2019 Fall

Introduction to Materials Science and Engineering

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Contents for previous class

CHAPTER 3:
Fundamentals of Crystallography

I. Crystal Structures

- Lattice, Unit Cells, Crystal system

II. Crystallographic Points, Directions, and Planes

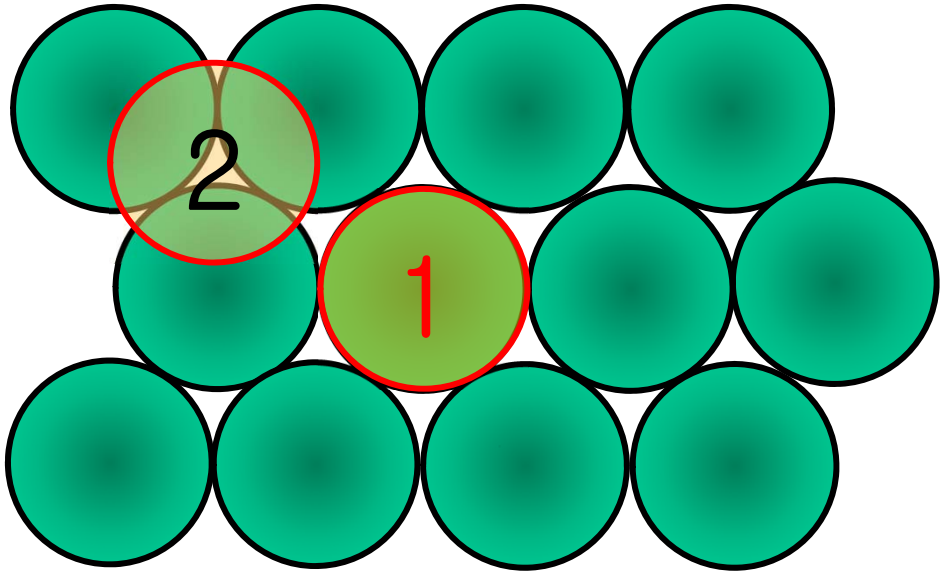
- Point coordinates, Crystallographic directions, Crystallographic planes

III. Crystalline and Noncrystalline Materials

- Single crystals, Polycrystalline materials, Anisotropy, Noncrystalline solids

Stacking of atoms in solid

Finding stable position



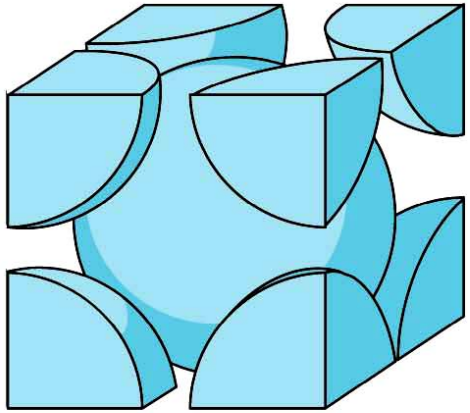
- Minimize energy configuration
  - Related to the bonding nature

I. Crystal structure

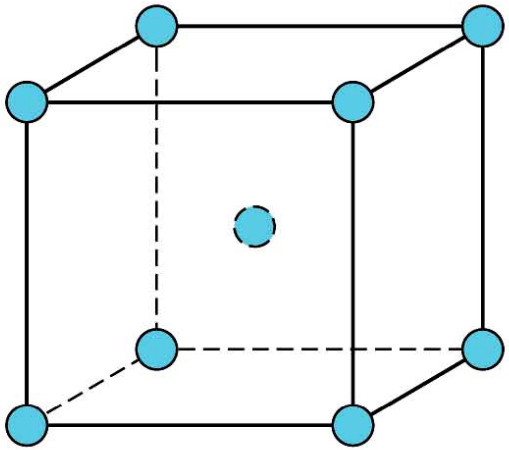
Lattice : 결정 공간상에서 점들의 규칙적인 기하학적 배열

- 3D point array in space, such that each point has identical surroundings. These points may or may not coincide with atom positions.
- Simplest case : each atom → its center of gravity → point or space lattice → pure mathematical concept

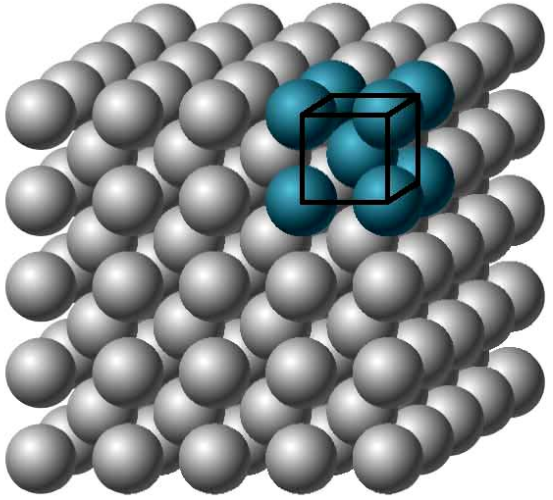
example: sodium (Na) ; body centered cubic



Hard-sphere unit cell



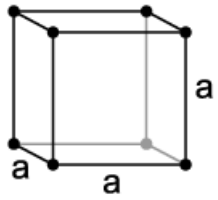
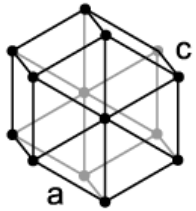
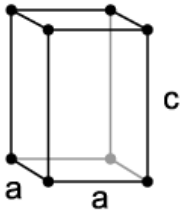
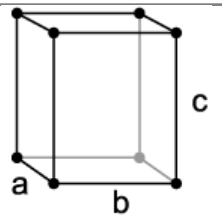
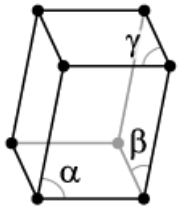
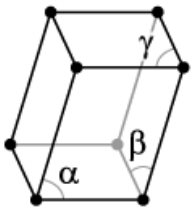
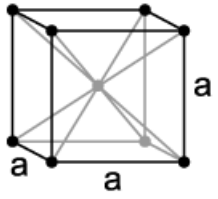
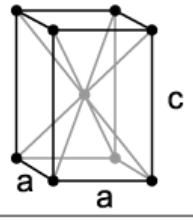
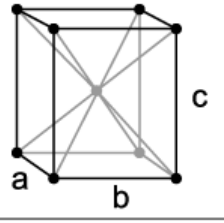
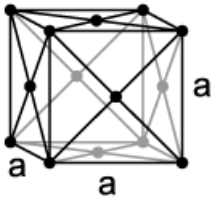
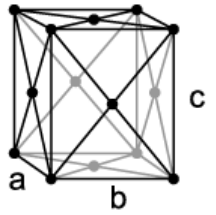
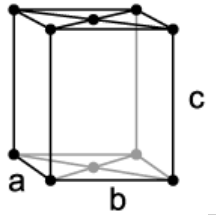
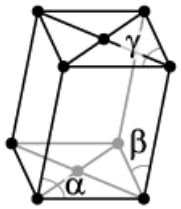
Reduced sphere unit cell



Aggregate of many atoms

I. Crystal structure : Unit cell

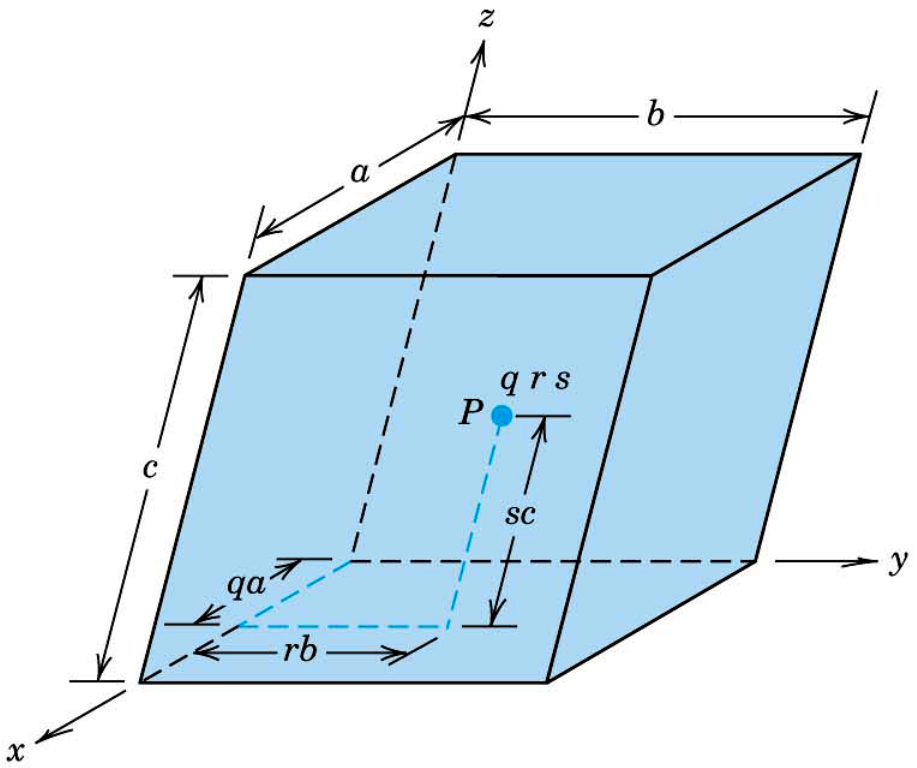
14 Bravais Lattice - Only 14 different types of unit cells are required to describe all lattices using symmetry

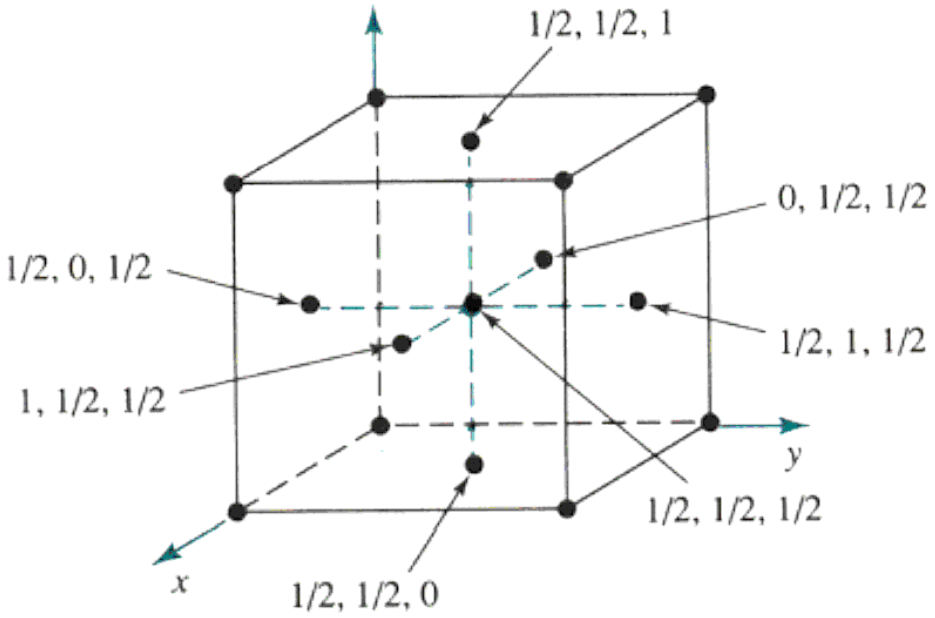
	cubic	hexagonal	rhombohedral (trigonal)	tetragonal	orthorhombic	monoclinic	triclinic
P							
I							
F							
C							

II. Crystallographic points, directions and planes

Chapter 3.5 Point coordinates

- **position: fractional multiples of the unit cell edge lengths**
  - **ex) P: q,r,s**

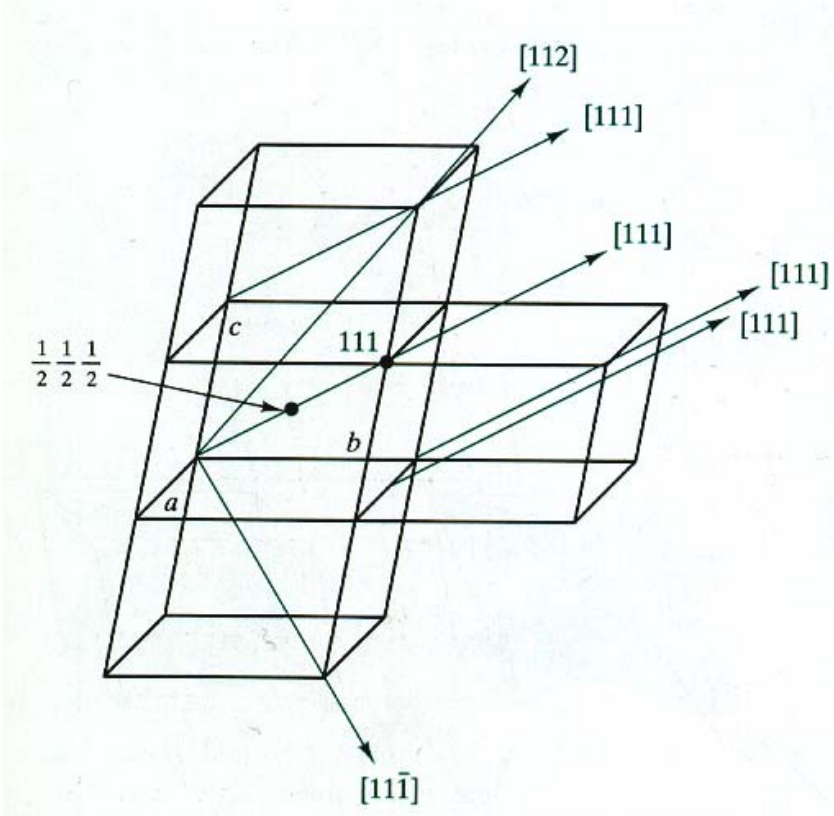




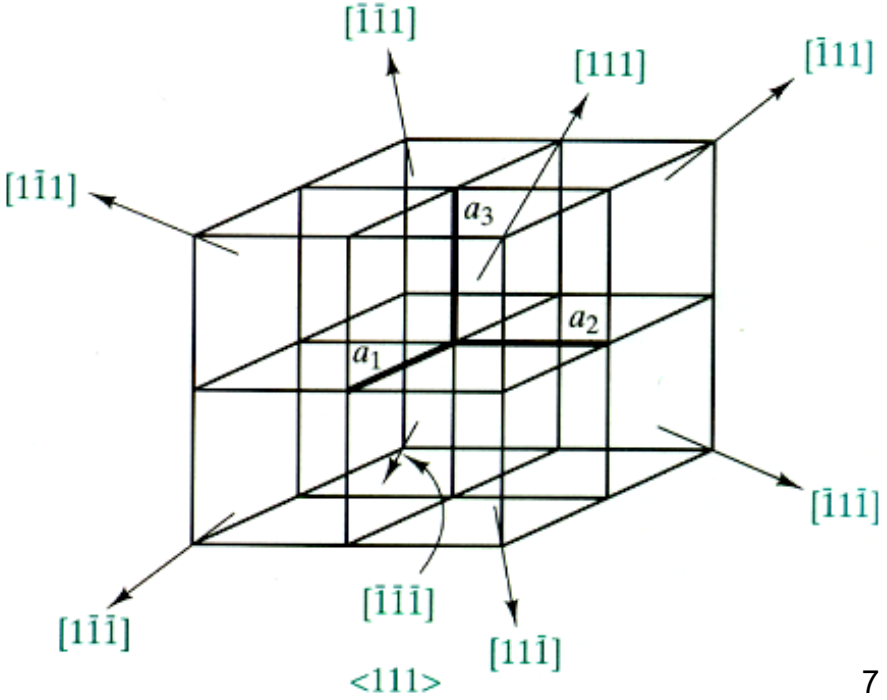
cubic unit cell

Crystallographic Directions

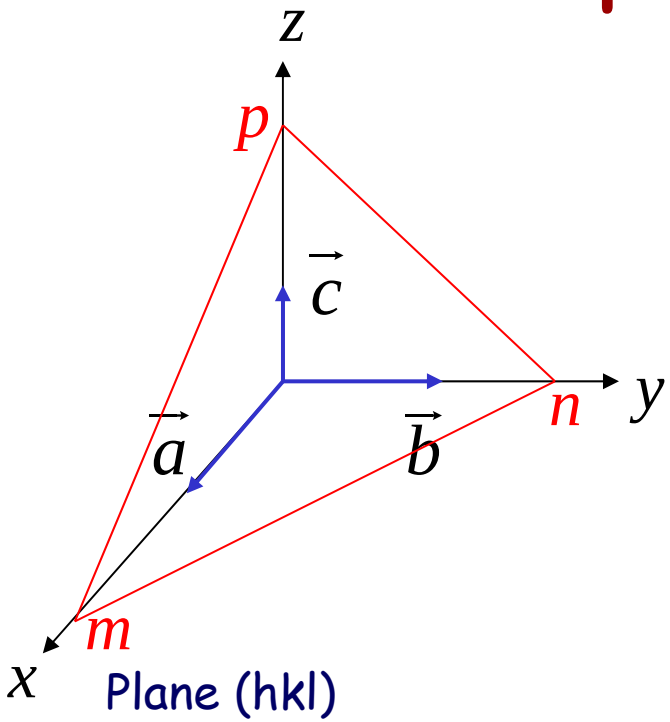
- a line between two points or a vector
- [uvw] square bracket, <u>smallest integer</u>
- families of directions: <uvw> angle bracket



cubic



Lattice plane (Miller indices)



