

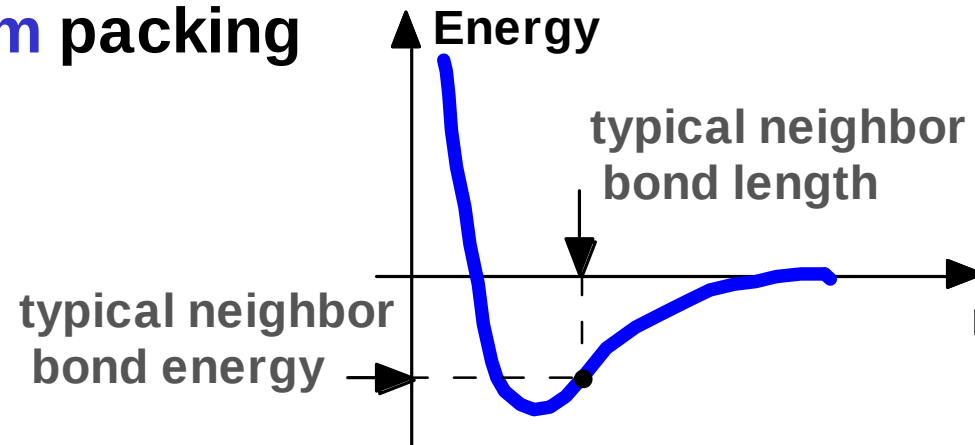
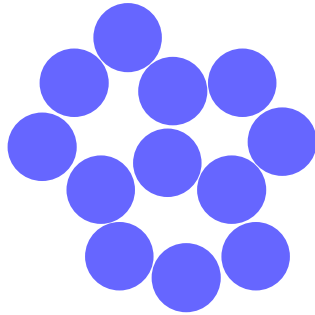
CHAPTER 3: CRYSTAL STRUCTURES & PROPERTIES

ISSUES TO ADDRESS...

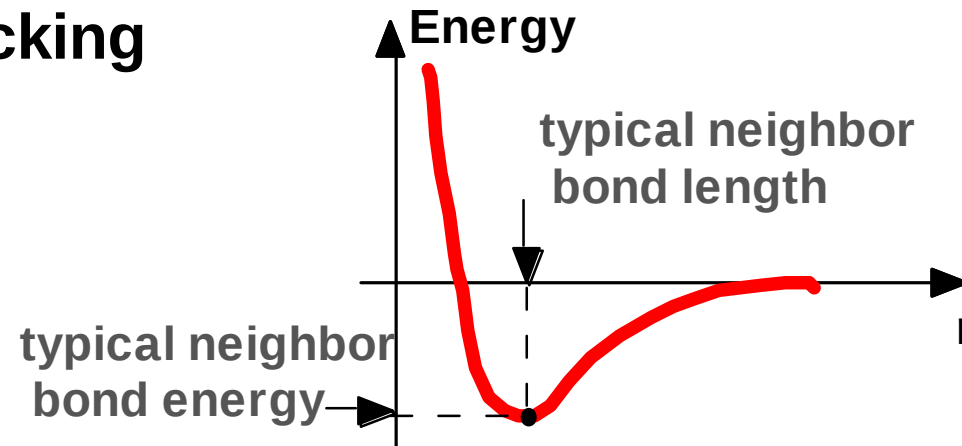
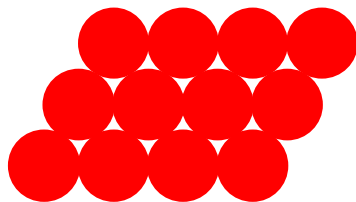
- **How do atoms assemble into solid structures?
(for now, focus on metals)**
- **How does the density of a material depend on
its structure?**
- **When do material properties vary with the
sample (i.e., part) orientation?**

ENERGY AND PACKING

- Non dense, **random** packing



- Dense, **regular** packing

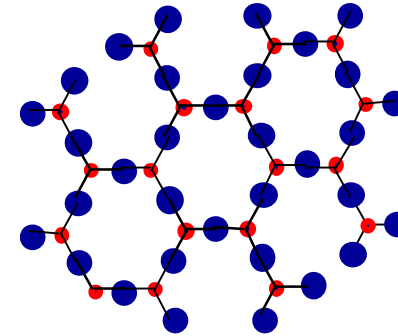


Dense, regular-packed structures tend to have lower energy.

MATERIALS AND PACKING

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
-many ceramics
-some polymers



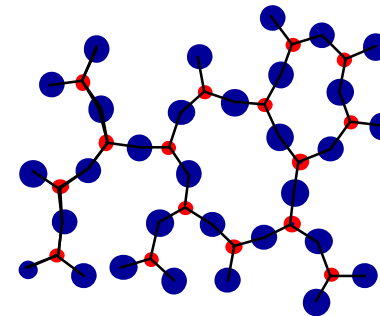
crystalline SiO₂

Adapted from Fig. 3.18(a),
Callister 6e.

• Si • Oxygen

Noncrystalline materials...

