Properties of Materials

Theme: Structure

Lecture 1: Atoms and Bonding

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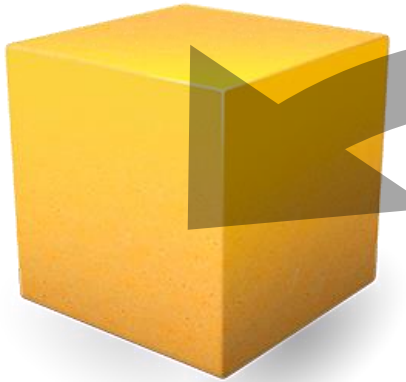
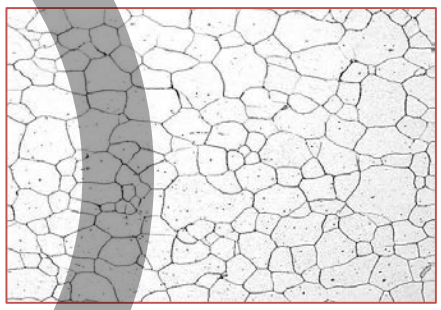
Scale

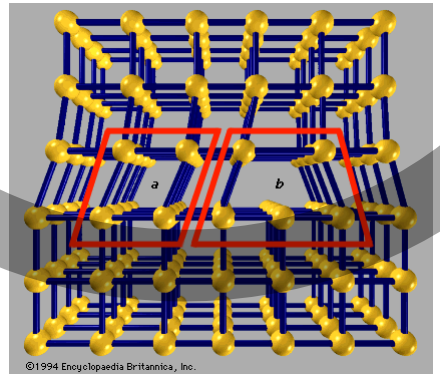
Continuum Mechanics
Perfect material with uniform properties



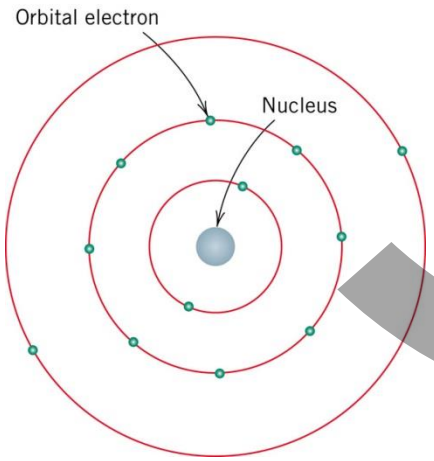
Macroscopic
Distinct regions with varying properties



Grain Structure
Real materials composed of many crystals stuck together

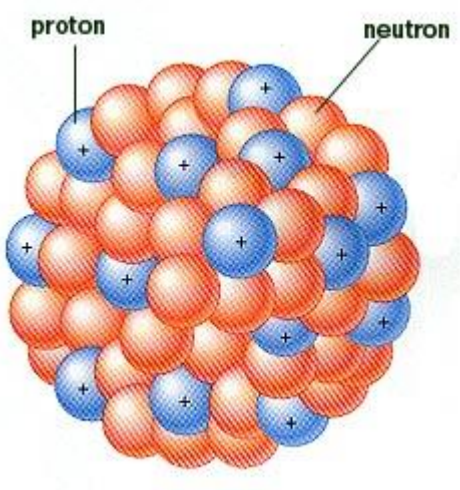


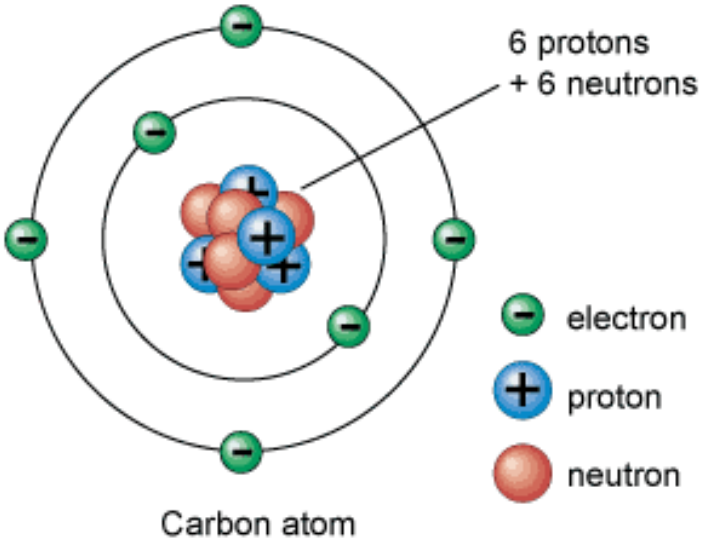
Crystal Structure
Arrangement of atoms (or lack of it)



Atoms
Intrinsic properties and bonding

Atomic Model



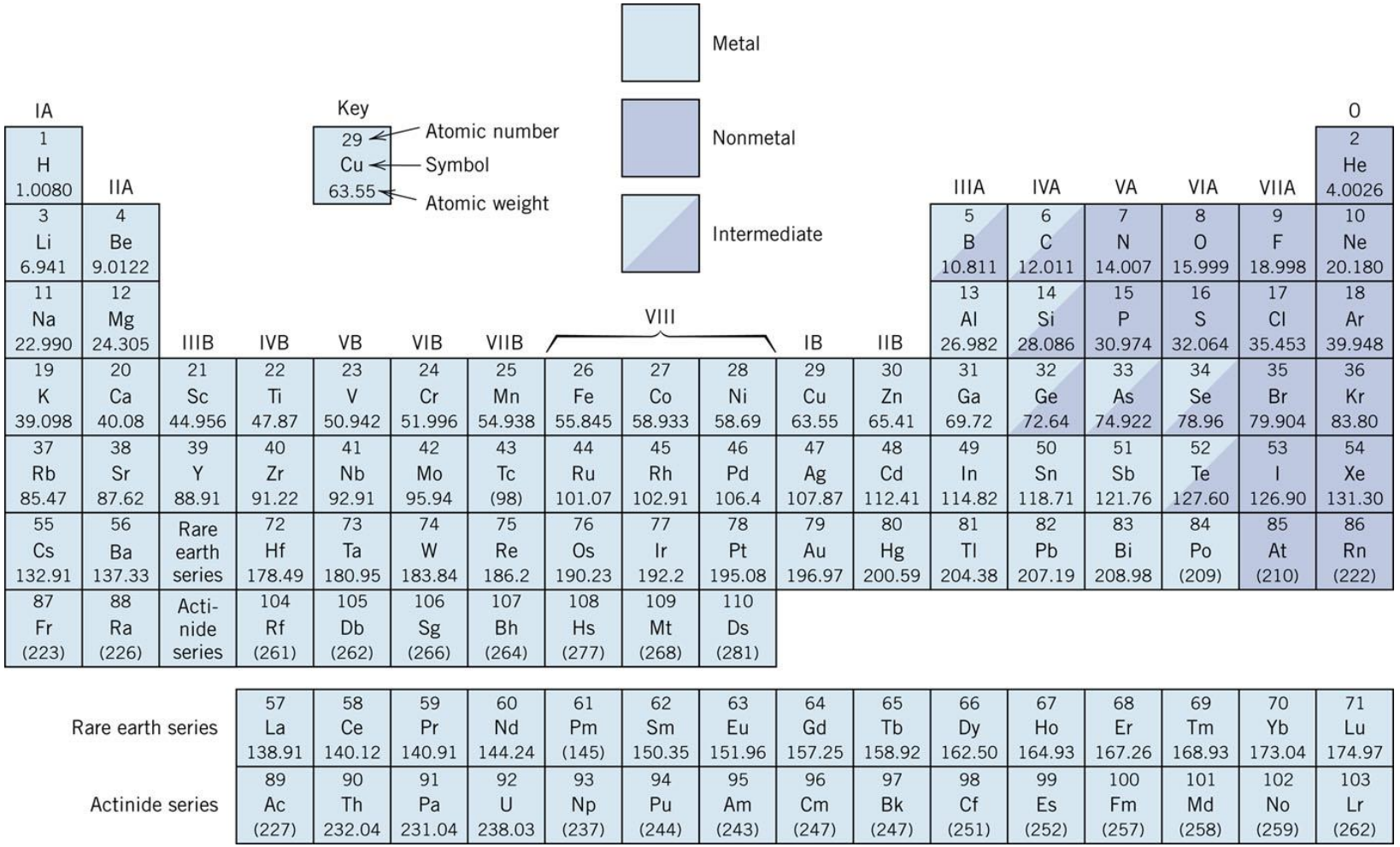


- Nucleus
  - Positive protons
  - Uncharged neutrons

"Protons give an atom its identity, electrons its personality"

- Electrons
  - Negatively charged
  - Same number as protons
  - Outermost layer govern interactions with other atoms (valence)

Bonding

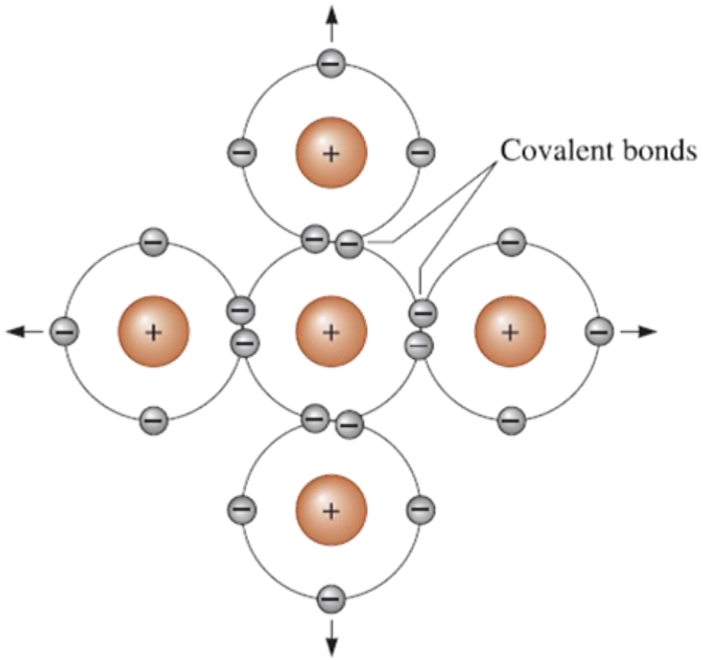


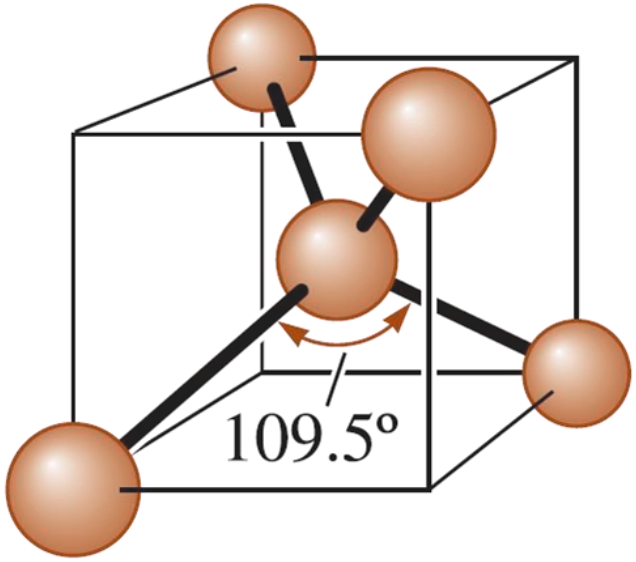
IA							VIII					IIIA	IVA	VA	VIA	VIIA	0
1 H 1.0080	IIA																2 He 4.0026
3 Li 6.941	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305	IIIB	IVB	VB	VIB	VIIB				IB	IIB	13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.87	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.33	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.2	76 Os 190.23	77 Ir 192.2	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.19	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	Acti-nide series	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (281)								

Rare earth series	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
Actinide series	89 Ac (227)	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

Covalent Bonding

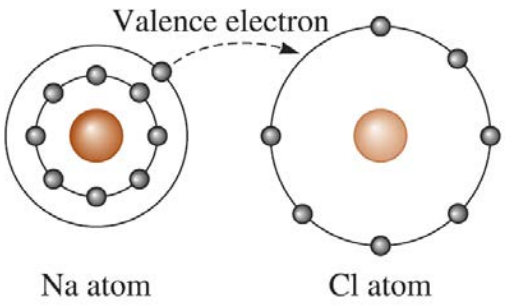
- ***Between 2 non-metals***
- ***Share*** valence electrons
  - Strong, directional bond between two atoms
- Breaking bond means fracturing material
  - brittle
- Electrons bound up
  - Poor electrical conductivity

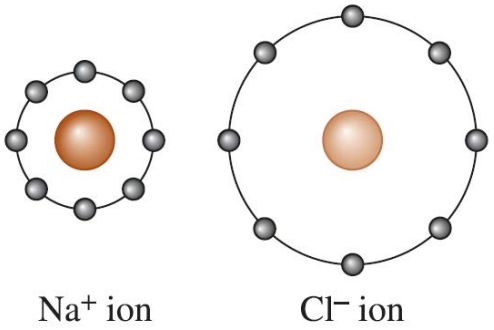


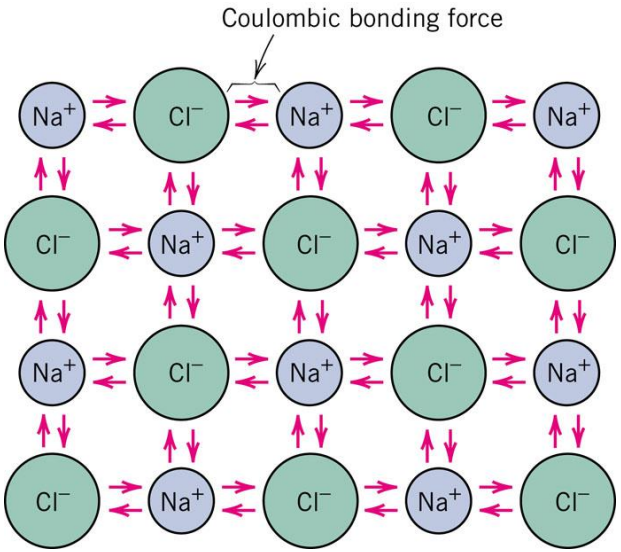


Ionic Bonding

- ***Between metal + non-metal***
- ***Exchange*** valence electrons
  - Unbalanced charges
  - Ordered structure with mutual attraction between opposite ions
  - Non directional bonds
- Ions immobile charge carriers
  - Poor electrical conductivity