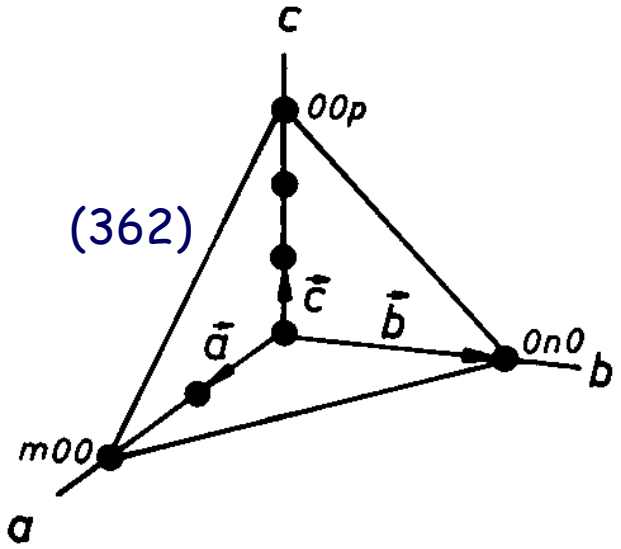
Plane (hkl)
Family of planes {hkl}

m00, 0n0, 00p: define lattice plane

m, n, ∞ : no intercepts with axes

Intercepts @ (mnp)	2	1	3
Reciprocals	½	1	1/3
Miller indicies	3	6	2
(362) plane			

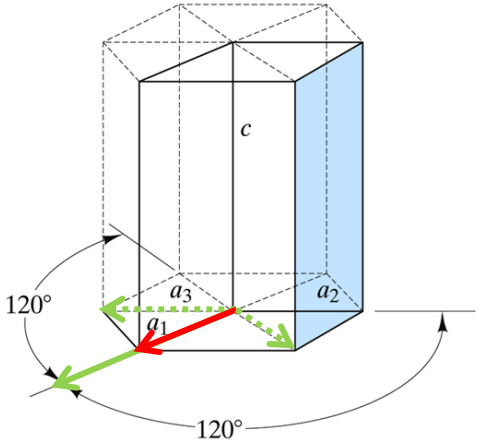
Miller indicies ; defined as the smallest integral multiples of the reciprocals of the plane intercepts on the axes



Miller-Bravais vs. Miller index system in Hexagonal system

Directions

Miller	Miller–Bravais	Miller	Miller–Bravais
[100]	$[2\bar{1}\bar{1}0]$	[010]	$[\bar{1}2\bar{1}0]$
[110]	[1120]	$[\bar{1}10]$	
[001]	[0001]		
[011]	$[\bar{1}2\bar{1}3]$	[111]	$[11\bar{2}3]$
[210]	$[10\bar{1}0]$	[120]	$[01\bar{1}0]$
[211]	$[10\bar{1}1]$	[112]	$[11\bar{2}6]$



Conversion of 4 index system (Miller-Bravais) to 3 index (Miller)

$$\vec{t} = u'\vec{a}_1 + v'\vec{a}_2 + w'\vec{c} = u\vec{a}_1 + v\vec{a}_2 + t\vec{a}_3 + w\vec{c}$$

Miller-Bravais to Miller
4 to 3 axis

$$u' = u - t = 2u + v$$
$$v' = v - t = 2v + u$$
$$w' = w$$

Miller to Miller-Bravais
3axis to 4 axis system

$$u = \frac{1}{3}(2u' - v')$$
$$v = \frac{1}{3}(2v' - u')$$
$$w = w'$$

Ex. M [100]
*u=(1/3)(2*1-0)=2/3*
*v=(1/3)(2*0-1)=-1/3*
w=0
=> 1/3[2 -1 -1 0]

Ex. M-B [1 0 -1 0]
*u'=2*1+0=2*
*v'=2*0+1=1*
w'=0
=> [2 1 0]

Contents for today's class

CHAPTER 3:
Fundamentals of Crystallography

III. Crystalline ↔ Noncrystalline Materials

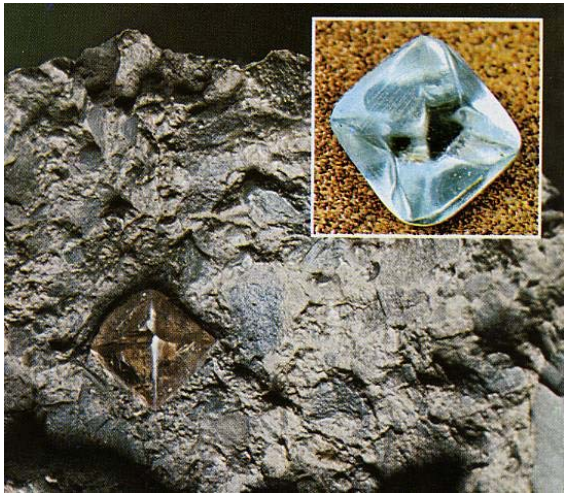
- Single crystals, Polycrystalline materials, Anisotropy
- Quasicrystals
- Noncrystalline solids : Amorphous solid

CHAPTER 4:
The Structure of Crystalline Solids

CRYSTALS AS BUILDING BLOCKS

- *Some* engineering applications require single crystals:

--diamond single crystals
Natural and artificial



(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

--turbine blades

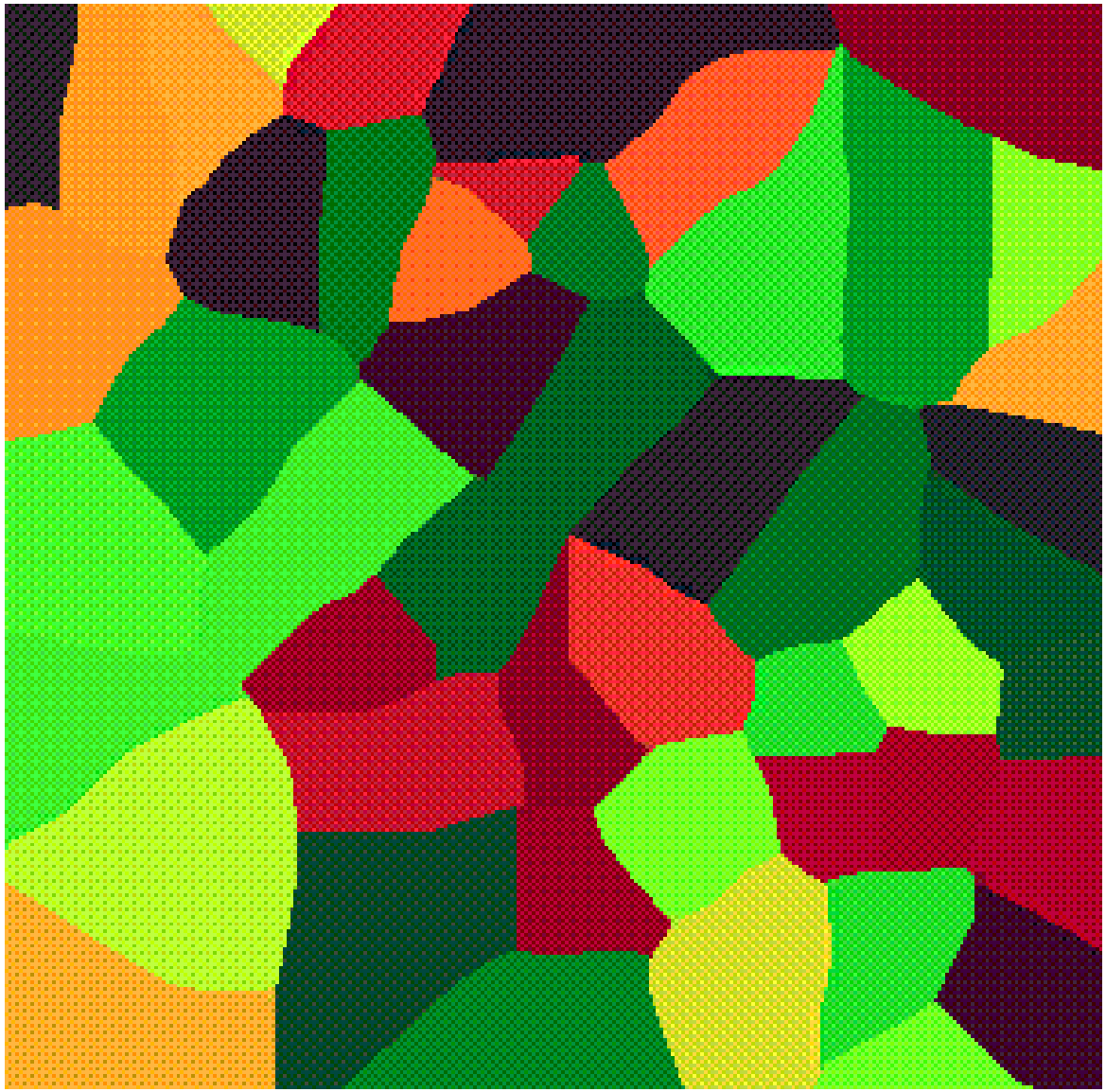
Fig. 8.30(c), *Callister 6e.* (Fig. 8.30(c) courtesy of Pratt and Whitney).

(Courtesy P.M. Anderson)

- Crystal properties reveal features of atomic structure.

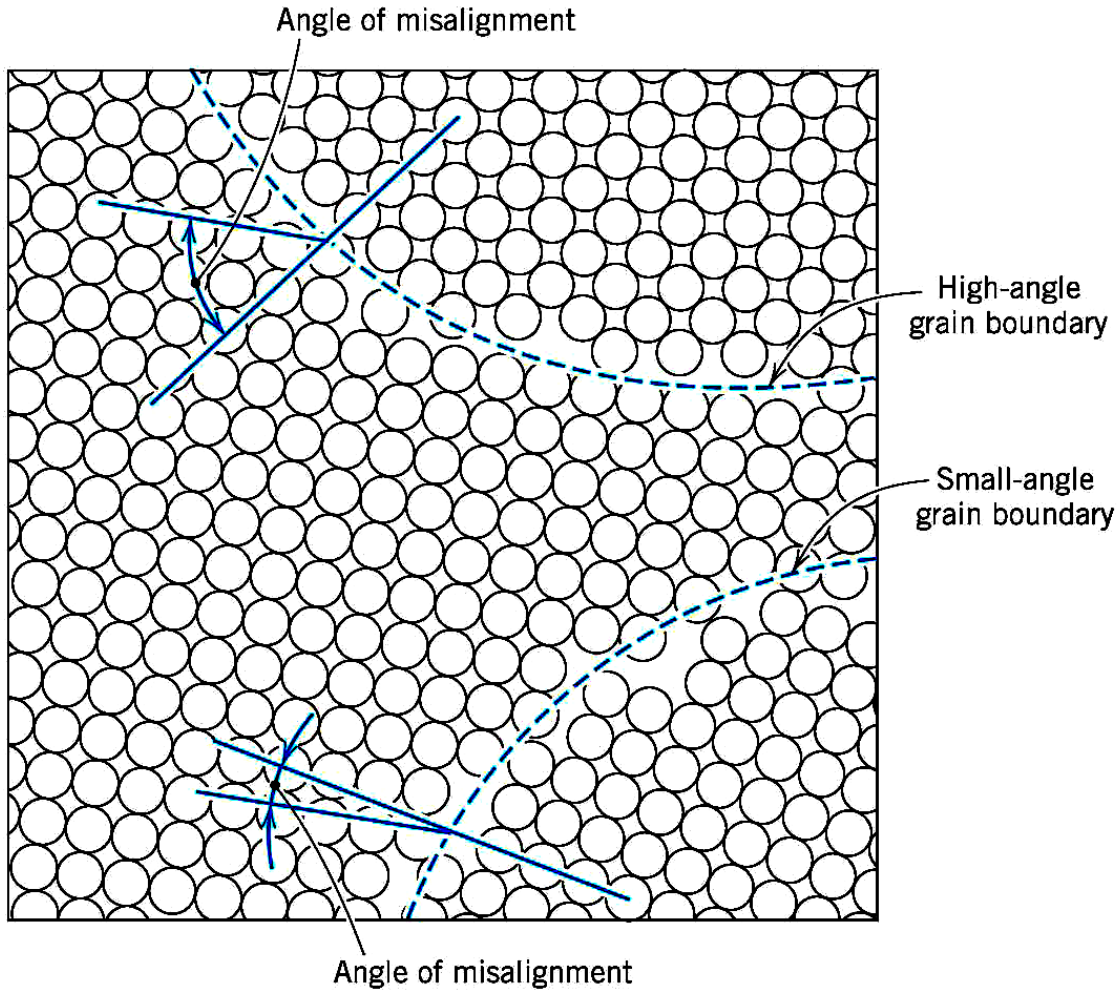
--Ex: Certain crystal planes in quartz fracture more easily than others.

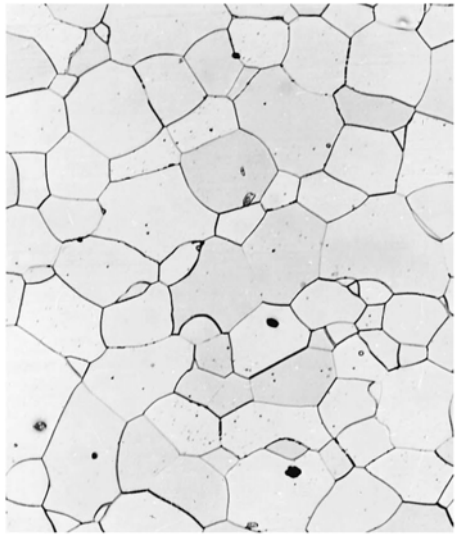
Solidification: Liquid → Solid

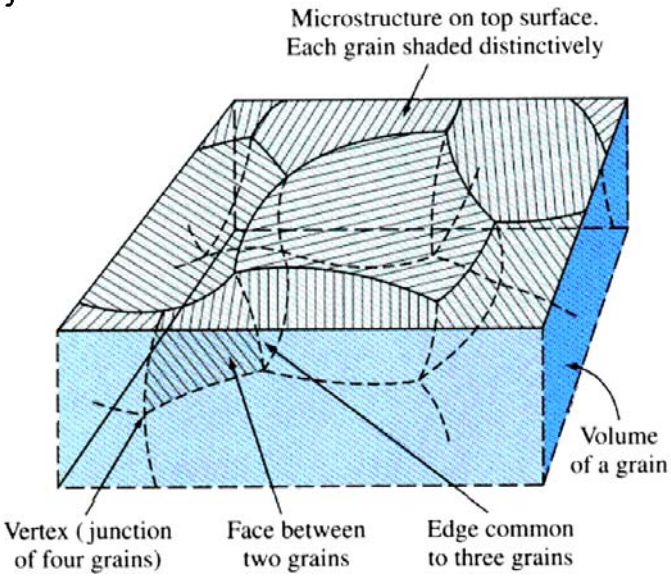


4 Fold Anisotropic Surface Energy/2 Fold Kinetics, Many Seeds

Grain Boundaries

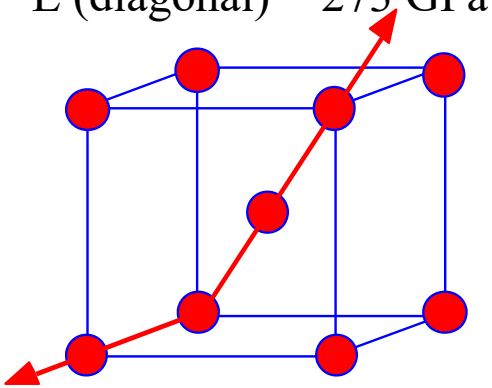






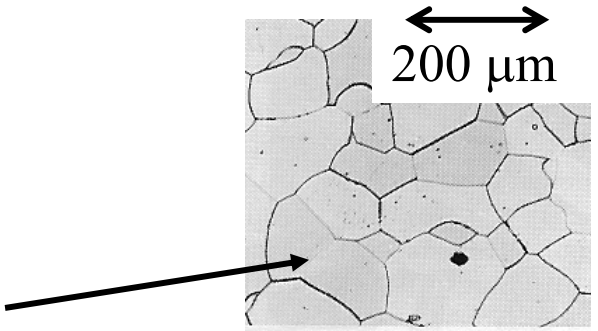
Single vs Polycrystals

- Single Crystals
  - -Properties vary with direction: anisotropic.
  - -Example: the modulus of elasticity (E) in BCC iron:



Data from Table 3.3, *Callister 7e*. (Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

- Polycrystals
  - -Properties may/may not vary with direction.
  - -If grains are randomly oriented: isotropic. ($E_{poly\ iron}$ = 210 GPa)
  - -If grains are textured, anisotropic.



Adapted from Fig. 4.14(b), *Callister 7e*. (Fig. 4.14(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

Polycrystals

- *Most* engineering materials are polycrystals.

Adapted from Fig. K, color inset pages of *Callister 5e*. (Fig. K is courtesy of Paul E. Danielson, Teledyne Wah Chang Albany)

- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- If grains are randomly oriented,
  overall component properties are not directional.
- Grain sizes typ. range from 1 nm to 2 cm
  (i.e., from a few to millions of atomic layers).