- atoms have no periodic packing
- occurs for: -complex structures
-rapid cooling



noncrystalline SiO₂

Adapted from Fig. 3.18(b),
Callister 6e.

"Amorphous" = Noncrystalline

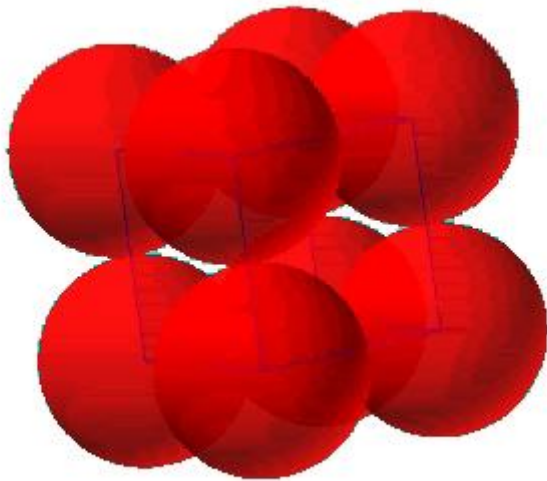
METALLIC CRYSTALS

- **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.**

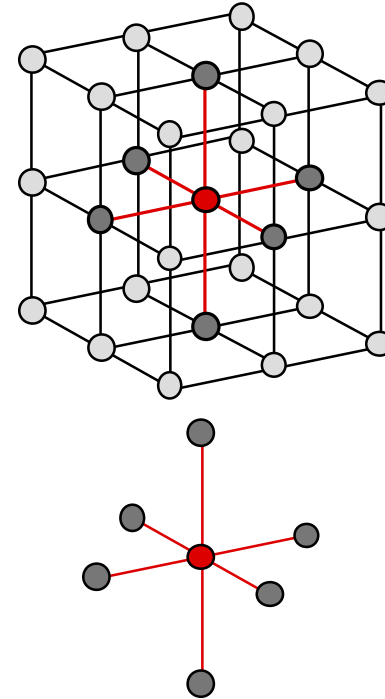
We will look at three such structures...

SIMPLE CUBIC STRUCTURE (SC)

- Rare due to poor packing (only Po has this structure)
- **Close-packed directions** are cube edges.
- **Coordination # = 6**
(# nearest neighbors)



(Courtesy P.M. Anderson)

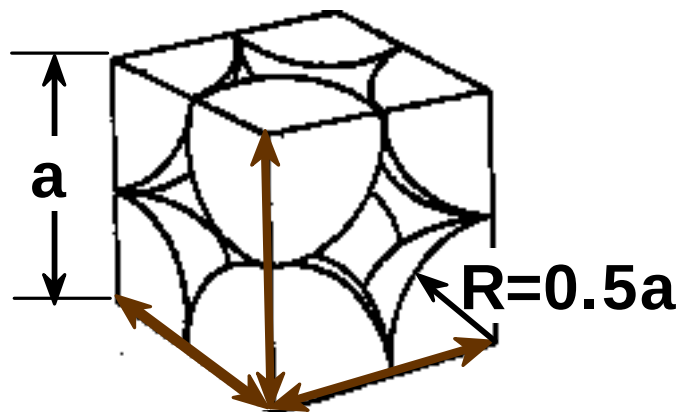


ATOMIC PACKING FACTOR

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

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains $8 \times 1/8 =$

1 atom/unit cell

Adapted from Fig. 3.19,
Callister 6e.

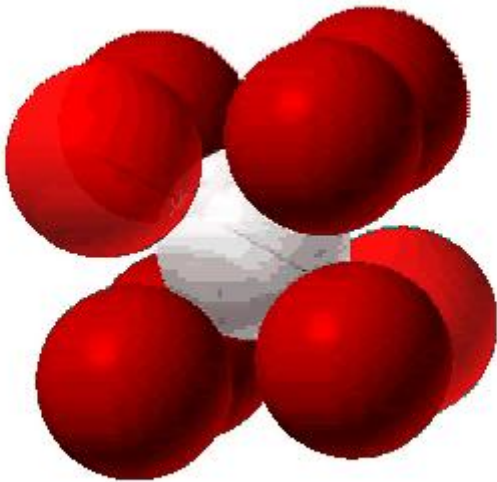
$$APF = \frac{\text{atoms unit cell} \times \frac{4}{3} \pi (0.5a)^3}{a^3}$$

volume
atom

volume
unit cell

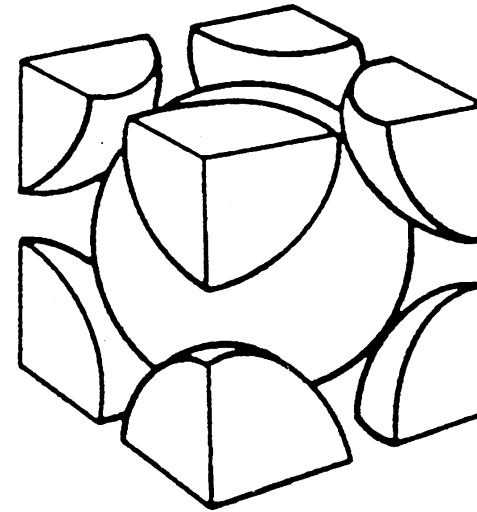
BODY CENTERED CUBIC STRUCTURE (BCC)

- Close packed directions are cube diagonals.
--Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.



