ATOMIC AND CRYSTAL STRUCTURE OF MATERIALS II

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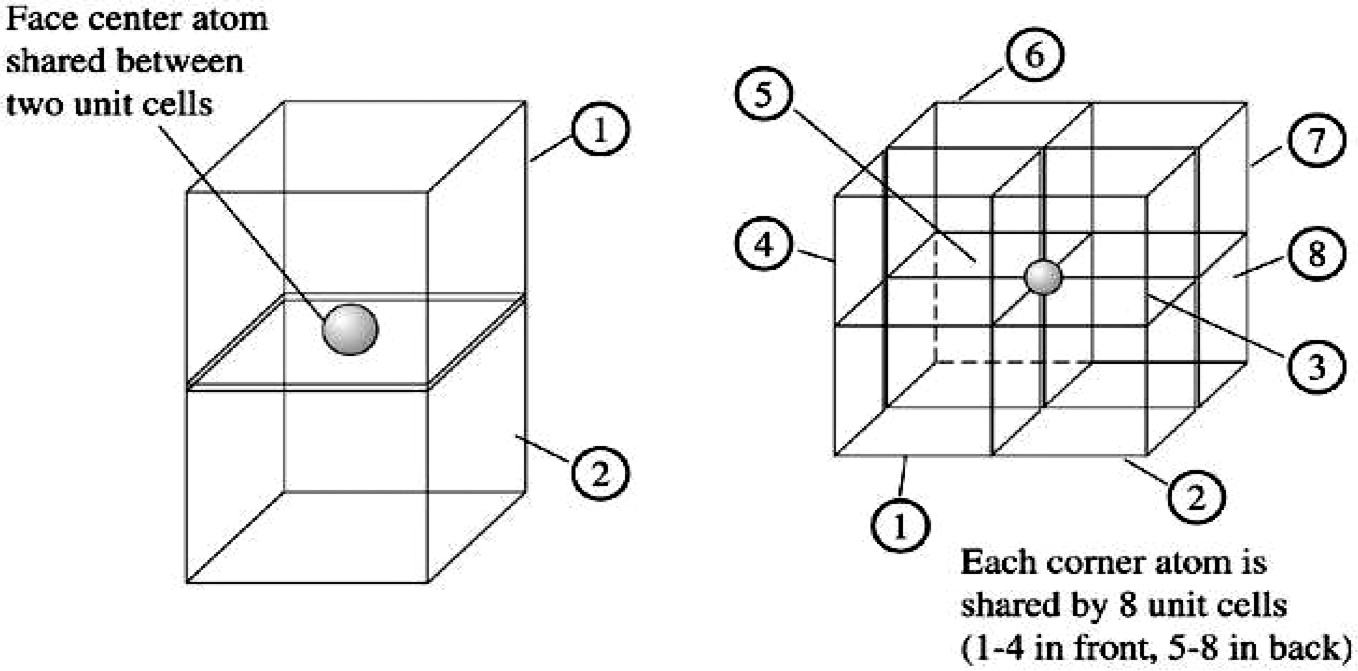
Common Crystal Lattices

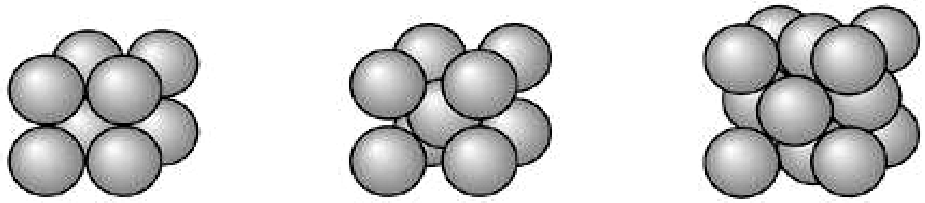
Most metals crystallise in one of the three structures:

- face-centred cubic (fcc)
- body-centred cubic (bcc) and
- hexagonal close packed structure (hcp or cph), (a special example of the hexagonal lattice.
- Very few metals crystallise in the simple cubic (sc) or the simple hexagonal (sh or hs) lattices.

Centered lattices and structures with more than one lattice point per unit cell



(a)



Simple cubic

Body-centered cubic

Face-centered cubic

(b)

(a)Illustration showing sharing of face and corner atoms.

(b)The models for simple cubic (SC), body centered cubic (BCC), and face- centered cubic (FCC) unit cells, ***assuming only one atom per lattice point*** .

Determining the Number of Lattice Points in Cubic Crystal Systems

Determine the number of lattice points per cell in the cubic crystal systems. If there is only one atom located at each lattice point, calculate the number of atoms per unit cell.

SOLUTION

In the SC unit cell : lattice point / unit cell = (8 corners)1/8 = 1

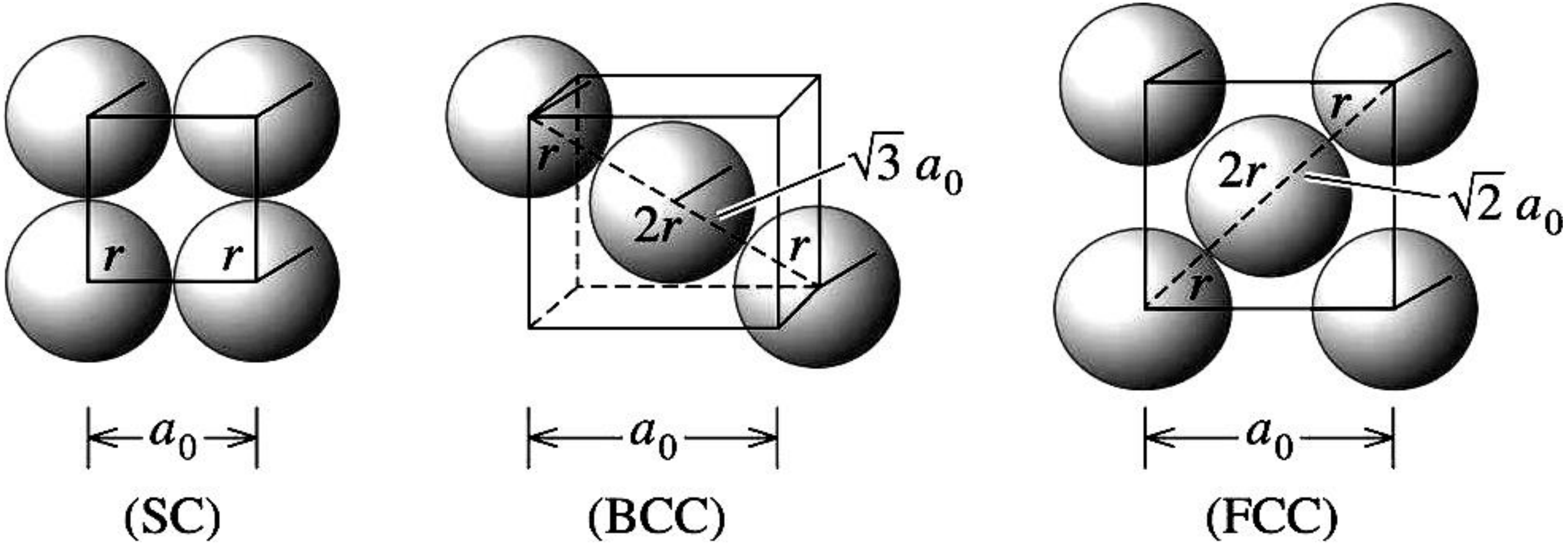
In BCC unit cells: lattice point / unit cell= (8 corners)1/8 + (1 center)(1) = 2

In FCC unit cells: lattice point / unit cell = (8 corners)1/8 + (6 faces)(1/2) = 4

If there is only on atom per lattice point, as in typical metal structures, the number of atoms per unit cell would be 1, 2, and 4, for the simple cubic, body-centered cubic, and face- centered cubic, unit cells, respectively. ***But there are also many structures with more than one atom per lattice point***

Determining the Relationship between Atomic Radius and Lattice Parameters

Determine the relationship between the atomic radius and the lattice parameter in SC, BCC, and FCC structures when one atom is located at each lattice point.



