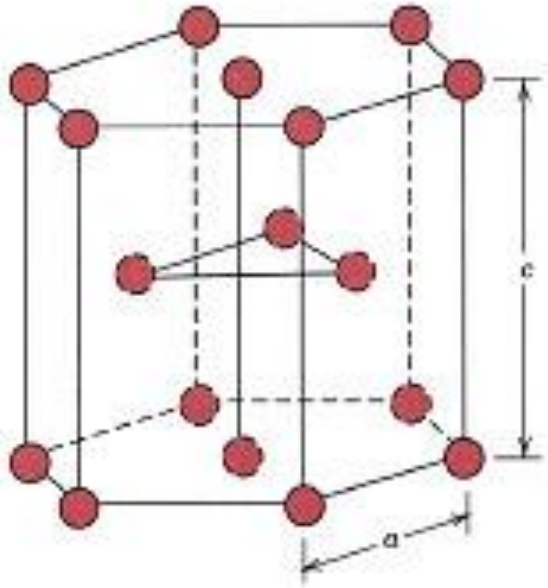
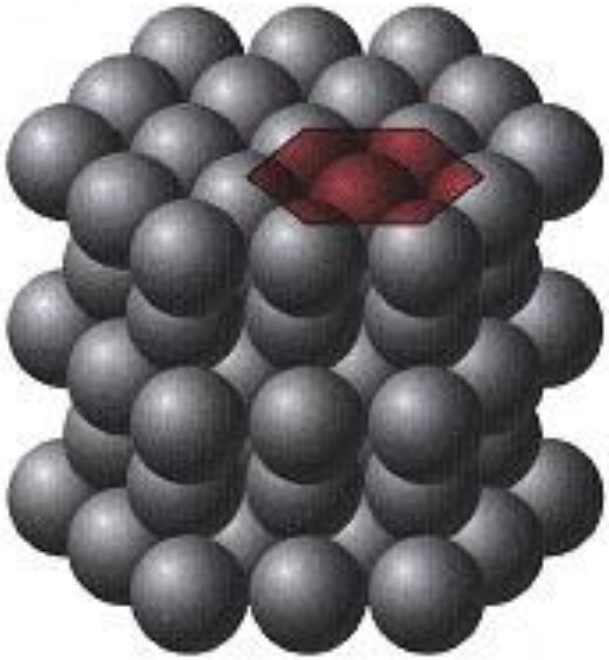
Crystal Structures

- **HEXAGONAL**

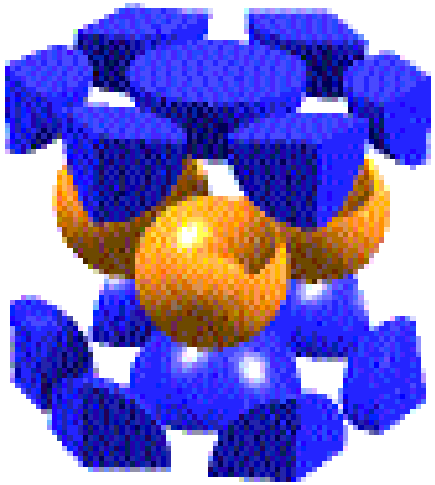
  $a = b \neq c;\ \alpha = \beta = 90;\ \gamma = 120$