Polymorphism

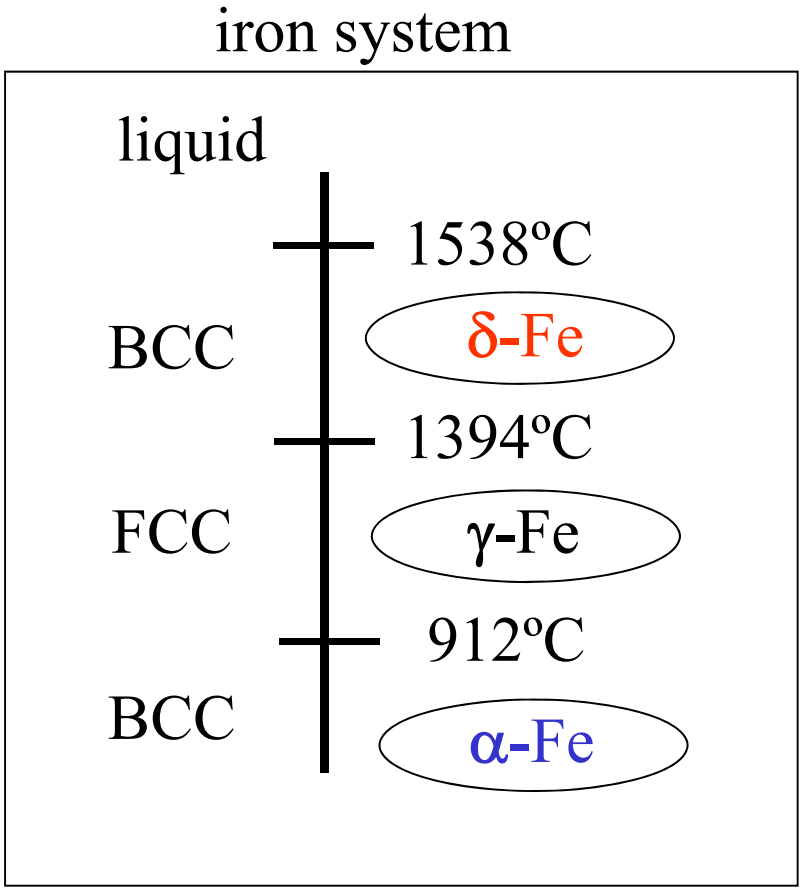
- **Two or more distinct crystal structures for the same material (allotropy/polymorphism)**

titanium

α, β-**Ti**

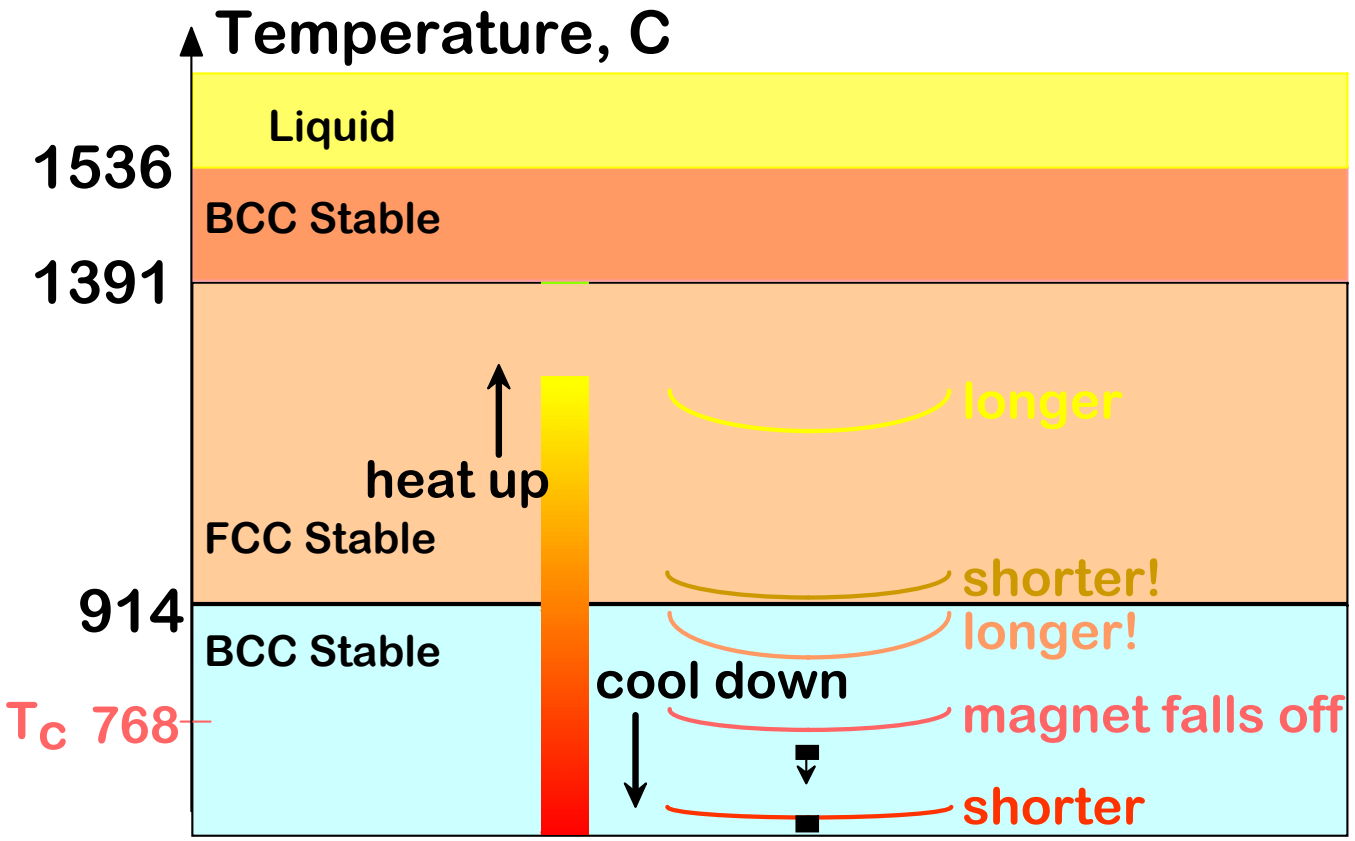
carbon

diamond, graphite



DEMO: HEATING AND COOLING OF AN IRON WIRE

- Demonstrates "polymorphism" ← The same atoms can have more than one crystal structure.



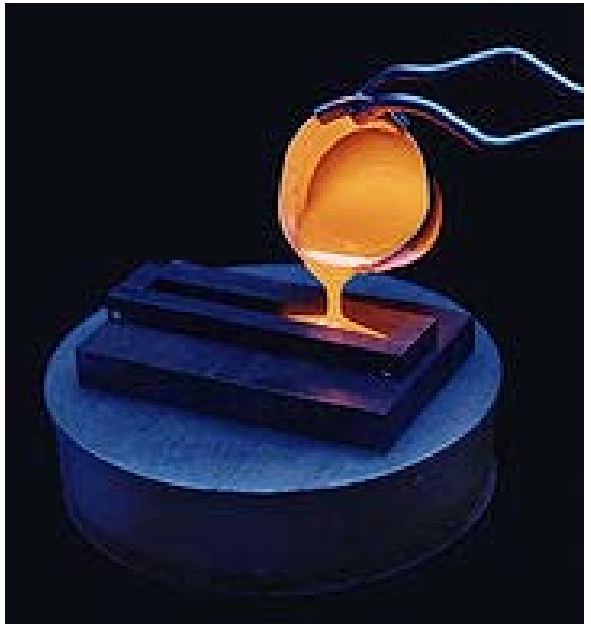
Non-crystalline Materials

- **Amorphous materials**

  a wide diversity of materials can be rendered amorphous indeed almost all materials can.

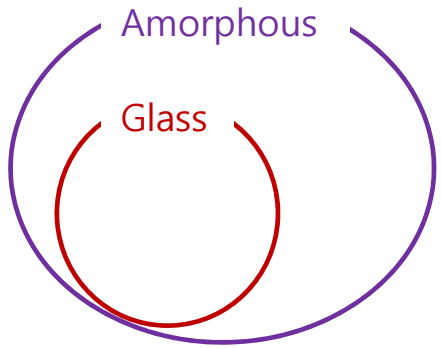
- metal, ceramic, polymer

ex) amorphous metallic alloy (1960)



- glassy/non-crystalline material

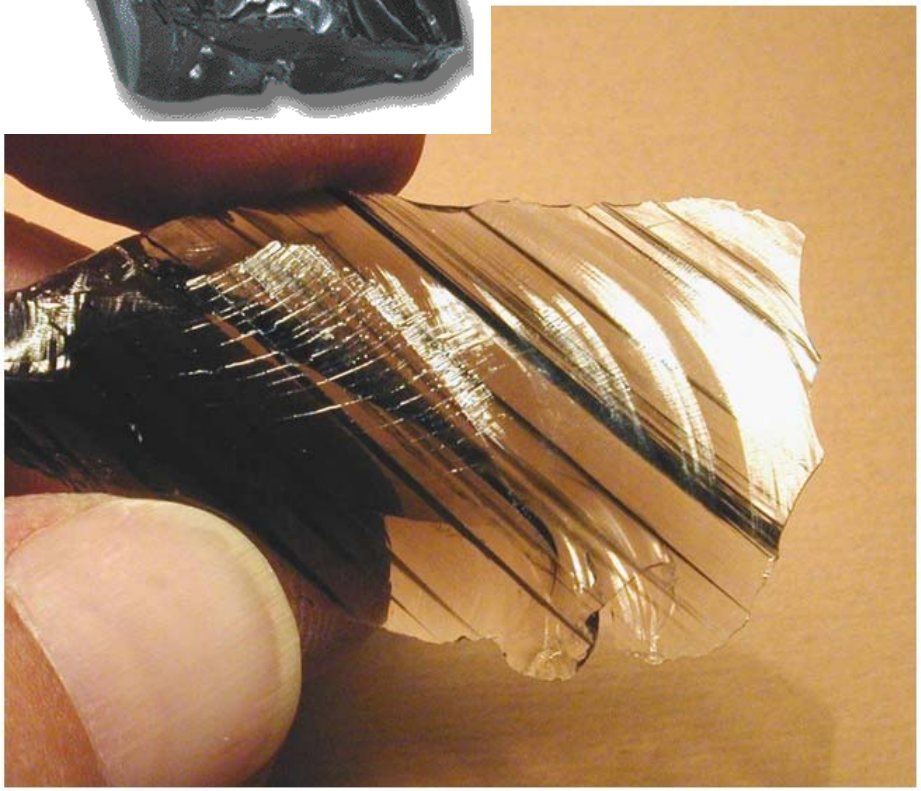
cf) amorphous vs glass
- random atomic structure (short range order)
- showing glass transition.



- retain liquid structure

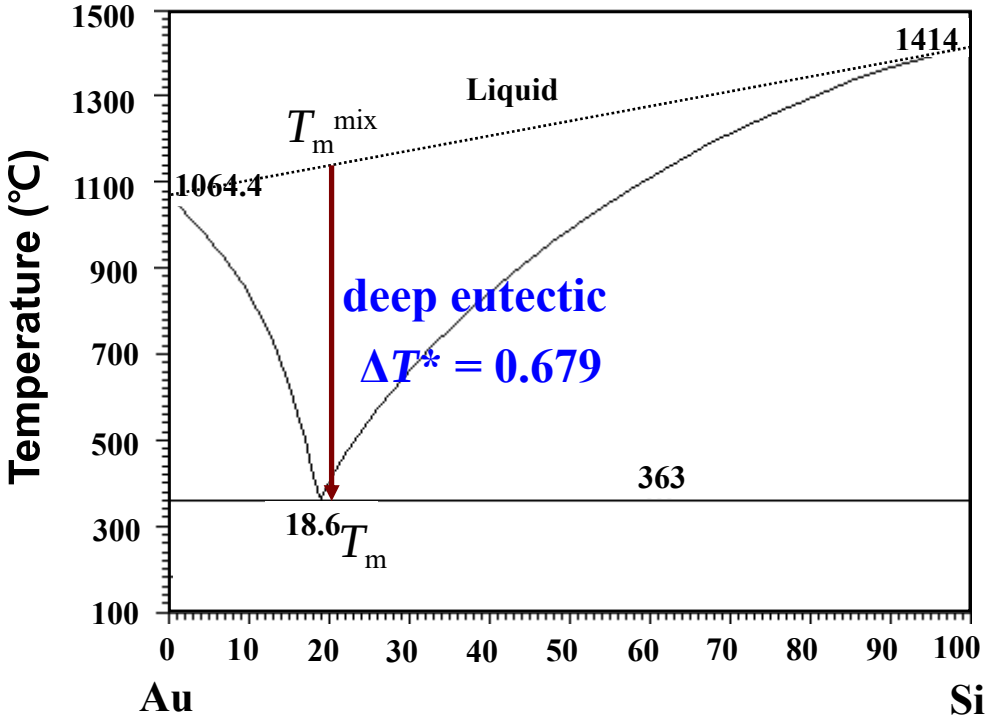
- rapid solidification from liquid state

Obsidian is a naturally occurring volcanic glass formed as an extrusive igneous rock. It is produced when felsic lava extruded from a volcano cools rapidly with minimum crystal growth. Obsidian is commonly found within the margins of rhyolitic lava flows known as **obsidian flows**, where the chemical composition (high silica content) induces a high viscosity and polymerization degree of the lava. The inhibition of atomic diffusion through this highly viscous and polymerized lava explains the lack of crystal growth. Because of this lack of crystal structure, obsidian blade edges can reach almost molecular thinness, leading to its ancient use as projectile points and blades, and its modern use as surgical scalpel blades.

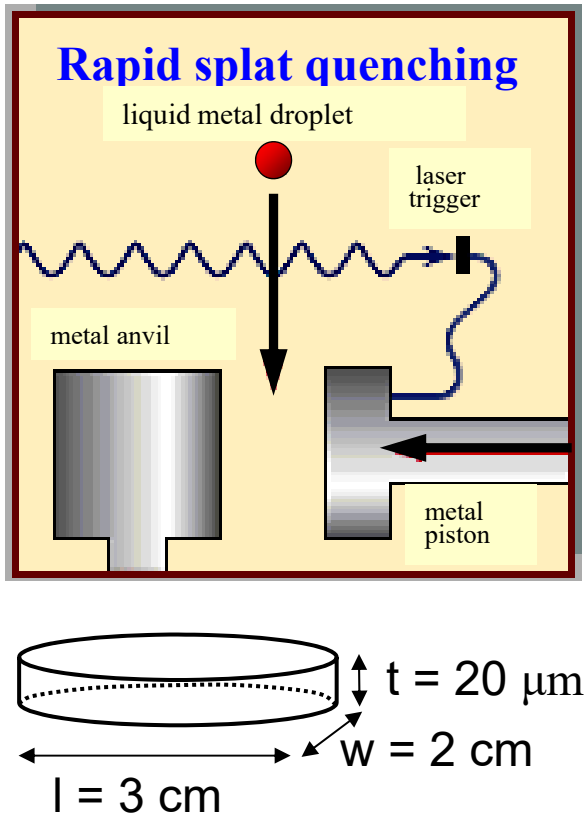


Glass formation: stabilizing the liquid phase

- First metallic glass ($Au_{80}Si_{20}$) produced by splat quenching at Caltech by Pol Duwez in 1957.



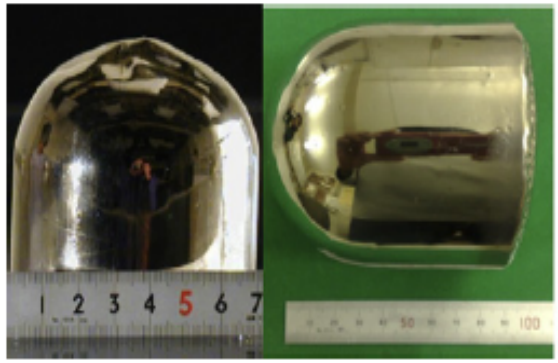
W. Klement, R.H. Willens, P. Duwez, Nature 1960; 187: 869.



