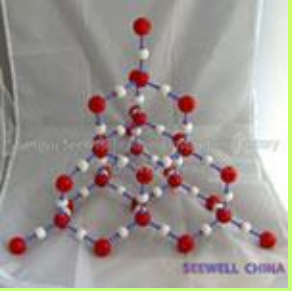
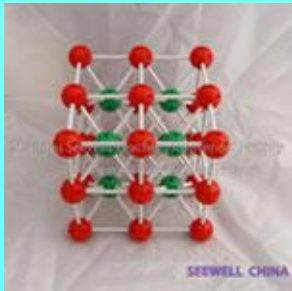


CHAPTER 3: CRYSTAL STRUCTURES & PROPERTIES



Metallic Crystals

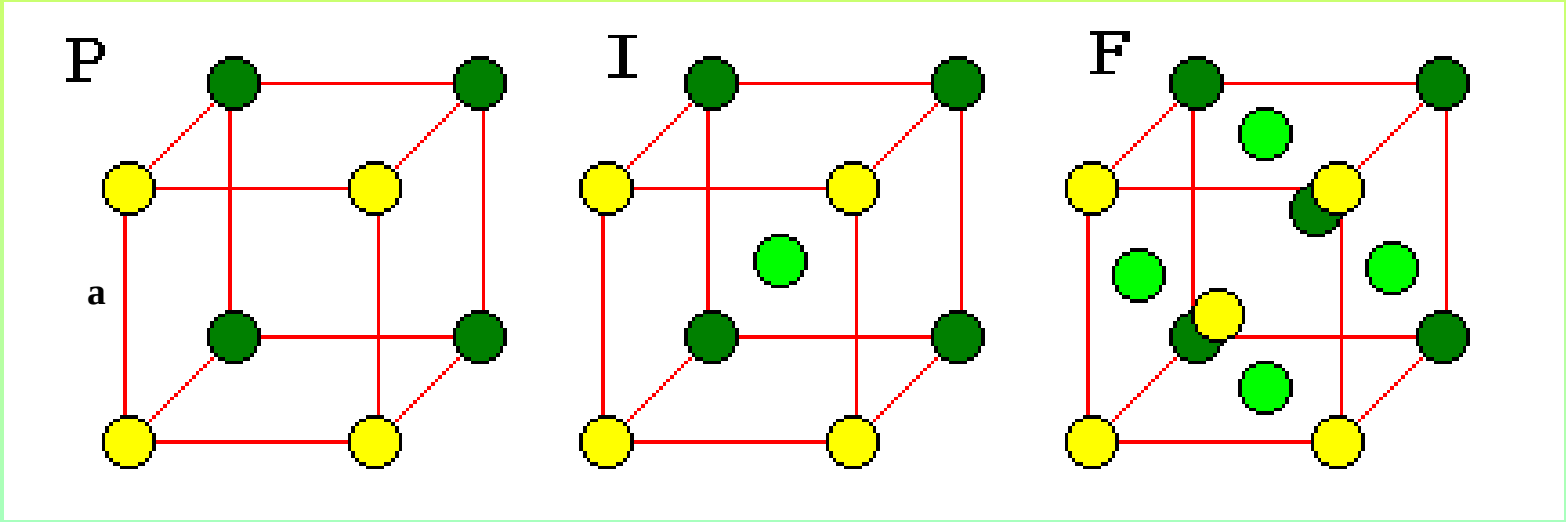
- tend to be densely packed.
- have several reasons for dense packing:

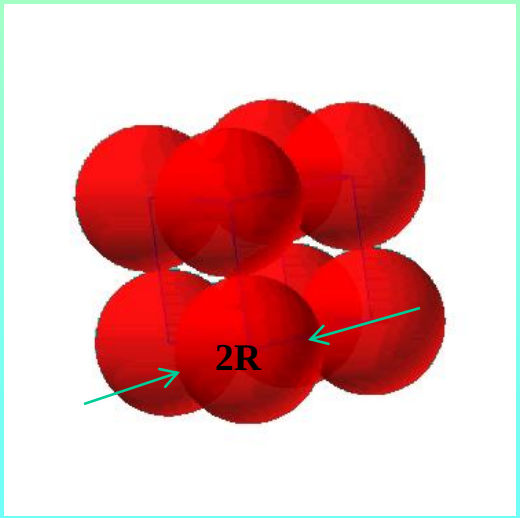
  -Typically, only one element is present, so all atomic radii are the same.
  -Metallic bonding is not directional.
  -Nearest neighbor distances tend to be small in order to lower bond energy.

