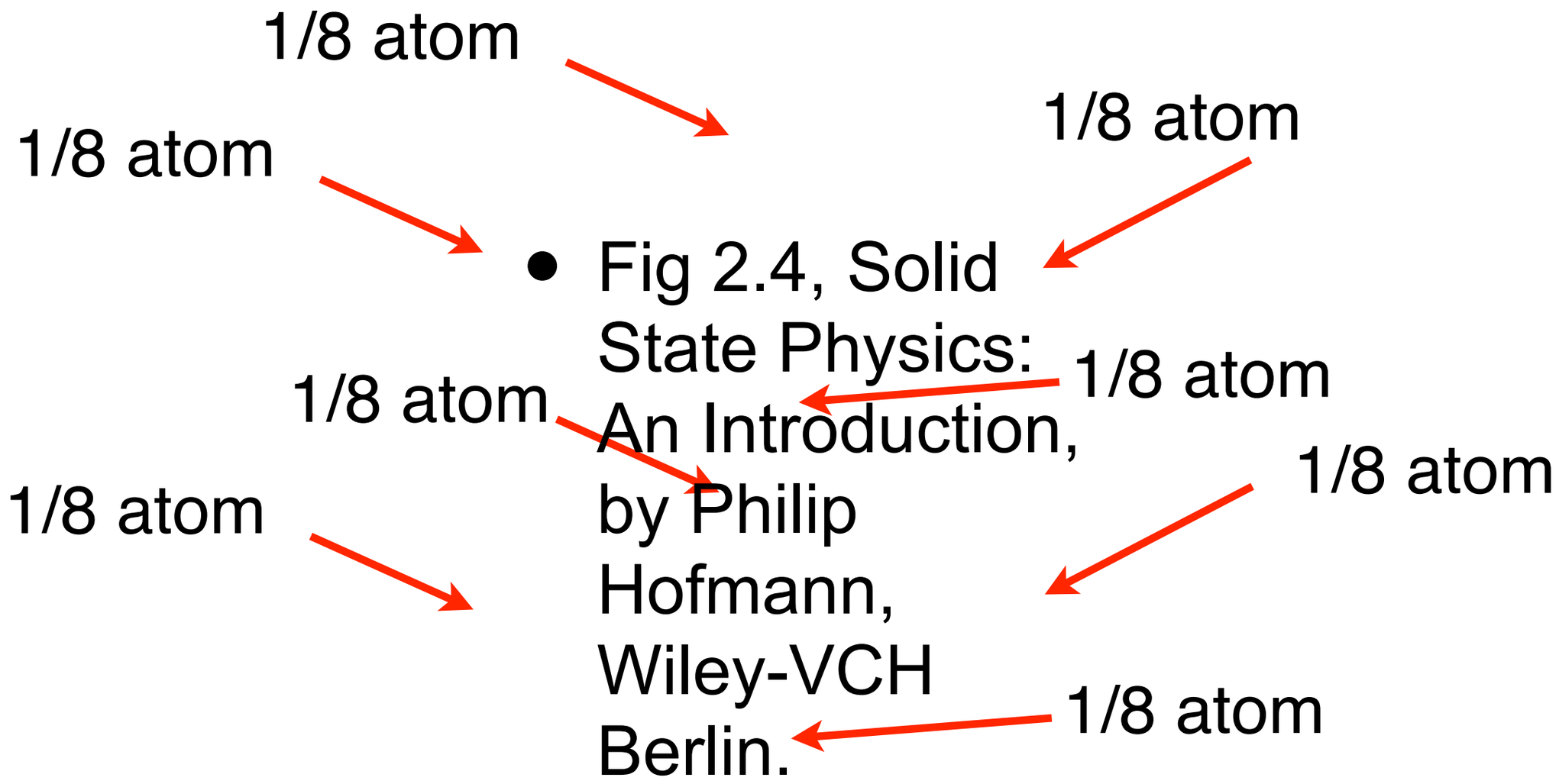
- The simple cubic structure is a Bravais lattice.
- The Wigner-Seitz cell is a cube
- The basis is one atom. So there is one atom per unit cell.

$$\mathbf{R}_{mno} = m\mathbf{a_1} + n\mathbf{a_2} + o\mathbf{a_3}$$

- Fig 2.4, Solid State Physics: An Introduction, by Philip Hofmann, Wiley-VCH Berlin.