Bulk glass formation in the Pd-/Ni-/Cu-/Zr- system

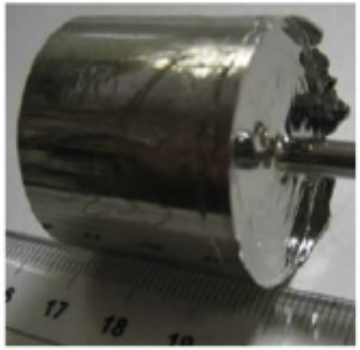
Massy Ingot Shape

(a) Pd-Cu-Ni-P



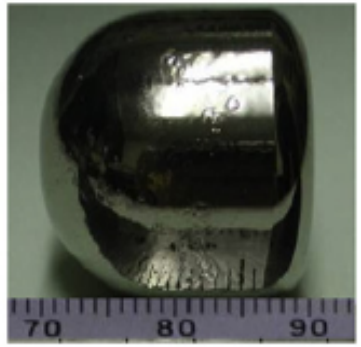
72ϕx 75 mm 80ϕx 85 mm

(b) Zr-Al-Ni-Cu



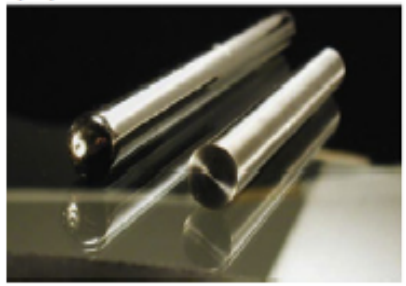
(c) Cu-Zr-Al-Ag

(d) Ni-Pd-P-B

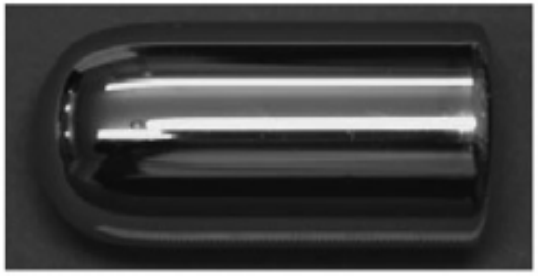


Cylindrical Rods

(e) Pd-Cu-Ni-P

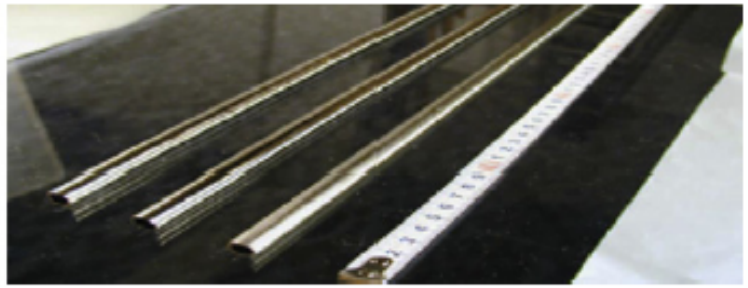


(f) Pt-Pd-Cu-P

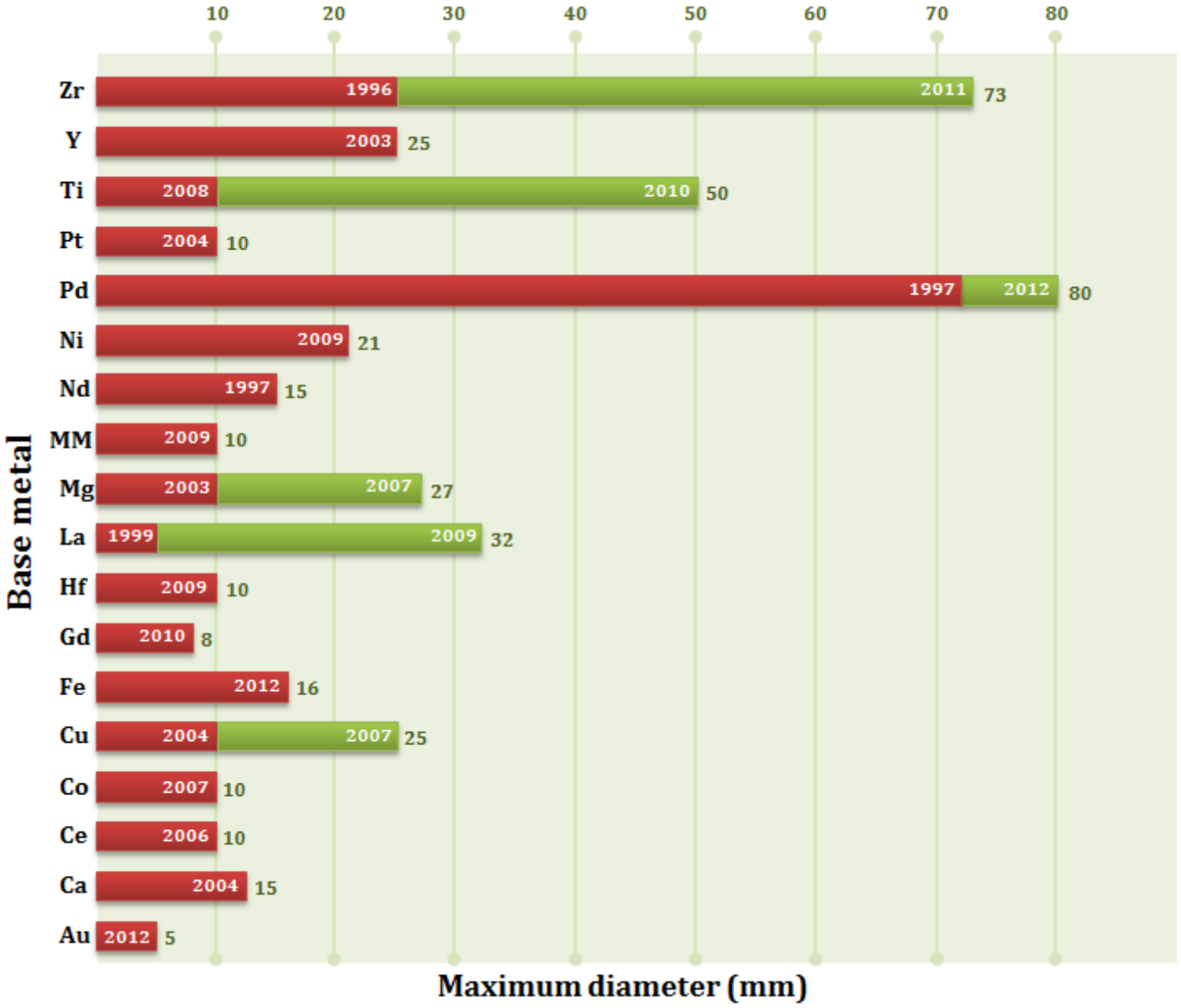


Hollow Pipes

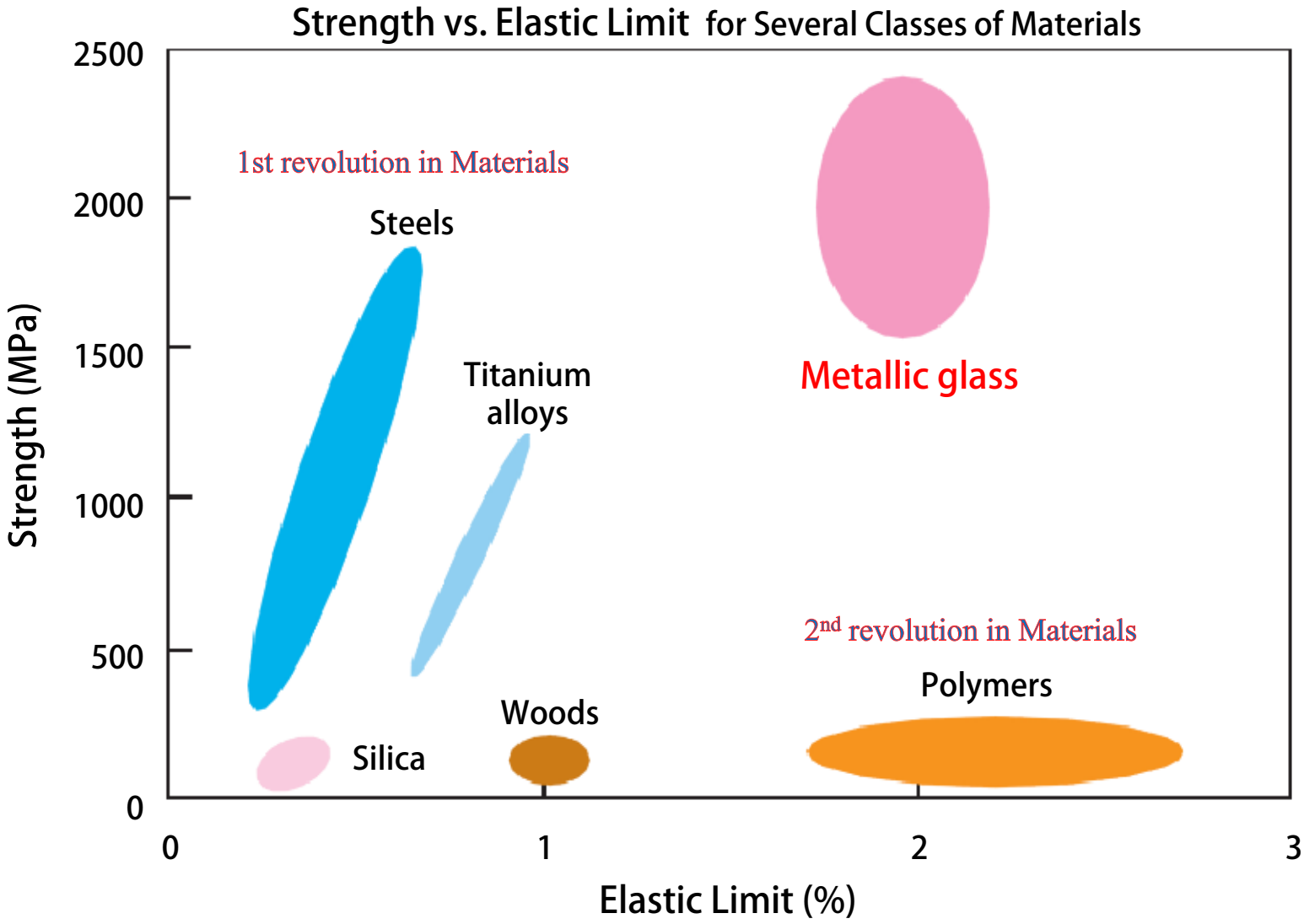
(g) Pd-Cu-Ni-P



Recent BMGs with critical size ≥ 10 mm



Bulk Metallic Glass: the 3rd Revolution in Materials?



: Metallic Glasses Offer a Unique Combination of High Strength and High Elastic Limit

Processing metals as efficiently as plastics: net-shape forming!

Seamaster Planet Ocean Liquidmetal® Limited Edition

- **Superior thermo-plastic formability**

  : possible to fabricate complex structure without joints

  - Multistep processing can be solved by simple casting
  - Ideal for small expensive IT equipment manufacturing

What are Quasicrystals?

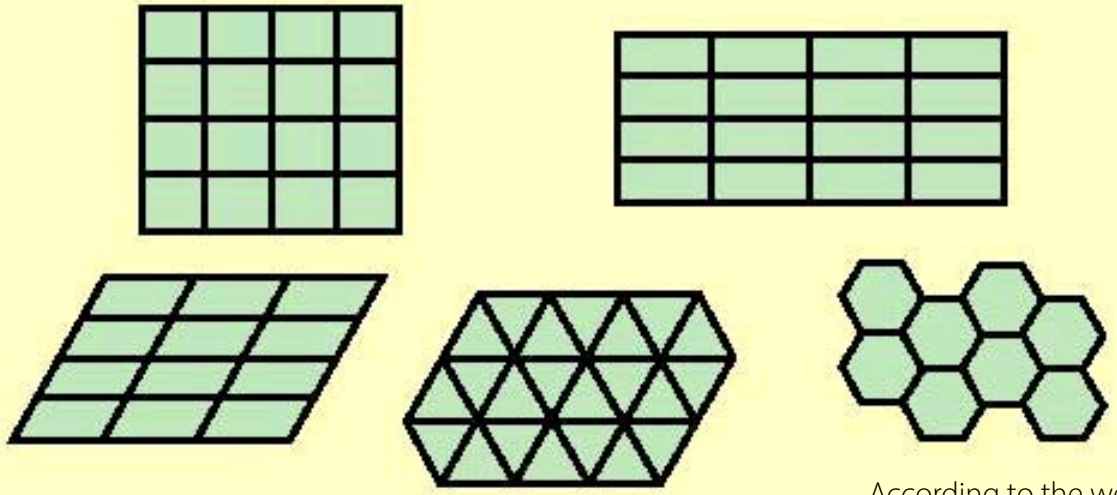
Crystals can only exhibit certain symmetries

In crystals, atoms or atomic clusters repeat periodically,
analogous to a tesselation in 2D
constructed from a single type of tile.

Try tiling the plane with identical units
… only certain symmetries are possible

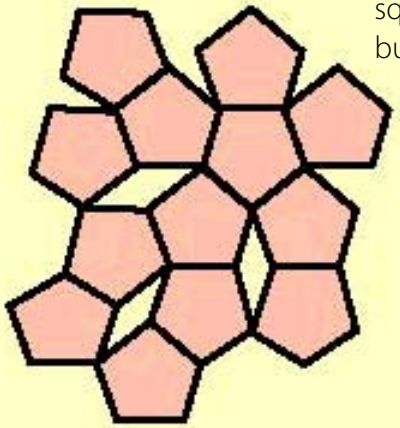
A tessellation or tiling of the plane is
a collection of plane figures that fills the plane with no overlaps and no gaps.

QUASICRYSTALS VIOLATE
Theorems of Crystallography



Symmetry axes compatible with periodicity

According to the well-known theorems of crystallography, only certain symmetries are allowed: the symmetry of a square, rectangle, parallelogram, triangle or hexagon, but not others, such as pentagons.



5-fold Symmetry is FORBIDDEN

Crystals can only exhibit certain symmetries

Crystals can only exhibit these
same rotational symmetries*

..and the symmetries determine
many of their physical properties and applications

* In 3D, there can be different rotational symmetries
along different axes, but they are restricted
to the same set (2-, 3-, 4-, and 6-fold)

Quasicrystals (Impossible Crystals)

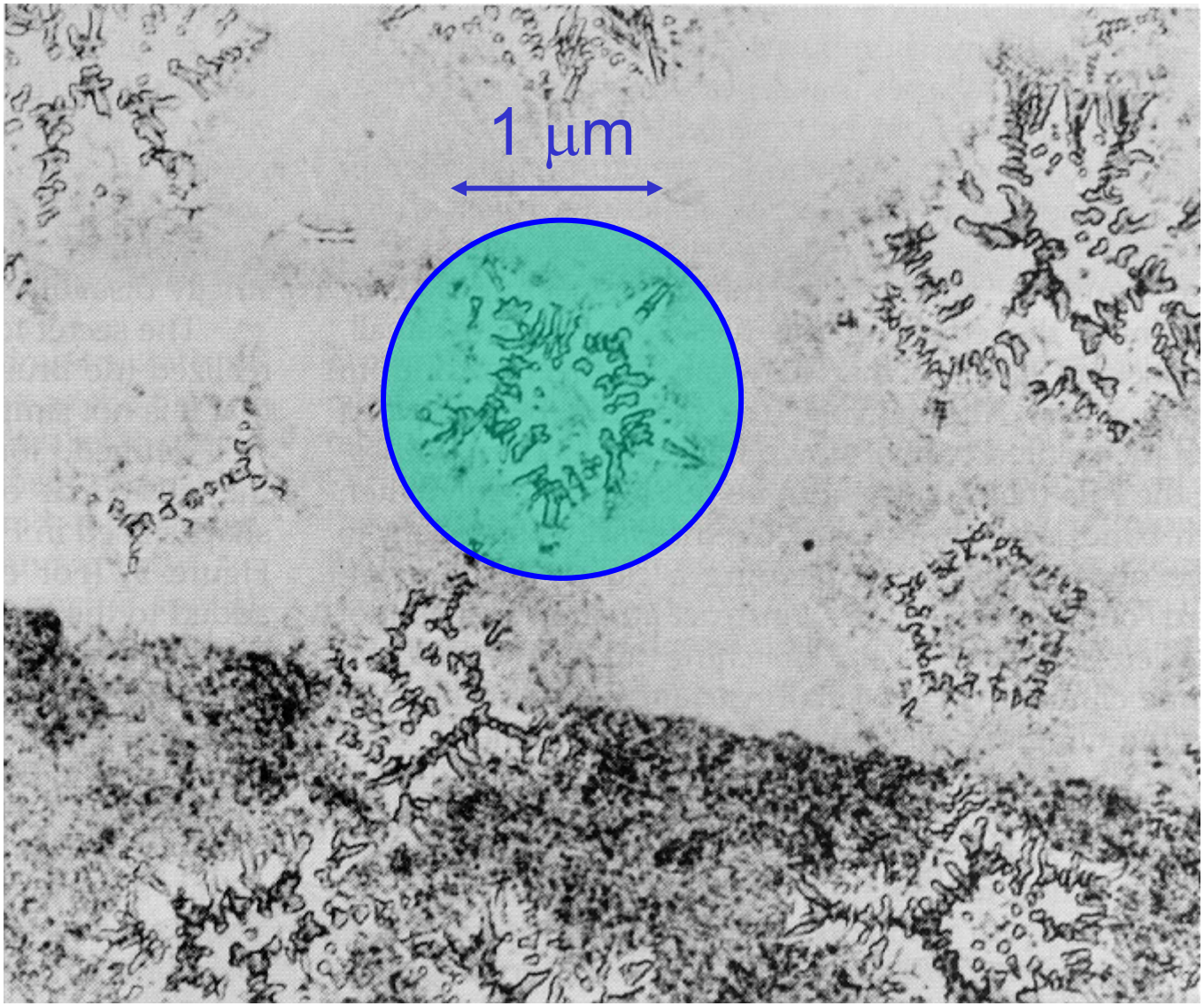
were first discovered in the laboratory by

Daniel Shechtman, Ilan Blech, Denis Gratias and John Cahn

in a beautiful study of an alloy of Al and Mn

D. Shechtman, I. Blech, D. Gratias, J.W. Cahn (1984)

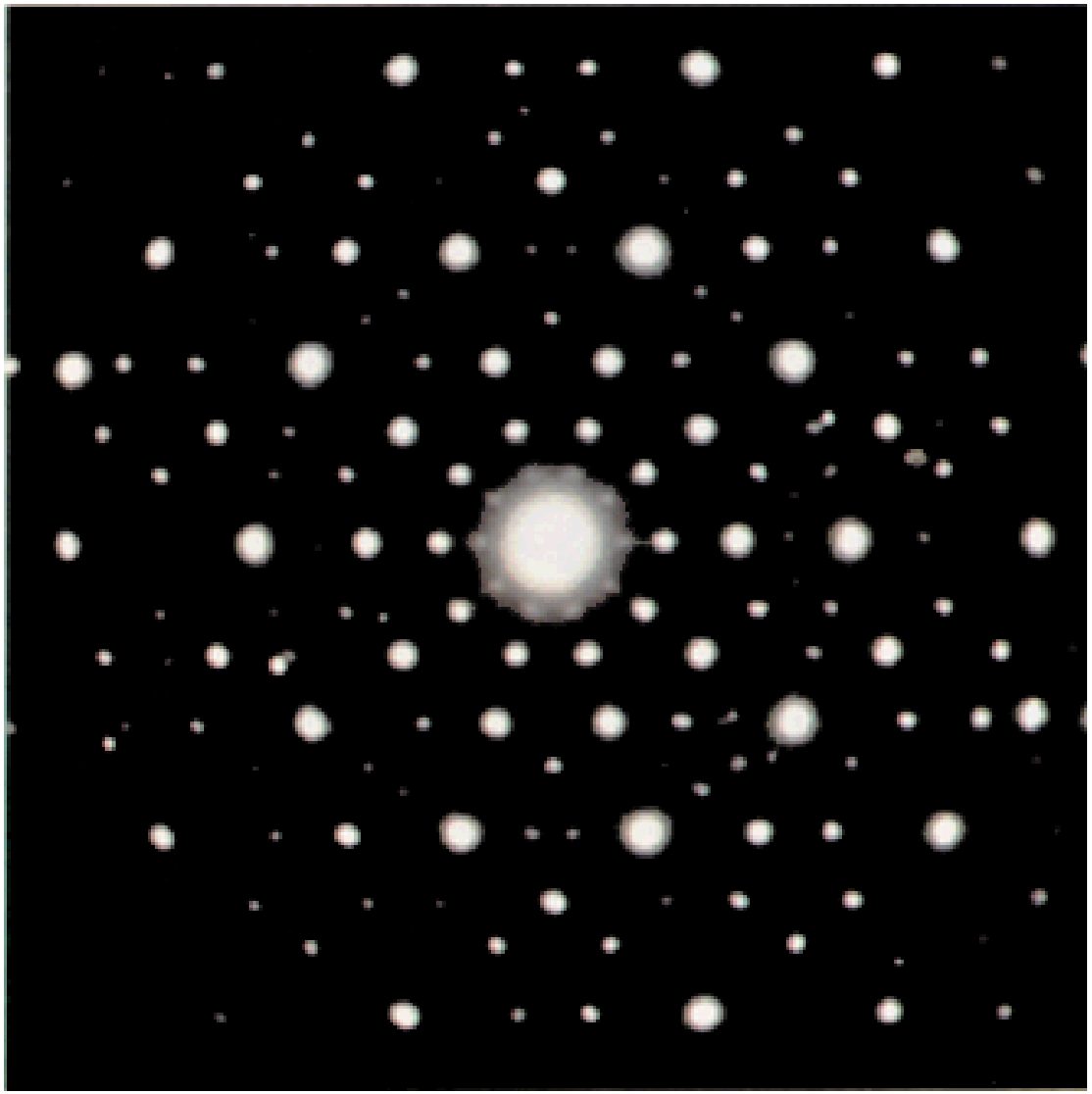
Al_6Mn



Their surprising claim:

"Diffracts electrons like a crystal . . .
But with a symmetry strictly forbidden for crystals"

Al_6Mn



QUASICRYSTALS

Similar to crystals, BUT…

- Orderly arrangement . . .
  But *QUASIPERIODIC* instead of *PERIODIC*

- Rotational Symmetry . . .
  But with *FORBIDDEN* symmetry

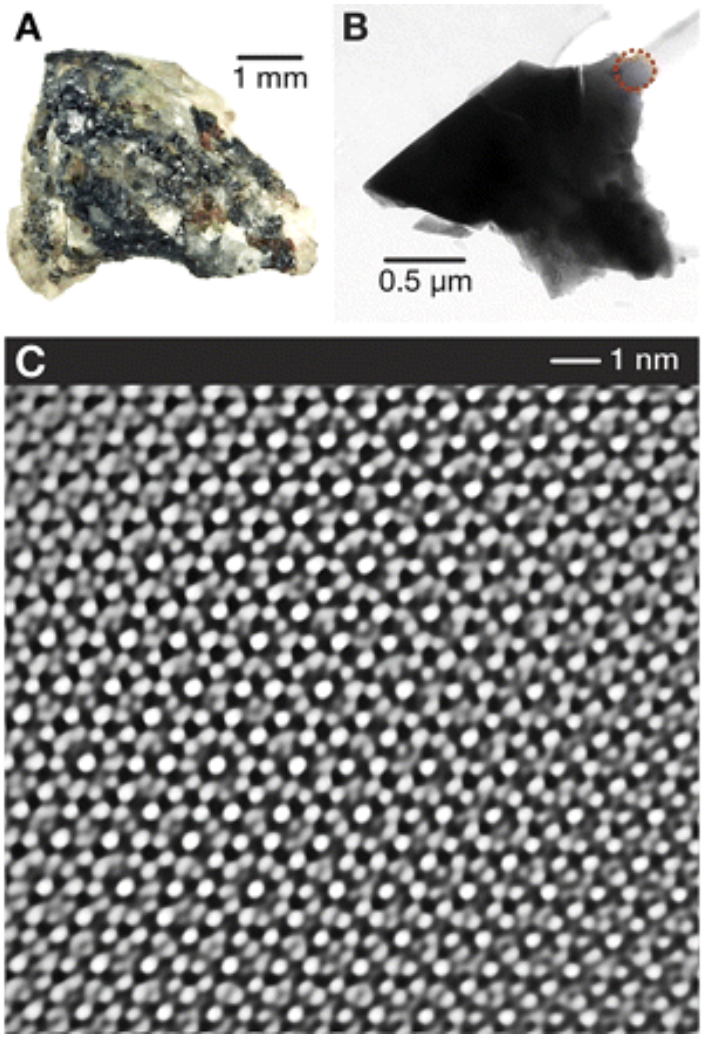
- Structure can be reduced to a finite number of repeating units

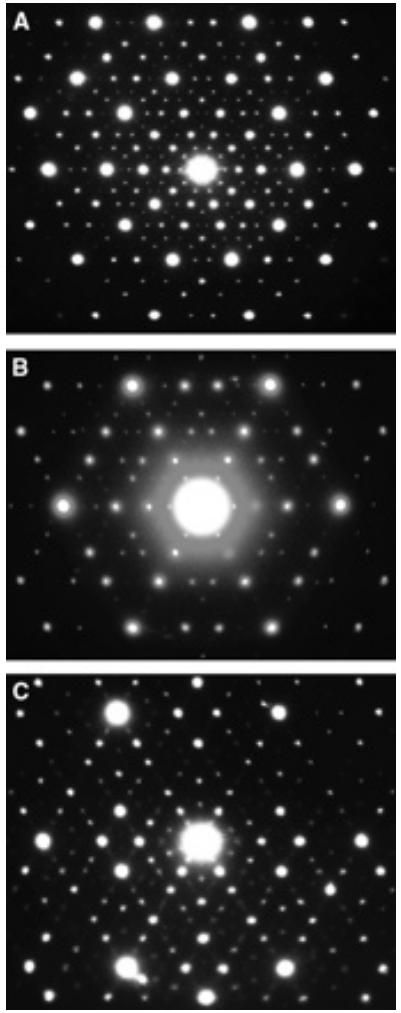
D. Levine and P.J. Steinhardt (1984)

Discovery of a Natural Quasicrystal

L Bindi, P. Steinhardt, N. Yao and P. Lu

Science 324, 1306 (2009)

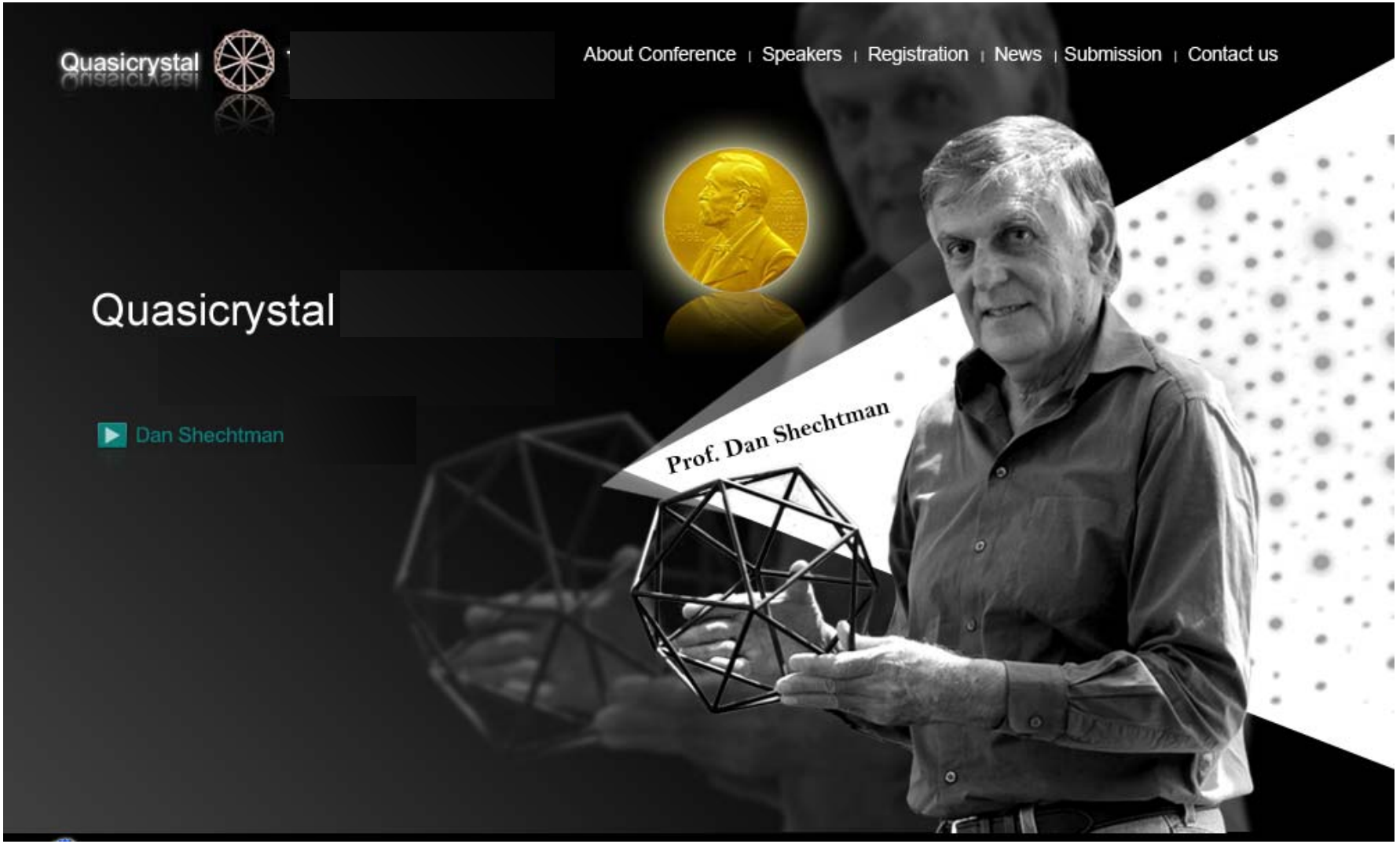




LEFT: Fig. 1 (A) The original khatyrkite-bearing sample used in the study. The lighter-colored material on the exterior contains a mixture of spinel, augite, and olivine. The dark material consists predominantly of khatyrkite ($CuAl_2$) and cupalite (CuAl) but also includes granules, like the one in (B), with composition $Al_{63}Cu_{24}Fe_{13}$. The diffraction patterns in Fig. 4 were obtained from the thin region of this granule indicated by the red dashed circle, an area 0.1 μm across. (C) The inverted Fourier transform of the HRTEM image taken from a subregion about 15 nm across displays a homogeneous, quasiperiodically ordered, fivefold symmetric, real space pattern characteristic of quasicrystals.

RIGHT: Diffraction patterns obtained from natural quasicrystal grain

2011 Nobel Prize in Chemistry: Quasicrystal



A new ordered phase showing the apparent fivefold symmetry was observed by Sastry et al. [Mater. Res. Bull. 13: 1065-1070] in 1978 in a rapidly solidified Al-Pd alloy, but was interpreted to arise from a microstructure Consisting of a series of fine twins. This was later shown to be a two-dimensional (or decagonal) qasicrystal.

Quasicrystals

Crystal with 5 fold symmetry *Mathematically impossible but exist*

1984 $Al_{86}Mn_{14}$ alloy : rapidly solidified ribbon_*Shectman et al.*

: materials whose structure cannot be understood within classical crystallography rules.

"Quasiperiodic lattices", with long-range order but without periodic translations in three dimensions

- long range order: quasiperiodic
- no 3-D translational symmetry
- sharp diffraction patterns

http://www.youtube.com/watch?v=k_VSpBI5EGM

Atomic arrangement in the solid state

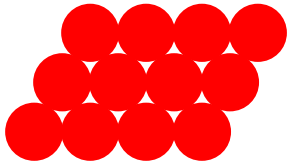
- Solid materials are classified according to the **regularity** with which atoms and ions are arranged with respect to one another.

- So, how are they arranged ?

  (a) **periodically** – having long range order in 3-D

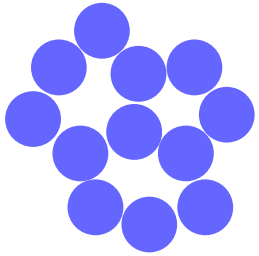
  (b) **quasi-periodically**

  (c) **randomly** – having short range order with the characteristics of bonding type but losing the long range order



Crystal

Quasicrystal



Amorphous

- **Crystal: Perfection → Imperfection**

CHAPTER 4:
The Structure of Crystalline Solids

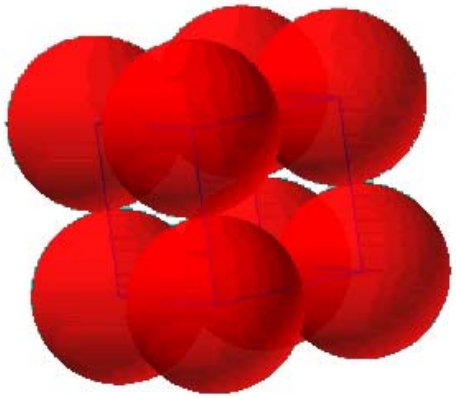
I. METALLIC CRYSTALS

- tend to be densely packed.
- have several reasons for dense packing:
  - Typically, only one element is present, so all atomic radii are the same.
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
- have the simplest crystal structures.

We will look at three such structures...

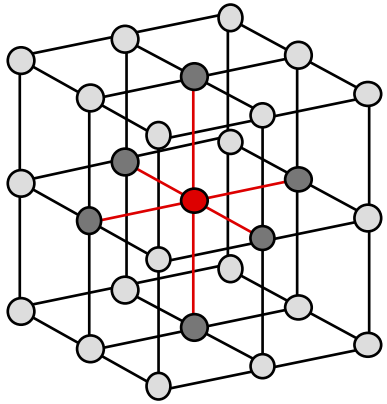
(1) SIMPLE CUBIC STRUCTURE (SC)

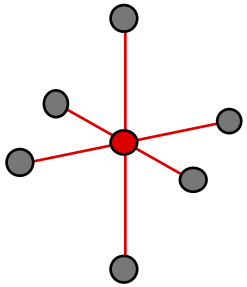
- Rare due to poor packing (only 84Polonium has this structure)
- Close-packed directions are cube edges.



(Courtesy P.M. Anderson)

- Coordination # = 6
  (# nearest neighbors)





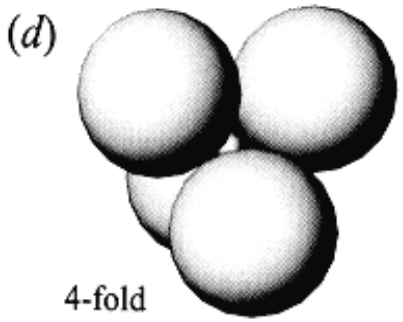
* Coordination Number

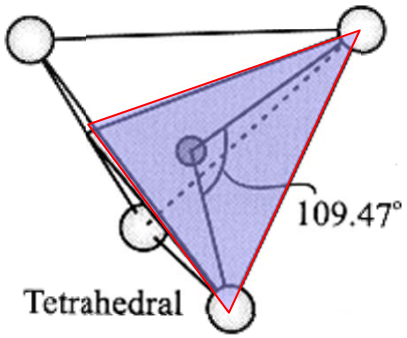
In chemistry and crystallography, the coordination number (CN) of a central atom in a molecule or crystal is **the number of its nearest neighbor.**

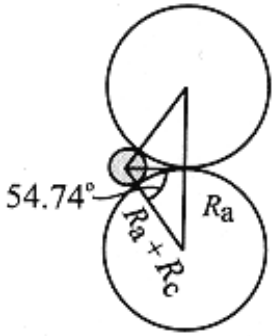
In chemistry the emphasis is on bonding structures in molecules or ions and the **CN of an atom** is determined by **simply counting** the other of atoms to **which it is bonded** (by either single or multiple bonds).

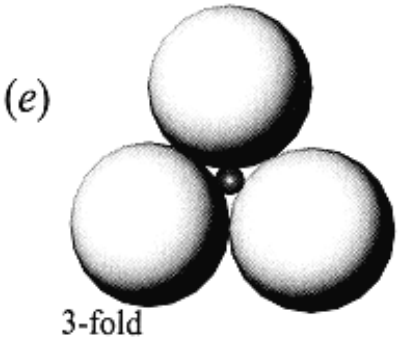
The **solid-state structure of crystals** often have less clearly defined bonds, so a simpler model is used, in which the atoms are represented by touching spheres. In this model the CN of an atom is the number of other atoms which it touches. For an atom in the interior of a crystal lattice, **the number of atoms touching the given atom** is the bulk coordination number, for an atom at a surface of a crystal this is the surface coordination number.