(Courtesy P.M. Anderson)

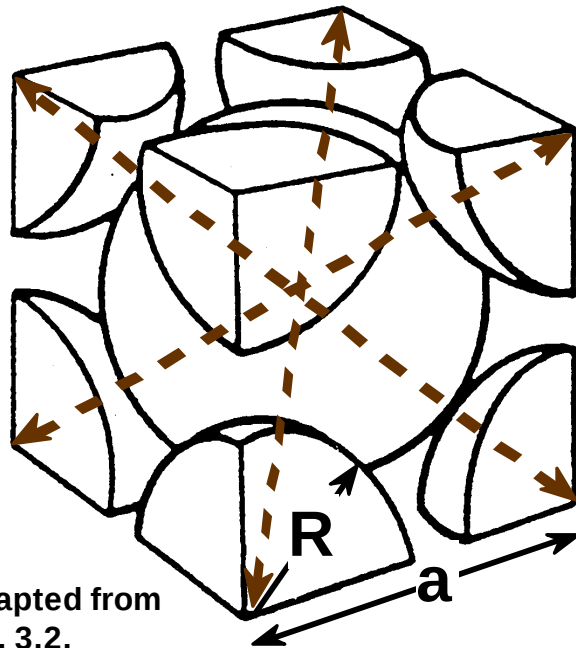
- Coordination # = 8



Adapted from Fig. 3.2,
Callister 6e.

ATOMIC PACKING FACTOR: BCC

- APF for a body-centered cubic structure = 0.68



Adapted from
Fig. 3.2,
Callister 6e.

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

Unit cell contains:
 $1 + 8 \times 1/8$
 $= 2 \text{ atoms/unit cell}$

$$\text{APF} = \frac{\text{atoms/unit cell} \times \text{volume/atom}}{\text{volume/unit cell}}$$

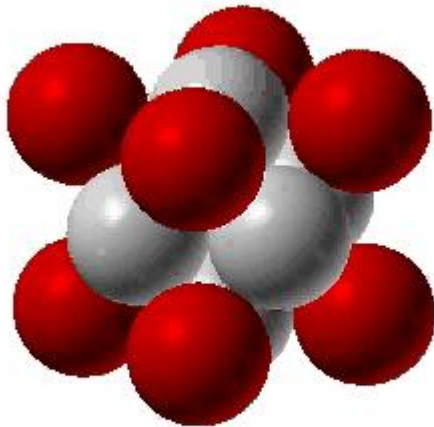
$$\text{APF} = \frac{2 \times \frac{4}{3} \pi (\sqrt{3}a/4)^3}{a^3}$$

The diagram shows the calculation of the Atomic Packing Factor (APF) for a BCC unit cell. The numerator represents the total volume of atoms in the unit cell, calculated as the number of atoms per unit cell (2) multiplied by the volume of a single atom ($\frac{4}{3} \pi R^3$, where $R = \sqrt{3}a/4$). The denominator represents the volume of the unit cell (a^3). Arrows indicate the correspondence between the text labels and the terms in the equation.

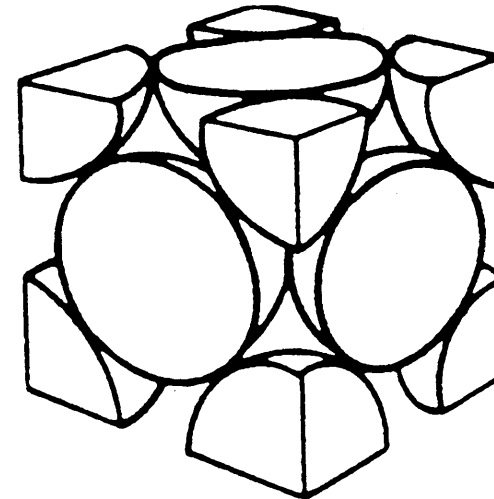
FACE CENTERED CUBIC STRUCTURE (FCC)

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

- Coordination # = 12



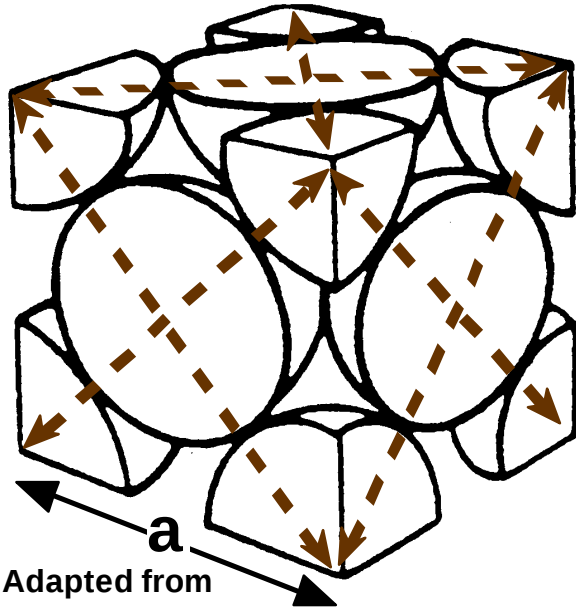
(Courtesy P.M. Anderson)