The relationships between the atomic radius and the lattice parameter in cubic systems

SOLUTION

Referring to Figure above, we find that atoms touch along the edge of the cube in SC structures.

$$a_0 = 2r$$

In BCC structures, atoms touch along the body diagonal. There are two atomic radii from the center atom and one atomic radius from each of the corner atoms on the body diagonal, so

$$a_0 = \frac{4r}{\sqrt{3}}$$

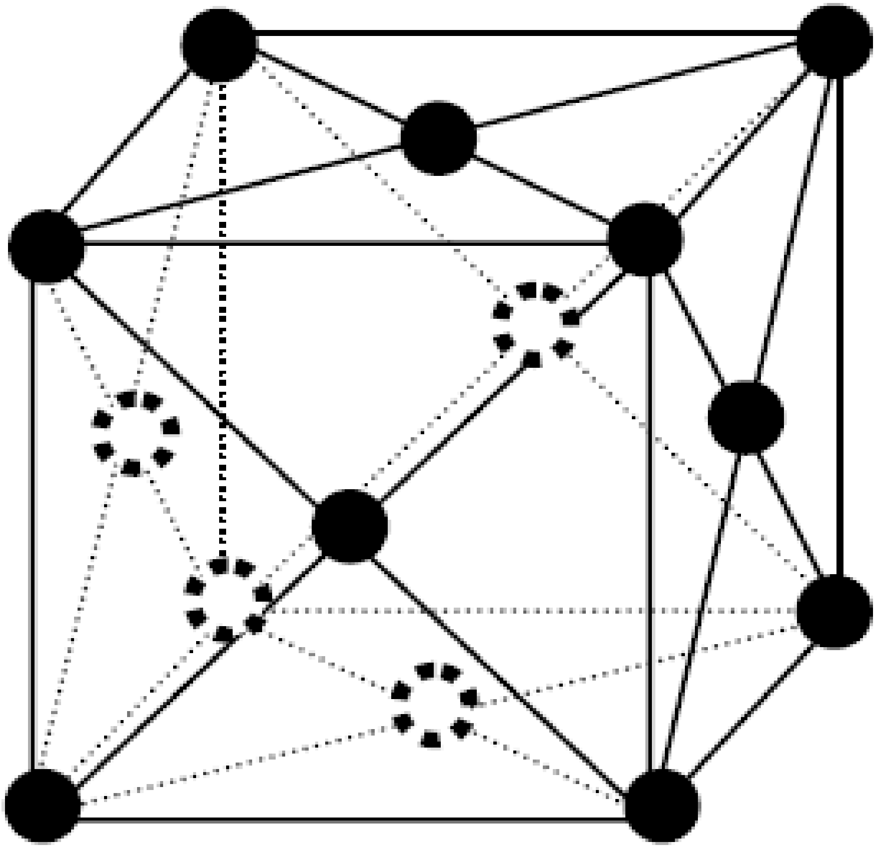
In FCC structures, atoms touch along the face diagonal of the cube. There are four atomic radii along this length—two radii from the face- centered atom and one radius from each corner, so:

$$a_0 = \frac{4r}{\sqrt{2}}$$

Atomic Structure of Materials

Face-centred cubic (fcc)system

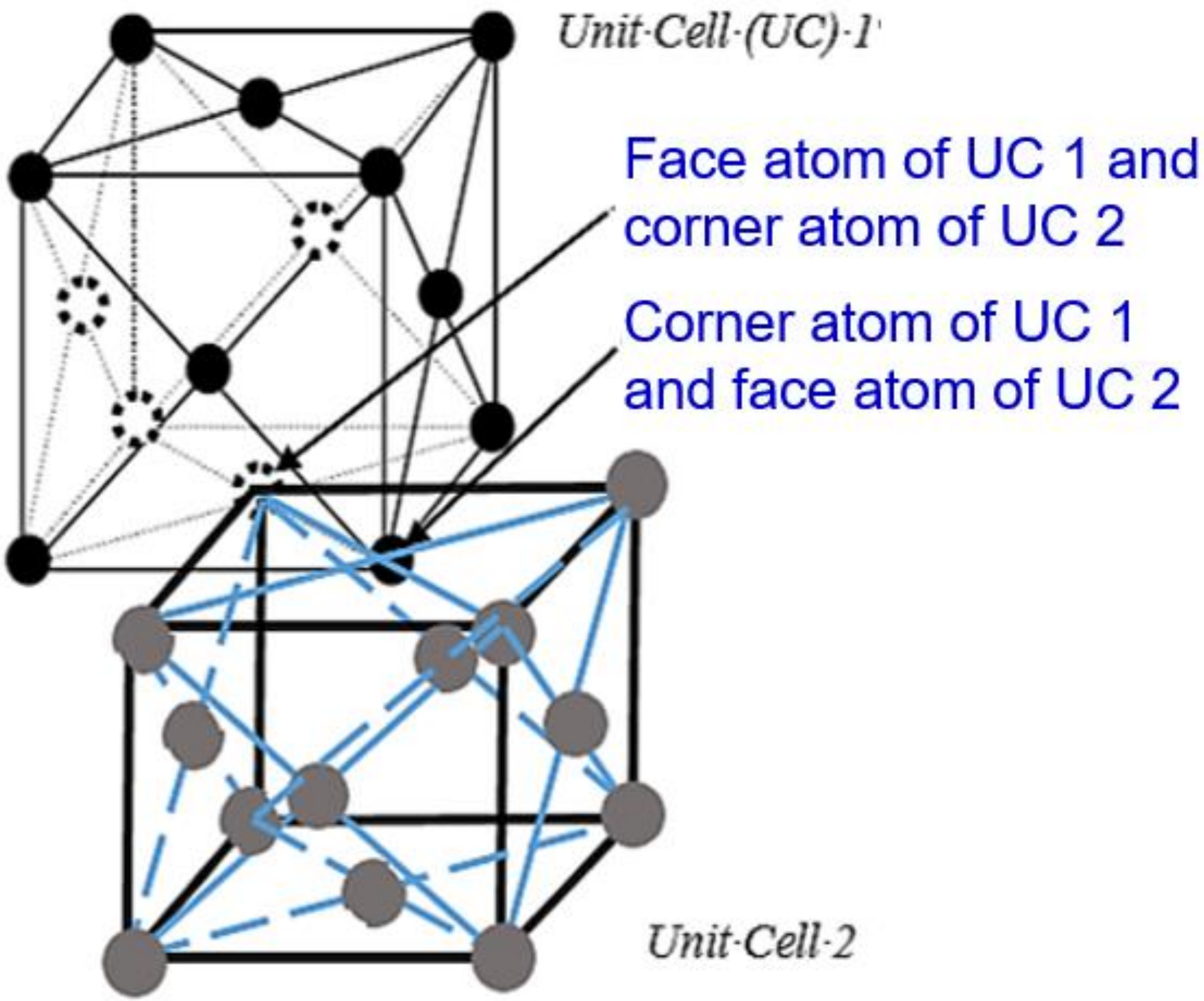
- Consider the unit cell given.
- Atom at corner and centre of each face.
- Now, let us make any one of the face atoms in this unit cell as a corner atom of a new unit cell.