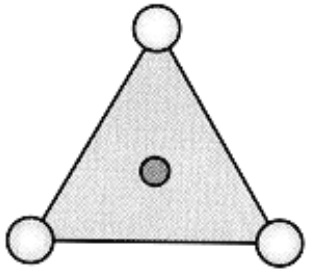
Coordination Number

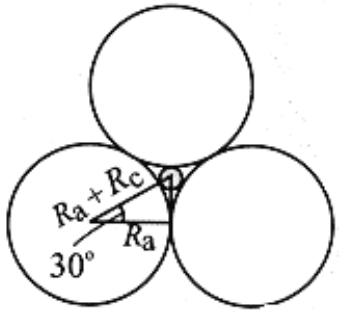


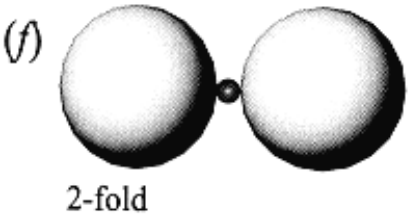


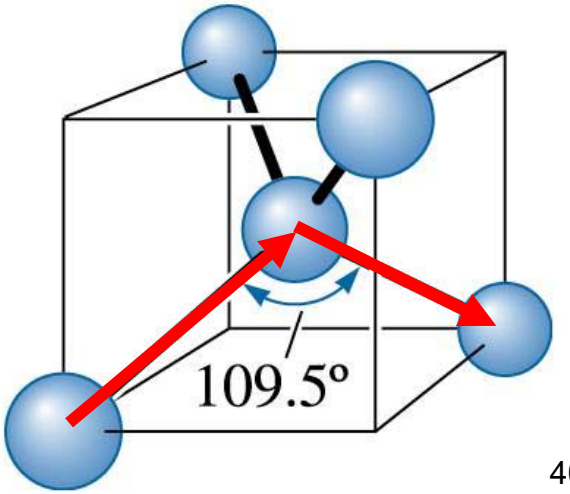




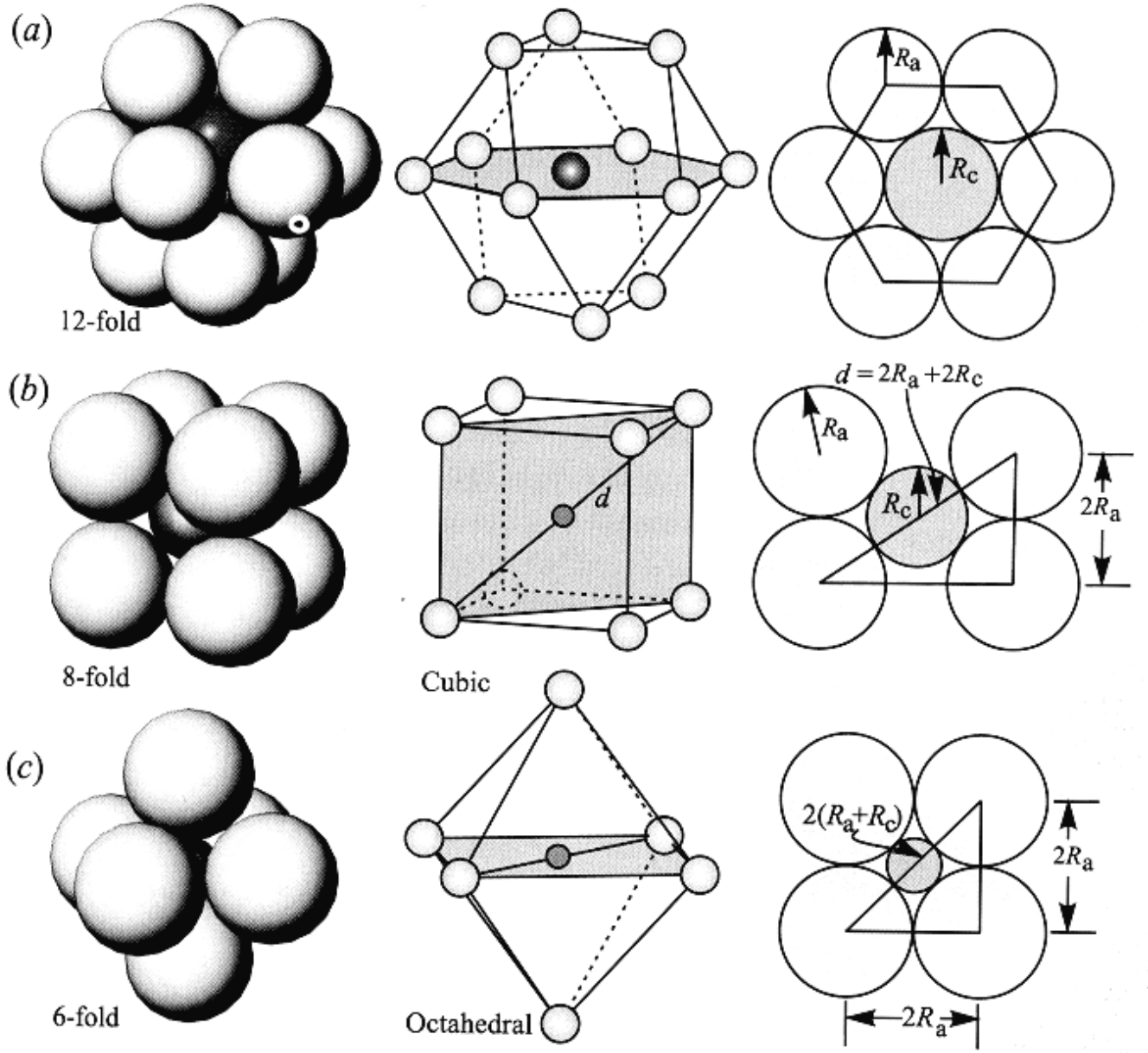








Coordination Number

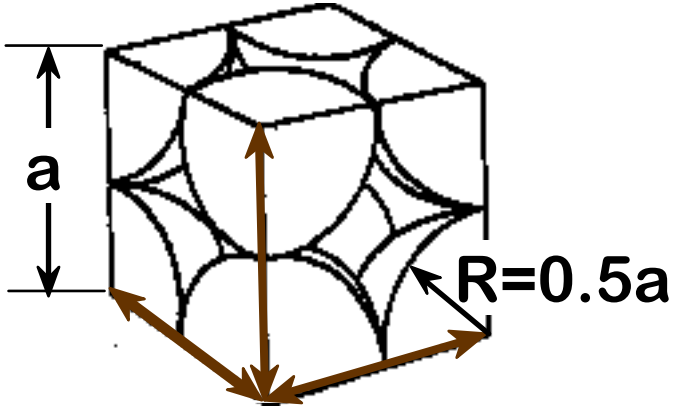


ATOMIC PACKING FACTOR : simple cubic

$$APF = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains 8 x 1/8 =

1 atom/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

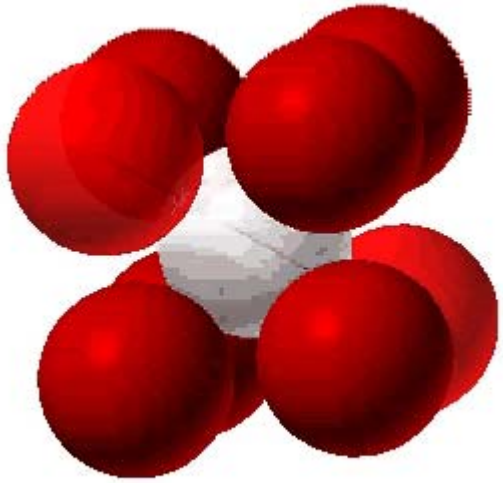
Adapted from Fig. 3.19, *Callister 6e.*

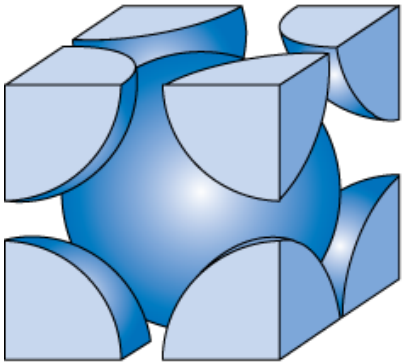
(2) Body Centered Cubic Structure (BCC)

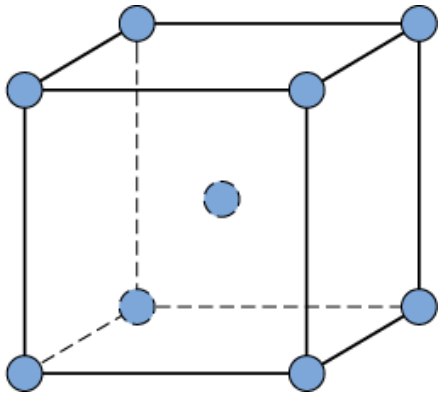
- Atoms touch each other along cube diagonals.
  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr, W, Fe (α), Tantalum, Molybdenum

- Coordination # = 8



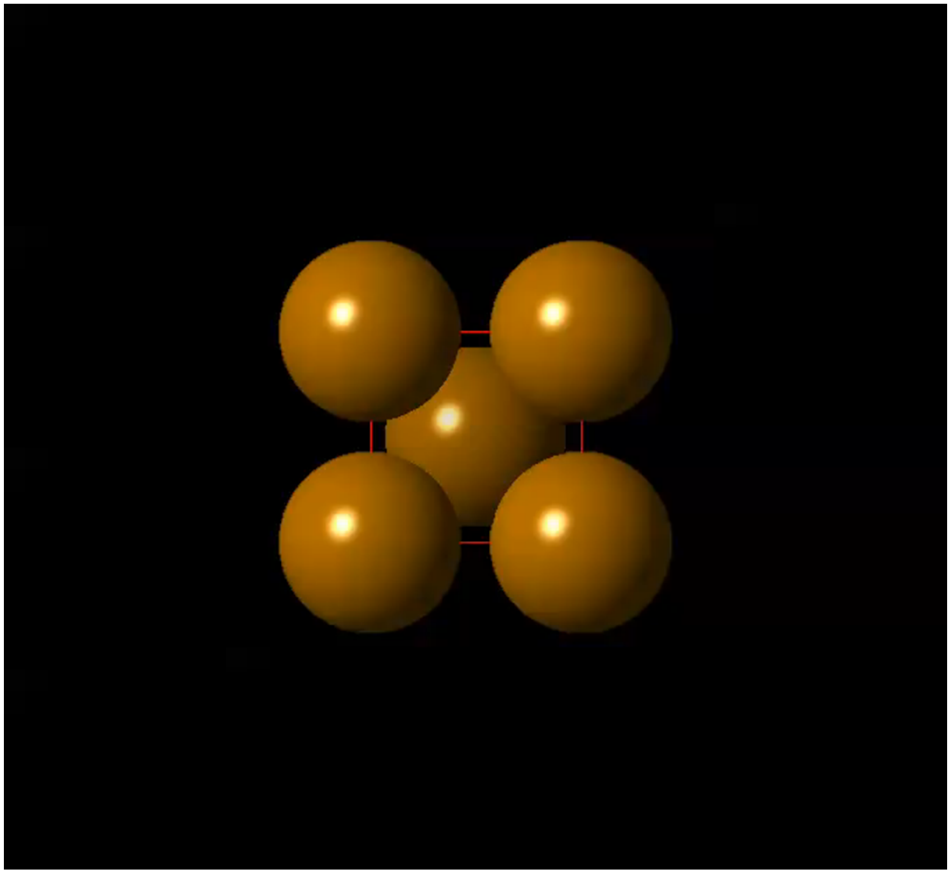




Adapted from Fig. 3.2, *Callister 7e.*

2 atoms/unit cell: 1 center + 8 corners x 1/8

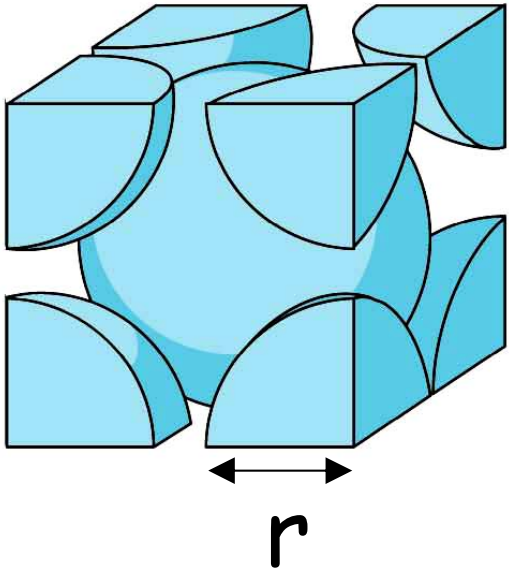
(Courtesy P.M. Anderson)

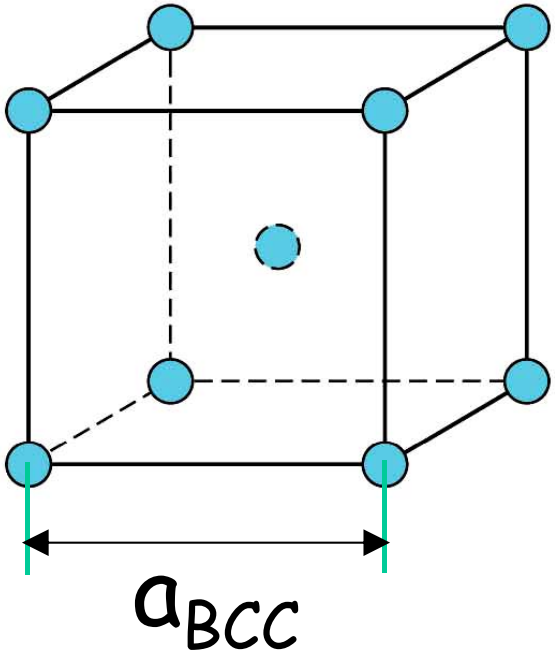


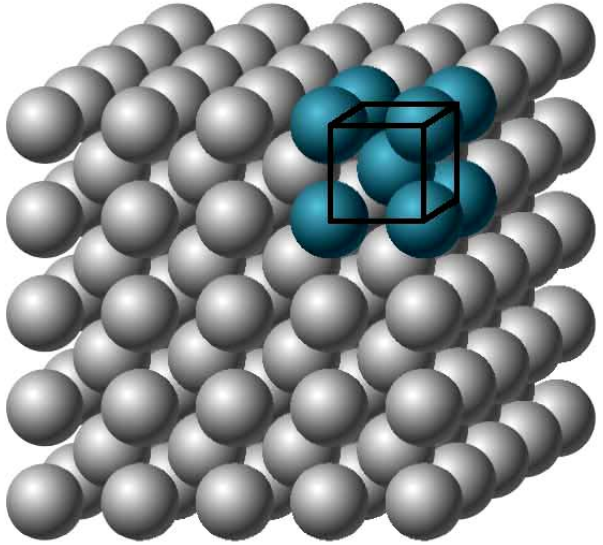
Body Centered Cubic (BCC)

- Close packed directions are cube diagonals <111>
- 2 atoms / unit cell (1 + 8 x 1/8) $a_{BCC} = 4r/3^{1/2}$
- Highest density plane {110} Coordination # = 8
- Cr, Fe, W, etc.

- Coordination # = 8

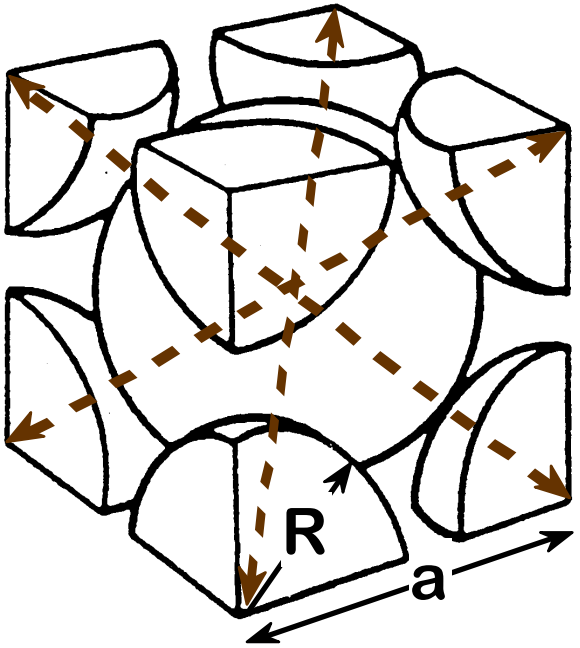






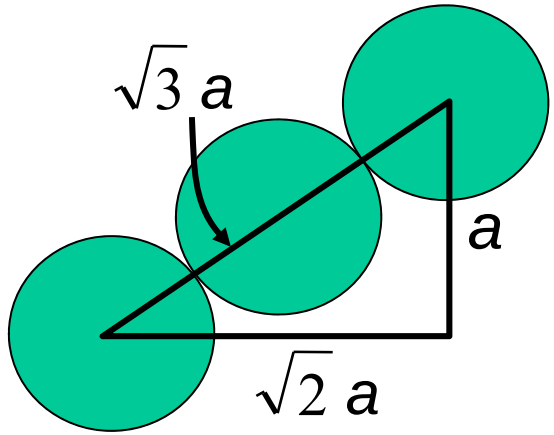
ATOMIC PACKING FACTOR: BCC

- APF for a body-centered cubic structure = 0.68



Close-packed directions:
length = 4R
$= \sqrt{3}\, a$

Unit cell contains:
1 + 8 x 1/8
= 2 atoms/unit cell



Close-packed directions
<111>

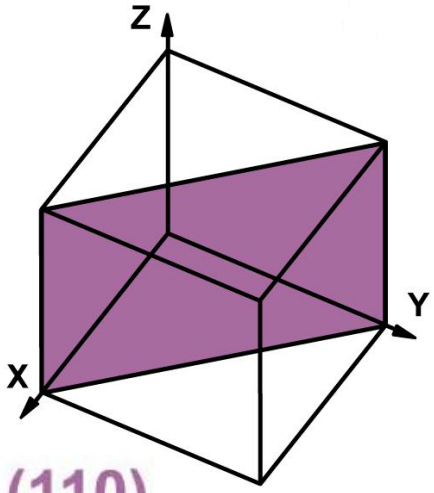
$$\text{APF} = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{2 \cdot \frac{4}{3}\pi (\sqrt{3}a/4)^3}{a^3}$$

$$\text{length} = 4R = \sqrt{3}\, a$$

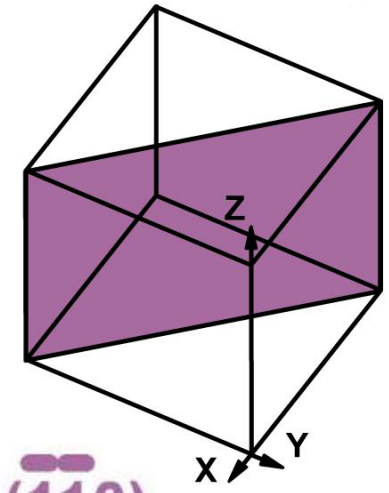
Highest density planes
{110}

Adapted from
Callister 6e.