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

ATOMIC PACKING FACTOR: FCC

- APF for a body-centered cubic structure = 0.74



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

Close-packed directions:
length = $4R$
 $= \sqrt{2} a$

Unit cell contains:
 $6 \times 1/2 + 8 \times 1/8$
 $= 4 \text{ atoms/unit cell}$

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

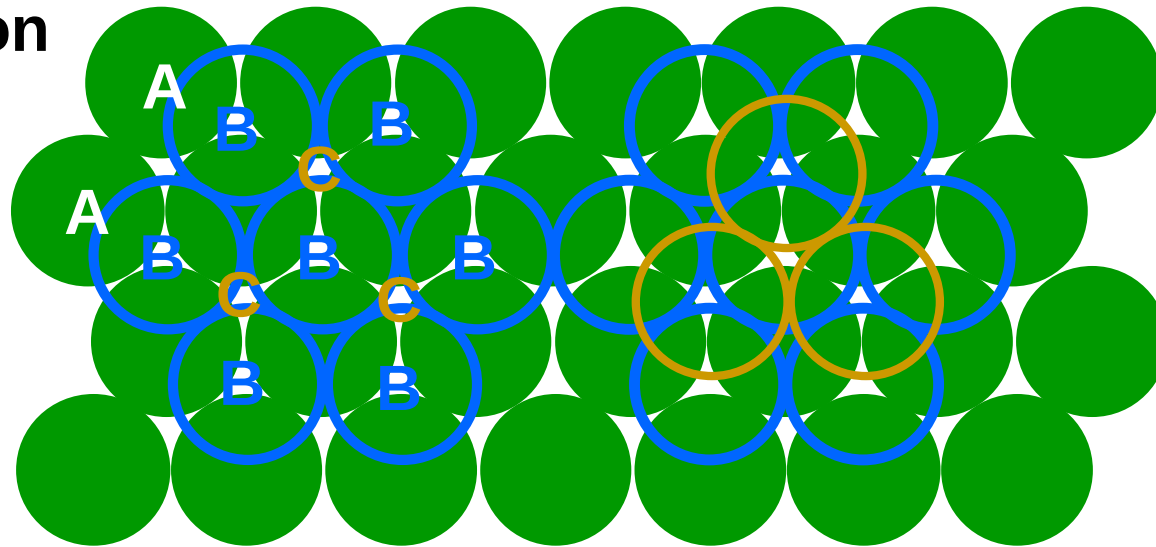
FCC STACKING SEQUENCE

- ABCABC... Stacking Sequence
- 2D Projection

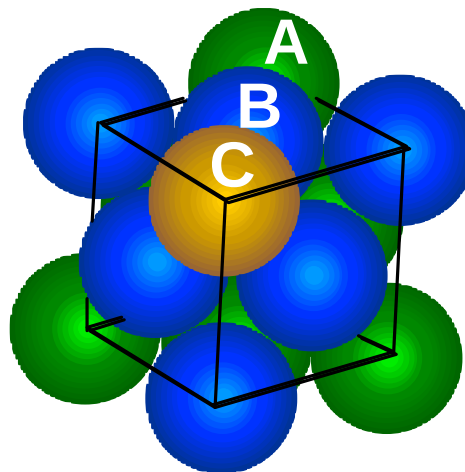
A sites

B sites

C sites

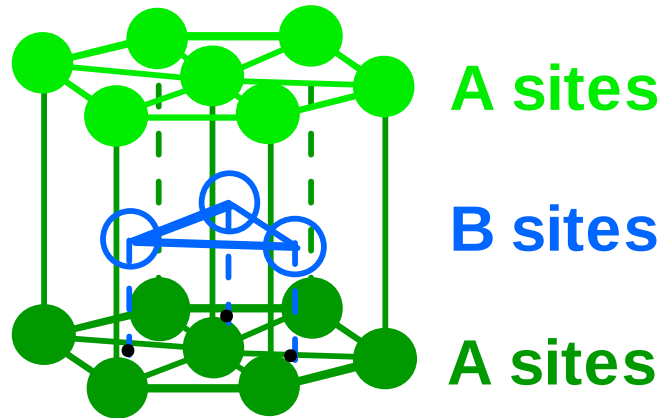


- FCC Unit Cell



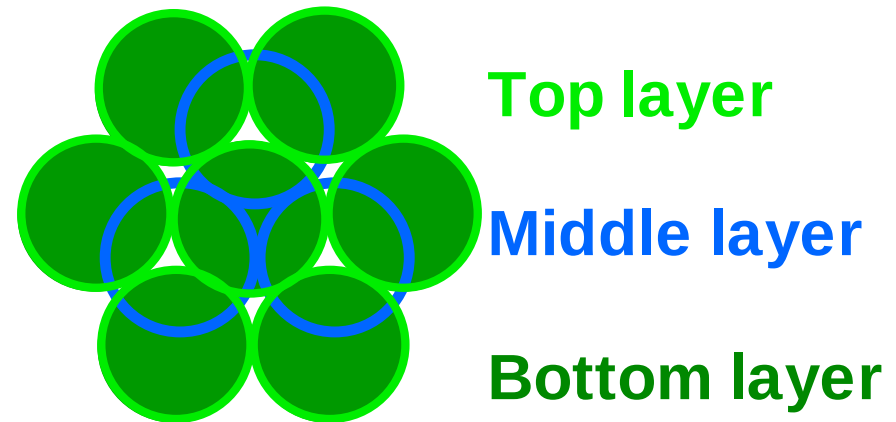
HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3,
Callister 6e.

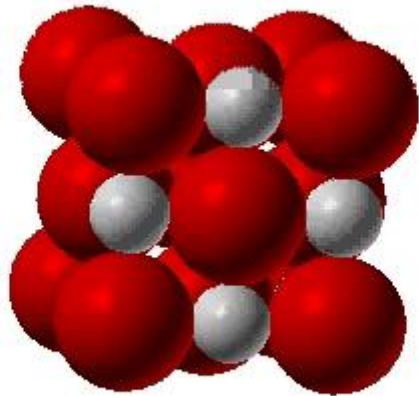
- 2D Projection



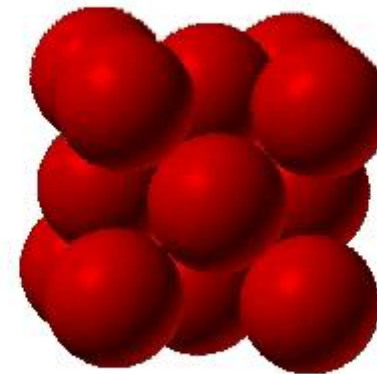
- Coordination # = 12
- APF = 0.74

STRUCTURE OF COMPOUNDS: NaCl

- Compounds: Often have similar close-packed structures.
- Structure of NaCl
 - Close-packed directions
--along cube edges.



(Courtesy P.M. Anderson)



(Courtesy P.M. Anderson)

THEORETICAL DENSITY, ρ

$$\rho = \frac{n A}{V_c N_A}$$

atoms/unit cell $\rightarrow$ n Atomic weight (g/mol) $\rightarrow$ A
 Volume/unit cell (cm³/unit cell) $\rightarrow$ V_c Avogadro's number (6.023 x 10²³ atoms/mol) $\rightarrow$ N_A

Example: Copper

Data from Table inside front cover of Callister (see next slide):