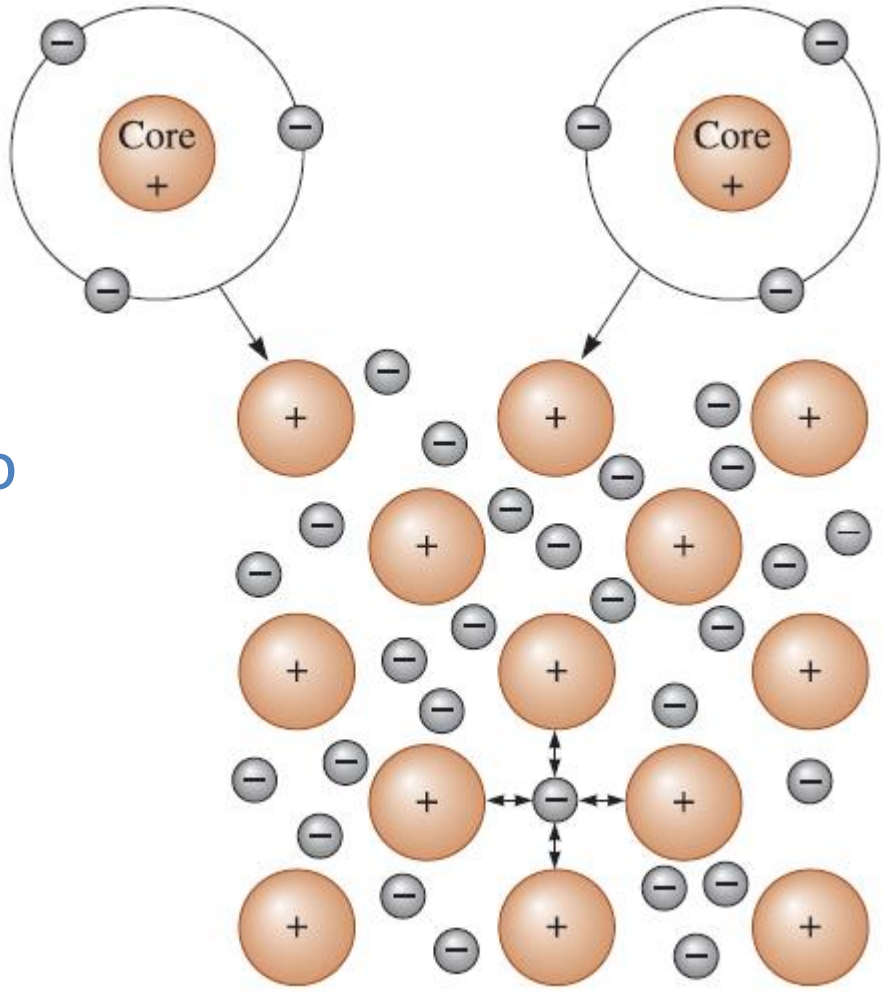




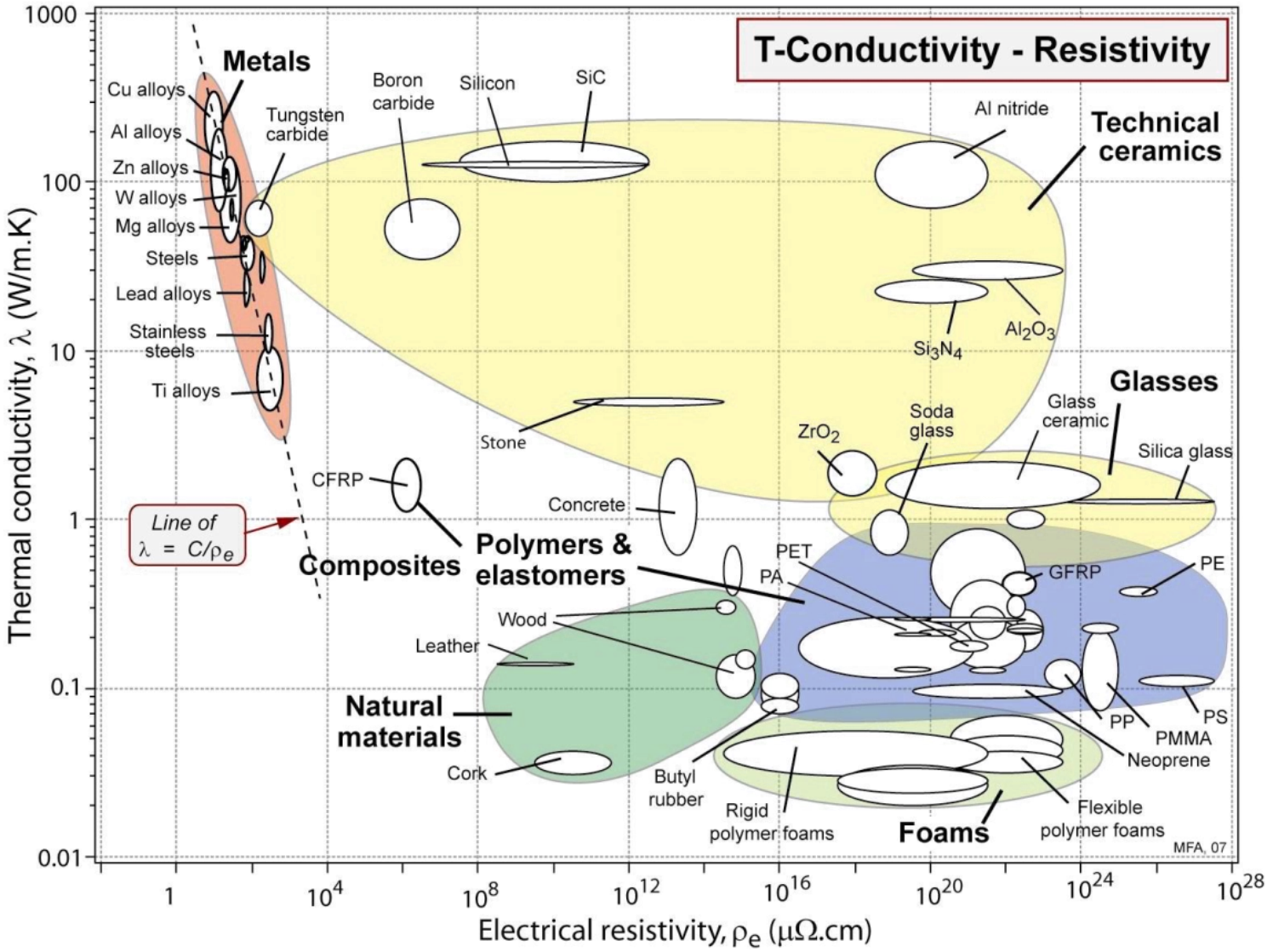


Metallic Bonding

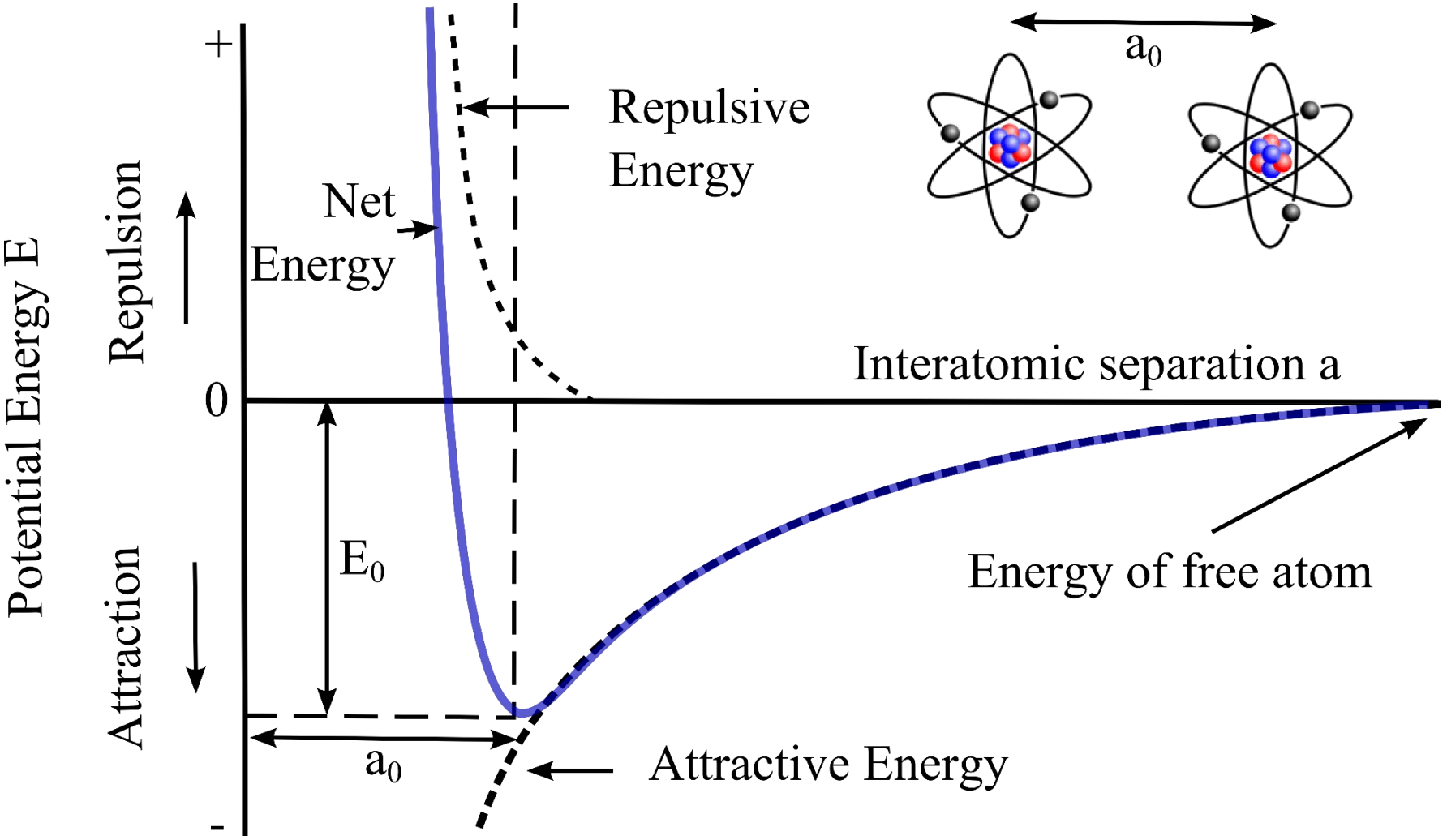
- Relatively electropositive atoms give up valance electrons
  - Form a sea of non-localised electrons
  - Positive ions attracted to negative sea
- Electrons are charge/heat carriers
  - Excellent conductivity