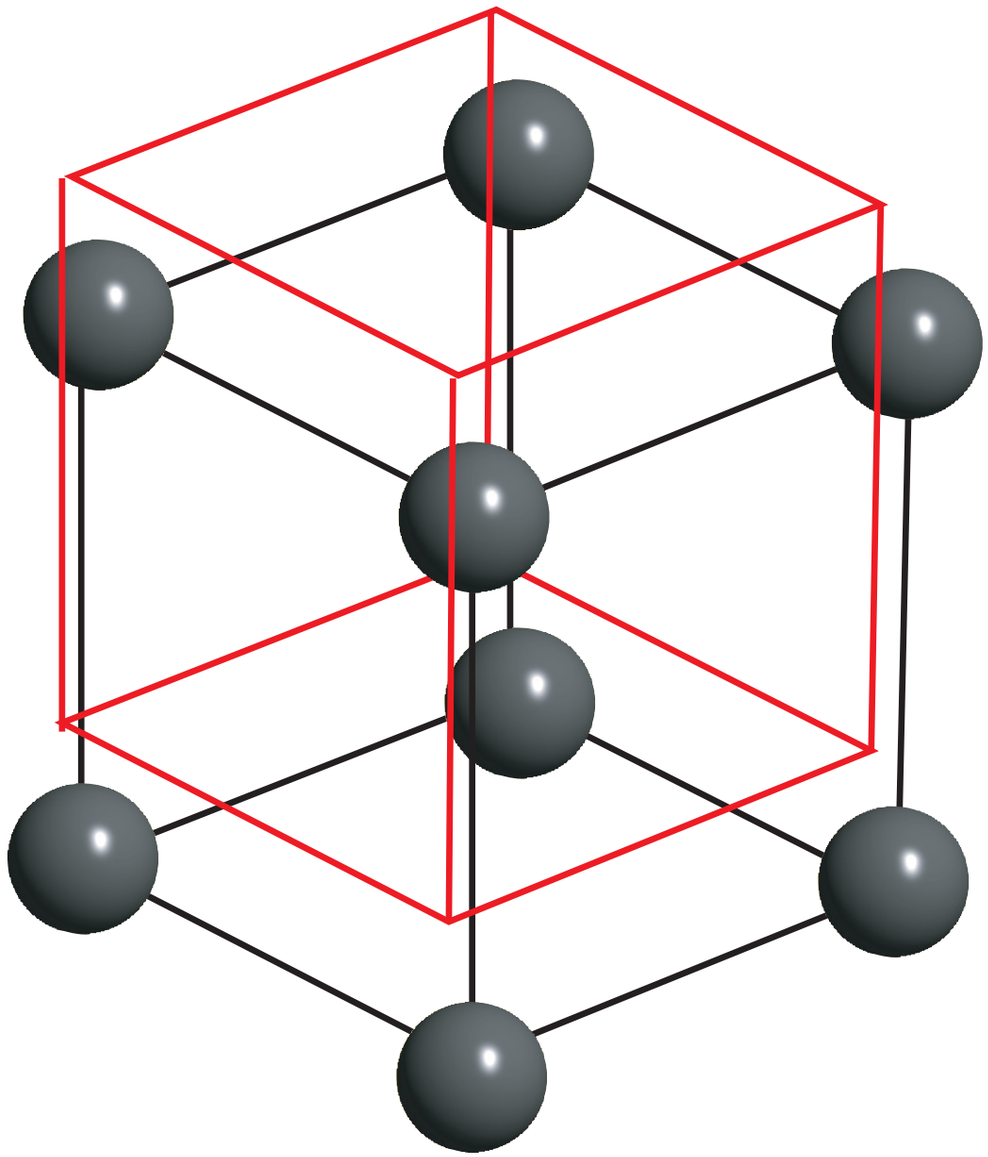
Simple cubic

- We can also simply count the atoms we see in one unit cell.
- But we have to keep track of how many unit cells share these atoms.