Face-centred cubic unit cell. The circles represent the nuclei of atoms

Face Centred Cubic System

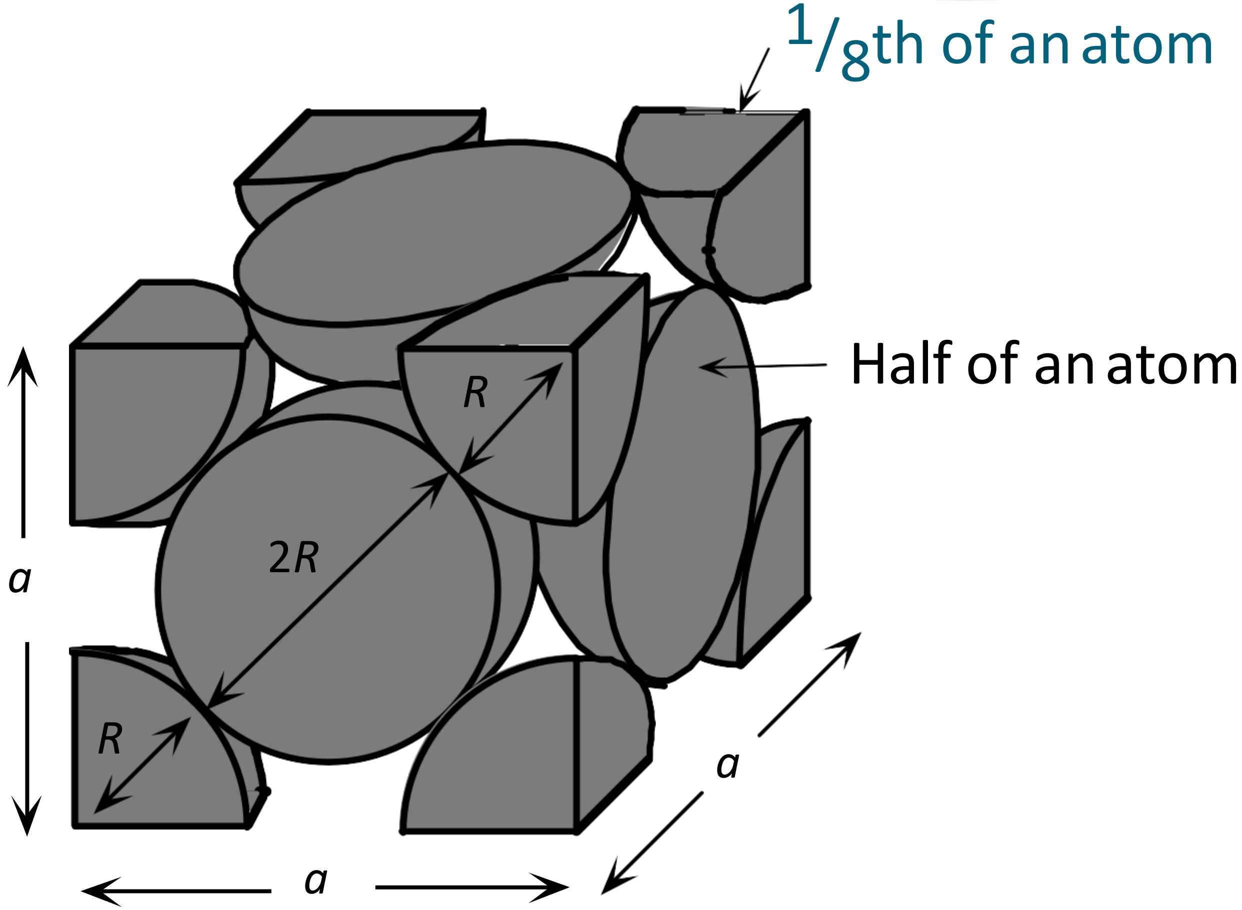
- By making any one face atom as a corner atom, all face atoms become corner atoms
- The corner atoms become face atoms as shown.
- Therefore, all the atoms in the fcc are lattice points.



Face atom of UC 1 and corner atom of UC 2

Corner atom of UC 1 and face atom of UC 2

Face Centred Cubic System



The FCC unit cell. The atomic radius is R and the lattice parameter is a

Atomic Structure of Materials
Face Centred Cubic System

- Each corner atom shared by eight (8) unit cells &
- Each face atom is shared by two (2) unit cells.
- Therefore the number of atoms per unit cell is:

$$(8 \times {}^{1}/_{8}) + (6 \times \tfrac{1}{2}) = 4$$

- Volume unit cell = a^3

Atomic Structure of Materials

- Therefore, the packing density, ***PD = 4/a^3*** atoms per unit cell.
- The material density for fcc is:

$$\rho = \frac{mass}{volume} = \frac{No.\,of\ atoms/unit\ cell\ \times mass\ of\ one\ atom}{Unit\ Cell\ Volume}$$