Conductivity



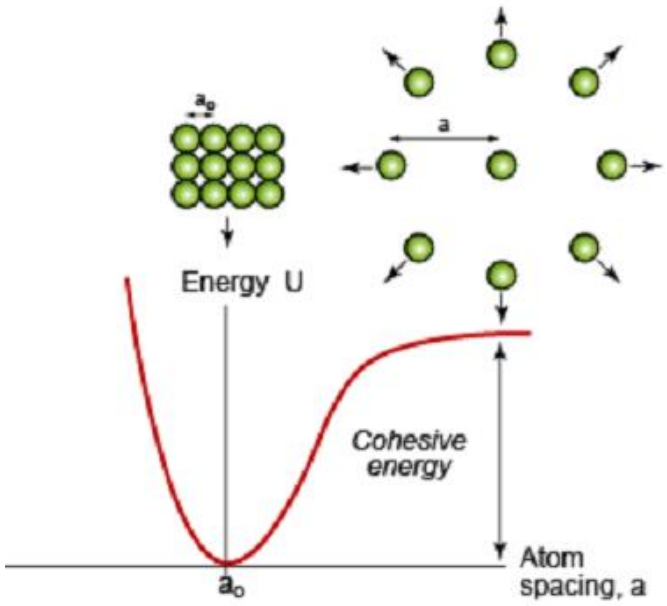
Bond stiffness

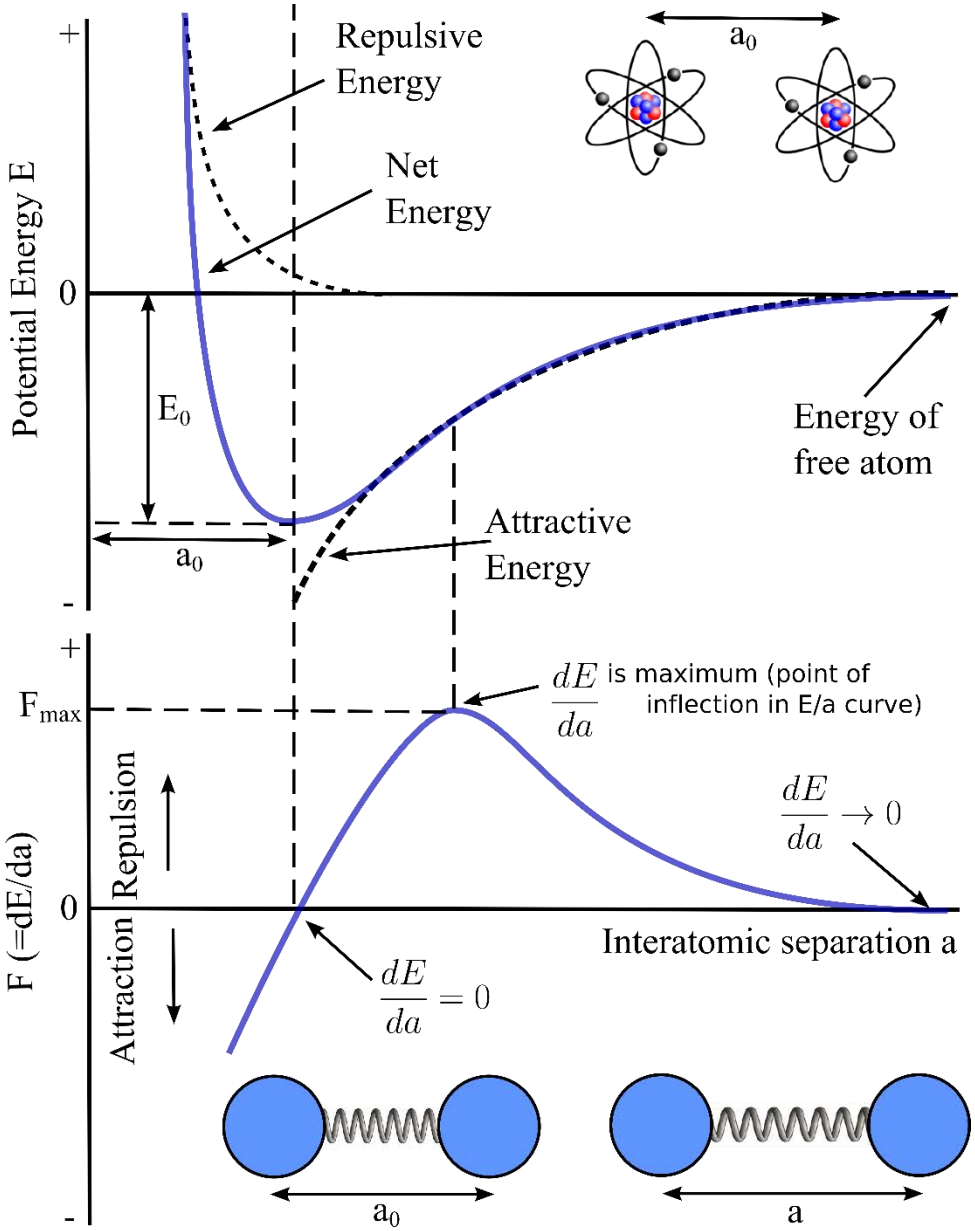


Bond stiffness

Cohesive energy – heat energy needed to turn solid to gas

More difficult if bonds are stronger (deeper potential well)





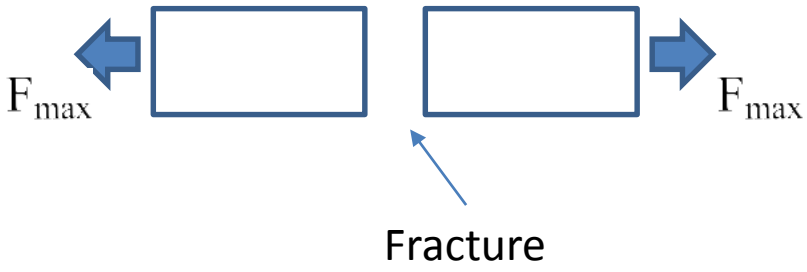
Bond stiffness

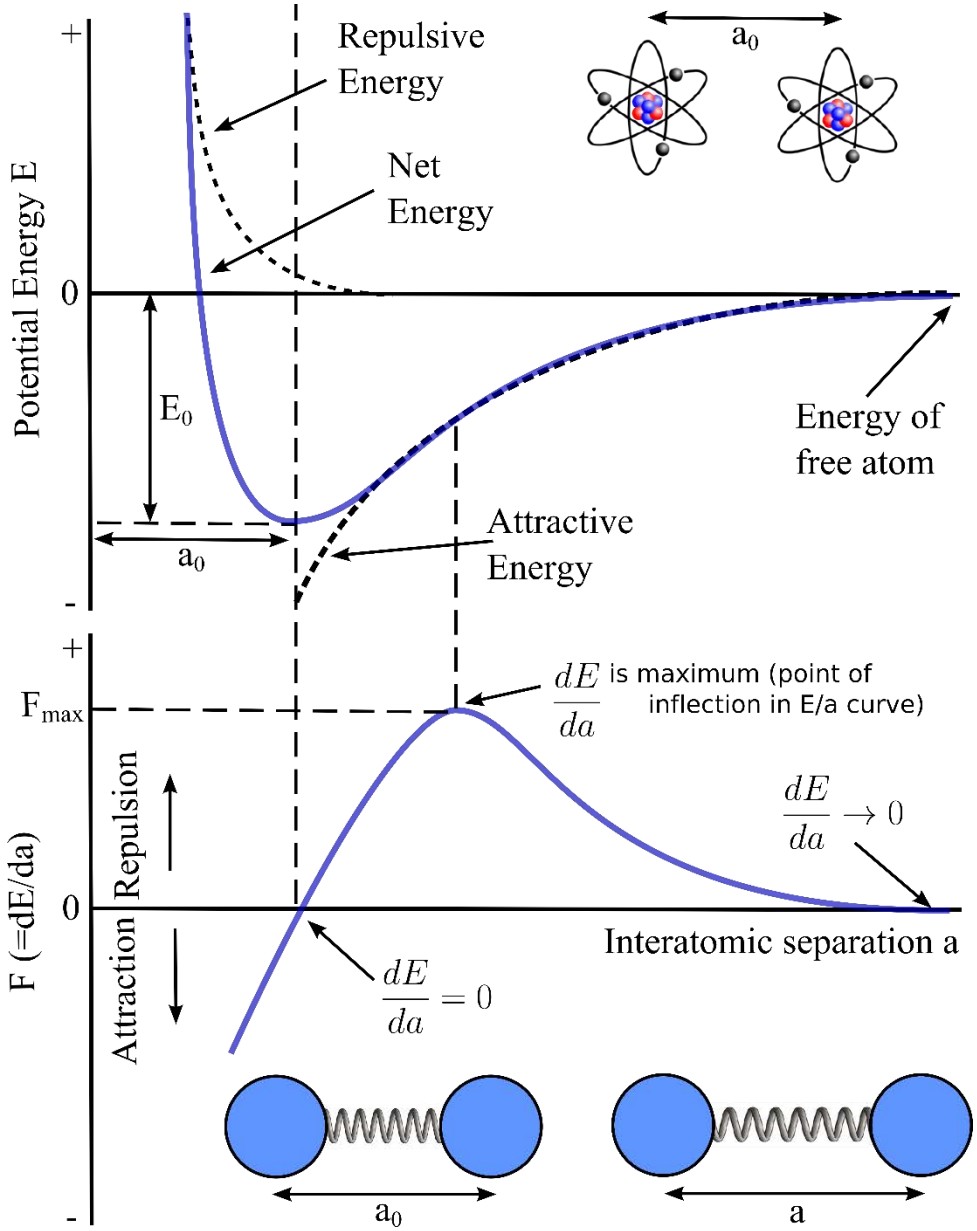
Force to displace atoms

$$F = \frac{dE}{da}$$

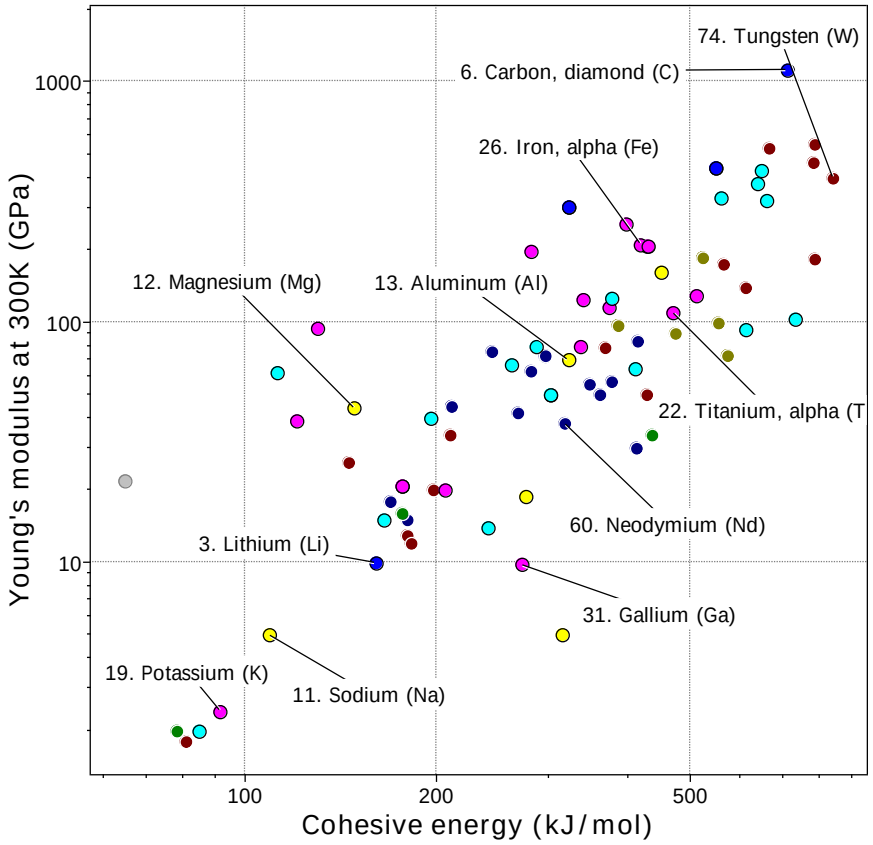
Stiffness of 'spring'

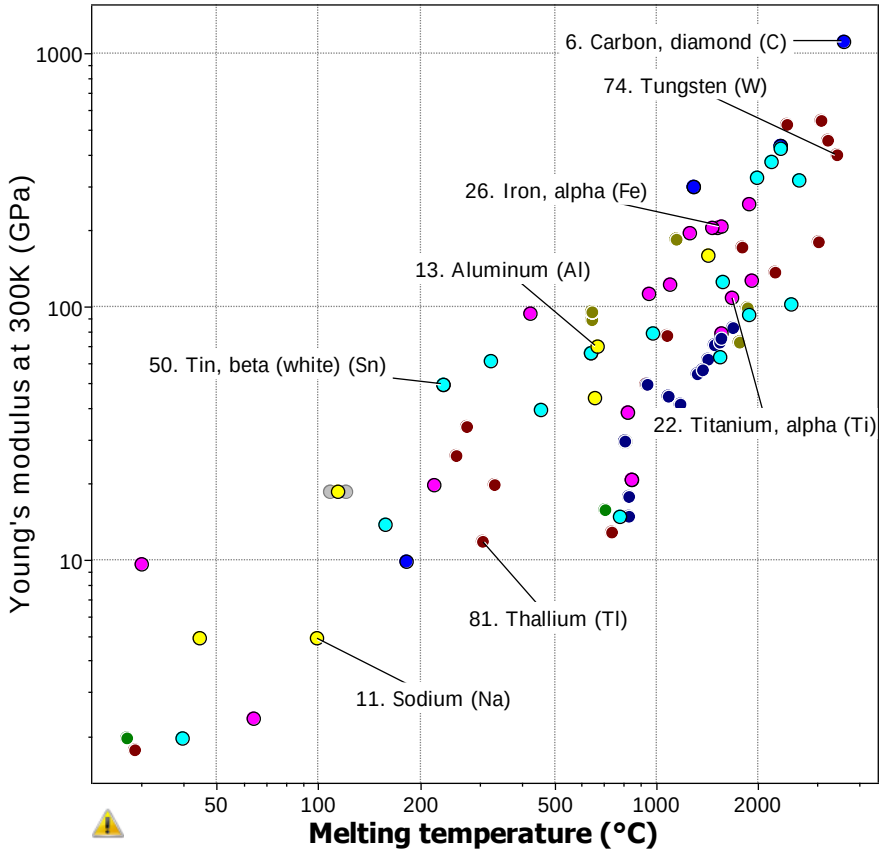
$$S = \frac{dF}{da} = \frac{d^2E}{da^2}$$