- have the simplest crystal structures.

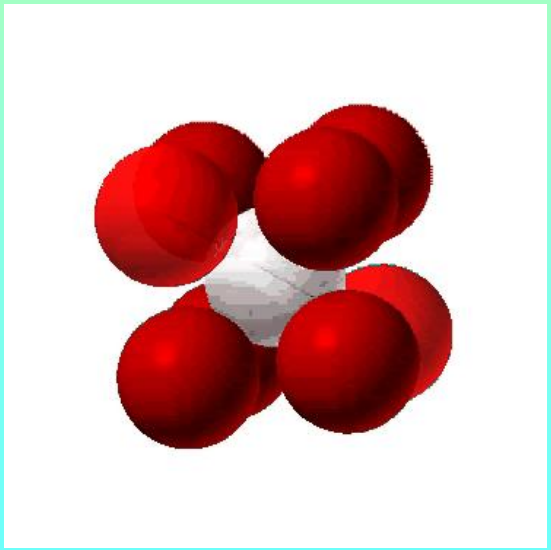
We will look at three such structures...

Cubic Unit Cells

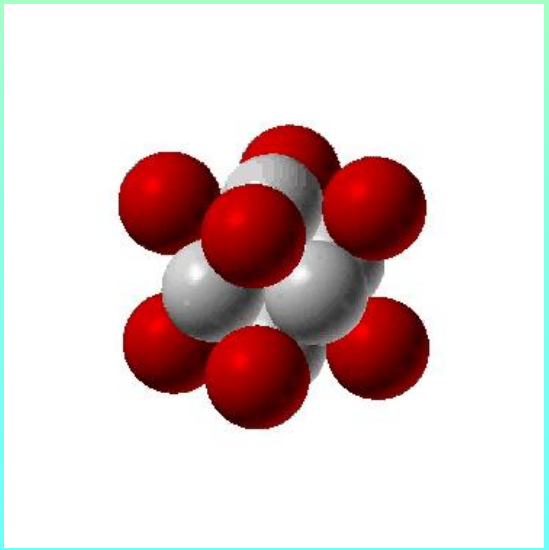




SIMPLE CUBIC STRUCTURE (SC)



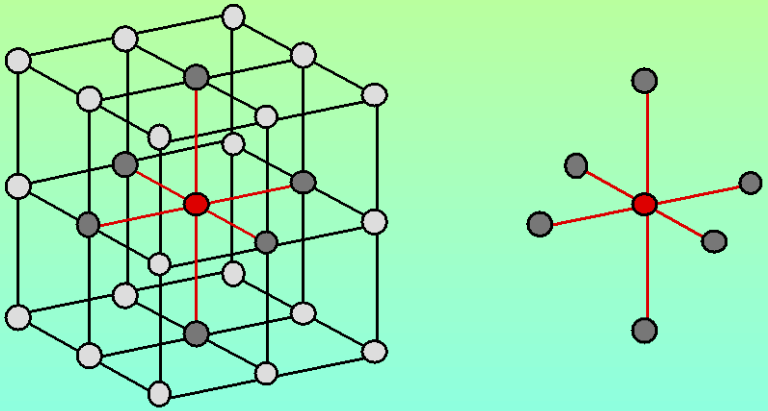
BODY CENTERED CUBIC STRUCTURE (BCC)