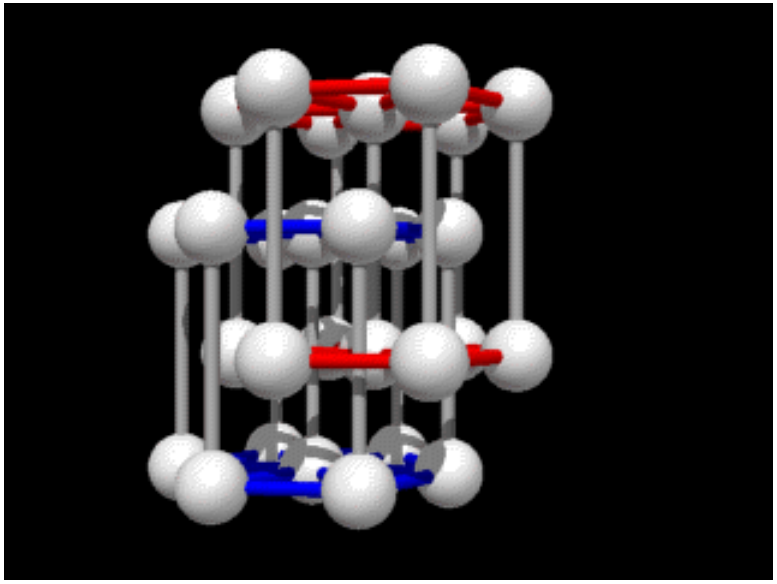




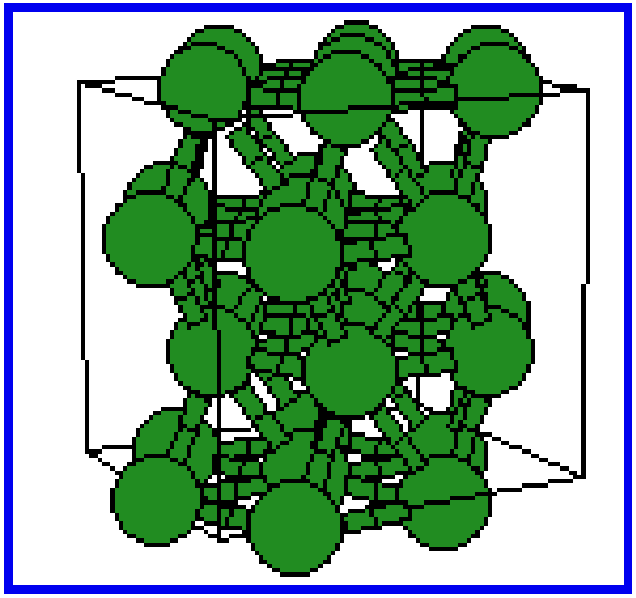
1- Hexagonal Close Packed (HCP) Lattice

- This is another structure that is common, particularly in metals. In addition to the two layers of atoms which form the base and the upper face of the hexagonal, there is also an intervening layer of arranged atoms.

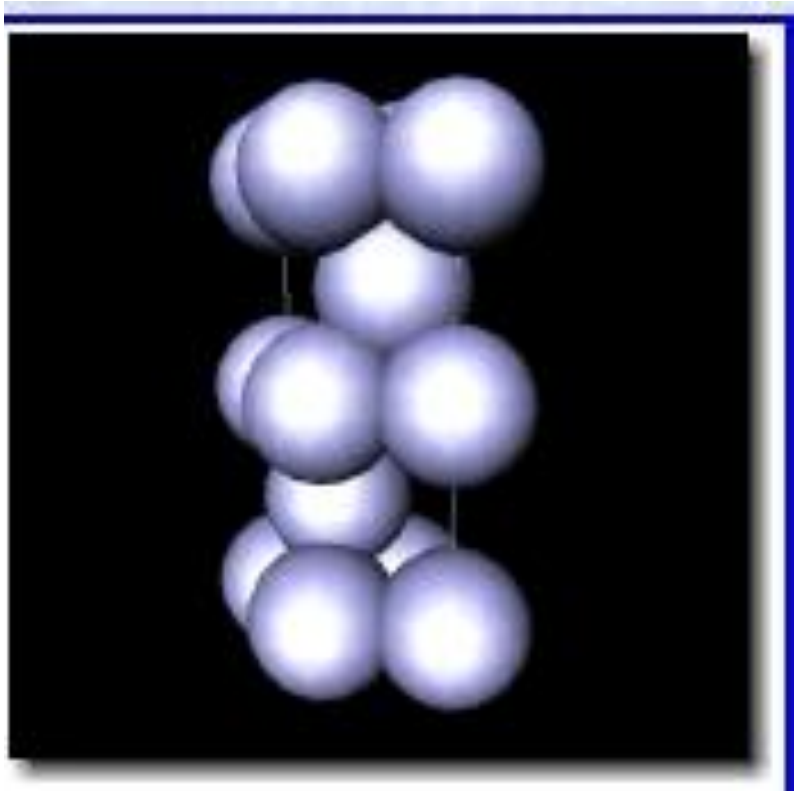




Hexagonal Close Packed (HCP) Lattice



Hexagonal Close Packed and related structures



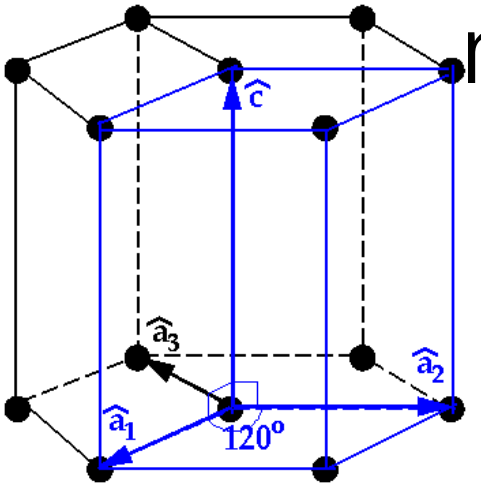
Crystal	*c/a*	Crystal	*c/a*	Crystal	*c/a*
He	1.633	Zn	1.861	Zr	1.594
Be	1.581	Cd	1.886	Gd	1.592
Mg	1.623	Co	1.622	Lu	1.586
Ti	1.586	Y	1.570		