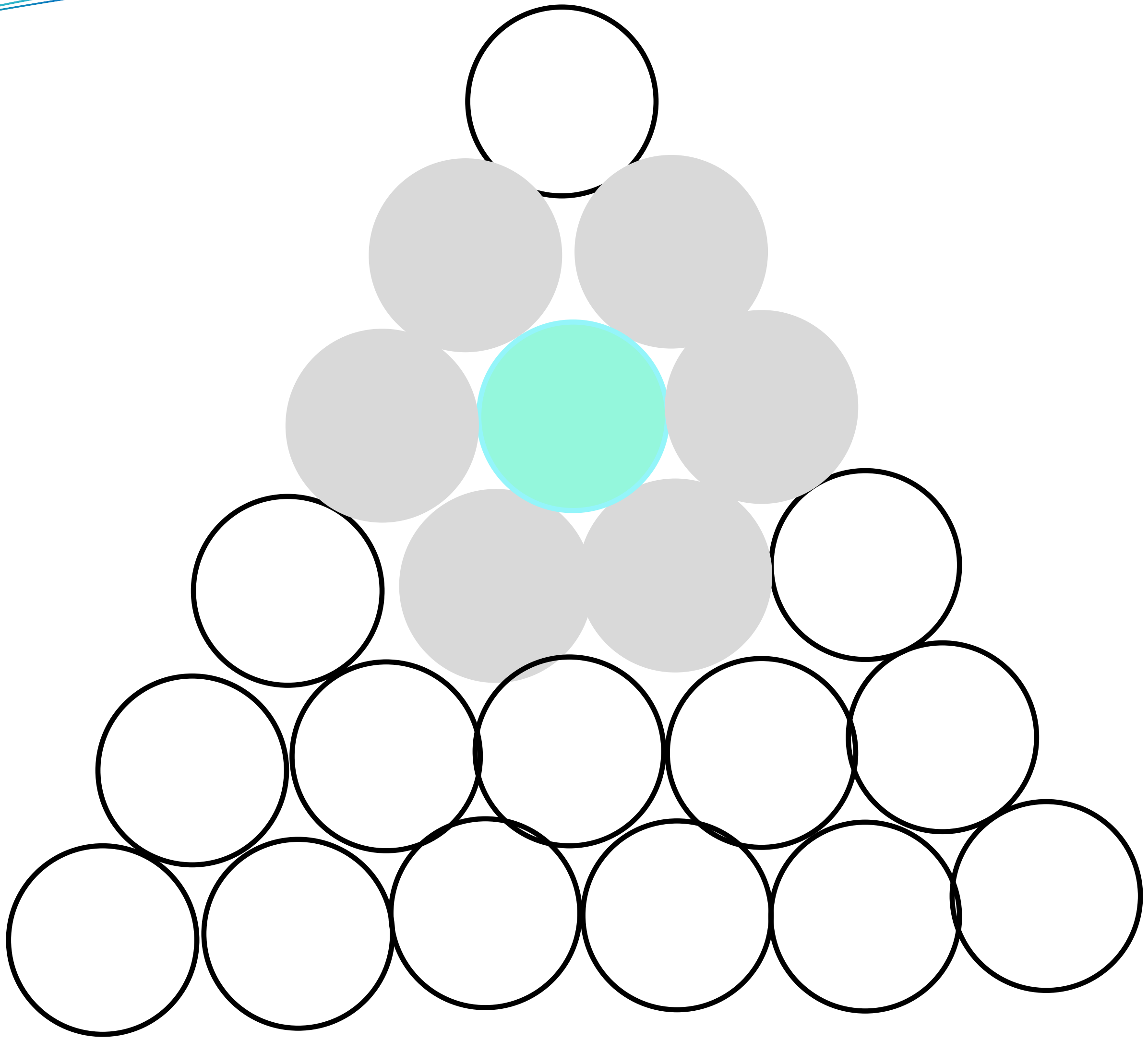
for fcc,

$$\rho = \frac{4\times \text{atomic mass}}{a^3}\ [\text{kg/m}^3]$$

Atomic Structure of Materials

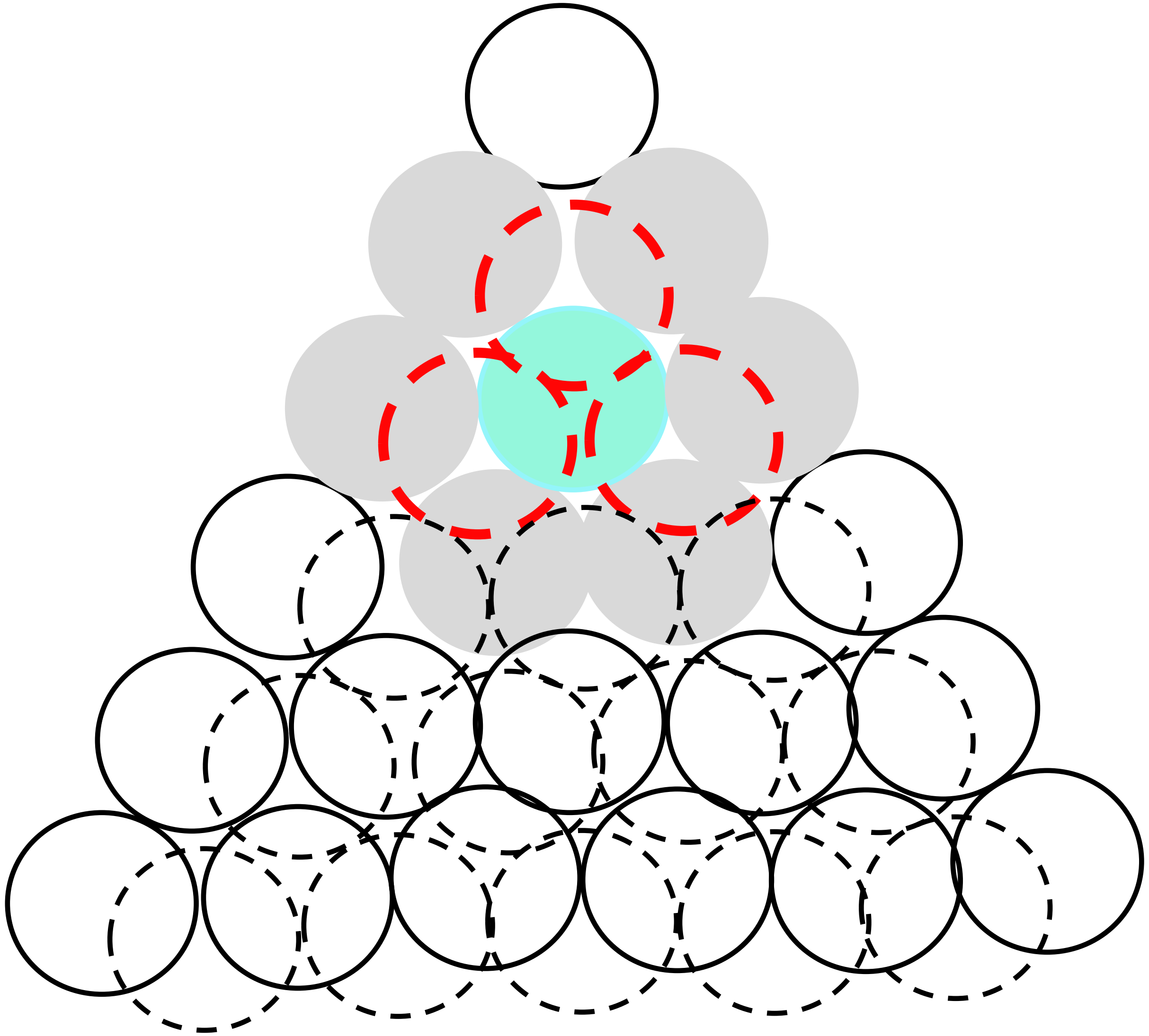
- Each atom has 12 near neighbours; $\Rightarrow$ the closest packing possible (Coordination No. = 12).
- Six of these in one plane form a hexagon around the centre atom,
- Three are in parallel planes on each side, this being (111) planes.
- All {111} planes are of closest packing.
- The spheres touch along the <111> directions, the directions of closest packing.

Atomic Structure of Materials



{111} Planes

Atomic Structure of Materials

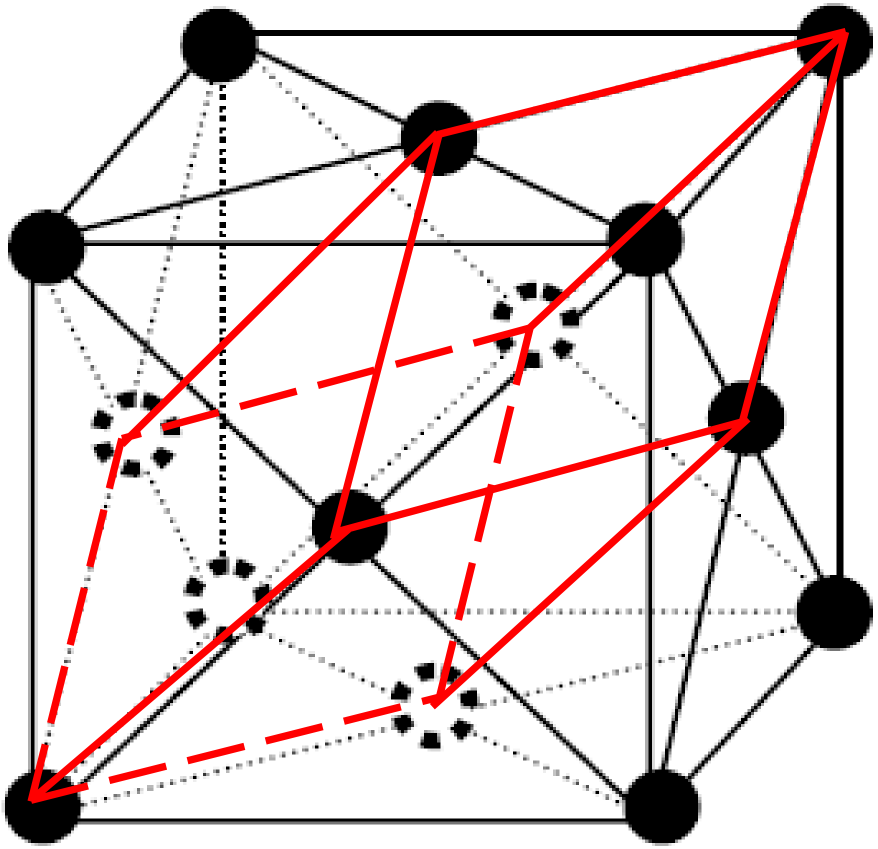


{111} Planes

Fcc Primitive Cell

- Taking the two corner atoms across the major diagonal and the six face atoms, such that each corner atoms is joined to the face atoms of its three adjacent faces, as shown, a new, **smaller** unit cell can be formed.