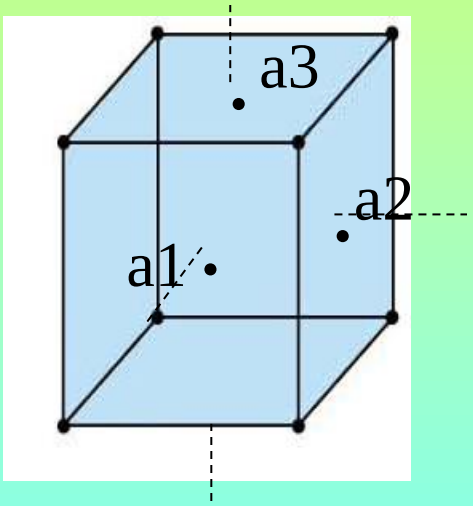
FACE CENTERED CUBIC STRUCTURE (FCC)

Simple Cubic (SC) Structure

- **Coordination number** is the number of nearest neighbors
- **Linear density** (LD) is the number of atoms per unit length along a specific crystallographic direction



Coordination number = 6



LD_{110} = 1 atoms/$2\sqrt{2}$ R

LD_{100}= 1 atoms/2R

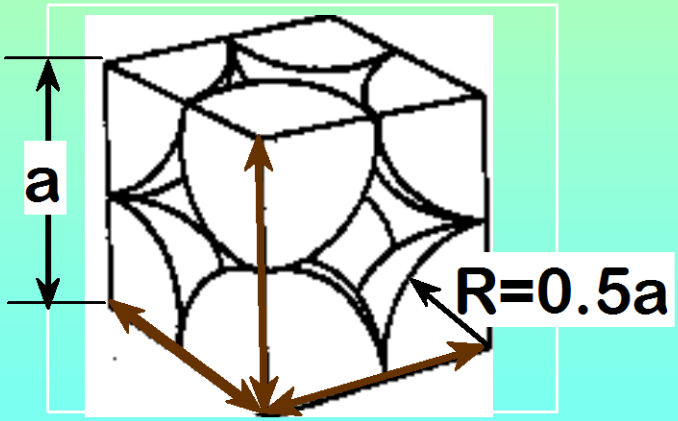
- **Rare due to poor packing (only Po [84] has this structure)**
- **Close-packed directions are cube edges.**

Atomic Packing Factor (APF)

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

*assume hard spheres

- APF for a simple cubic structure = 0.52



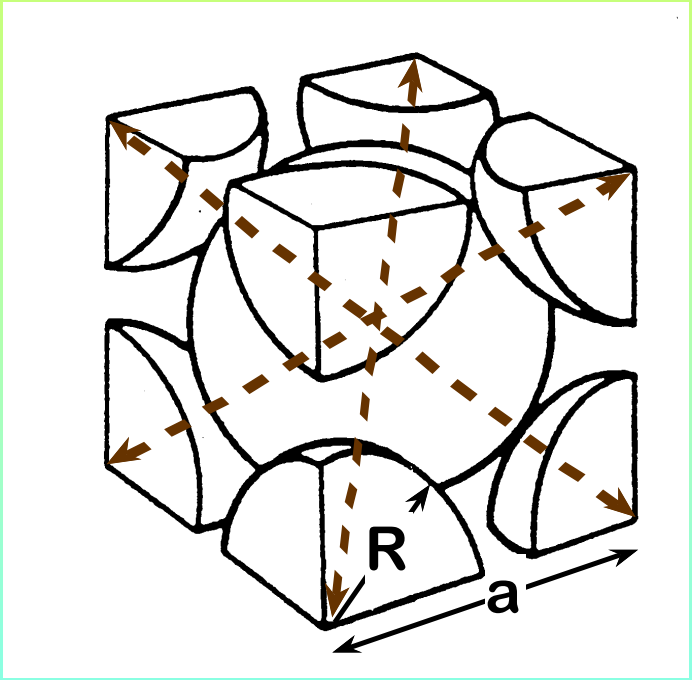
close-packed directions

contains 8 x 1/8 =

1 atom/unit cell

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

Body Centered Cubic (BCC) Structure



- **Coordination number** = 8
- **Close packed directions** are cube diagonals:

LD_{110}= 1 atom/(4R√(2/3))=1/(2R√8/3)

LD_{001} = 1 atom/(4R/√3))= 1/(2R √4/3)

LD_{111} = 2 atoms/4R = 1/(2R)

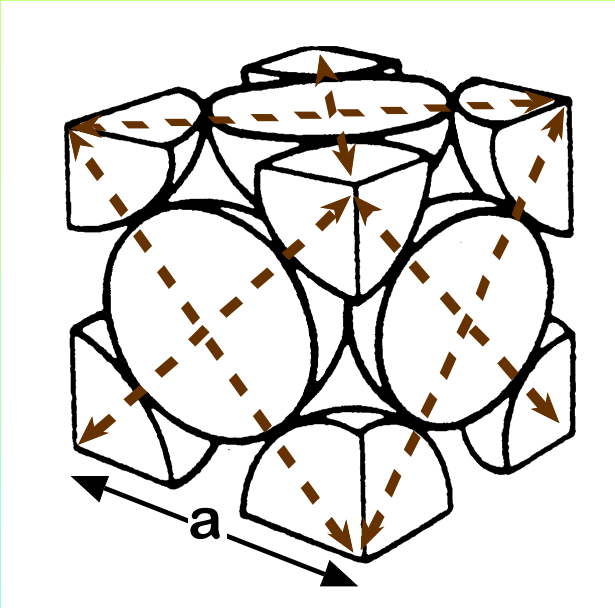
- **Unit cell contains:**

1 + 8 x 1/8 = **2** atoms/unit cell

- **APF** = 0.68:

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

Face-Centered Cubic (FCC) Structure



- **Coordination number** = 12
- **Close packed directions** are face diagonals:

LD_{110}= 2 atom/(4R)= 1/2R

LD_{001} = 1 atom/(2R√2))= 1/(2R √2)

LD_{111} = 1 atoms/4R = 1/(2R √6)

- **Unit cell contains**:

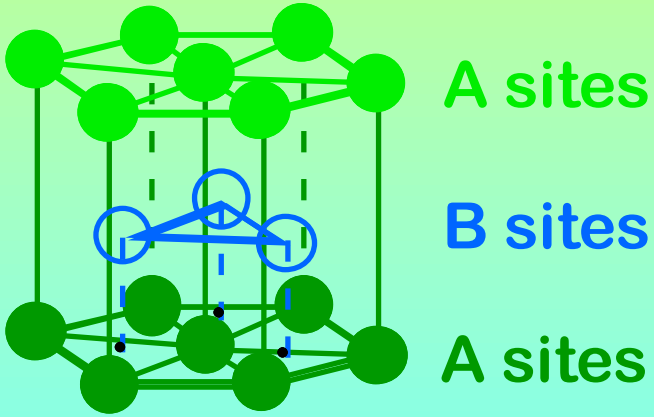
6 x 1/2 + 8 x 1/8 = **4** atoms/unit cell