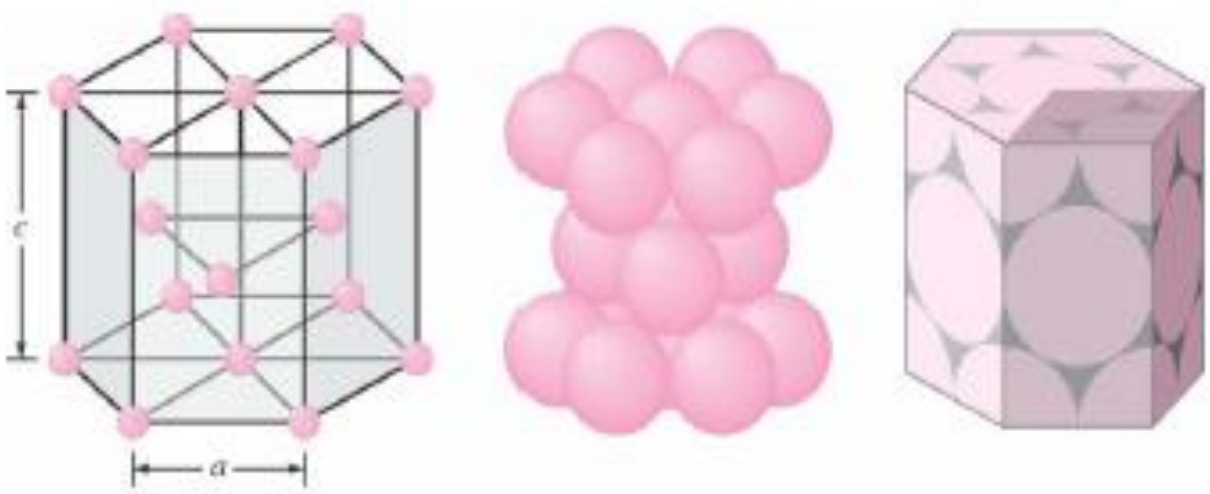
1) Hexagonal close-packed (HCP)

- **Unit cell has two lattice parameters a and c.**
  Ideal ratio c/a = 1.633
- **The coordination number, CN = 12 (same as in FCC)**
- **Number of atoms per unit cell, n = 6.**
  3 mid-plane atoms not shared: 3 x 1 = 3
  12 hexagonal corner atoms shared by 6 cells:
  12 x 1/6 = 2
  2 top/bottom plane center atoms shared by 2 cells:
  2 x 1/2 = 1
- **Atomic packing factor, APF = 0.74 (same as in FCC)**

2- HEXAGONAL CRYSTAL SYSTEMS

- In a *Hexagonal Crystal System*, three equal coplanar axes intersect at an angle of 60°, and another axis is perpendicular to the others and of a



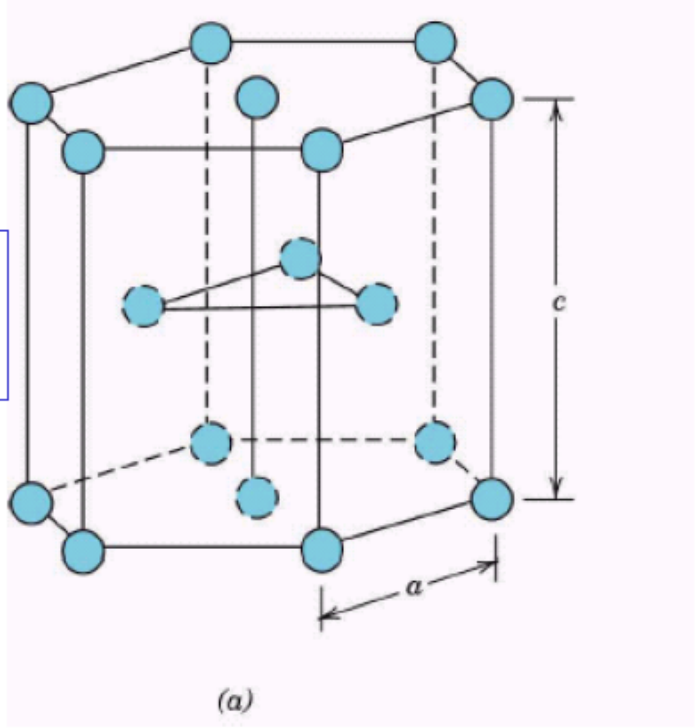


The atoms are all the same.

Hexagonal close packed (HCP) crystal structure

c/a = 1.63

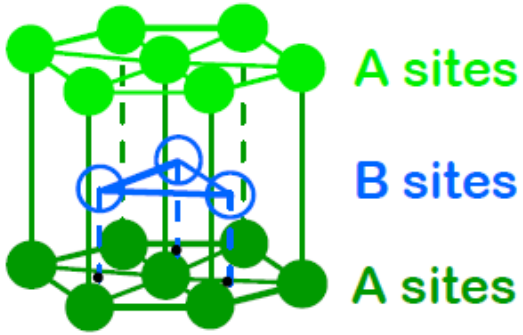
For most HCP metals



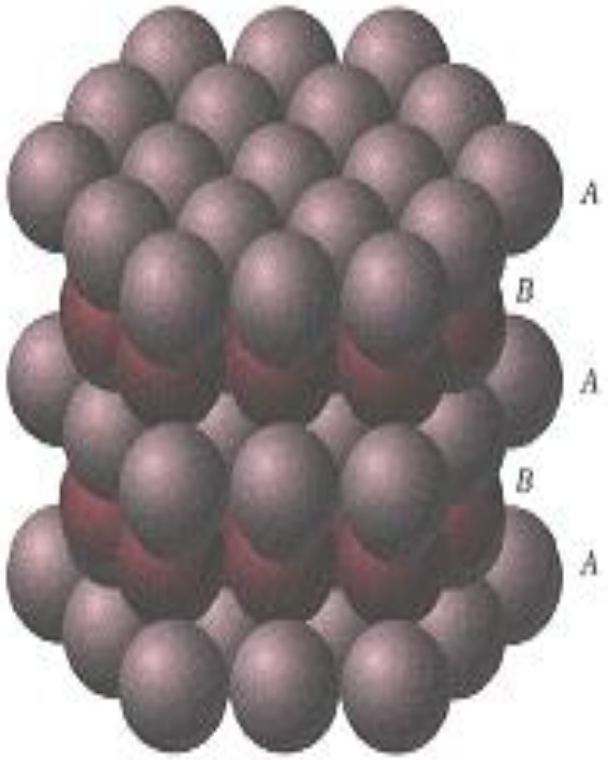
Number of atoms per unit cell :