- It is **different from** in shape and orientation and **smaller than** the actual unit cell of the fcc.

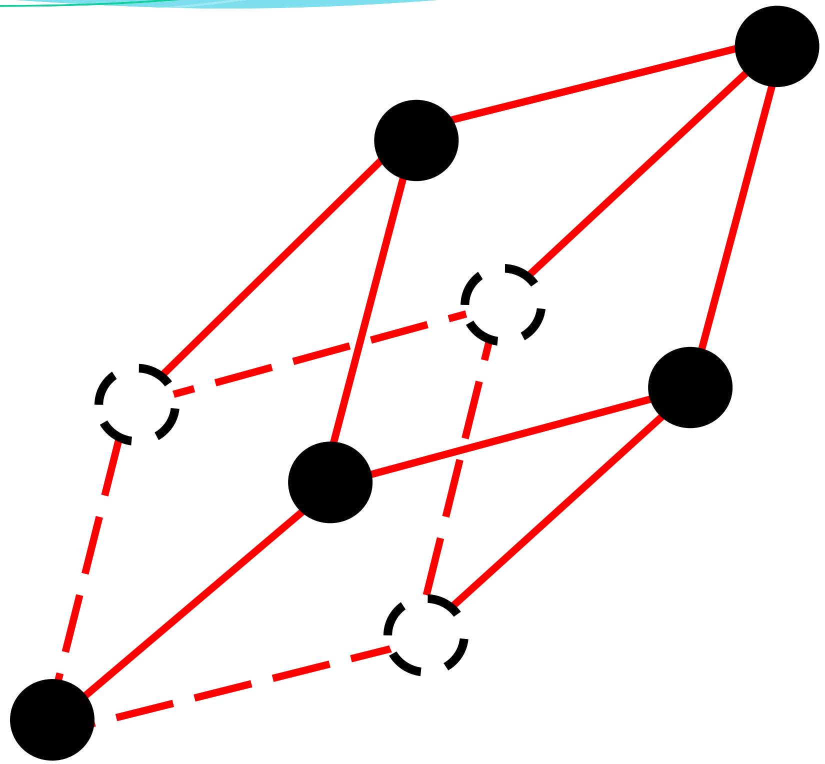


FCC Primitive Cell

- Taking two corner atoms across the major diagonal and the six face atoms, a new, **smaller** unit cell can be formed

- It is different from actual unit cell of the fcc.

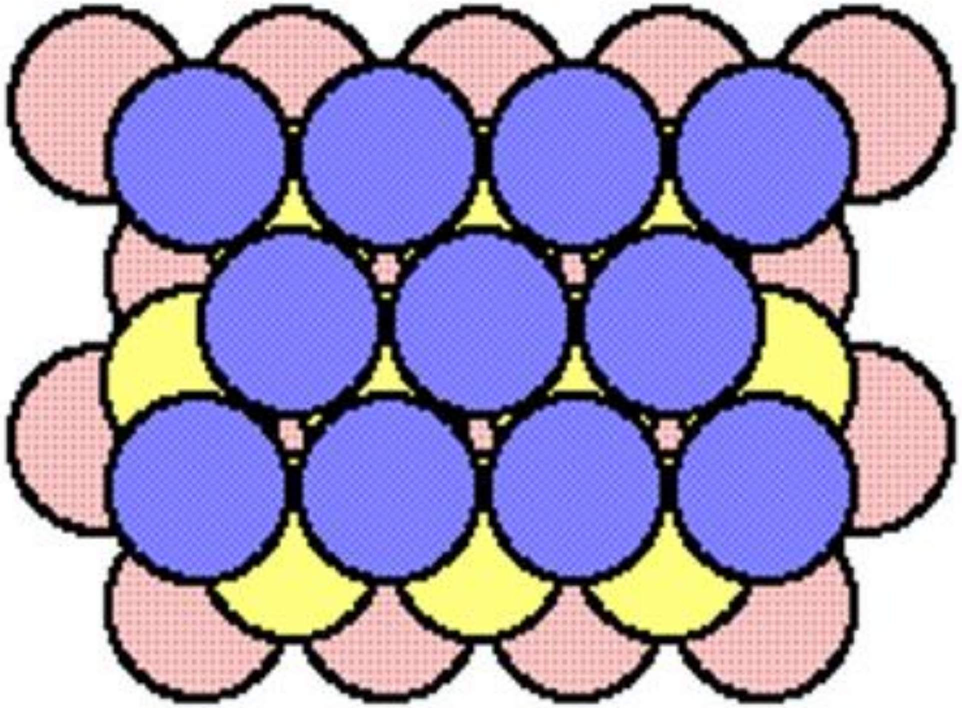
- It is called a ***primitive cell***, the ***smallest unit*** that the lattice can be divided into.