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius $R = 0.128$ nm (1 nm = 10⁻⁷cm)

$$V_c = a^3 ; \text{ For FCC, } a = 4R/\sqrt{2} ; V_c = 4.75 \times 10^{-23} \text{ cm}^3$$

Result: theoretical $\rho_{\text{Cu}} = 8.89 \text{ g/cm}^3$

Compare to actual: $\rho_{\text{Cu}} = 8.94 \text{ g/cm}^3$

Characteristics of Selected Elements at 20C

Element	Symbol	At. Weight (amu)	Density (g/cm ³)	Crystal Structure	Atomic radius (nm)
Aluminum	Al	26.98	2.71	FCC	0.143
Argon	Ar	39.95	-----	-----	-----
Barium	Ba	137.33	3.5	BCC	0.217
Beryllium	Be	9.012	1.85	HCP	0.114
Boron	B	10.81	2.34	Rhomb	-----
Bromine	Br	79.90	-----	-----	-----
Cadmium	Cd	112.41	8.65	HCP	0.149
Calcium	Ca	40.08	1.55	FCC	0.197
Carbon	C	12.011	2.25	Hex	0.071
Cesium	Cs	132.91	1.87	BCC	0.265
Chlorine	Cl	35.45	-----	-----	-----
Chromium	Cr	52.00	7.19	BCC	0.125
Cobalt	Co	58.93	8.9	HCP	0.125
Copper	Cu	63.55	8.94	FCC	0.128
Flourine	F	19.00	-----	-----	-----
Gallium	Ga	69.72	5.90	Ortho.	0.122
Germanium	Ge	72.59	5.32	Dia. cubic	0.122
Gold	Au	196.97	19.32	FCC	0.144
Helium	He	4.003	-----	-----	-----
Hydrogen	H	1.008	-----	-----	-----

Adapted from
Table, "Charac-
teristics of
Selected
Elements",
inside front
cover,
Callister 6e.

DENSITIES OF MATERIAL CLASSES

ρ_{metals} ρ_{ceramics} ρ_{polymers} Metals/Alloys Graphite/Ceramics/Semicond Polymers Composites/fibers

Why?

Metals have...