12 (corner atoms) x 1/6 + 3 (interior atoms)

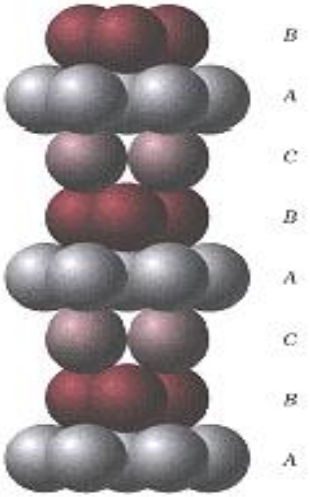
+ 2 (face atoms) x 1/2= 6 atoms / unit cell

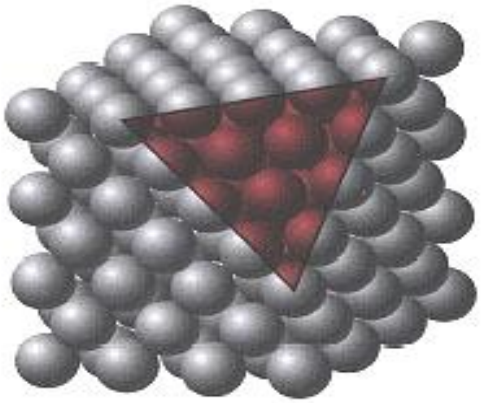


- **FCC and HCP: APF =0.74 (maximum possible value)**
- **FCC and HCP may be generated by the stacking of close-packed planes**
- **Difference is in the stacking sequence**



HCP: Stacking Sequence ABABAB...



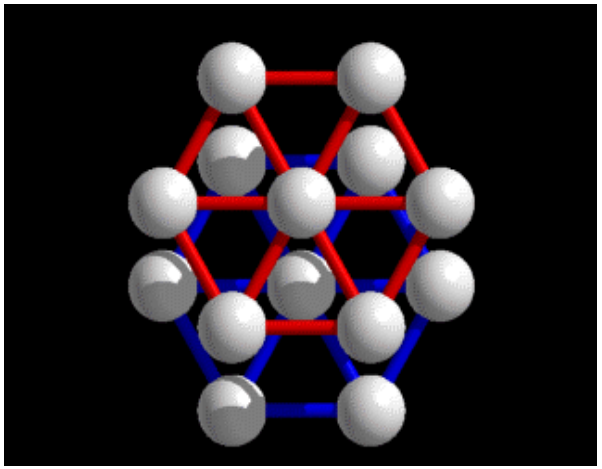


FCC: Stacking Sequence ABCABCABC...

For more clarity:

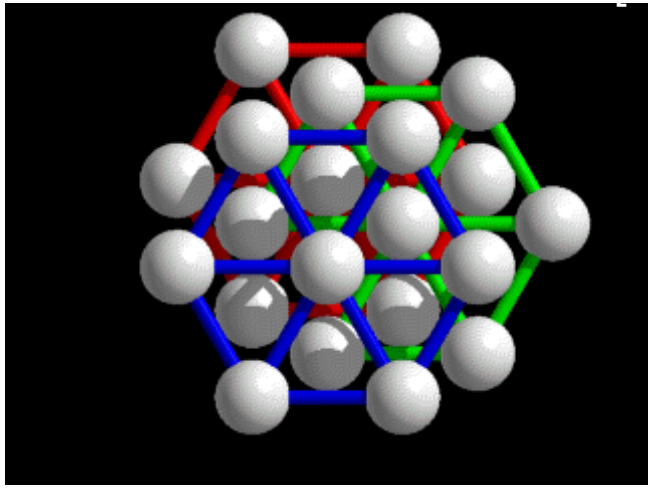
The FCC and hexagonal closed-packed structures (HCP) are formed from packing in different ways. FCC (sometimes called the cubic closed-packed structure, or CCP) has the stacking arrangement of ABCABCABC… HCP has the arrangement ABABAB….