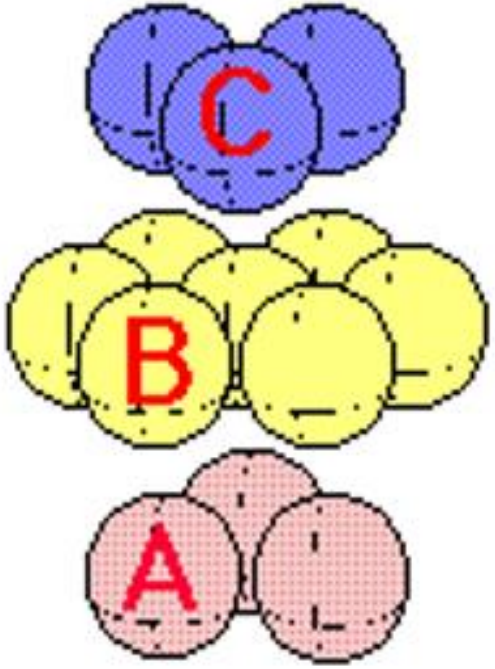


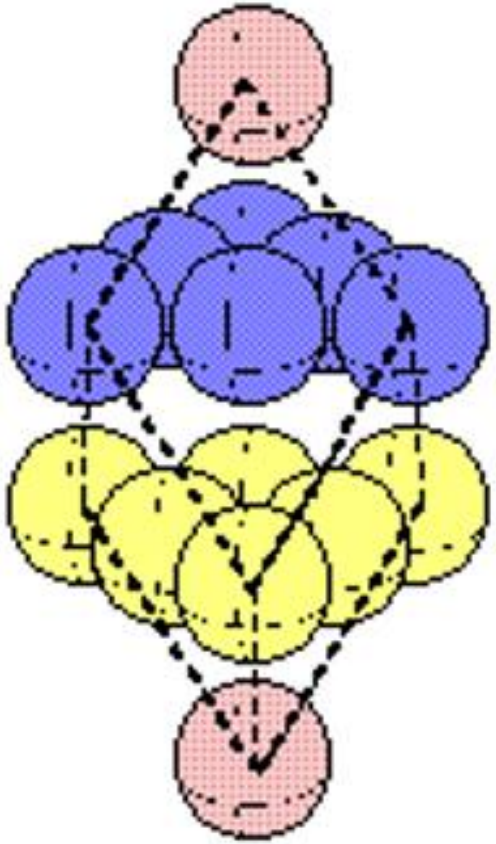
FCC Primitive Cell

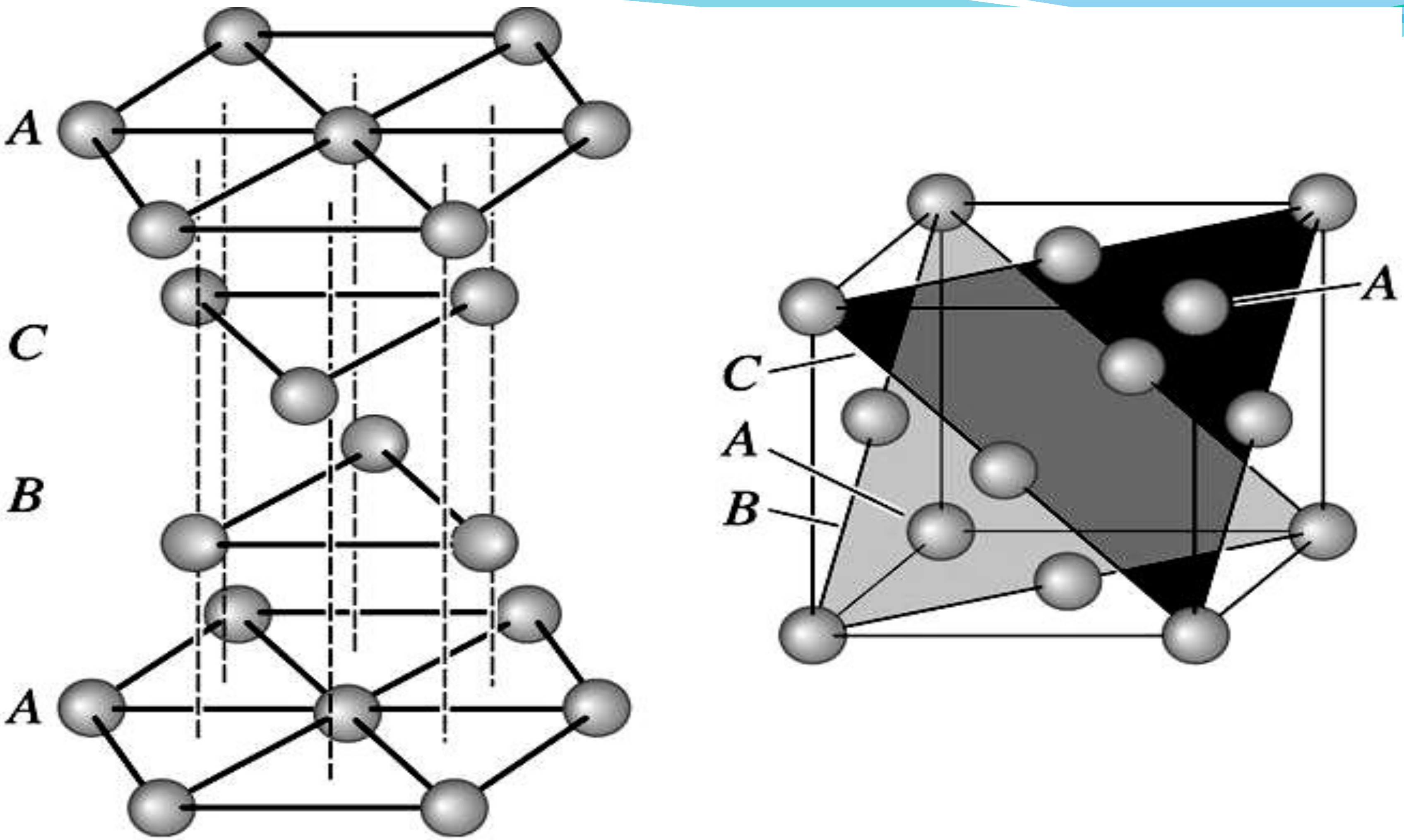
- It runs along the major diagonal of the unit cell (so, it has four possible orientations since the cube has four major diagonals.

Cubic close packing (ABCABC…)









The *ABCABCABC* stacking sequence of close- packed planes produces the FCC structure.

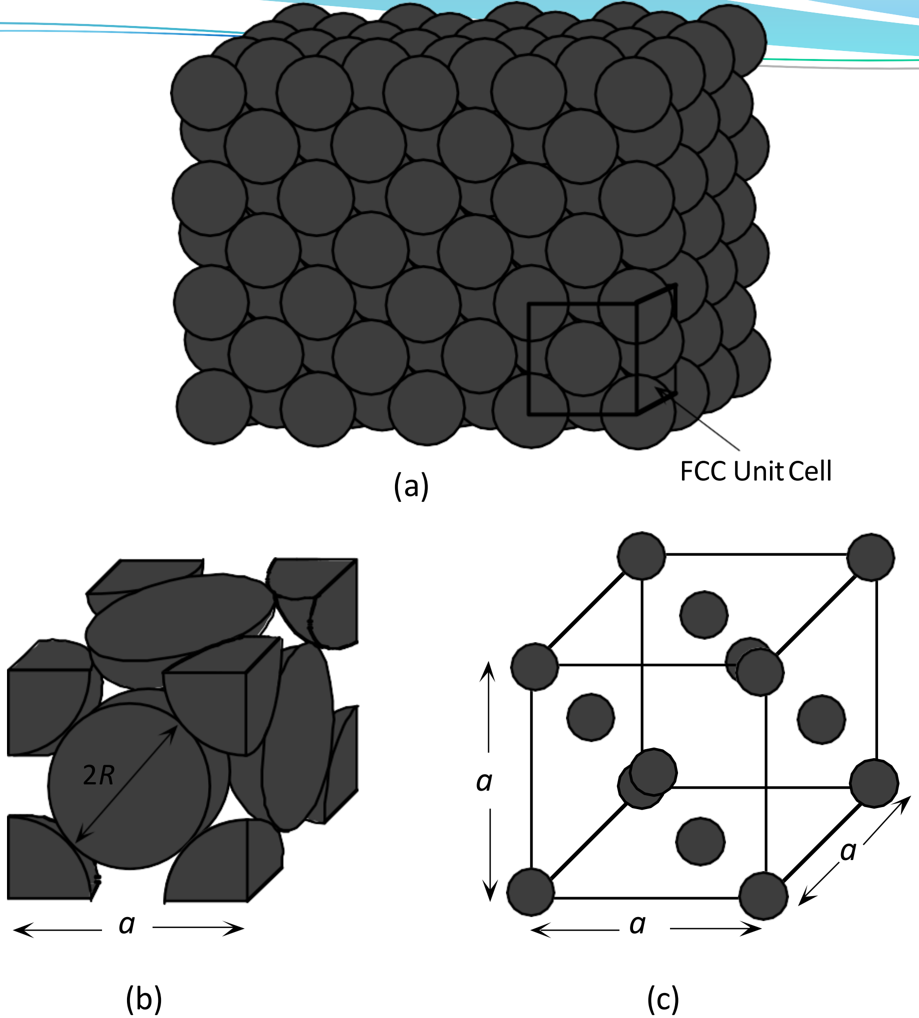
Atomic Structure of Materials

Metals that crystallise in fcc include:

Copper (Cu), Nickel (Ni), Aluminium (Al), Iron (Fe), Silver (Ag) and Gold (Au).