- close-packing (metallic bonding)
- large atomic mass

Ceramics have...

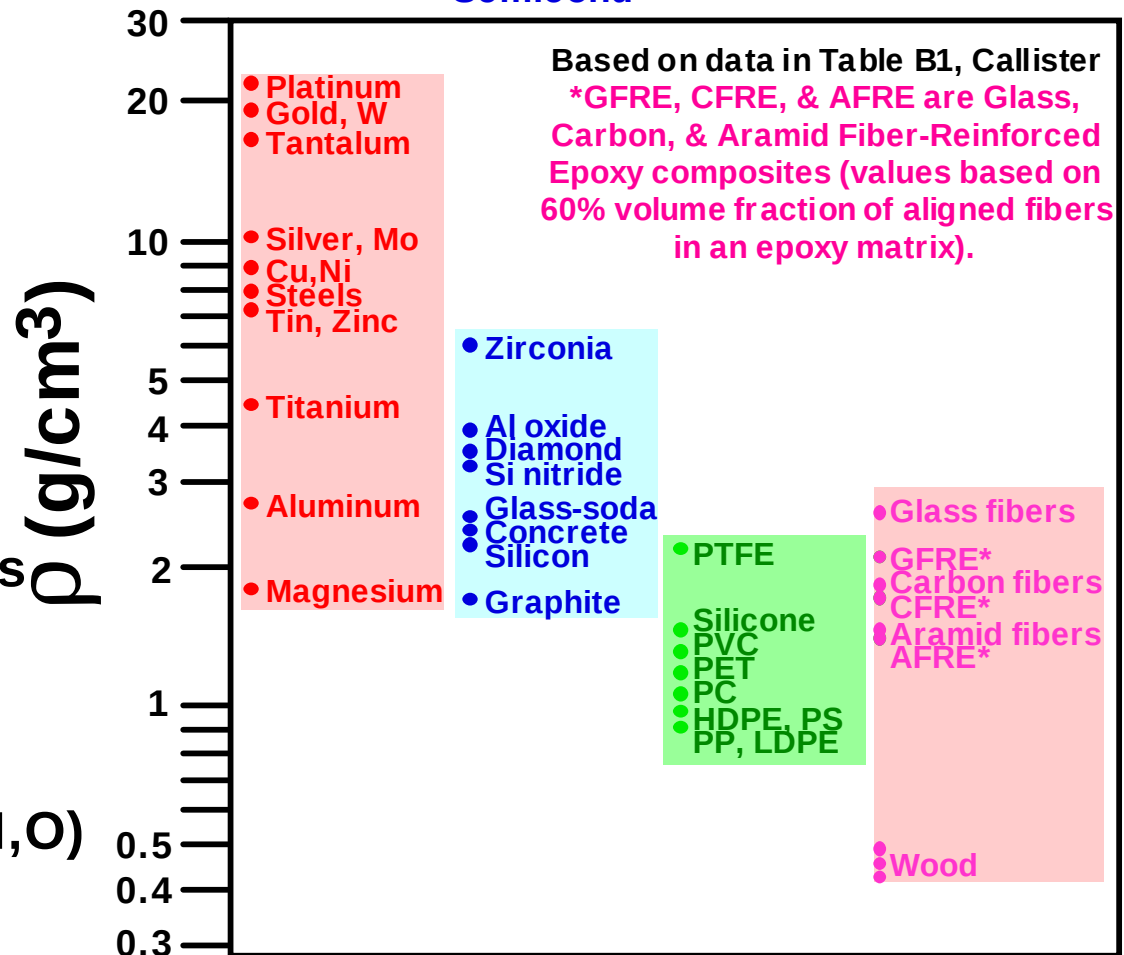
- less dense packing (covalent bonding)
- often lighter elements

Polymers have...

- poor packing (often amorphous)
- lighter elements (C,H,O)

Composites have...

- intermediate values

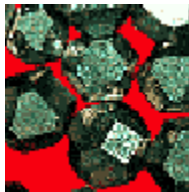


Data from Table B1, Callister 6e.

CRYSTALS AS BUILDING BLOCKS

- **Some engineering applications require single crystals:**
 - diamond single
 - turbine blades

crystals for abrasives



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

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



- **Crystal properties reveal features of atomic structure.**
 - Ex: Certain crystal planes in quartz fracture more easily than others.



(Courtesy P.M. Anderson)

POLYCRYSTALS

- *Most* engineering materials are polycrystals.



Adapted from Fig. K, color inset pages of *Callister 6e*.
(Fig. K is courtesy of Paul E. Danielson, Teledyne Wah Chang Albany)

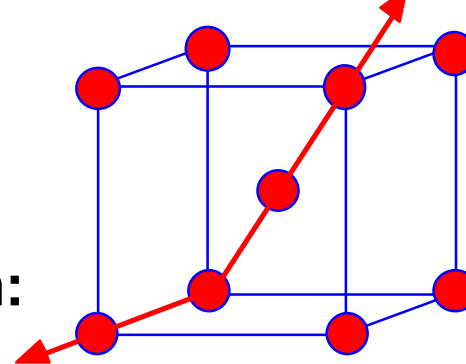
- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- If crystals are randomly oriented, overall component properties are not directional.
- Crystal sizes typ. range from 1 nm to 2 cm (i.e., from a few to millions of atomic layers).