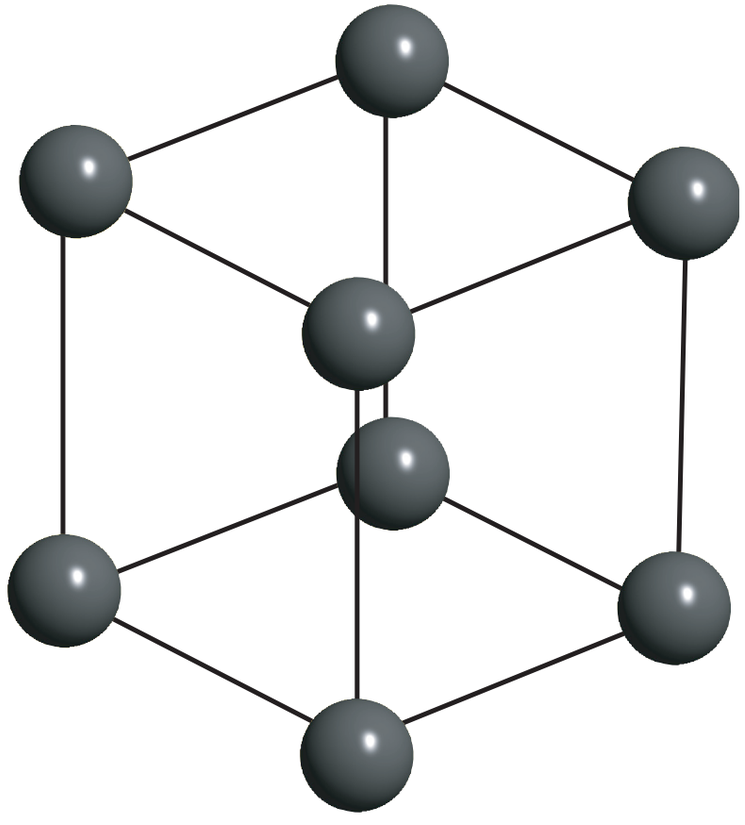
Simple cubic

- Or we can define the unit cell like this



Simple cubic

- A simple cubic structure is not a good idea for packing spheres (they occupy only 52% of the total volume).
- Only two elements crystallise in the simple cubic structure (F and O).



Better packing

- Fig 2.4, Solid State Physics: An Introduction, by Philip Hofmann, Wiley-VCH Berlin.

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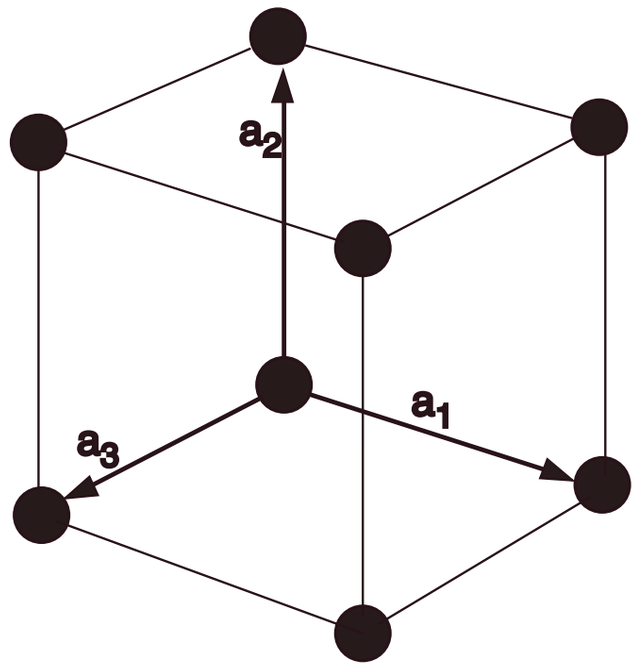

- In the body-centred cubic (bcc) structure 68% of the total volume is occupied.
- The bcc structure is also a Bravais lattice but the edges of the cube are (obviously) not the Bravais lattice vectors.