HCP



ABAB
sequence

FCC



ABCABC
sequence

2) Isotropic and Anisotropic crystals

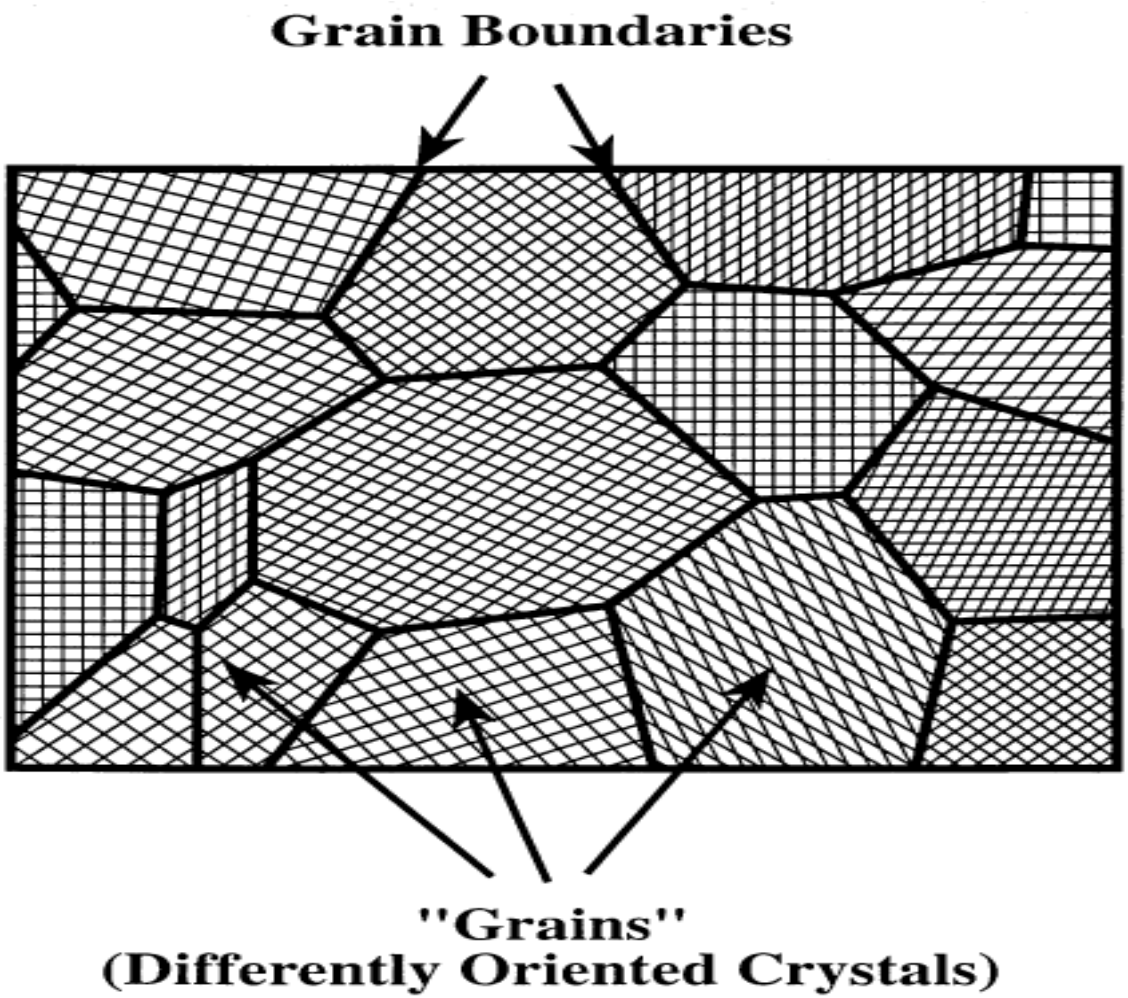
Different directions in a crystal have different packing.

For instance: atoms along the edge of FCC unit cell are more separated than along the face diagonal → causes anisotropy in crystal properties.

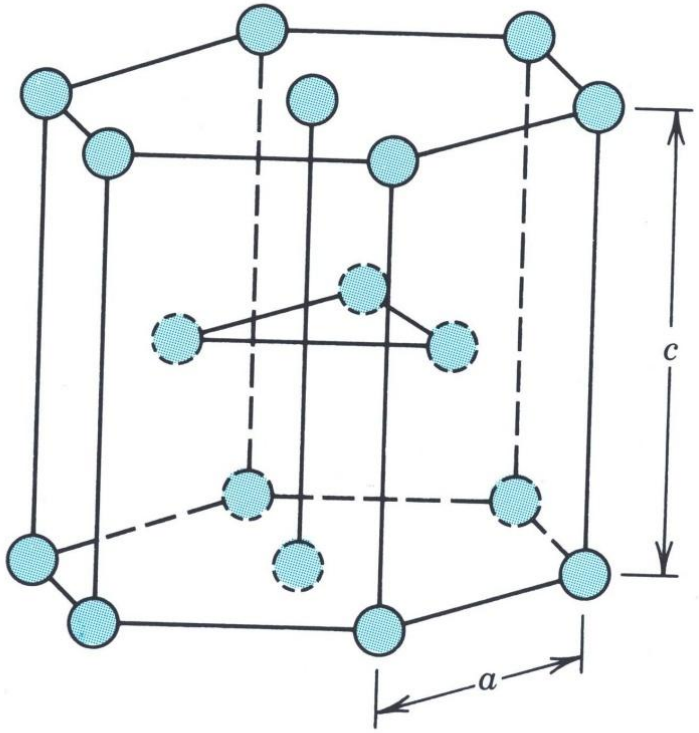
Deformation depends on direction of applied stress