SINGLE VS POLYCRYSTALS

- Single Crystals

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

E (diagonal) = 273 GPa

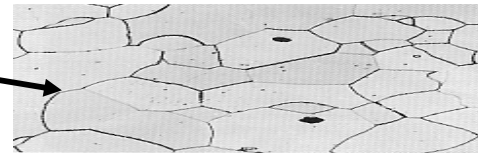
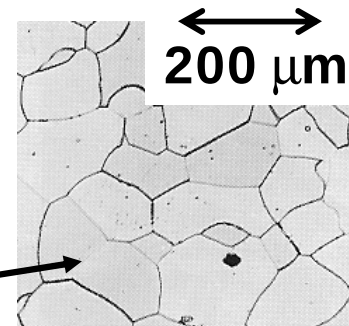


E (edge) = 125 GPa

Data from Table 3.3, *Callister 6e*.
(Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

- Polycrystals

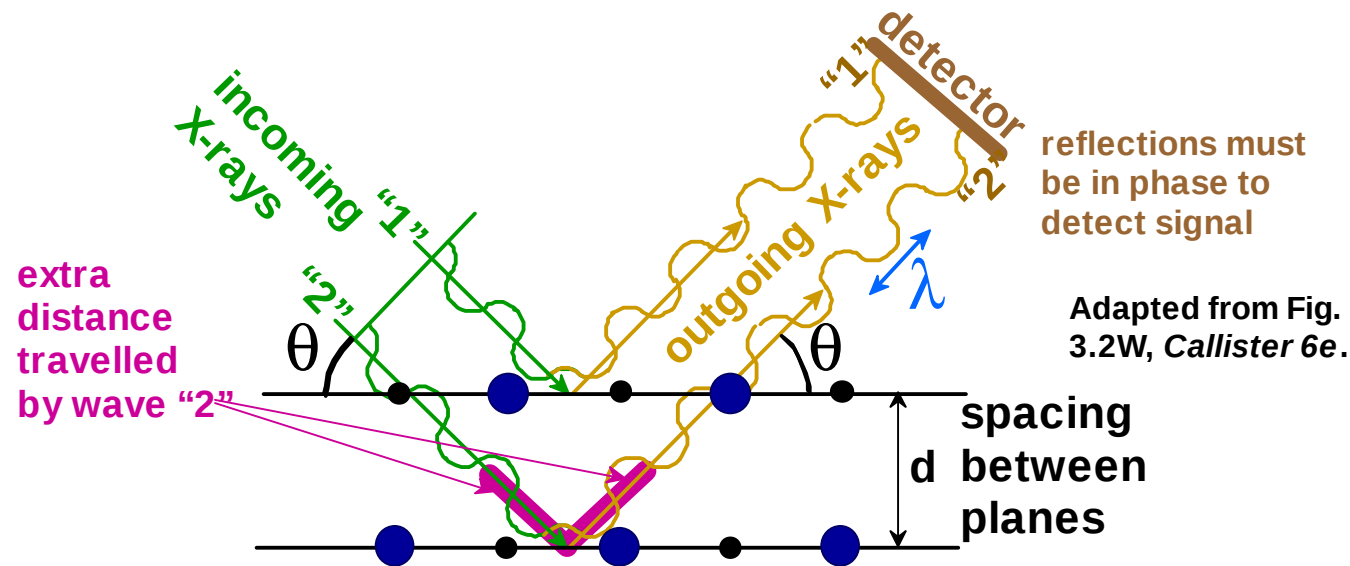
- Properties may/may not vary with direction.
- If grains are randomly oriented: **isotropic**.
($E_{\text{poly iron}} = 210$ GPa)
- If grains are **textured**, anisotropic.



Adapted from Fig. 4.12(b), *Callister 6e*.
(Fig. 4.12(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].)

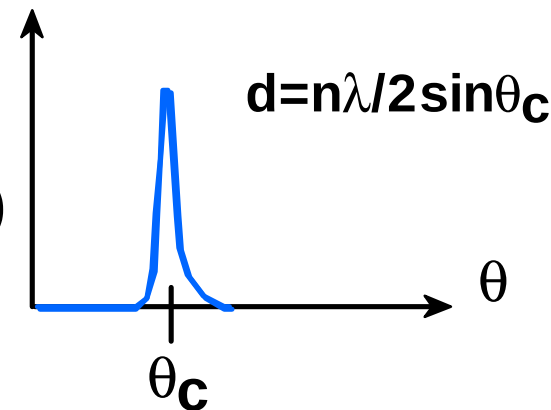
X-RAYS TO CONFIRM CRYSTAL STRUCTURE

- Incoming X-rays **diffract** from crystal planes.