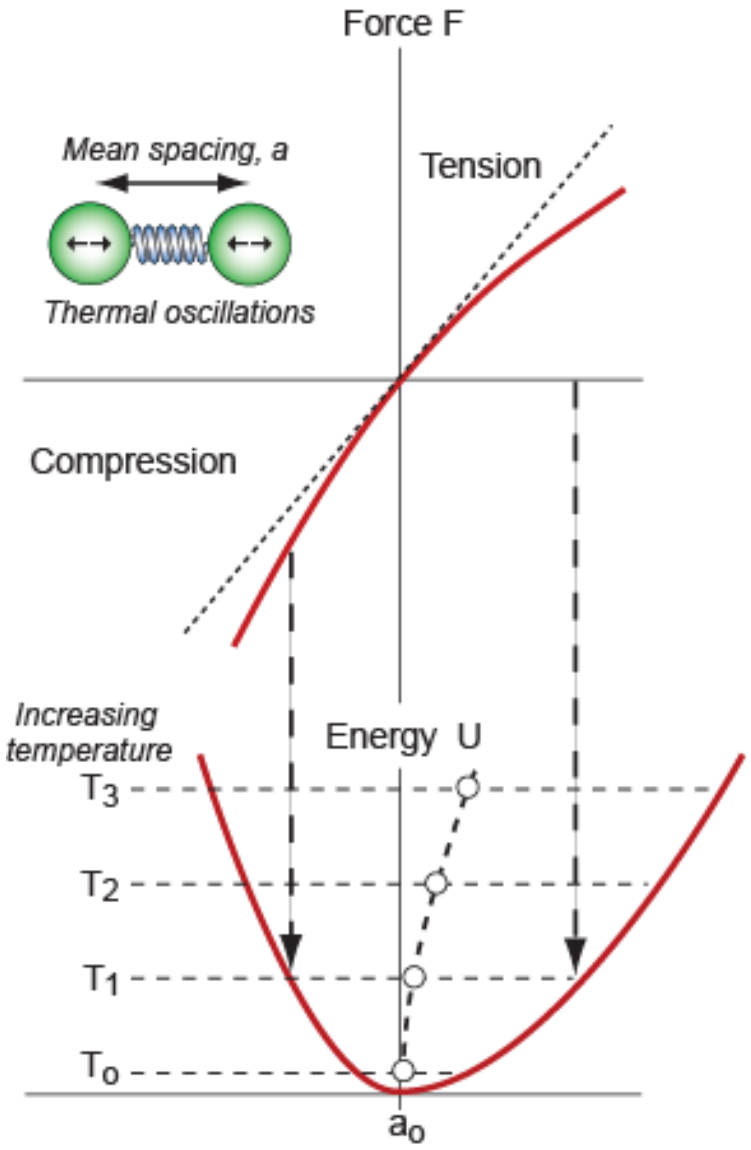


Bond stiffness



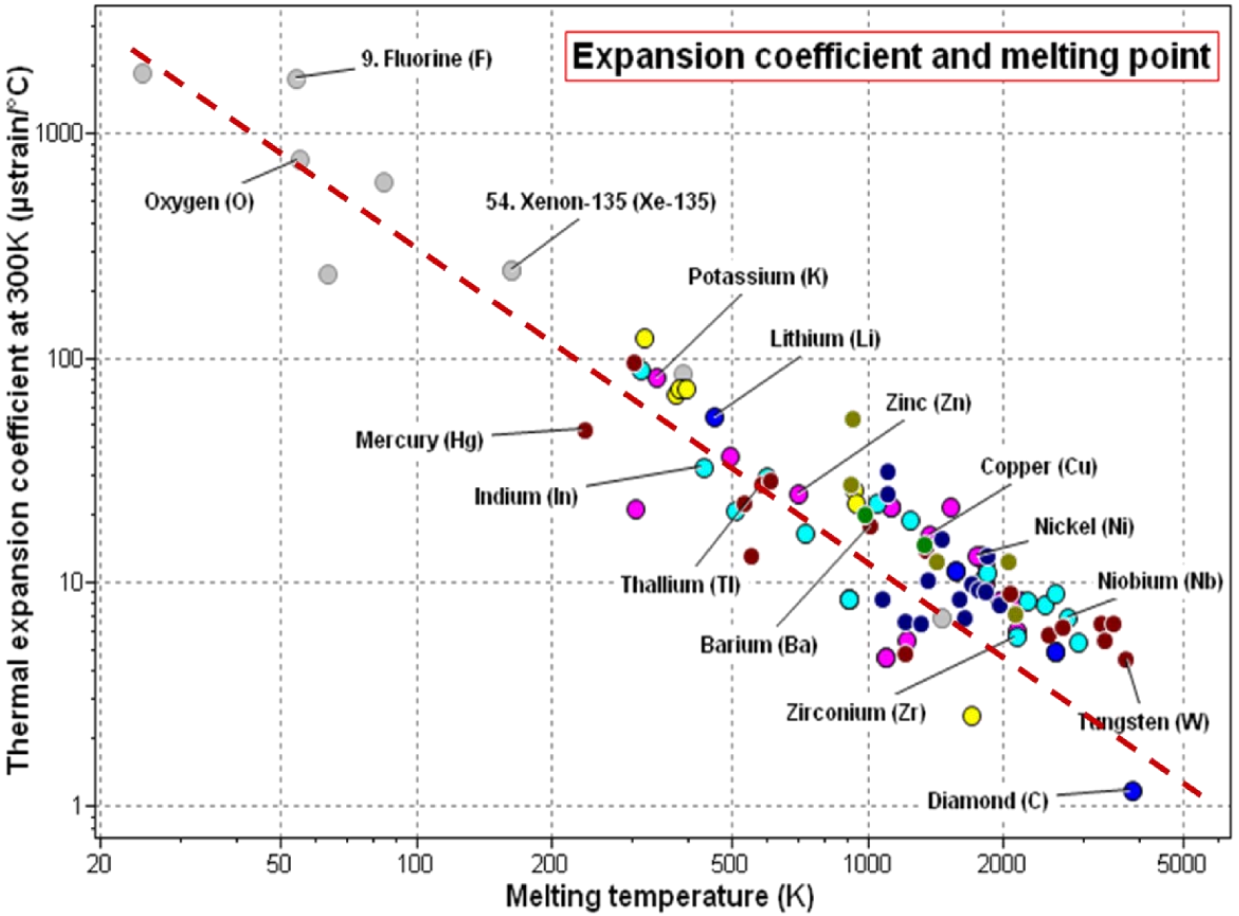


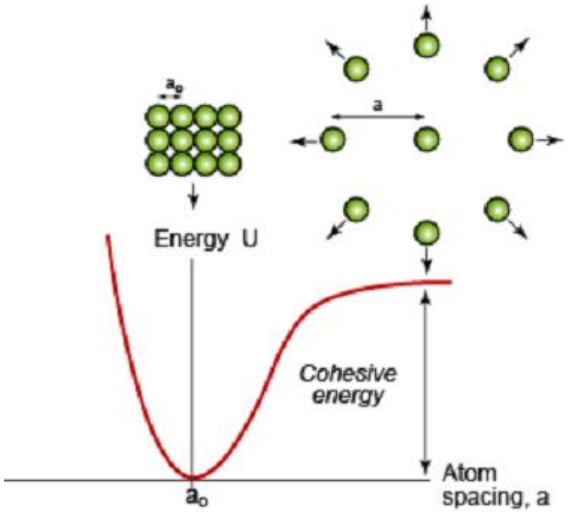
Thermal Expansion



- Thermal energy = more atomic vibration
  - Atoms still at absolute zero
- Potential well not really symmetric
  - A bit harder to compress than extend
  - Vibrating more means moving up-down potential well
  - Shift in origin = expansion

Cohesive energy and properties





Cohesive energy = thermal energy needed to break all bonds

$$\alpha = \frac{1.6 \times 10^{-3}}{E}$$

Higher melting point

=

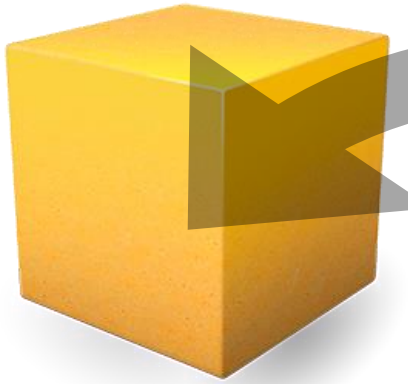
lower thermal expansion

Summary

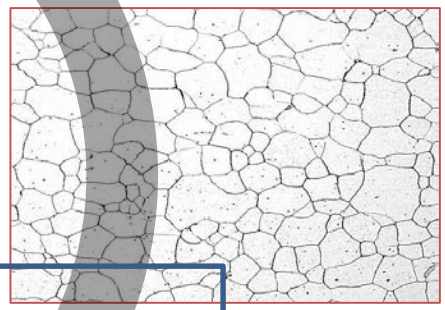
- Aim of these lectures is to introduce the science of material behaviour
  - Atomic bonding alters many properties
  - Metals vs Non-metals (continues later)
  - Strong atomic bonds correlate with melting point, high modulus, low thermal expansion
- Next
  - Examine how the way in which packing in crystals is described

Scale

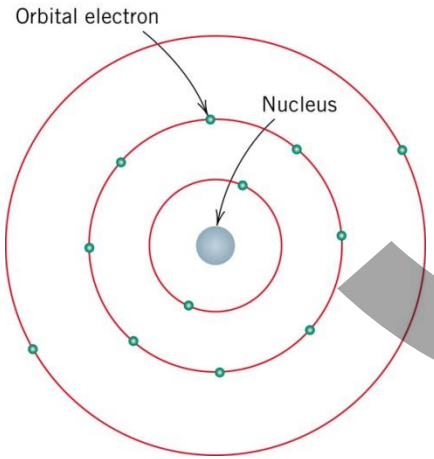
Continuum Mechanics
Perfect material with uniform properties



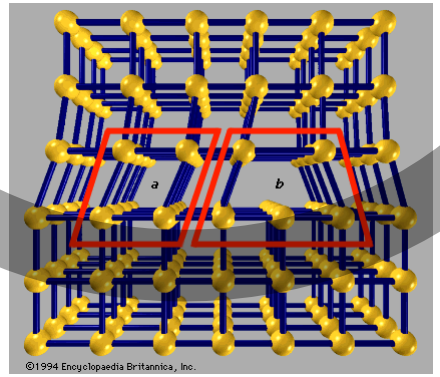
Macroscopic
Distinct regions with varying properties



Grain Structure
Real materials composed of many crystals stuck together



Atoms
Intrinsic properties and bonding



Crystal Structure
Arrangement of atoms (or lack of it)

Properties of Materials

Theme: Structure

Lecture 2: Crystals

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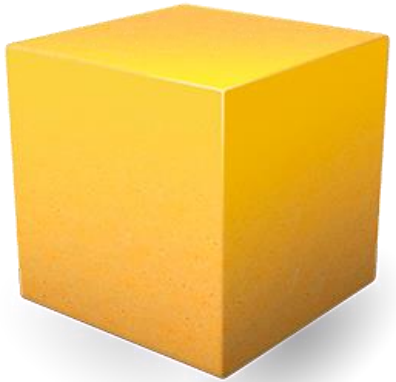

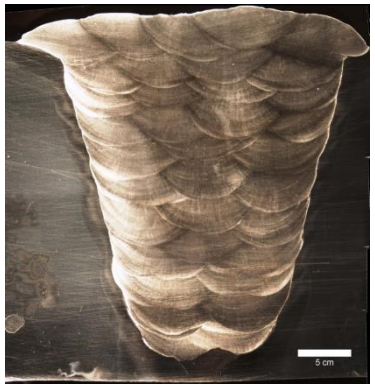

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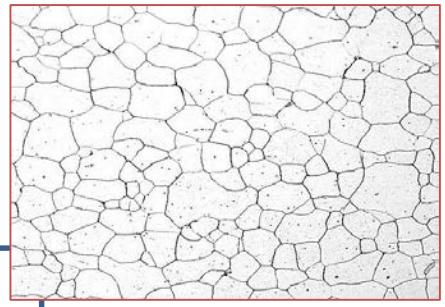

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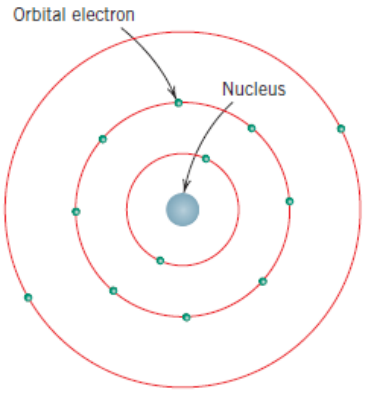