If grain orientations are random → bulk properties are isotropic

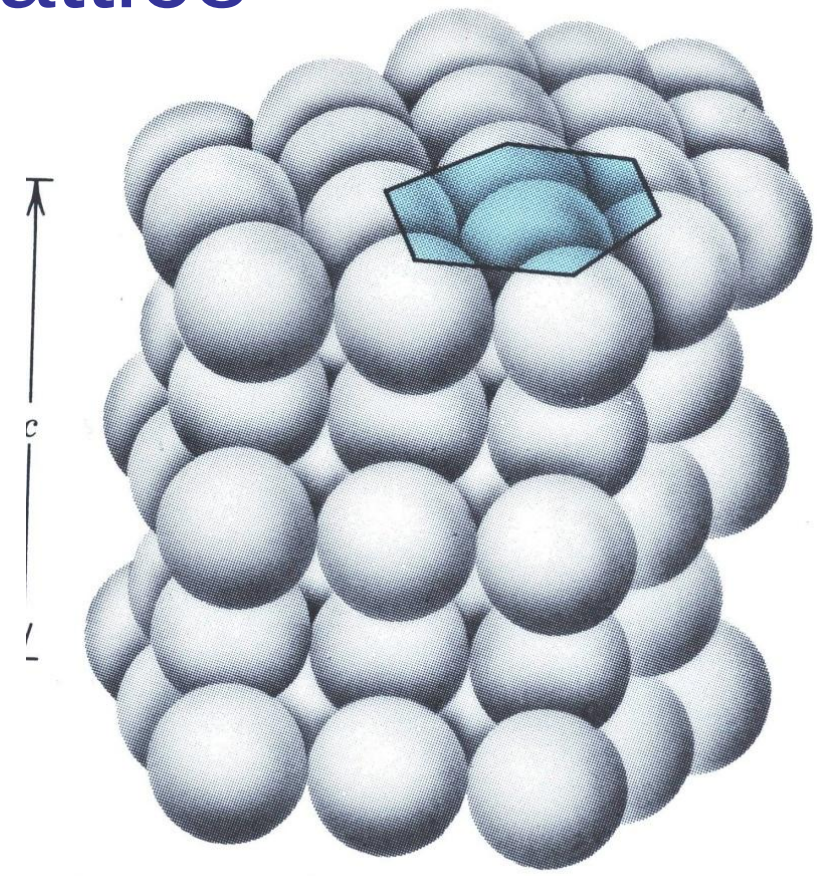
Some polycrystalline materials have grains with preferred orientations (texture): material exhibits anisotropic properties


Grain Boundaries
"Grains"
(Differently Oriented Crystals)

Hexagonal Close Packed (HCP) Lattice



(a)

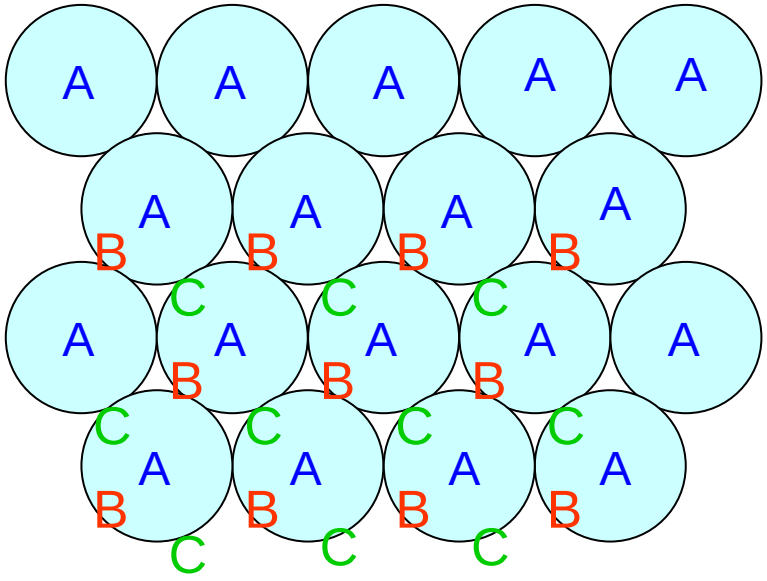


(b)

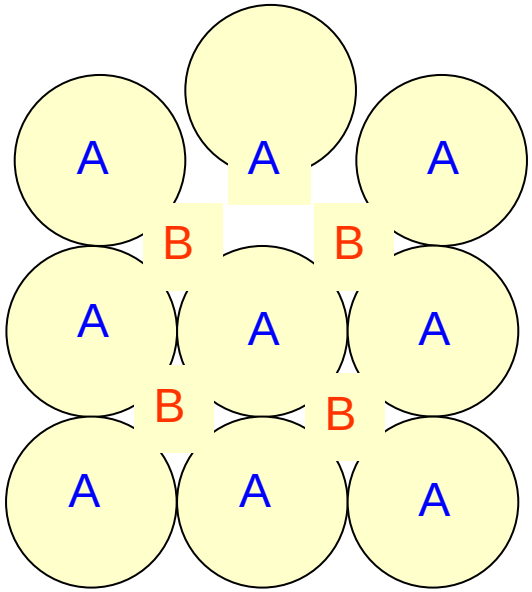
The HCP lattice is not a Bravais lattice, because orientation of the environment of a point varies from layer to layer along the c-axis.