Properties:

Generally soft, ductile and easy to form.



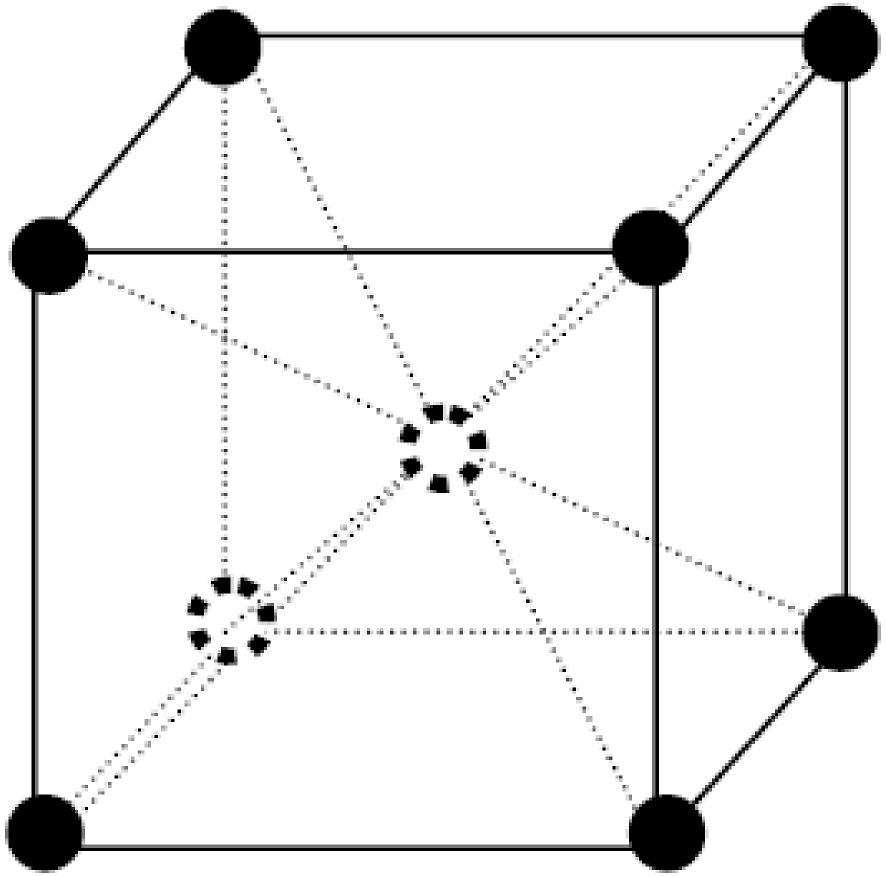
(a) The crystal structure of copper is Face Centered Cubic (FCC). The atoms are positioned at well defined sites arranged periodically. (b) An FCC unit cell with closed packed spheres. (c) Reduced sphere representation of the FCC unit cell. Examples: Ag, Al, Au, Ca, Cu, γ-Fe (>912• C), Ni, Pd, Pt, Rh

Body-centred cubic (bcc) unit cell.

- One atom at each corner and also
- One atom at the centre.
- The number of atoms per unit cell:

$(8 \times {}^{1}/_{8}) + (1) = 2$

- The volume of the unit cell is a^3.



Body-centred cubic unit cell.

- As in fcc, each atomic site in bcc is a lattice point.

Atomic Structure of Materials

- Therefore, the packing density, ***PD = 2/a³*** atoms per unit cell.
- The material density for bcc is:

$$\rho = \frac{mass}{volume} = \frac{No.\,of\ atoms/unit\ cell\ \times mass\ of\ one\ atom}{Unit\ Cell\ Volume}$$

for bcc,

$$\boldsymbol{\rho = \frac{2 \times atomic\ mass}{a^3}}\ [\mathrm{kg/m^3}]$$

Atomic Structure of Materials

- Each atom has eight (8) near neighbours (Coordination No. = 8), so that this system is ***not*** one of closest packing.

- There is no close-packed plane in this system.

- In bcc, primitive cell is the same as the unit cell.

Atomic Structure of Materials

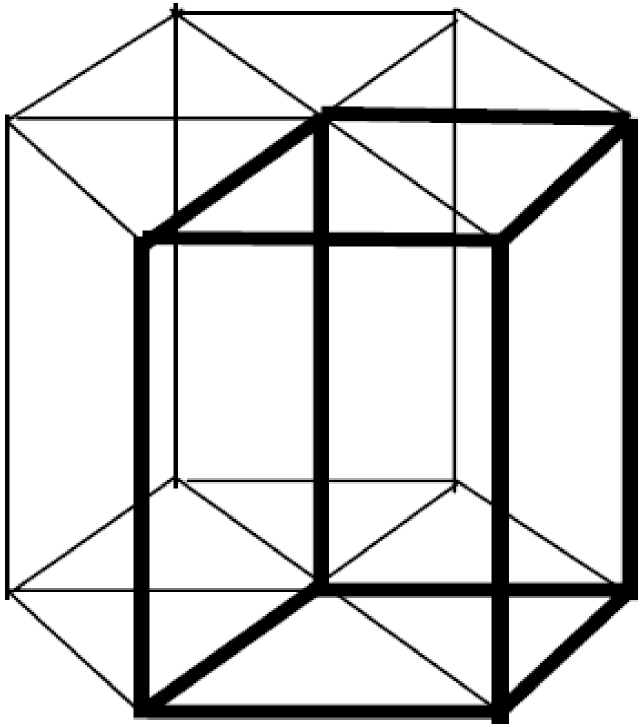
Metals that crystallise in bcc include:

Sodium (Na), Potassium (K), Iron (Fe), Chromium (Cr), Molybdenum (Mo), Wolfram or Tungsten (W).

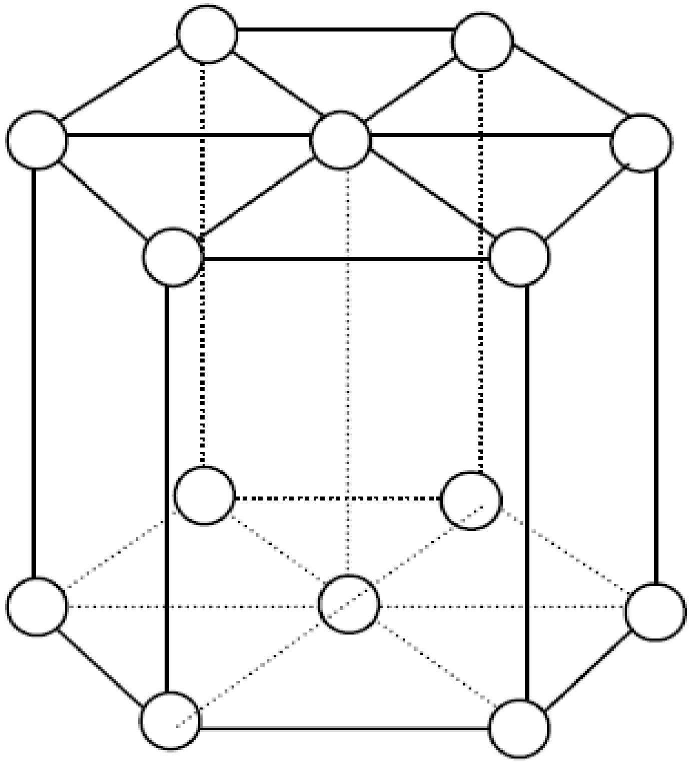
Properties:

Brittle and difficult to form.