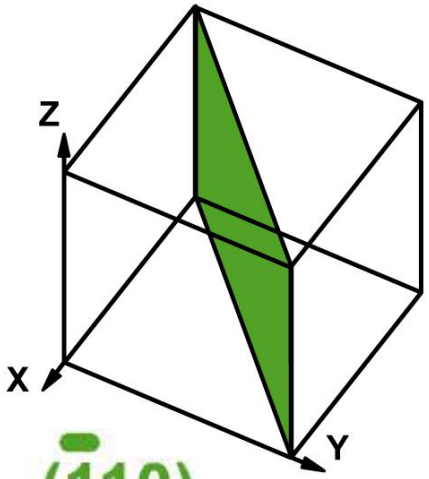
{110} Family



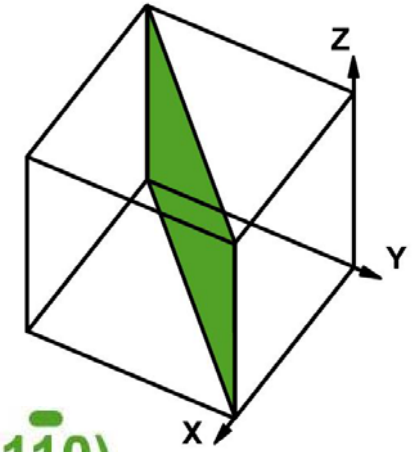
(110)



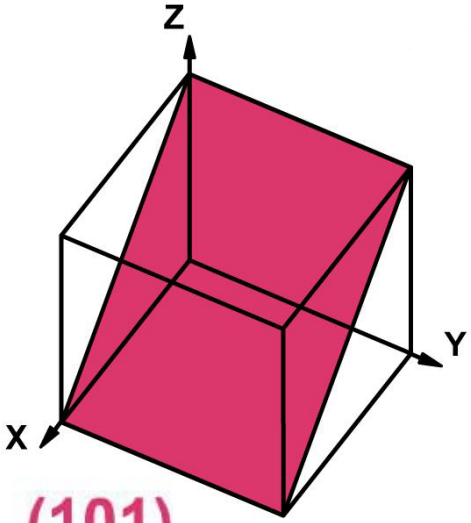
$(\bar{1}\bar{1}0)$



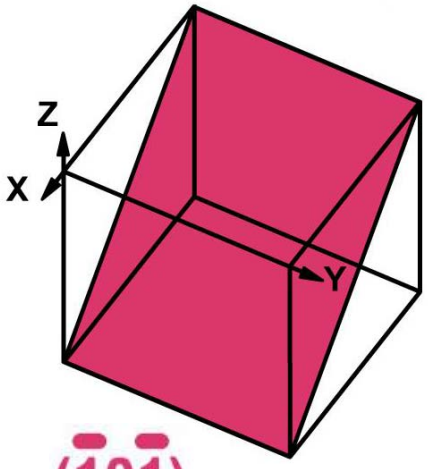
$(\bar{1}10)$



$(1\bar{1}0)$

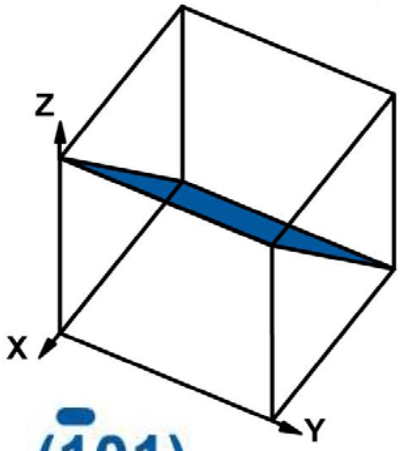


(101)

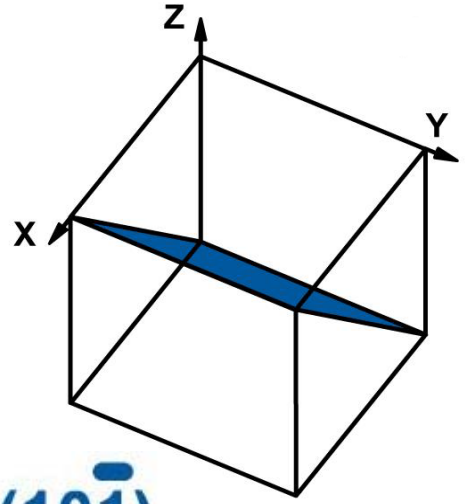


$(\bar{1}0\bar{1})$

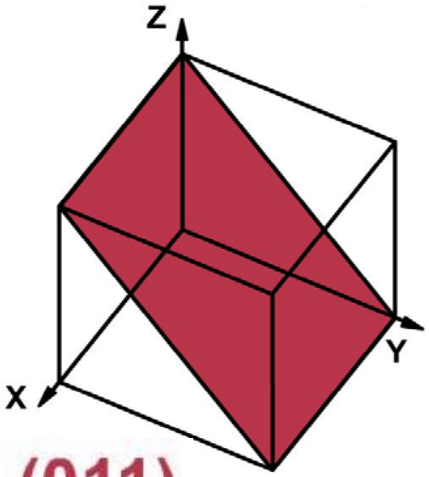
{110} Family



$(\bar{1}01)$



$(10\bar{1})$



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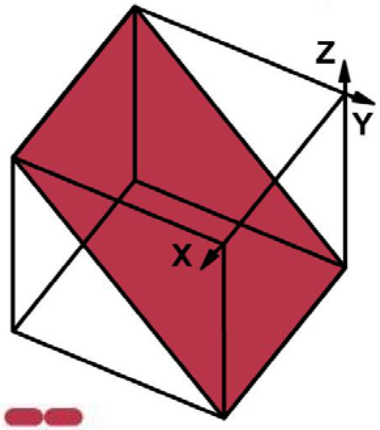
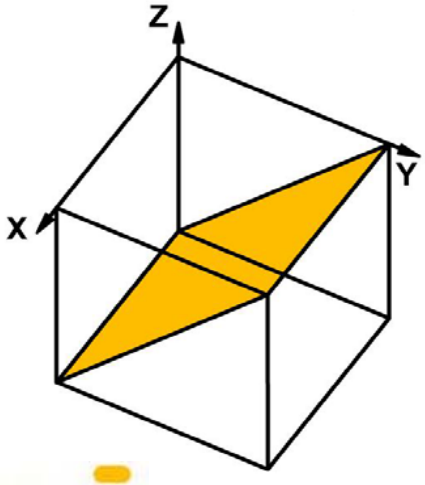
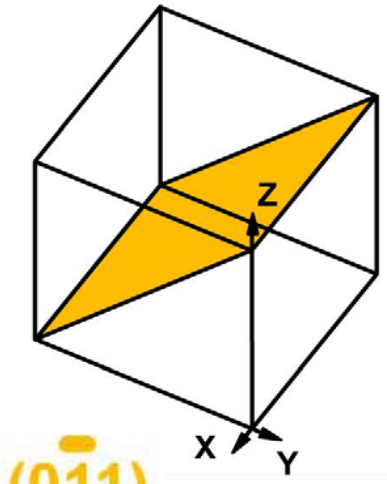


$(0\bar{1}\bar{1})$



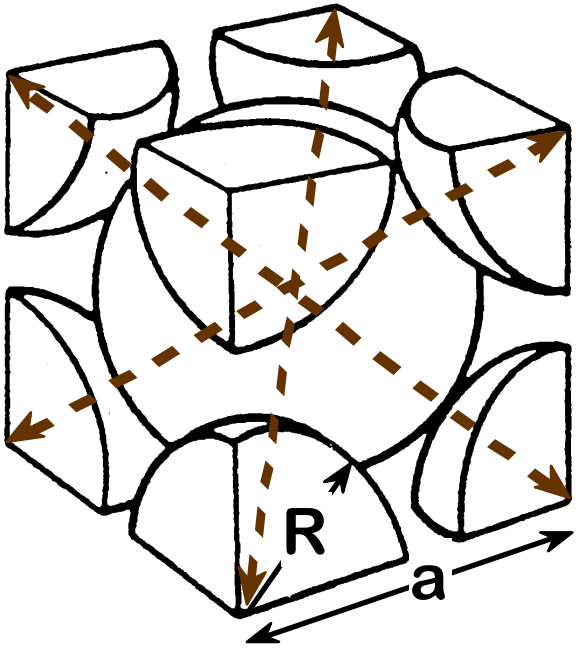
$(01\bar{1})$



$(0\bar{1}1)$

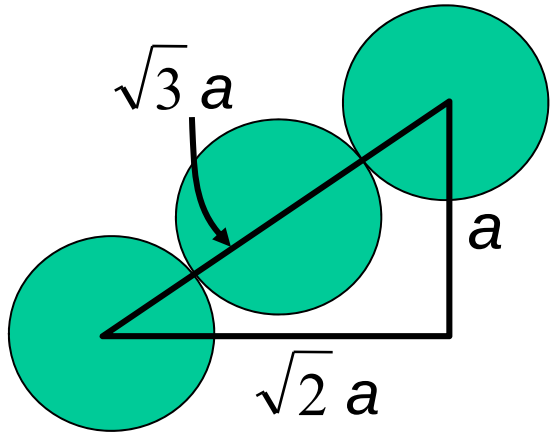
ATOMIC PACKING FACTOR: BCC

- APF for a body-centered cubic structure = 0.68



Close-packed directions:
length = 4R
$= \sqrt{3}\, a$

Unit cell contains:
1 + 8 x 1/8
= 2 atoms/unit cell



Close-packed directions
<111>

$$\text{APF} = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{2 \cdot \frac{4}{3}\pi (\sqrt{3}a/4)^3}{a^3}$$

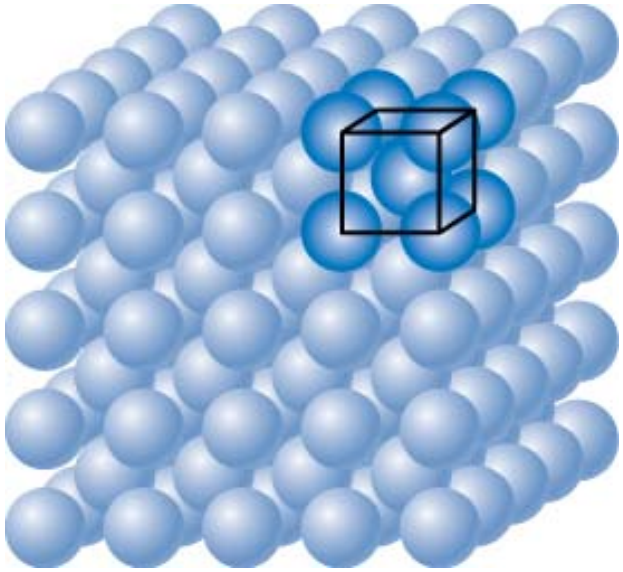
$$\text{length} = 4R = \sqrt{3}\, a$$

Highest density planes
{110}

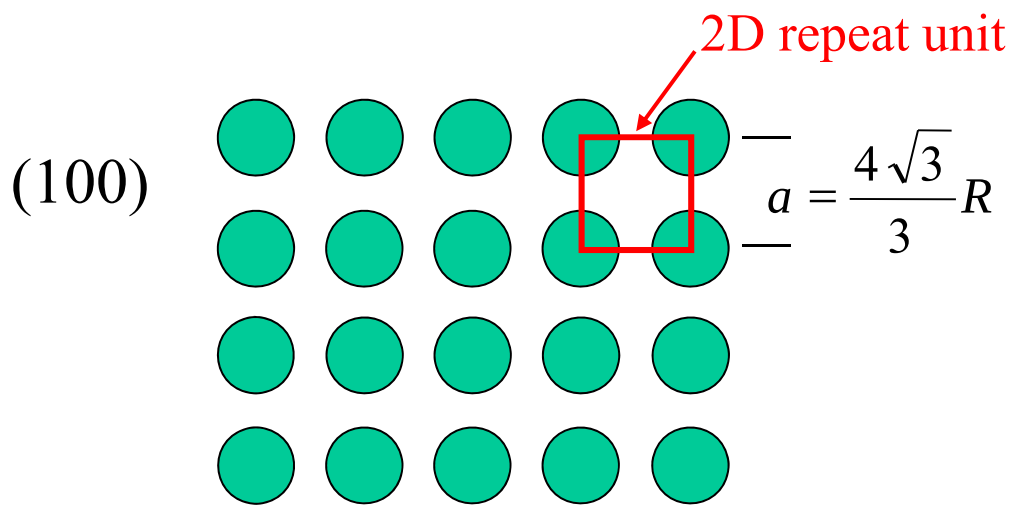
Adapted from
Callister 6e.

Planar Density of (100) Iron

At T < 912°C iron has the BCC structure.



Adapted from Fig. 3.2(c), *Callister 7e.*

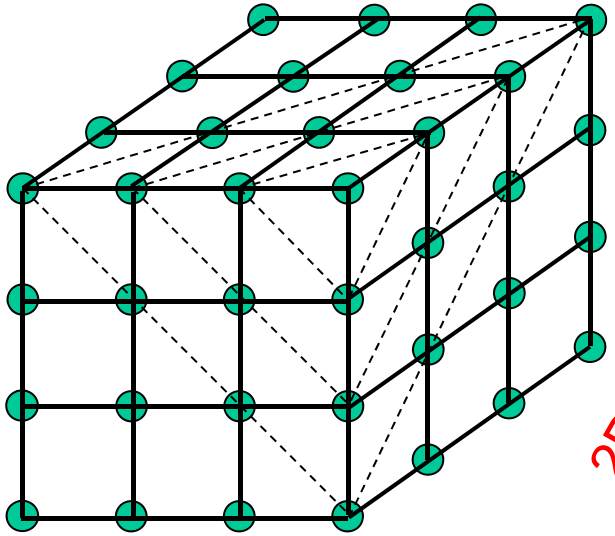


Radius of iron $R = 0.1241$ nm

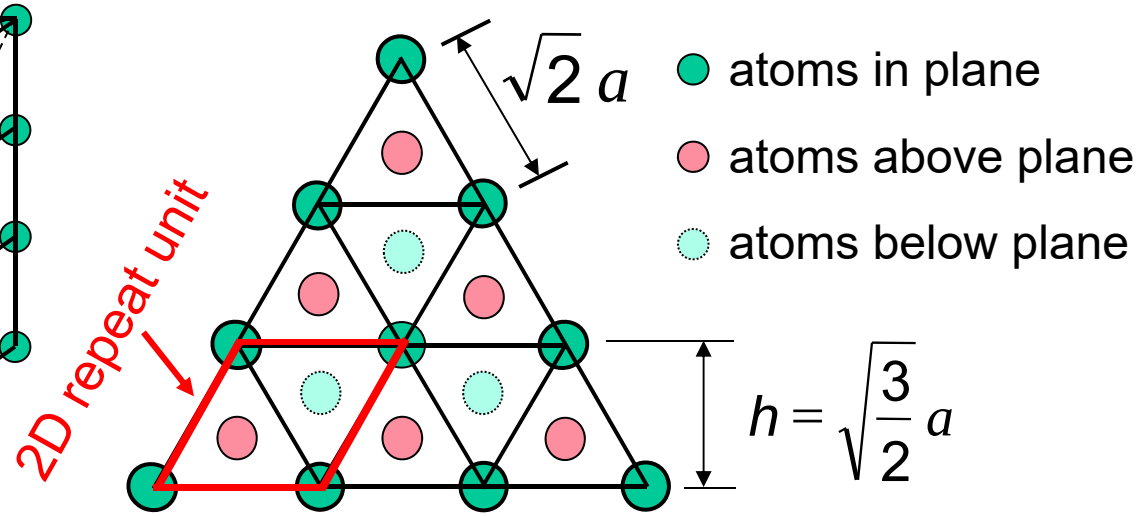
$$\text{Planar Density} = \frac{\dfrac{\text{atoms}}{\text{2D repeat unit}}}{\dfrac{\text{area}}{\text{2D repeat unit}}} = \frac{1}{a^2} = \frac{1}{\left(\frac{4\sqrt{3}}{3}R\right)^2} = 12.1 \frac{\text{atoms}}{\text{nm}^2} = 1.2 \times 10^{19} \frac{\text{atoms}}{\text{m}^2}$$

Planar Density of (111) Iron

(111) plane



1 atom in plane/ unit surface cell

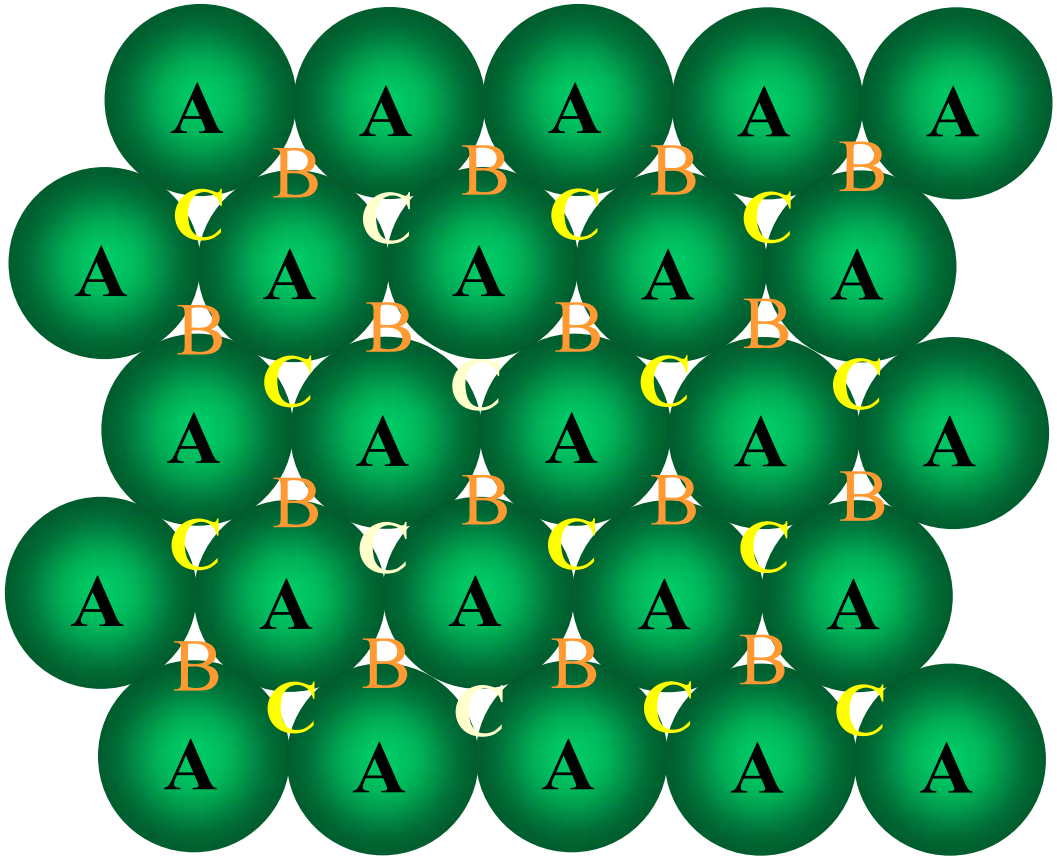


$$\text{area} = \sqrt{2}\,ah = \sqrt{3}\,a^2 = \sqrt{3}\left(\frac{4\sqrt{3}}{3}R\right)^2 = \frac{16\sqrt{3}}{3}R^2$$

$$\text{Planar Density} = \frac{\dfrac{\text{atoms}}{\text{2D repeat unit}}}{\dfrac{\text{area}}{\text{2D repeat unit}}} = \frac{1}{\frac{16\sqrt{3}}{3}R^2} = 7.0\,\frac{\text{atoms}}{\text{nm}^2} = 0.70 \times 10^{19}\,\frac{\text{atoms}}{\text{m}^2}$$