Comments on Close Packing

Close Packed



Sequence ABABAB: Hexagonal Close Packed



Sequence ABCABCAB: Face Centered Cubic Close Packed

Sequence ABAB: Body Centered Cubic

Sequence AAA: Simple Cubic

HCP Lattice ≡
Hexagonal Bravais Lattice with a 2 Atom Basis

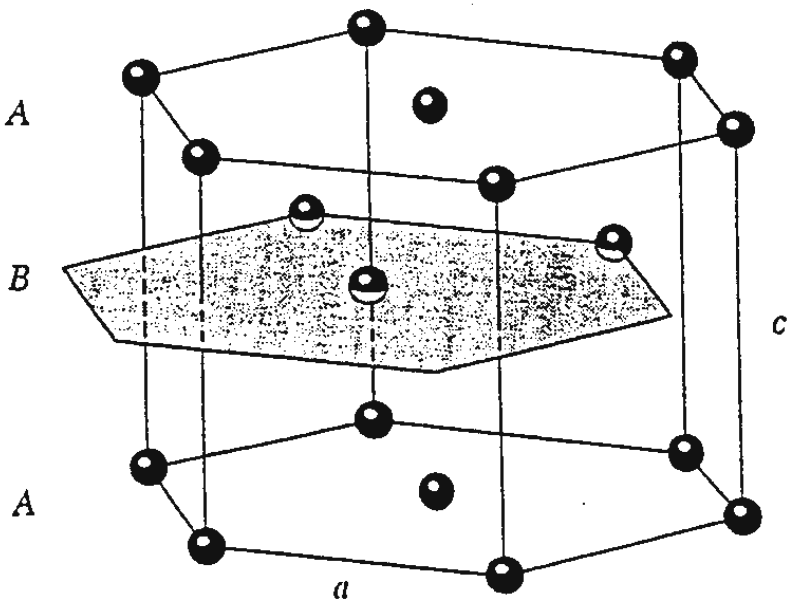
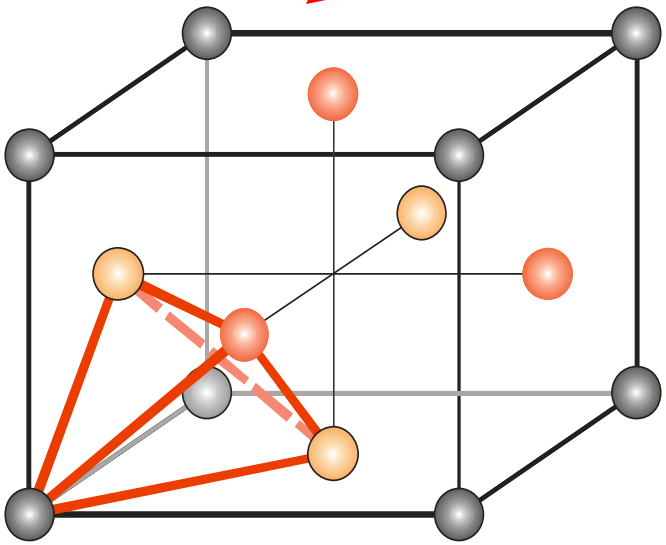


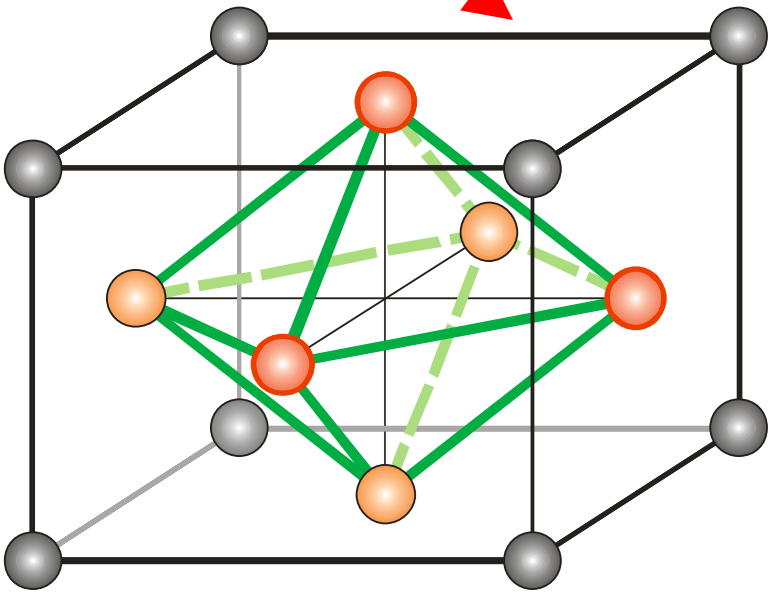
Figure 22 The hexagonal close-packed structure. The atom positions in this structure do not constitute a space lattice. The space lattice is simple hexagonal with a basis of two identical atoms associated with each lattice point. The lattice parameters a and c are indicated, where a is in the basal plane and c is the magnitude of the axis $\mathbf{a}_3$ of Fig. 14.