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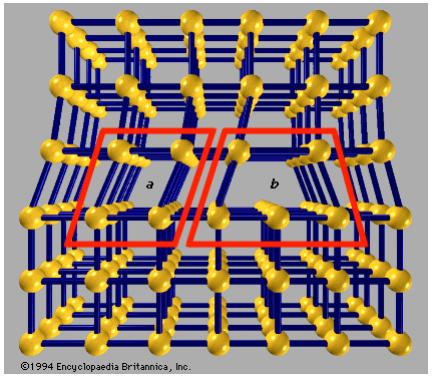
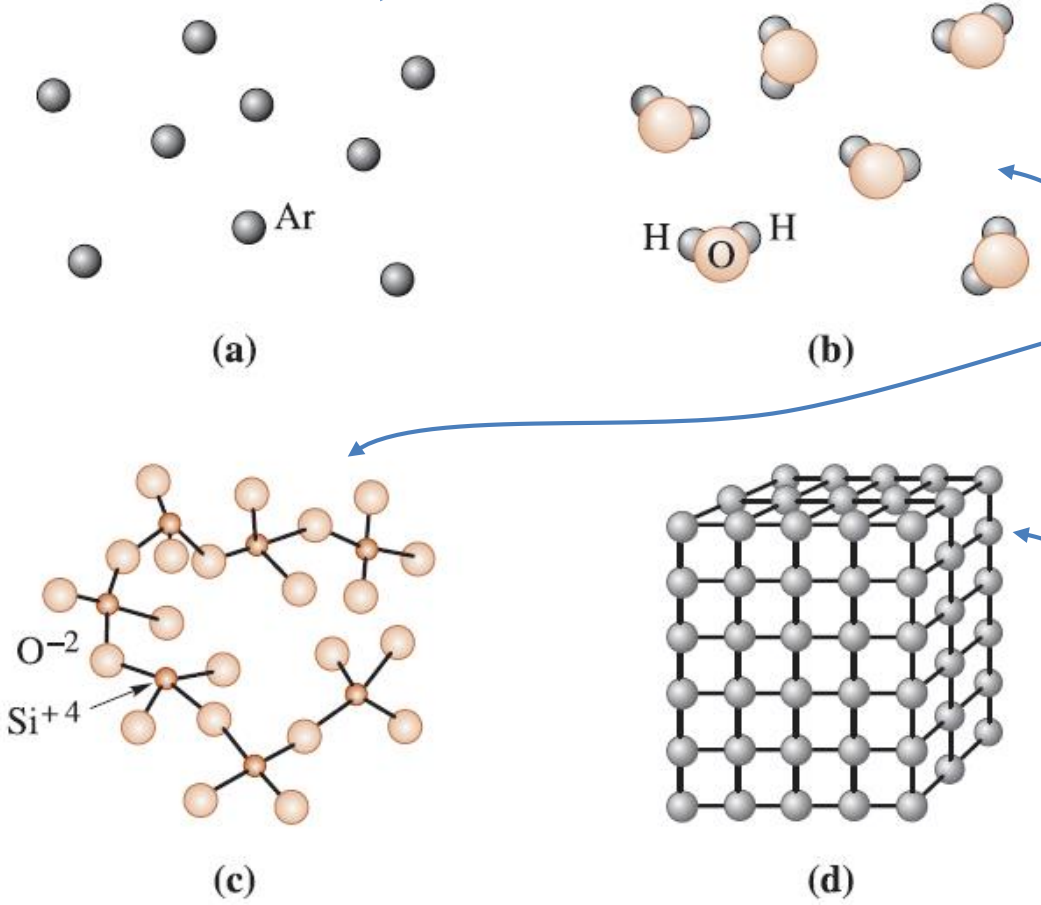
Intrinsic properties and bonding



Crystal Structure
Arrangement of atoms

Order



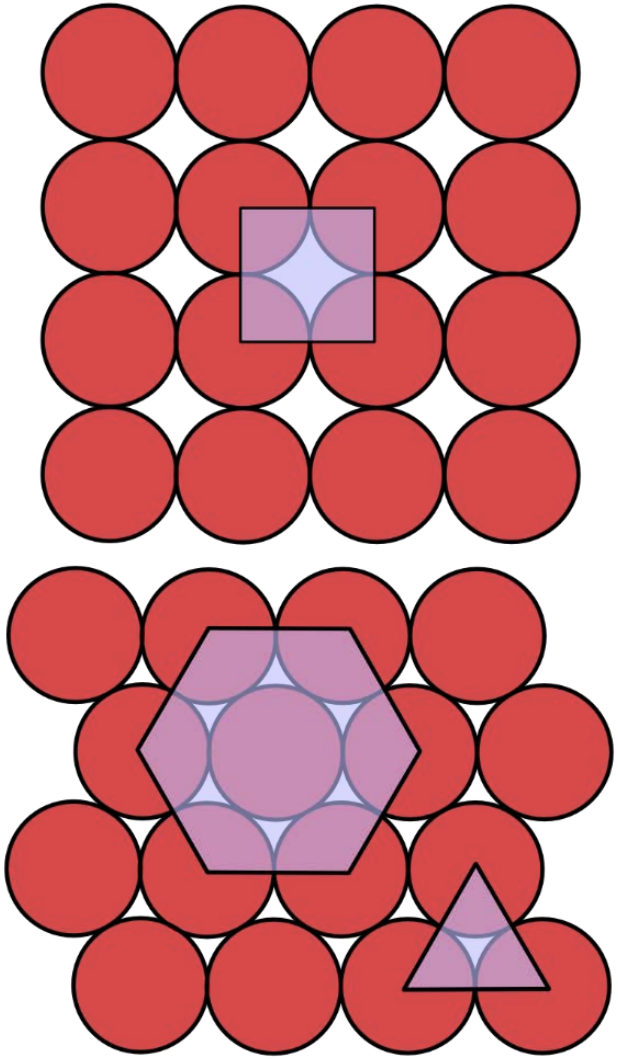
No Order
All atoms are random in space.
e.g. Gases

Short range order
Order extends only to nearest neighbours
e.g. water molecules in steam, amorphous silica (SiO_2)

Long range order
Order extends over many atomic distances in the form of a crystal
e.g. steel, diamond

2D packing

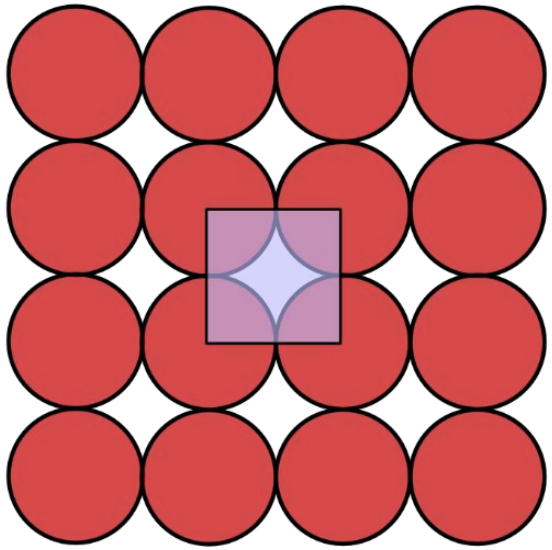
- 3D crystals are made up of 2D crystal *planes*
  - These built up of densely packed atoms
  - Essentially problem of equal circle packing in (infinite) plane
- Square *vs.* hexagonal (triangular) lattice

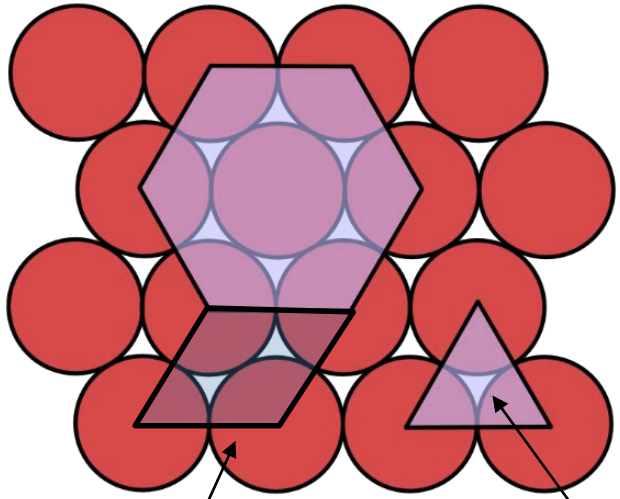


Unit Cell

Smallest block of a crystal that contains all information required to create crystal

Reconstruct crystal by repeated translation of unit cell (no rotation, etc)
e.g. building a wall with bricks





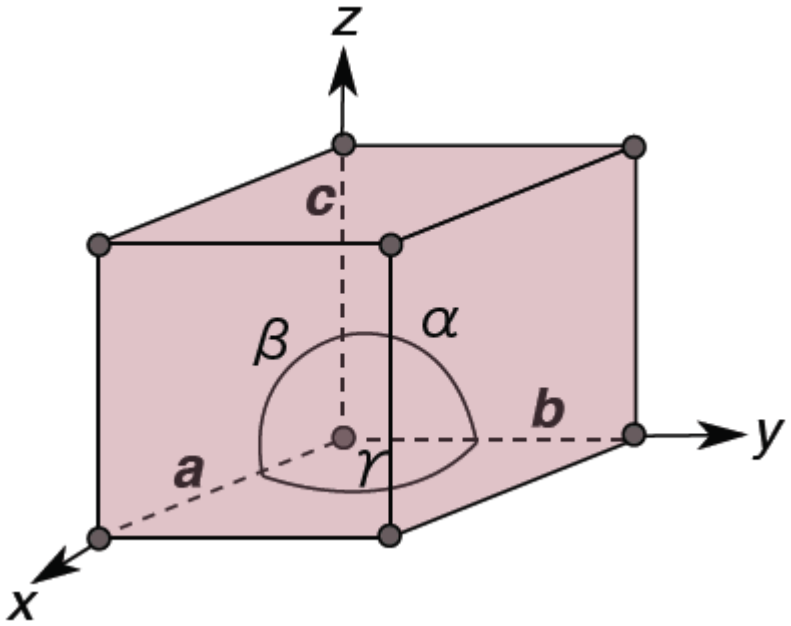
Simplest representation but less intuitive

Can't be unit cell (rotation needed)

Unit Cell

Smallest block of a crystal that contains all information required to create crystal

Reconstruct crystal by repeated translation of unit cell (no rotation, etc)
e.g. building a wall with bricks



Often quite complex but we limit to

Cubic ($a = b = c$,
$\alpha = \beta = \gamma = 90°$)

Hexagonal ($a = b \neq c$,
$\alpha = \beta = 90°, \gamma = 120°$)

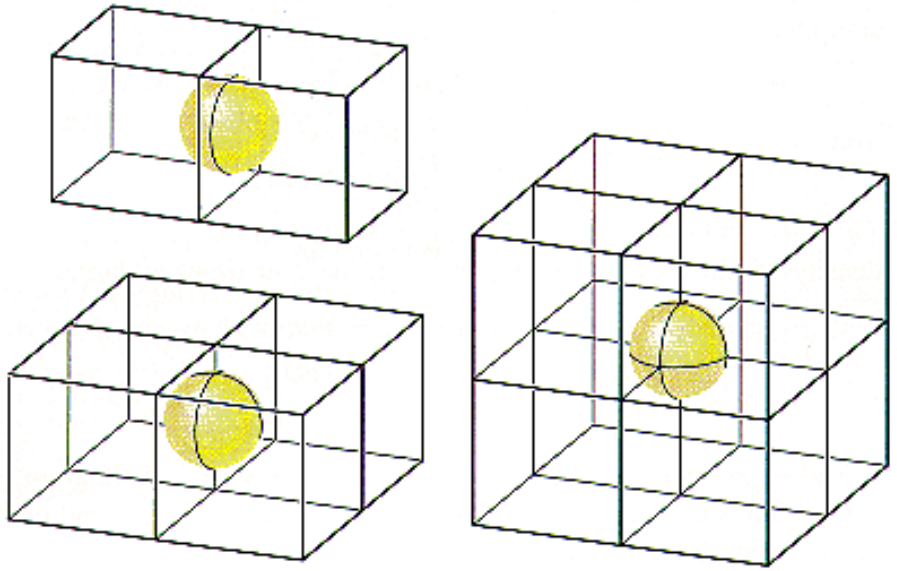
Atomic Packing Factor

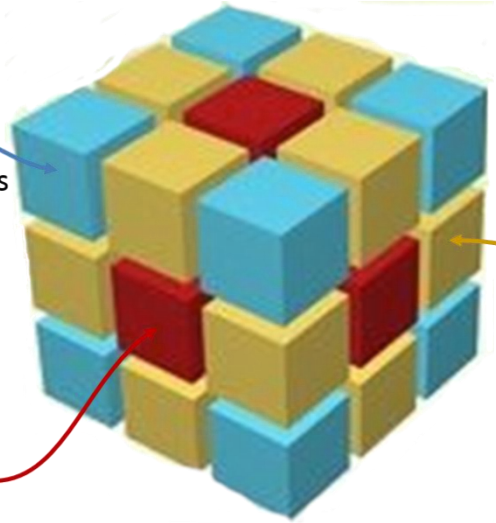
How efficient are crystals?

Volume of spherical atoms (hard-sphere model) *within* unit cell

$$APF = \frac{volume\ of\ atoms\ in\ cell}{volume\ of\ total\ cell}$$

Volume of unit cell (cubic for now)





Dictates the density of crystalline materials

Primitive cubic

$$APF = \frac{volume\ of\ atoms\ in\ cell}{volume\ of\ total\ cell}$$

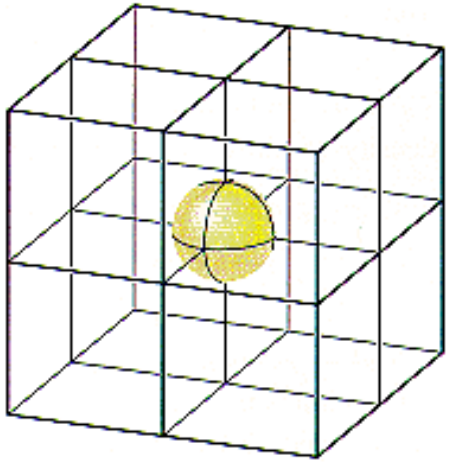
Primitive cubic
Simple layers of square lattice