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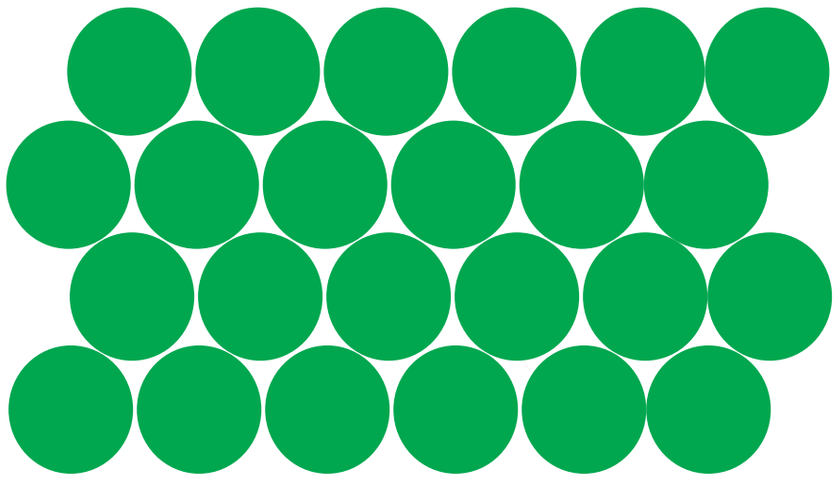
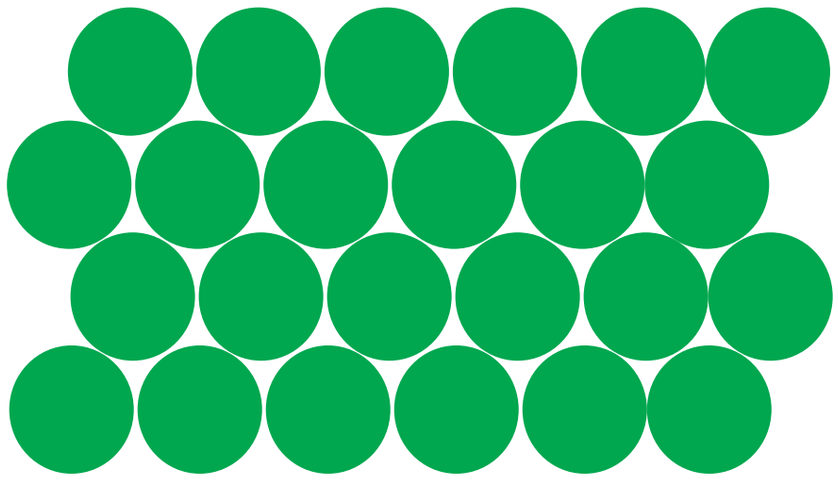
Close-packed structures

Close-packed structures: fcc and hcp

hcp
ABABAB...



fcc
ABCABCABC...