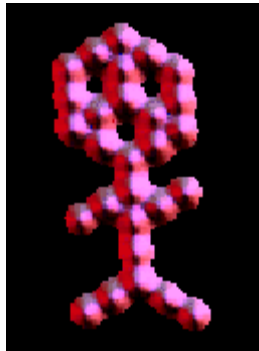
- Measurement of: Critical angles, θ_c , for X-rays provide atomic spacing, d .

x-ray intensity
(from detector)

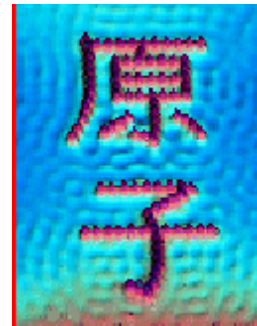


SCANNING TUNNELING MICROSCOPY

- Atoms can be arranged and imaged!



Carbon monoxide molecules arranged on a platinum (111) surface.

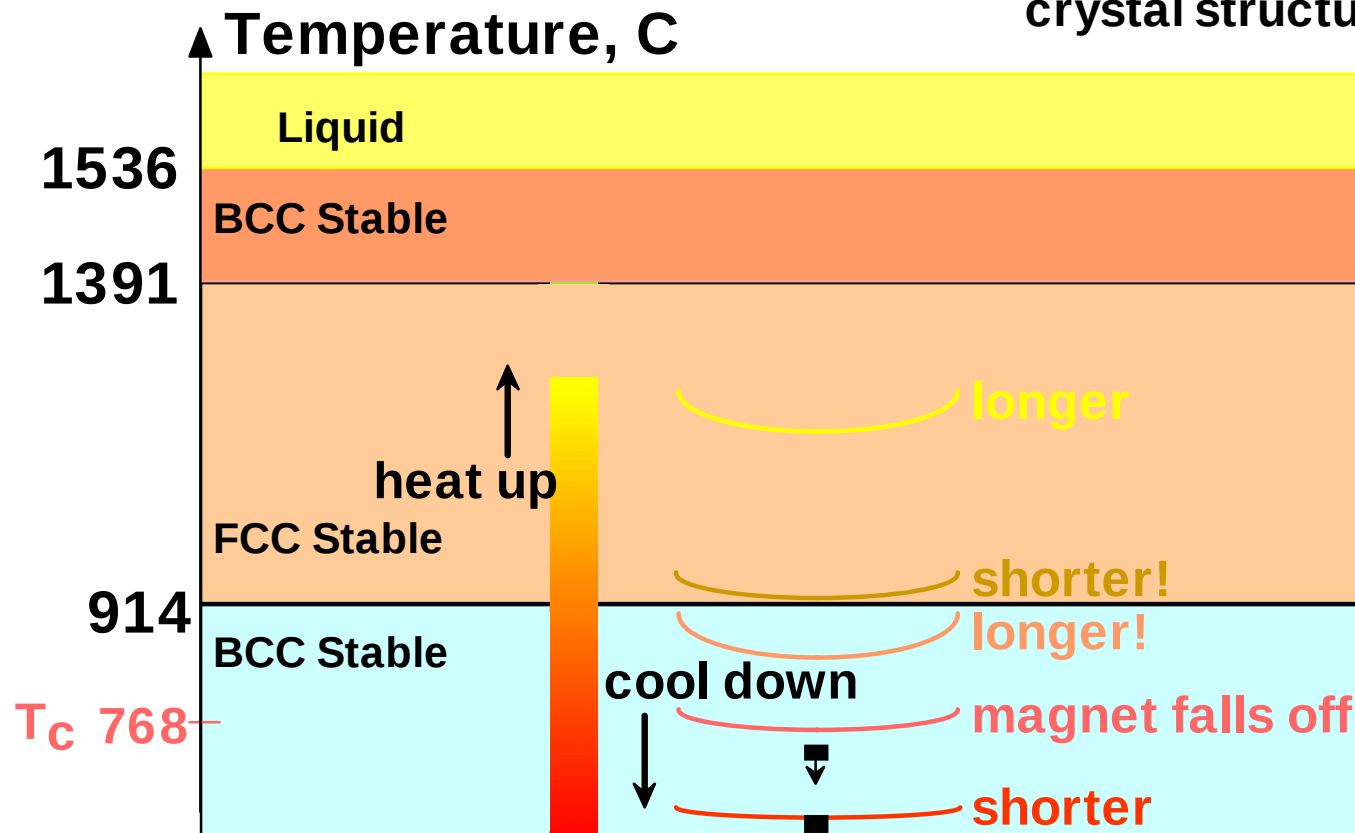


Iron atoms arranged on a copper (111) surface. These Kanji characters represent the word “atom”.

Photos produced from the work of C.P. Lutz, Zeppenfeld, and D.M. Eigler. Reprinted with permission from International Business Machines Corporation, copyright 1995.

DEMO: HEATING AND COOLING OF AN IRON WIRE

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



SUMMARY

- Atoms may assemble into **crystalline** or **amorphous** structures.
- 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 generally non-directional (i.e., they are **isotropic**) in polycrystals with randomly oriented grains.