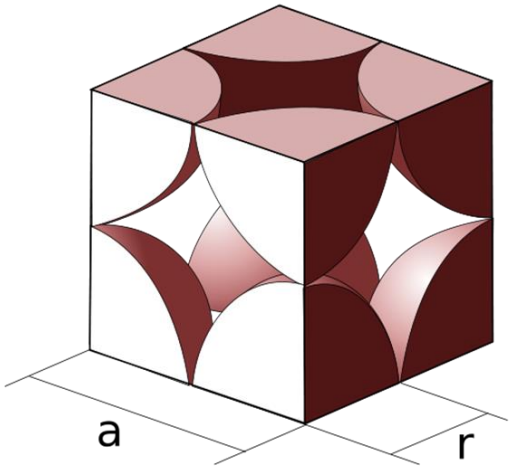
Number of atoms in cell

Atomic radius

$$APF = \frac{n\frac{4}{3}\pi r^3}{V_{cell}}$$

$$APF = \frac{1\times\frac{4}{3}\pi r^3}{(2r)^3} = \frac{\pi}{6}$$

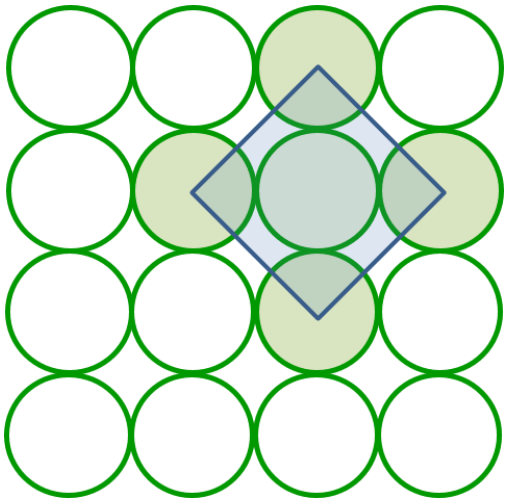


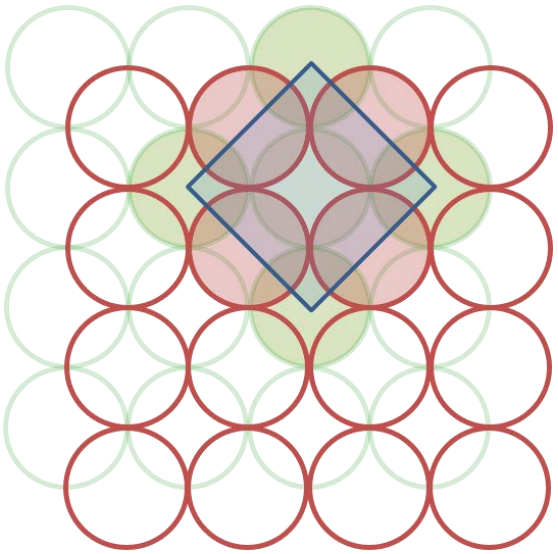


1 atom per cell (8 corners x 1/8 atom per corner)

Close Packing

- Simple stacking of square lattice not efficient
  - Stagger so that atoms sit in dimples of lower layer





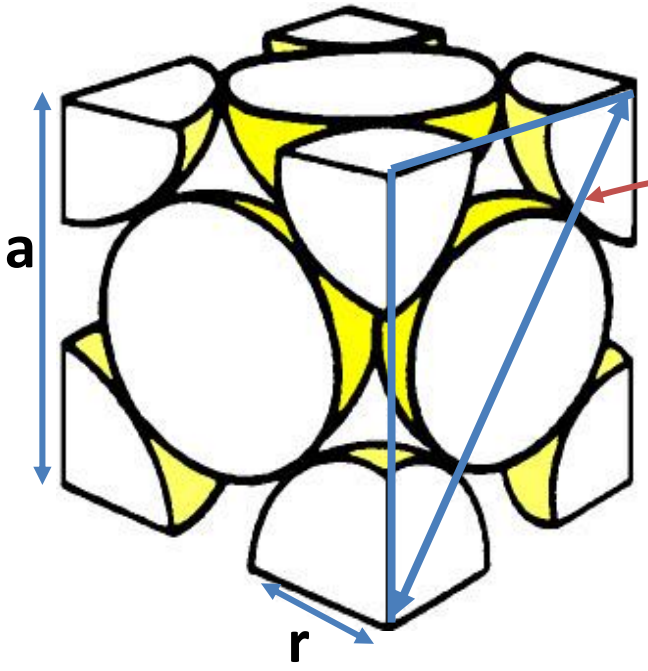
Face centred cubic

Face Centred Cubic

There are **4** atoms per unit cell

8 corner atoms = 1

6 face atoms = 3



Line of contact = 4r

$$(4r)^2 = a^2 + a^2$$

$$a = 2r\sqrt{2}$$

$$V_{\text{cell}} = a^3 = (2r\sqrt{2})^3 = 16r^3\sqrt{2}$$

volume of 1 atom

Number of atoms

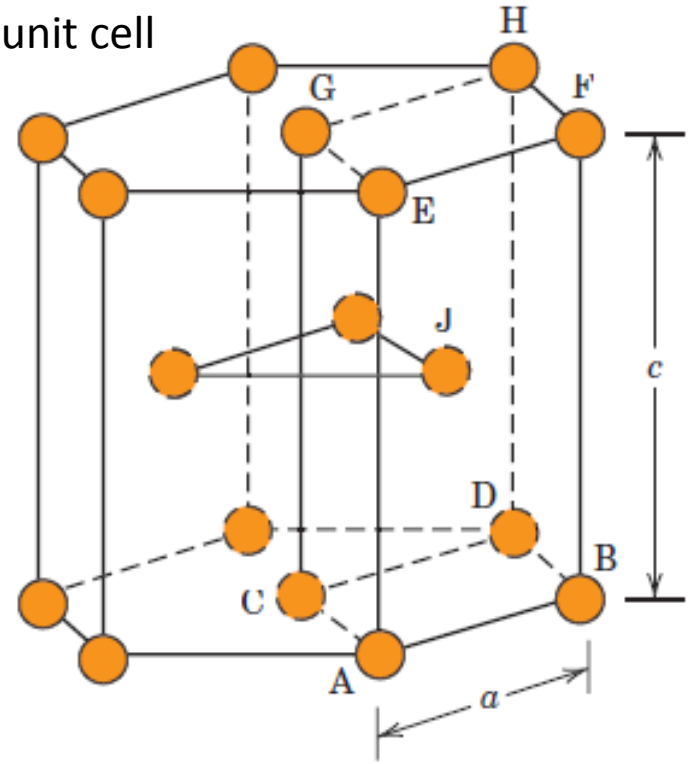
$$APF = \frac{4 \cdot \frac{4}{3}\pi r^3}{a^3} = \frac{\frac{16}{3}\pi r^3}{16r^3\sqrt{2}} = \frac{\pi}{3\sqrt{2}} = 0.74$$

volume of cell

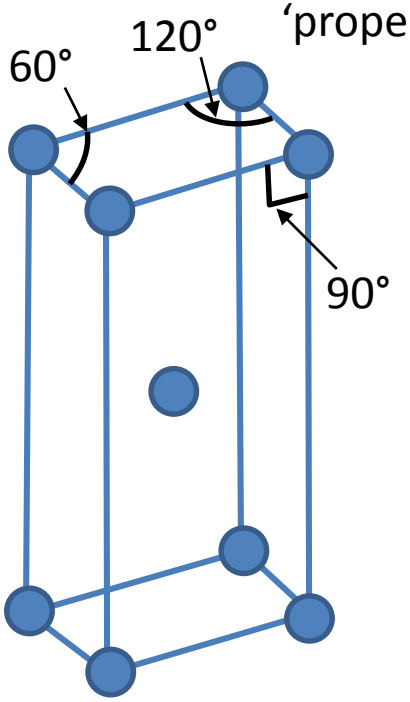
Very efficient packing

Hexagonal Close Packed (HCP)

‘hexagonal’ unit cell



$$c = \sqrt{\frac{8}{3}}\,a$$



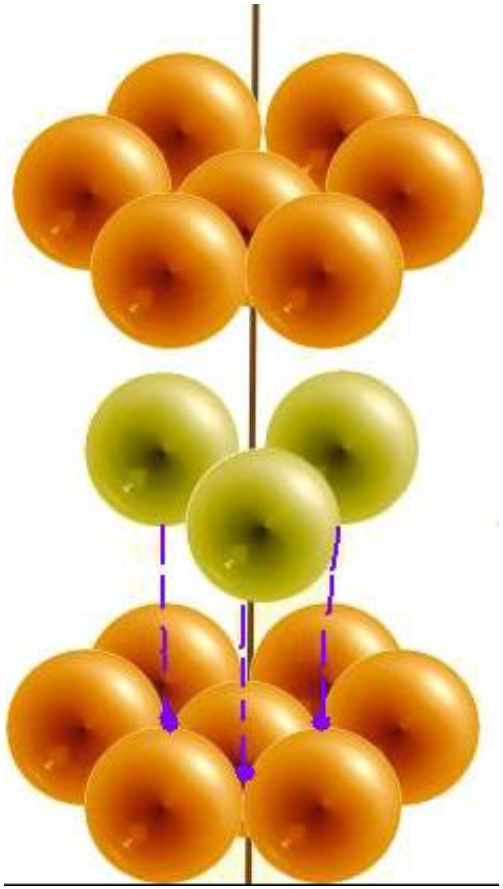
‘proper’ unit cell

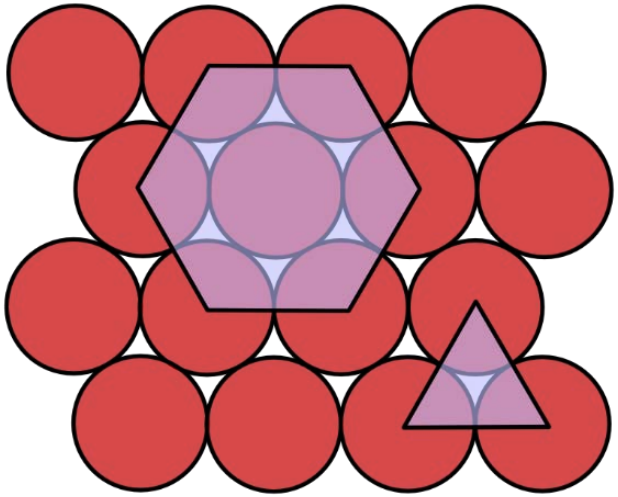
6 atoms per hexagonal unit
12 corner atoms shared with **6** cells
2 face atoms shared with **2** cells
3 internal atoms

2 atoms per unit cell
8 corner atoms shared with **8** cells
1 internal atom
(There are **3** of these cells per hexagonal unit)

Close Packing

HCP – obtained by stacking hexagonal lattice





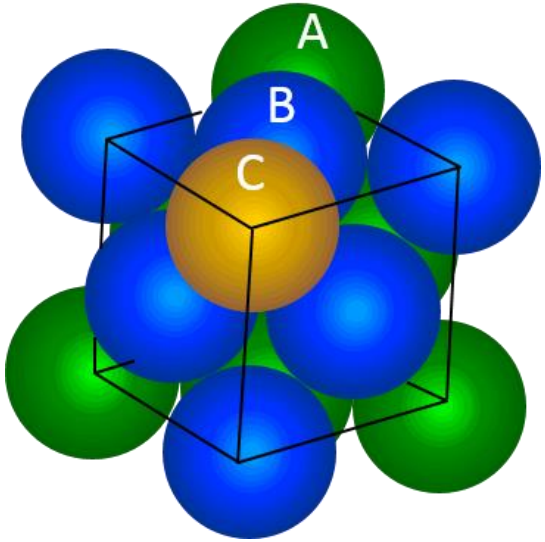
Hexagonal lattice
Closest packed 2D structure