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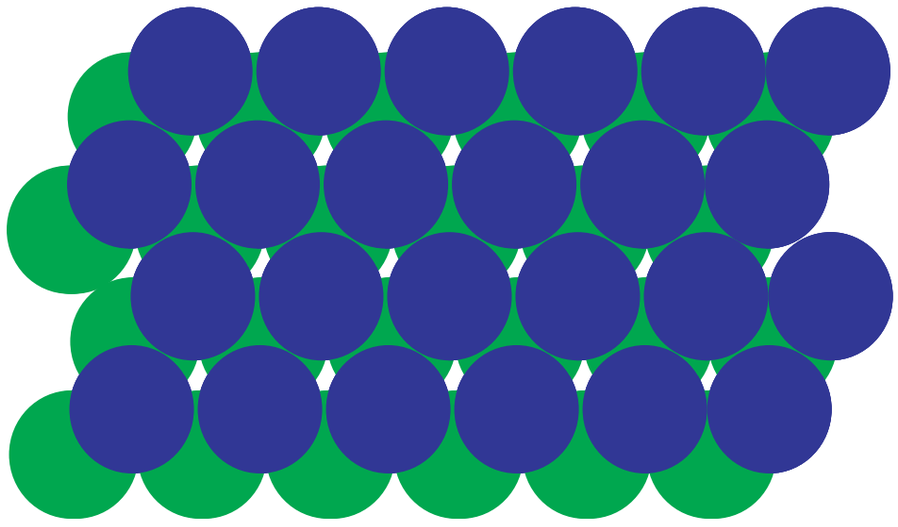

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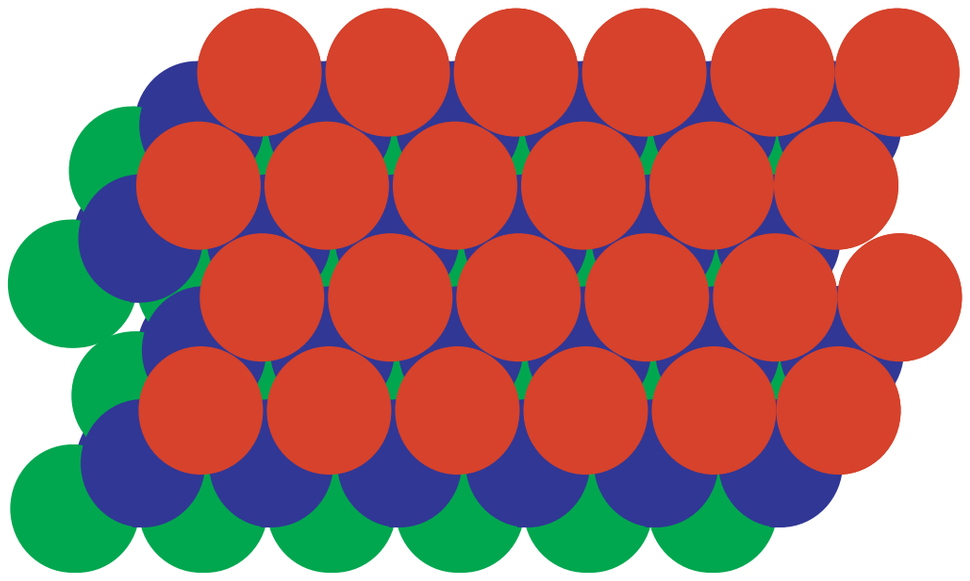

- The hexagonal close-packed (hcp) and face-centred cubic (fcc) and structure have the same packing fraction

The fcc structure

- Fig 2.4, Solid State Physics: An Introduction, by Philip Hofmann, Wiley-VCH Berlin.

- In the face-centred cubic (fcc) structure 74% of the total volume is occupied (slightly better than bcc with 68%)
- This is probably the optimum (Kepler, 1611) and grocers.

The fcc lattice: Bravais lattice (3D)

- The fcc lattice is also a Bravais lattice but the edges of the cube are not the correct lattice vectors.
- The cubic unit cell contains more than one atom.

$$\mathbf{R}_{mno} = m\mathbf{a_1} + n\mathbf{a_2} + o\mathbf{a_3}$$

- Fig 2.3, Solid State Physics: An Introduction, by Philip Hofmann, Wiley-VCH Berlin.