- **APF = 0.74**

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

Hexagonal Close-Packed (HCP) Structure

- ABAB… Stacking Sequence
- 3D Projection



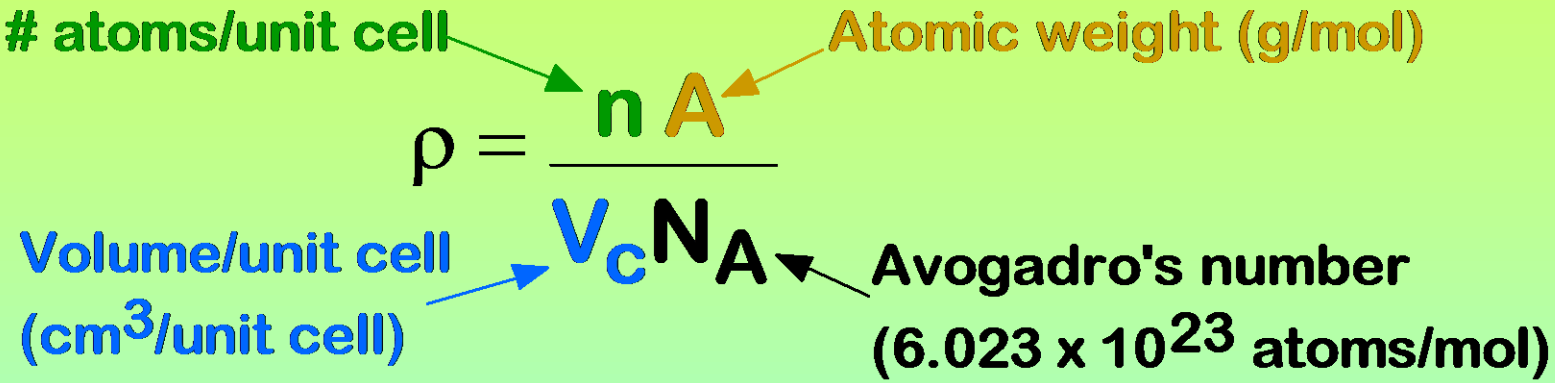
- 2D Projection

- Coordination number = ?
- APF = ?

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	------	-----	------

Theoretical Density, ρ



Example: Copper

- crystal structure **FCC**
- # atoms/unit cell **= 4**
- atomic weight = **63.55 g/mol**
- atomic radius R = **0.128 nm**
- for FCC **a = 2R√2**; $V_c = a^3$; $V_c = 4.75\ 10^{-23}\ cm^3$

Result: theoretical $\rho_{Cu} = 8.89\ g/cm^3$
Compare to actual: $\rho_{Cu} = 8.94\ g/cm^3$

Densities of Materials Classes

$\rho_{metal} > \rho_{ceramics} > \rho_{polymers}$

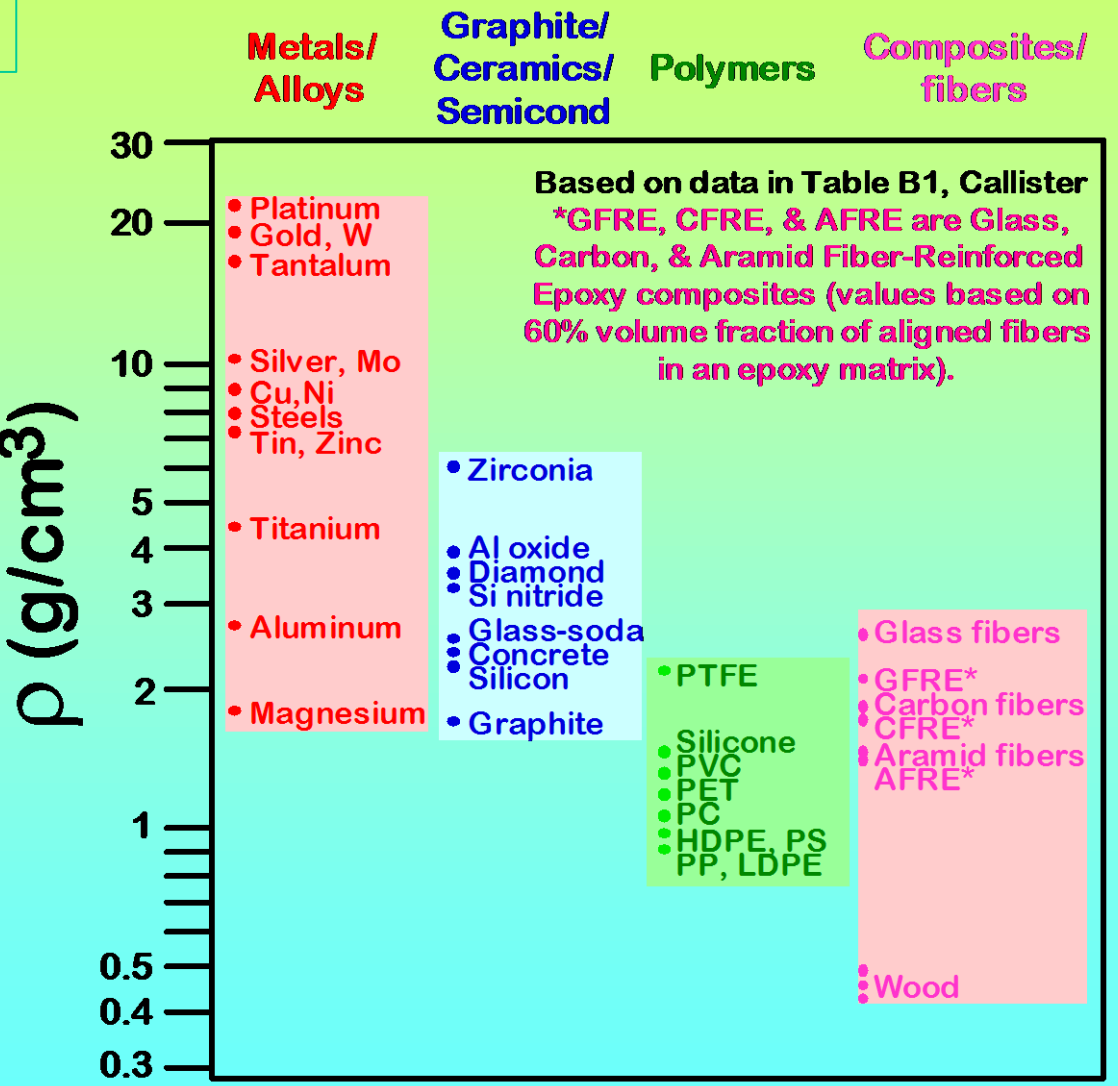
Why?