$$APF = 0.74$$

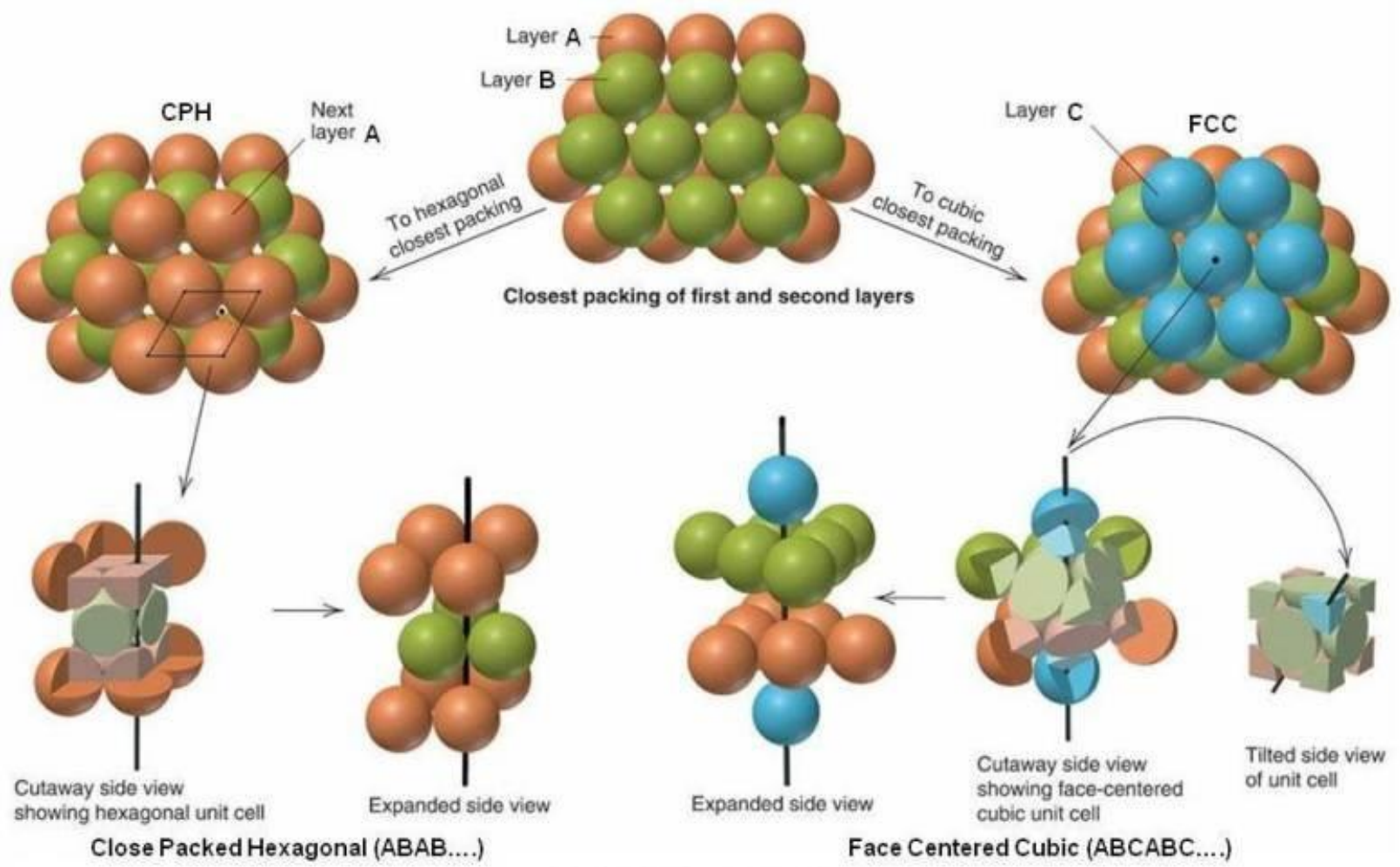
For both FCC and HCP

Most dense and so most common

FCC – obtained by stacking square lattice or hexagonal lattice



Close Packing



ABA and ABC Packing

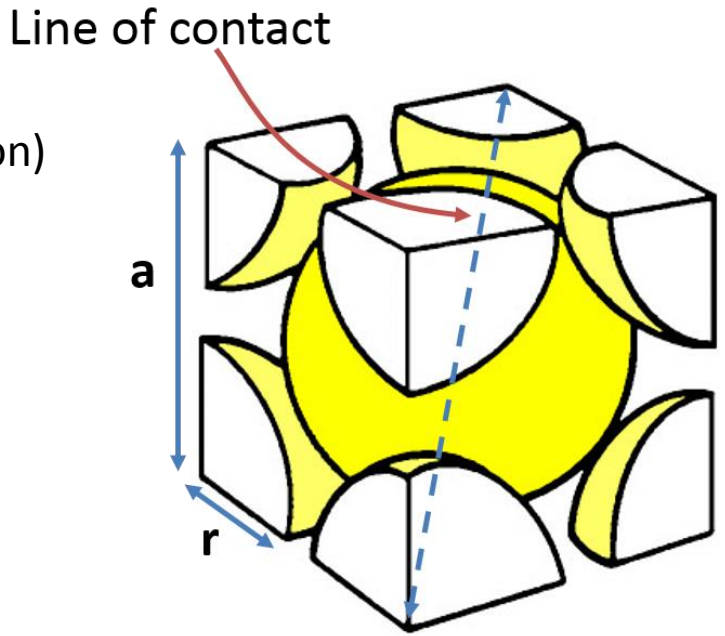
Body Centred Cubic

- Composed of square lattices with simple translation
- No close packed planes

$$V_{cell} = \frac{64}{3\sqrt{3}} r^3$$

$$APF = \frac{\sqrt{3}\pi}{8} = 0.68$$ (tutorial question)

- Less densely packed
  - Only occurs due to bonding



Common examples

Metal	*Crystal Structure*[a]	*Atomic Radius*[b] *(nm)*	*Metal*	*Crystal Structure*	*Atomic Radius (nm)*
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

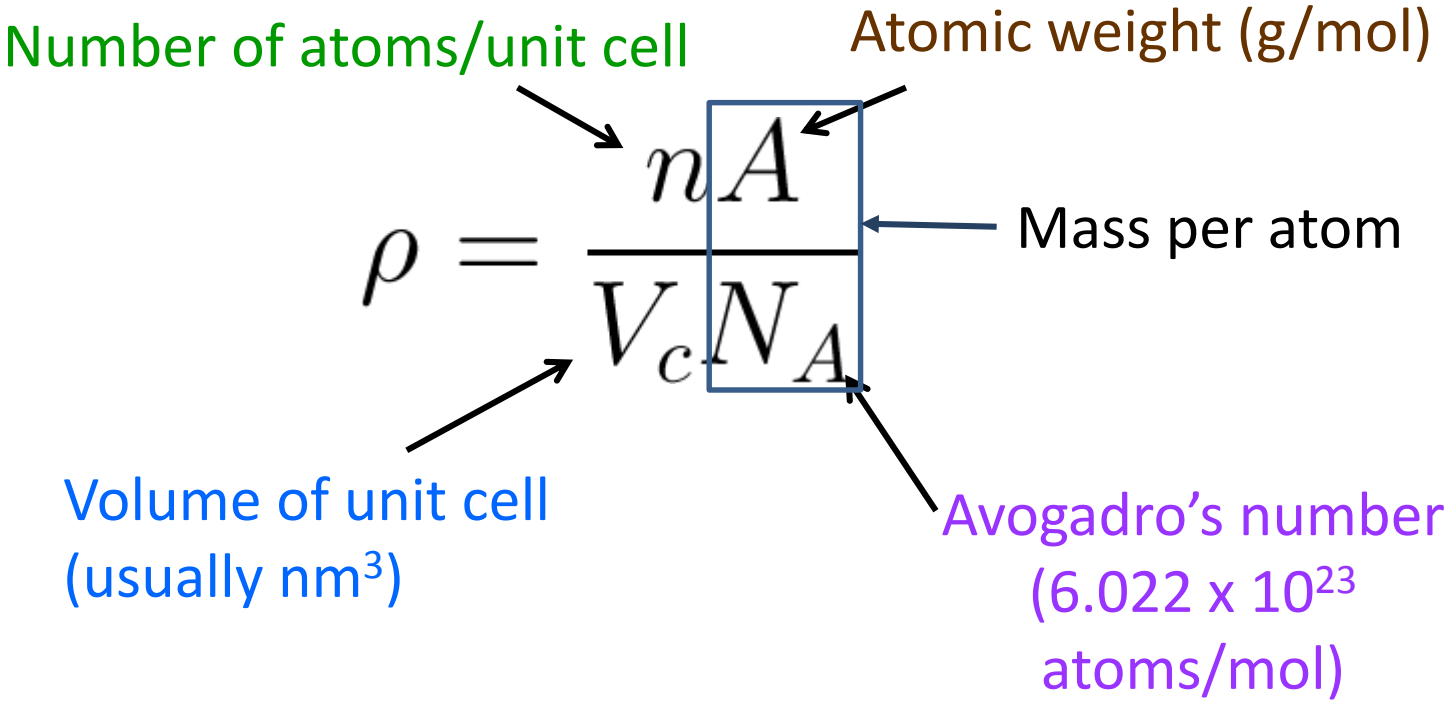
[a] FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.

[b] A nanometer (nm) equals 10^{-9} m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.

- FCC and HCP are the most closely packed structures – most common

Theoretical Density

$$\text{Density} = \rho = \frac{\text{Mass of atoms in cell}}{\text{Volume of cell}}$$



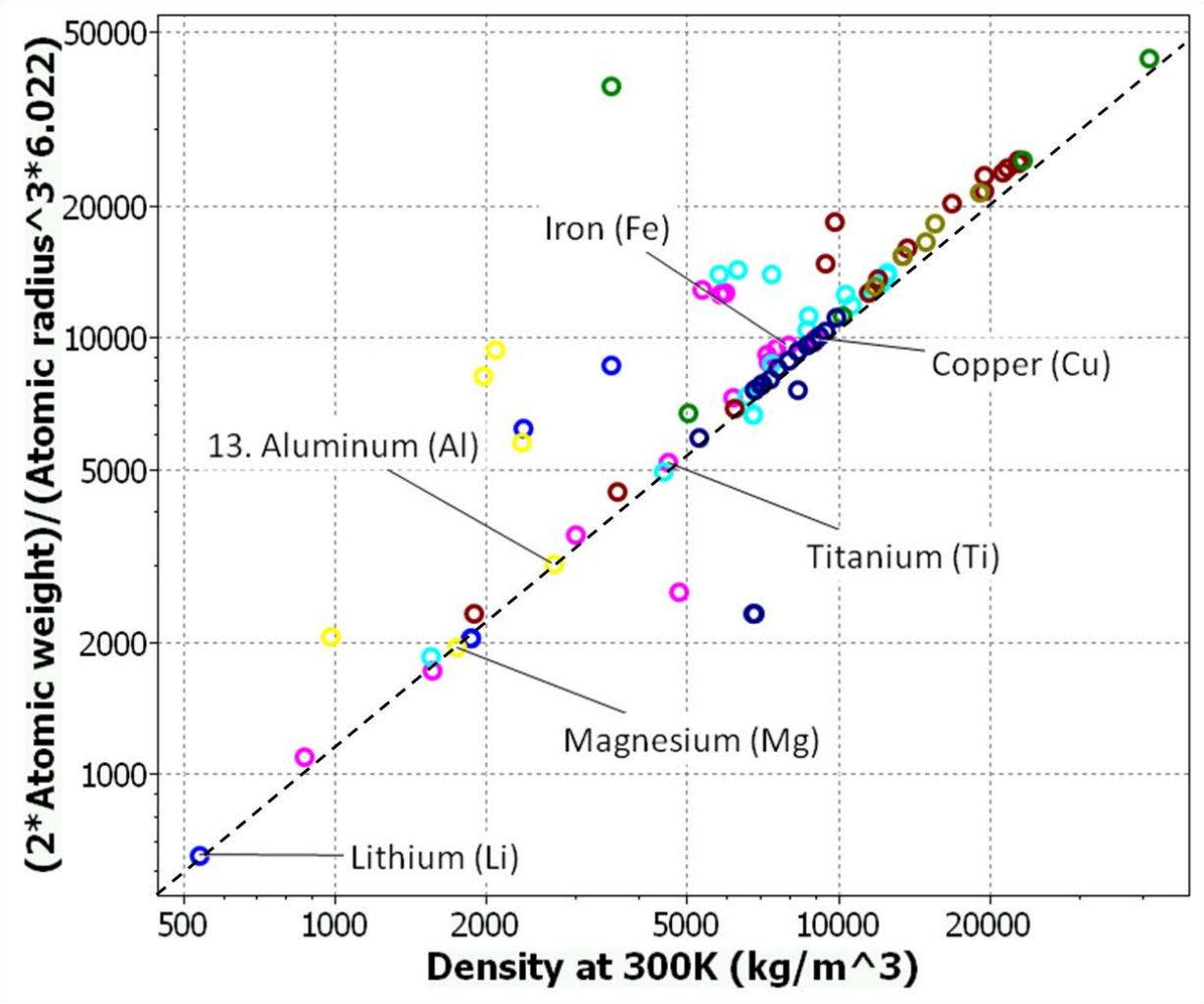
Theoretical Density

Approximations

$$V_c \approx r^3$$

$$n = 2$$

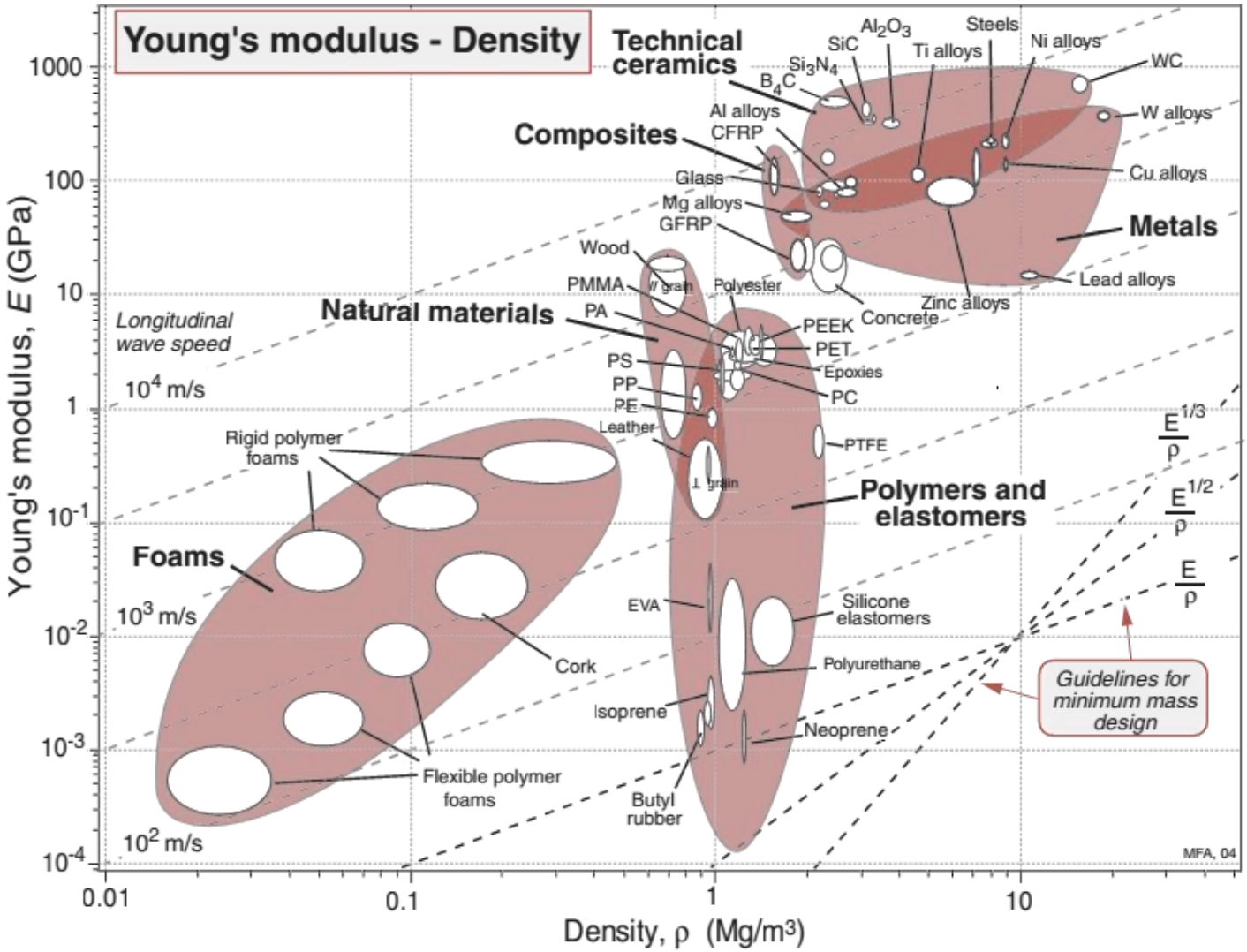
$$\rho = \frac{nA}{V_c N_A}$$



Real elemental density

Density

Density dictated by atoms and crystal structure – little possibility of altering density of metals and ceramics