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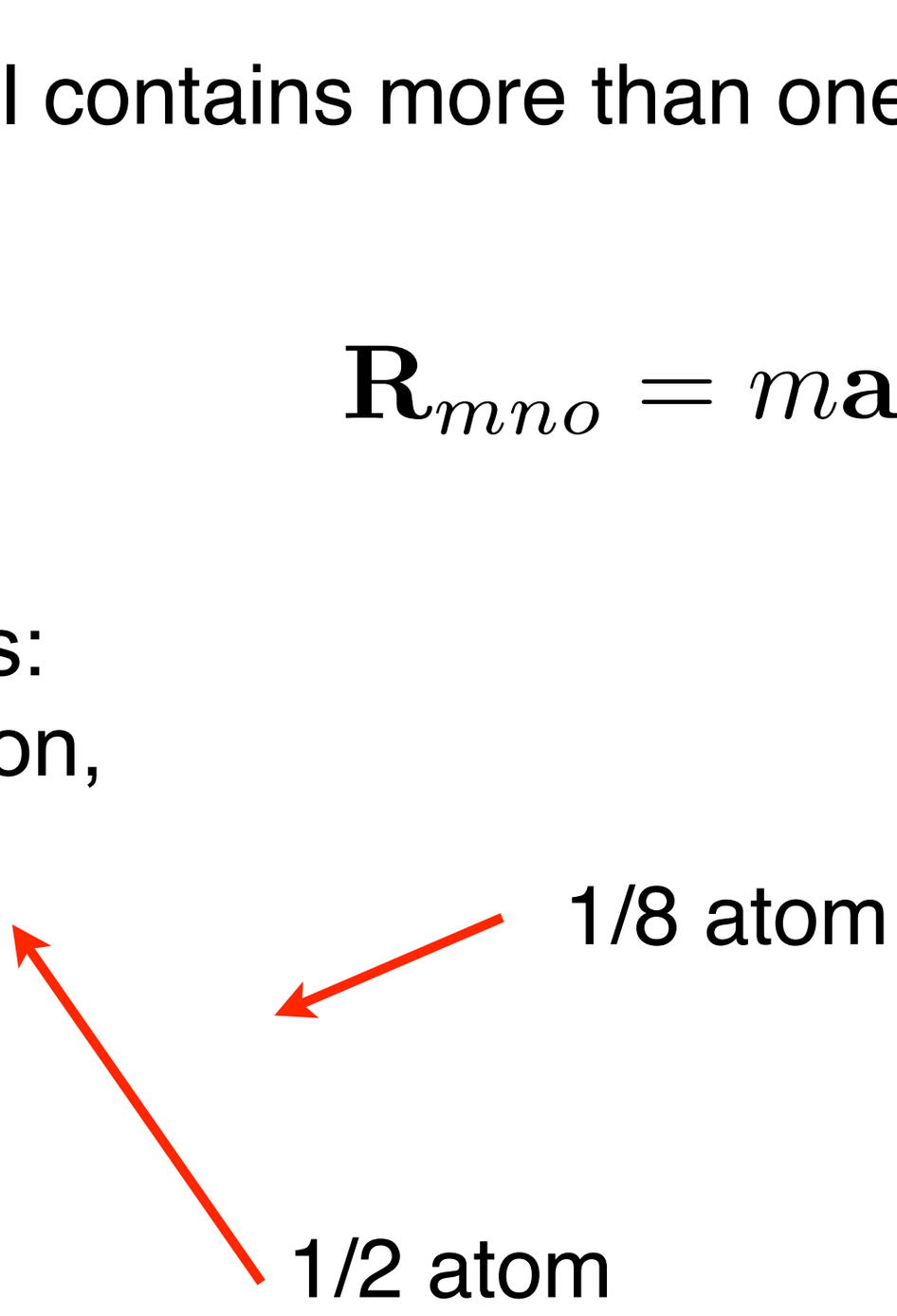

The fcc lattice: Bravais lattice (3D)

- The fcc and bcc lattices are also Bravais lattices but the edges of the cube are not the correct lattice vectors.
- When choosing the correct lattice vectors, one has only one atom per unit cell.

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