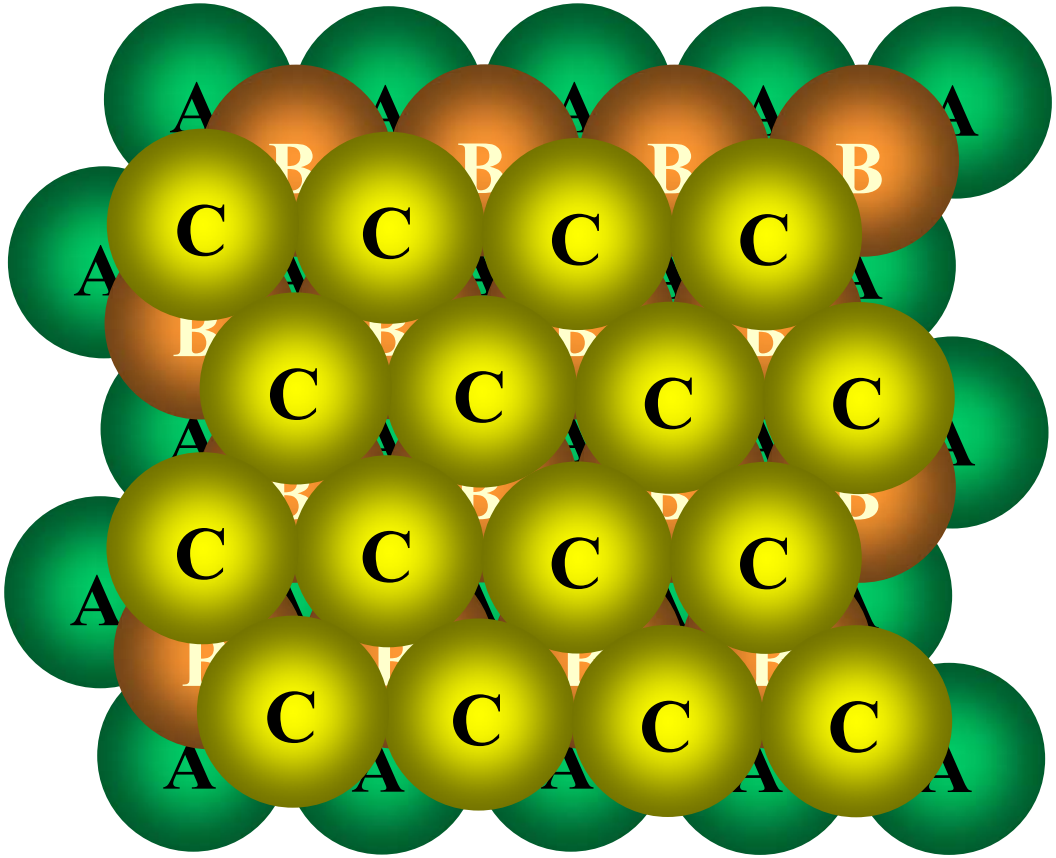
Metallic crystal system

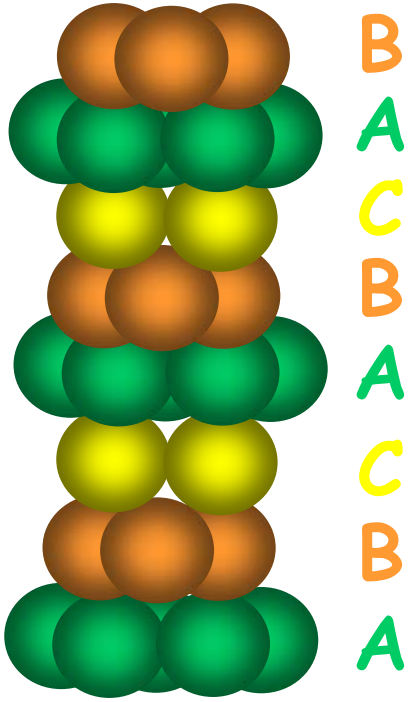
- Stacking sequence



Metallic crystal system

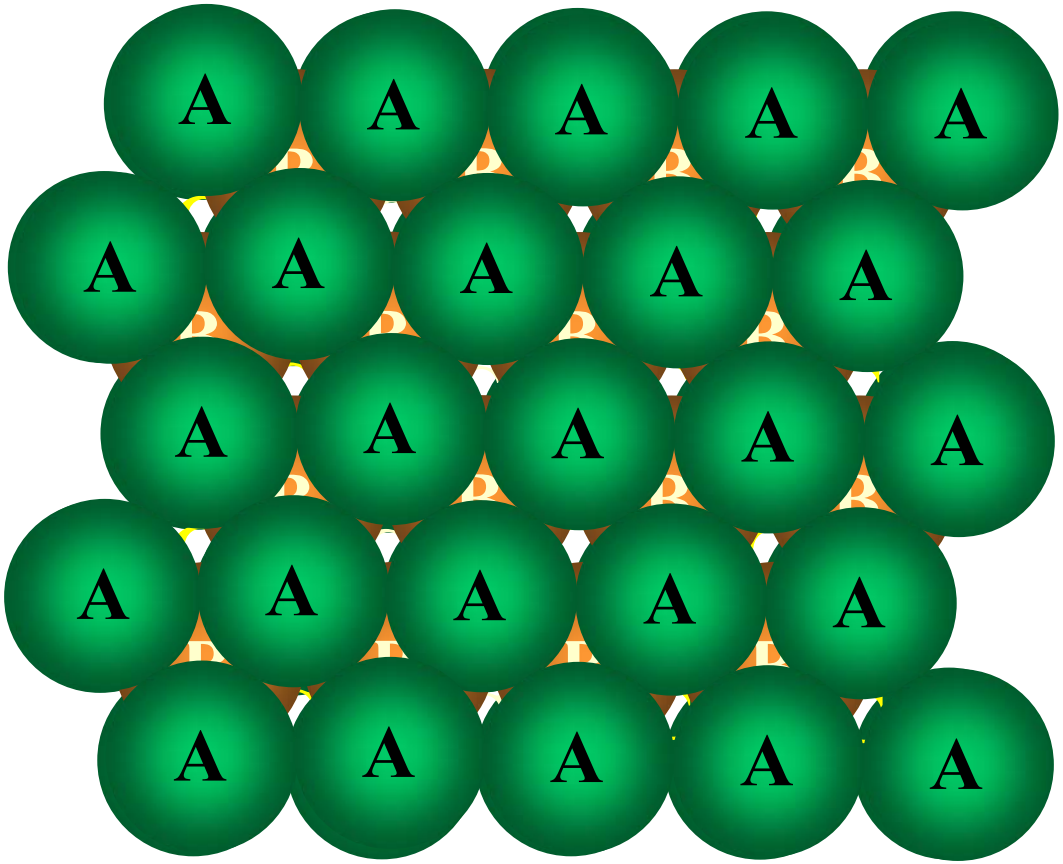
- A – B – C – A stacking sequence → FCC

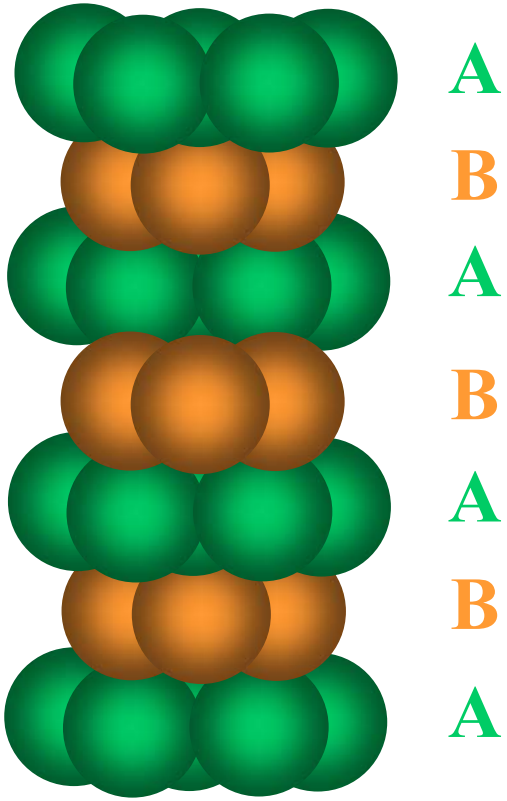




Metallic crystal system

- A – B – A – B stacking sequence → HCP





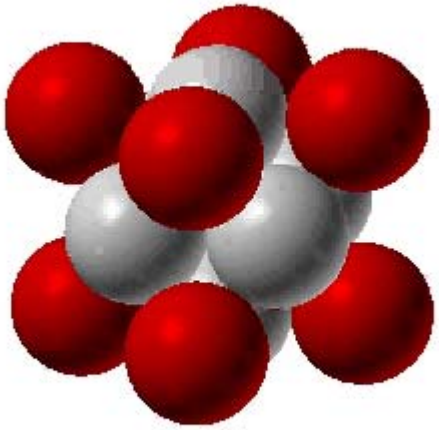
(3) Face Centered Cubic Structure (FCC)

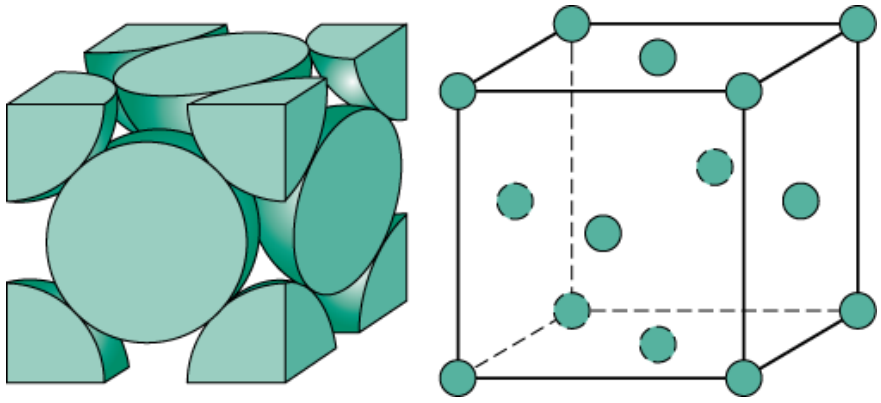
- Atoms touch each other along face diagonals.

  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ex: Al, Cu, Au, Pb, Ni, Pt, Ag

- Coordination # = 12





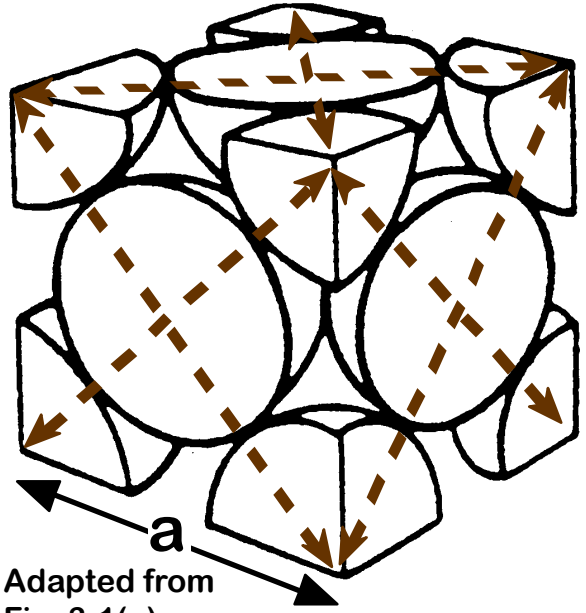
Adapted from Fig. 3.1, *Callister 7e.*

4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

(Courtesy P.M. Anderson)

ATOMIC PACKING FACTOR: FCC

- APF for a face-centered cubic structure = 0.74



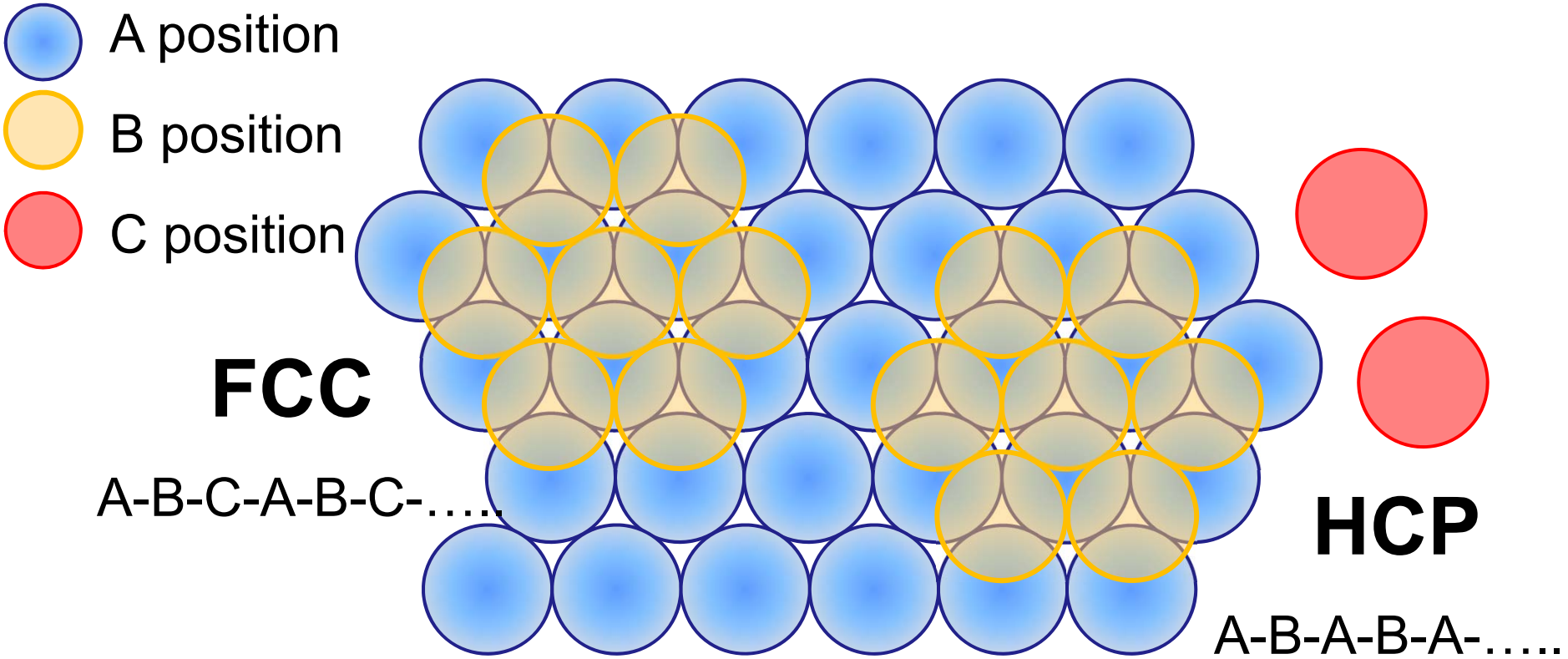
Adapted from Fig. 3.1(a), *Callister 6e.*

Close-packed directions: <110>
length = 4R {111}
$= \sqrt{2}\,a$

Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{4 \cdot \frac{4}{3}\pi\left(\sqrt{2}a/4\right)^3}{a^3}$$

Two closely packed stackings

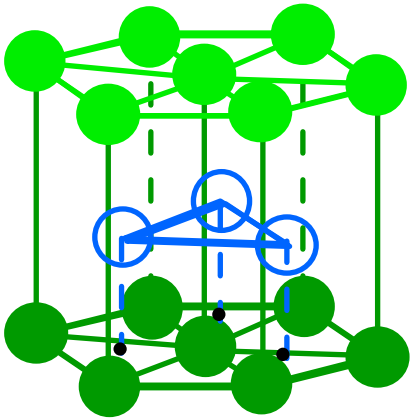


FCC : Al, Ni, Cu, Ag, Ir, Pt, Au

HCP : Be, Mg, Sc, Ti, Co, Zn, Y, Zr, Se, Te, Ru

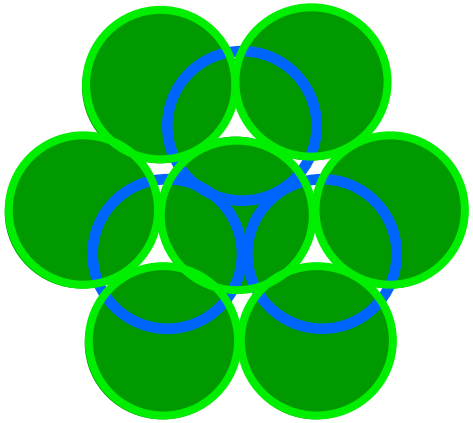
HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3, *Callister 6e.*

- 2D Projection



- Coordination # = 12
- APF = 0.74

Close-packed direction : $<11\bar{2}0>$

plane : (0001)

Contents for today's class

I. Atomic arrangement in the solid state

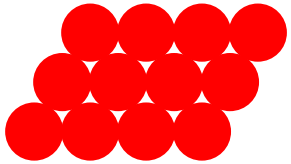
- Solid materials are classified according to the **regularity** with which atoms and ions are arranged with respect to one another.

- So, how are they arranged ?

  (a) **periodically** – having long range order in 3-D

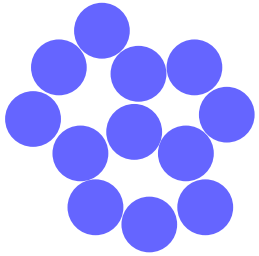
  (b) **quasi-periodically**

  (c) **randomly** – having short range order with the characteristics of bonding type but losing the long range order



Crystal

Quasicrystal



Amorphous

- **Crystal: Perfection → Imperfection**

Contents for today's class

II. Metallic crystal system

TABLE 3-2 ■ *Crystal structure characteristics of some metals*

Structure	a_0 versus r	Atoms per Cell	Coordination Number	Packing Factor	Examples
Simple cubic (SC)	$a_0 = 2r$	1	6	0.52	Polonium (Po), α-Mn
Body-centered cubic	$a_0 = 4r/\sqrt{3}$	2	8	0.68	Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Zr, Cr
Face-centered cubic	$a_0 = 4r/\sqrt{2}$	4	12	0.74	Fe, Cu, Au, Pt, Ag, Pb, Ni
Hexagonal close-packed	$a_0 = 2r$ $c_0 \approx 1.633a_0$	2	12	0.74	Ti, Mg, Zn, Be, Co, Zr, Cd