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



CRYSTALS AS BUILDING BLOCKS

- ***Some*** **engineering applications require single crystals:**

diamond single crystals for abrasives

turbine blades

- **Crystal properties reveal features of atomic structure.**

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

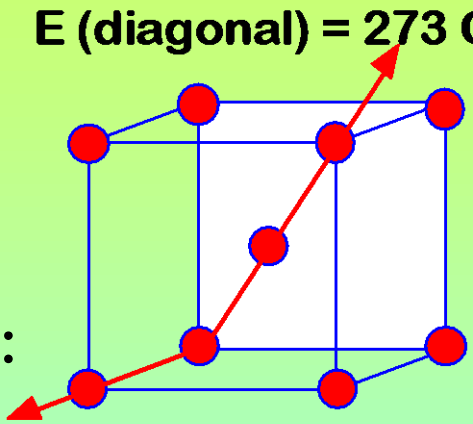
POLYCRYSTALS

- ***Most*** **engineering materials are polycrystals.**

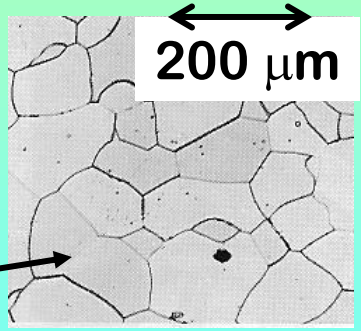
- **Nb-Hf-W plate with an electron beam weld.**
- **Each "grain" is a single crystal.**
- **If crystals are randomly oriented,**
  overall component properties are not directional.
- **Crystal sizes typ. range from 1 nm to 2 cm**
  (i.e., from a few to millions of atomic layers).

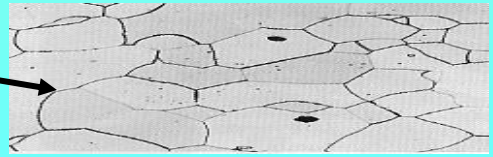
SINGLE VS POLYCRYSTALS

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



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





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.