4- Tetrahedral and octahedral voids

TV

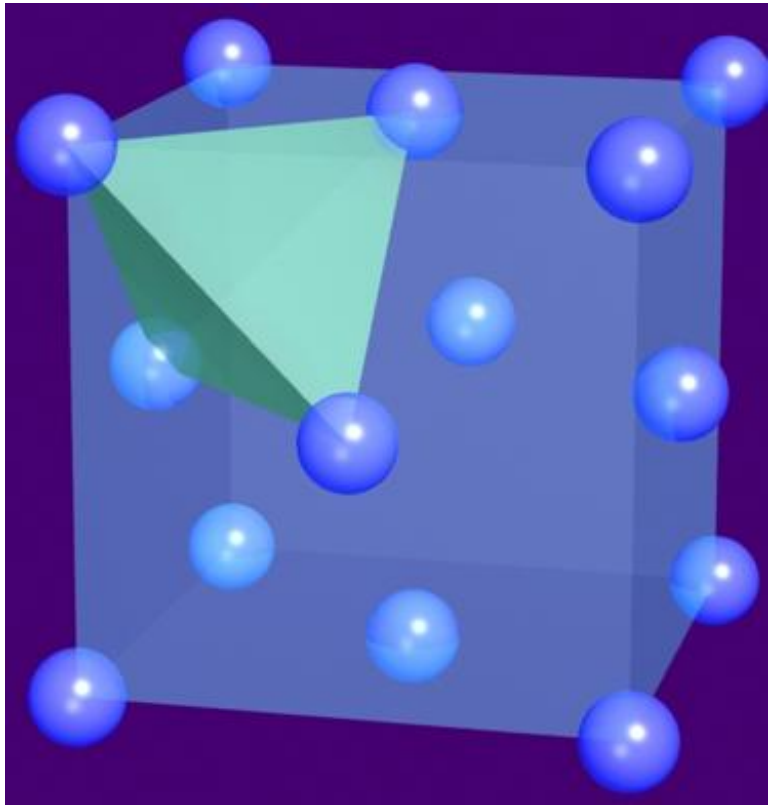


OV

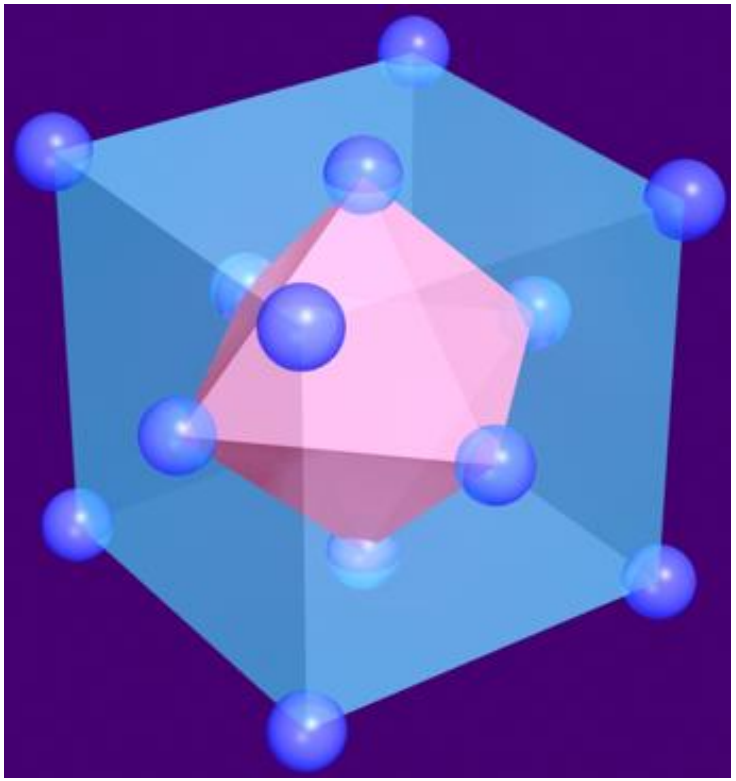


More views

Tetrahedral TV



Octahedral OV



Comments on Close Packing

A *second layer* of spheres is placed in the **indentations** left by the first layer

- **space** is trapped between the layers that is not filled by the spheres
- **TWO** different types of **HOLES** (so-called ***INTERSTITIAL*** sites) are left
  - **OCTAHEDRAL (O)** holes with **6** nearest sphere neighbours
  - **TETRAHEDRAL (T±)** holes with **4** nearest sphere neighbours

When a *third layer* of spheres is placed in the indentations of the second layer there are TWO choices

- The third layer lies in indentations directly in line (***eclipsed***) with the 1st layer
  - Layer ordering may be described as ABA
- The third layer lies in the alternative indentations leaving it ***staggered*** with respect to both previous layers
  - Layer ordering may be described as ABC

- **More Complex close-packing sequences** than simple HCP & CCP are possible
  - HCP & CCP are merely the simplest close-packed stacking sequences, others are possible!
    - All spheres in an HCP or CCP structure have **identical** environments
  - Repeats of the form **ABCB**.... are the next simplest
    - There are **two** types of sphere environment
      - surrounding layers are both of the same type (*i.e.* **anti-cuboctahedral** coordination) like HCP, so labelled **h**
      - surrounding layers are different (*i.e.* **cuboctahedral** coordination) like CCP, so labelled **c**
    - Layer environment repeat is thus **hchc**...., so labelled **hc**
    - ***Unit cell*** is alternatively labelled **4 H**
      - Has **4 layers** in the *c*-direction
      - **Hexagonal**
    - The **hc (4 H)** structure is adopted by early lanthanides