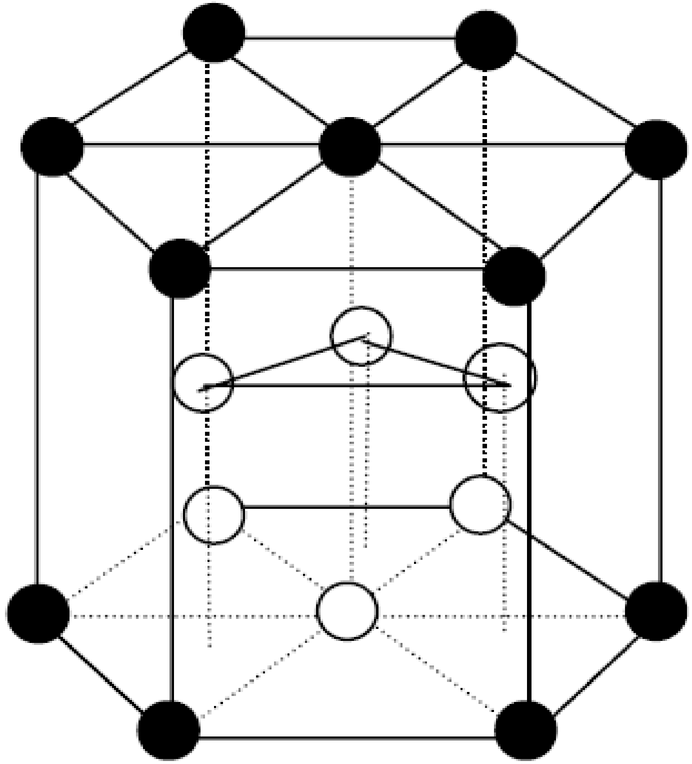
Close-packed hexagonal system



Relationship of unit cell to hexagon in the hexagonal close-packed structure



Lattice points of hexagonal system



Atom sites of hexagonal close-packed structure

Atomic Structure of Materials

- In hcp system, close-packed layers are packed on top of one another.
- Unit cell (which is a primitive cell) is related to the hexagonal structure as shown in the first figure.
- One corner atom is common to eight (8) unit cells,
- One body atom is unique to each unit cell.
- Thus number of atoms per unit cell:

$$(8 \times {}^{1}/_{8}) + (1) = 2$$

- The volume of the unit cell is $\boldsymbol{a_1 \cdot a_2 \cdot c \cdot \sin 120^o = \frac{1}{2}\sqrt{3} \cdot a^2 c}$

Atomic Structure of Materials

- Therefore, the packing density,

$$PD = \frac{2}{\frac{1}{2}\sqrt{3}\cdot a^2 c} = \frac{4}{\sqrt{3}\cdot a^2 c}$$ atoms per unit cell.

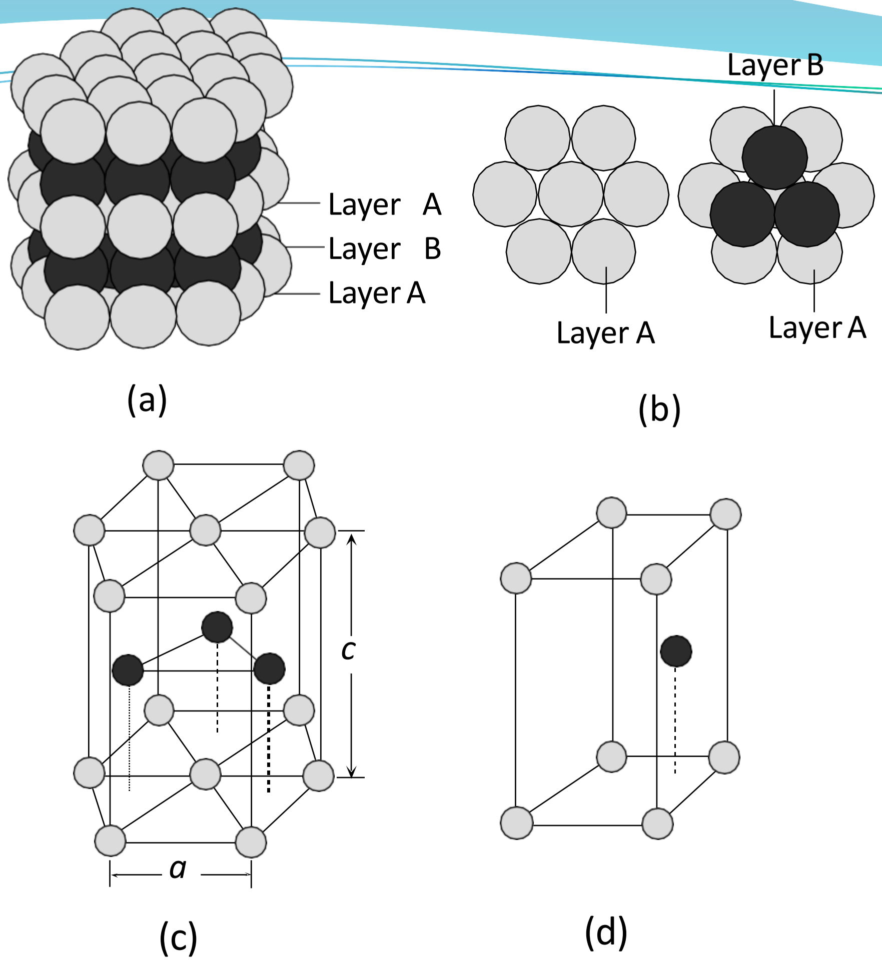
- The material density for hcp is:

$$\rho = \frac{mass}{volume} = \frac{No.\,of\ atoms/unit\ cell\ \times mass\ of\ one\ atom}{Unit\ Cell\ Volume}$$

$$\rho = \frac{2\times \text{atomic mass}}{\left(\frac{1}{2}\sqrt{3}\cdot a^2 c\right)}$$ [kg/m^3]

Atomic Structure of Materials

- Each atom has twelve (12) near neighbours (Coordination No. = 12), so that this system **is** one of closest packing
- hcp has three primitive cells in each unit cell, at 120° orientation with each other.
- Metals that crystallise in hcp include
- Cobalt (Co), Zinc (Zn), Titanium (Ti), Manganese (Mn) and Magnesium (Mg).
- Properties:
- Metals that crystallise in hcp structures are also brittle and difficult to form.



Be very careful, the black and grey spheres represent one and the same type of atoms

(a) The Hexagonal Close Packed (HCP) Structure. A collection of many Zn atoms. Color difference distinguishes layers (stacks).

(b)The stacking sequence of closely packed layers is ABAB

(c)A unit cell with reduced spheres (d) The smallest unit cell with reduced spheres.

Atomic Structure of Materials

Crystal Defects

- Almost all crystals contain defects, i.e. the atoms are not perfectly arranged according to their crystal structures.

- Defects affect the properties of materials.

Crystal Defects

- Crystal defects can be classified into the following categories:
  - Point defects (vacancy, interstitial, etc.)
  - Line defects (dislocations)
  - Surface defects (grain boundaries)
  - Volume defects (voids)

SUMMARY Crystals

- Atoms typically assemble into crystals some materials e.g. glass are amorphous

- We can predict the density of a material, provided we know the atomic weight, atomic radius, and crystal geometry (e.g., FCC, BCC, HCP).

- Material properties generally vary with single crystal orientation (i.e., they are anisotropic), but properties are frequently quite non-directional (i.e., they are isotropic) in polycrystals with randomly oriented grains as e.g. in steel and other engineering materials

The End