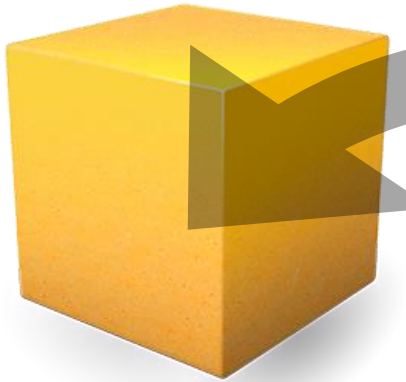


Quench cracking

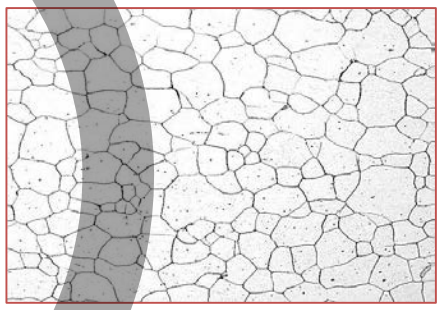
- Blades are quenched (quick cool) to make hard
- Thermal stresses + transformation stress
  - Results in cracking
- Common when welding old structural steels

Scale

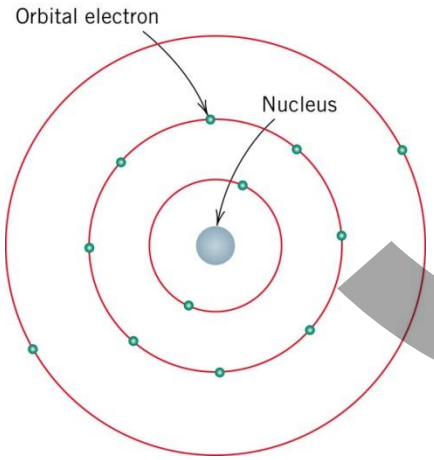
Continuum Mechanics
Perfect material with uniform properties



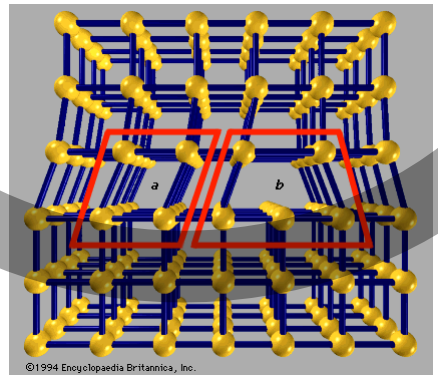
Macroscopic
Distinct regions with varying properties



Grain Structure
Real materials composed of many crystals stuck together



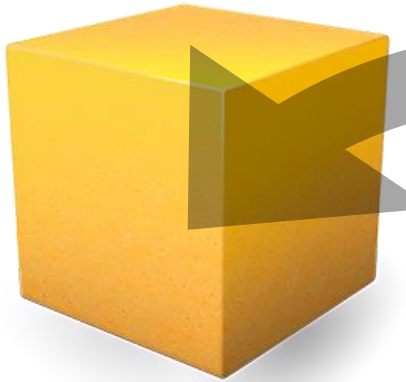
Atoms
Intrinsic properties and bonding



Crystal Structure
Arrangement of atoms (or lack of it)

Scale

Continuum Mechanics
Perfect material with uniform properties



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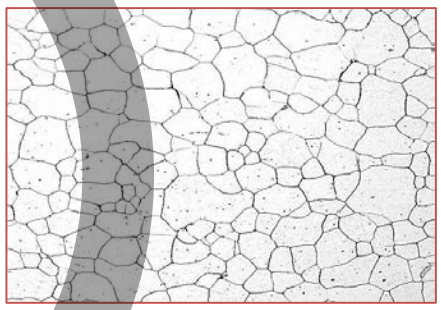
Distinct regions with varying properties



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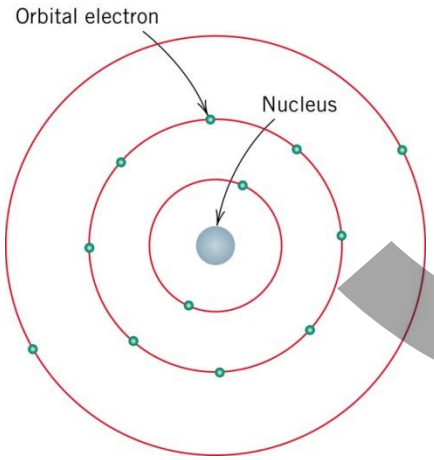

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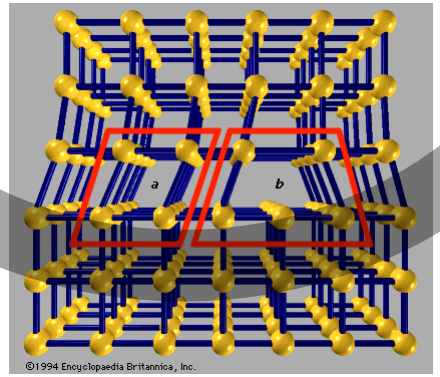
Intrinsic properties and bonding



Crystal Structure
Arrangement of atoms (or lack of it)

Properties of Materials

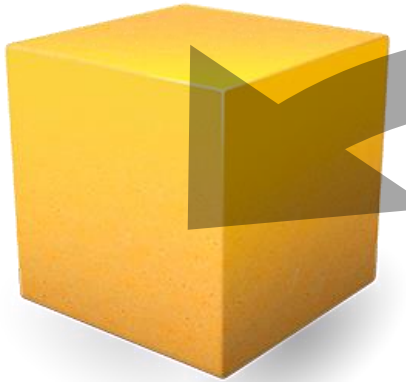
Theme: Structure

Lecture 3: Crystal Directions and Planes

Professor Steve Eichhorn
s.j.eichhorn@bristol.ac.uk
Room 0.115, Queen's Building

Scale

Continuum Mechanics
Perfect material with uniform properties



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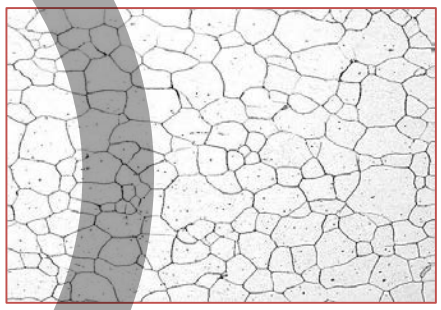
Distinct regions with varying properties



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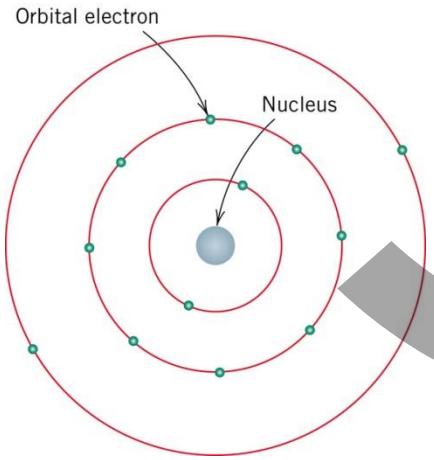
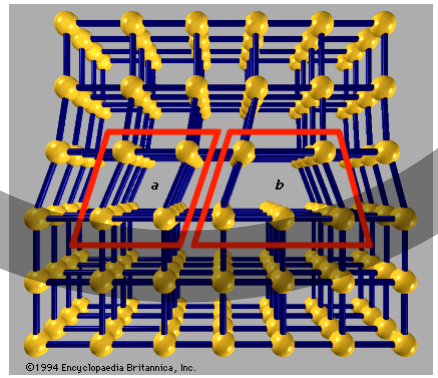


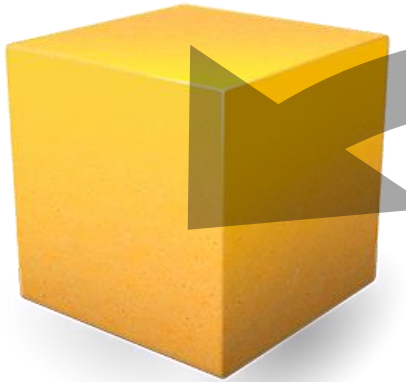
Atoms
Intrinsic properties and bonding



Crystal Structure
Arrangement of atoms (or lack of it)

Scale

Continuum Mechanics
Perfect material with uniform properties



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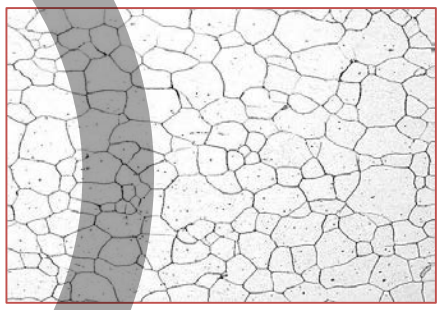
Distinct regions with varying properties



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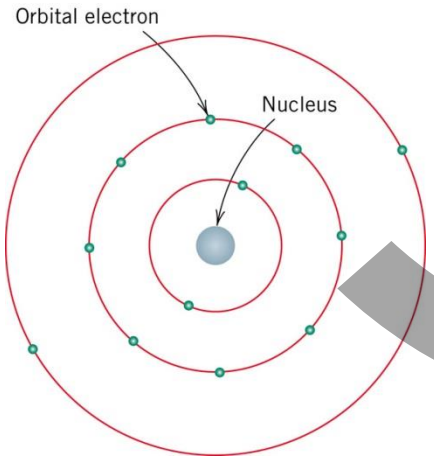
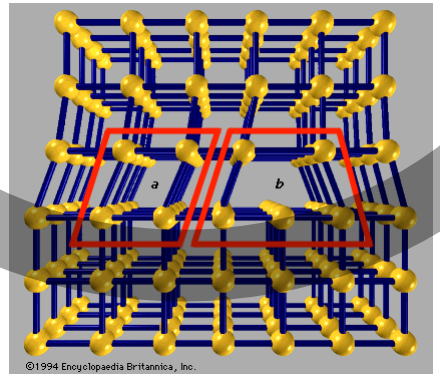
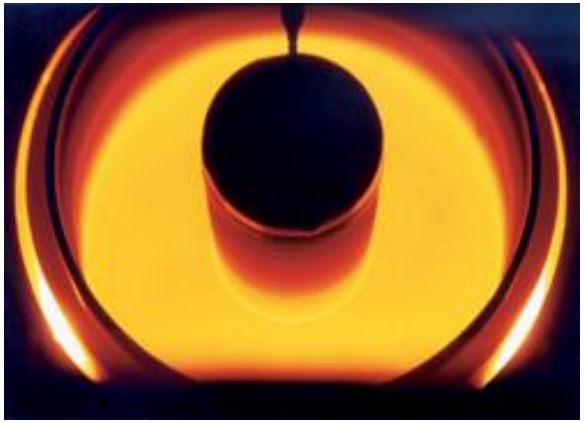


Atoms
Intrinsic properties and bonding

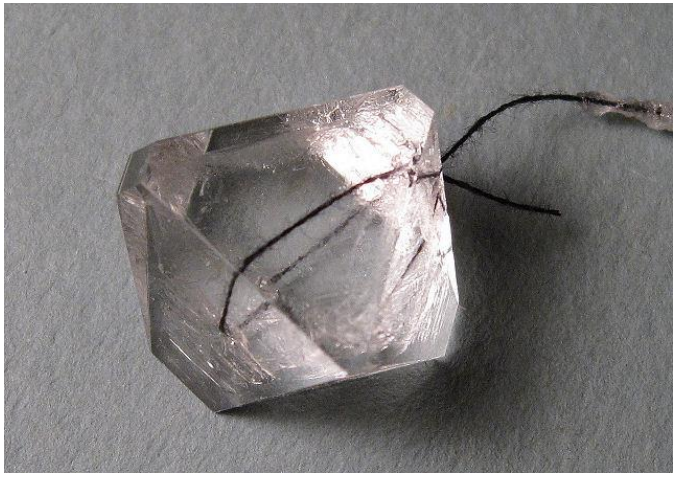


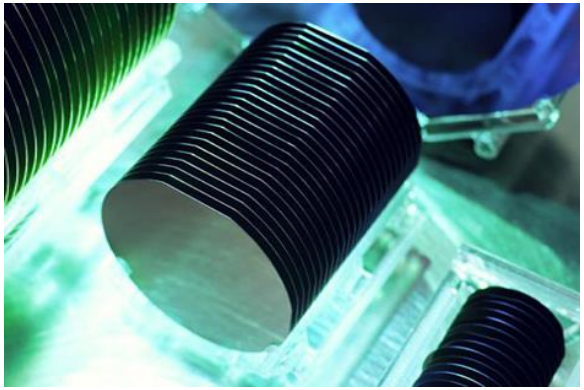
Crystal Structure
Arrangement of atoms (or lack of it)

Introduction



Growth of single crystals occurs on specific planes

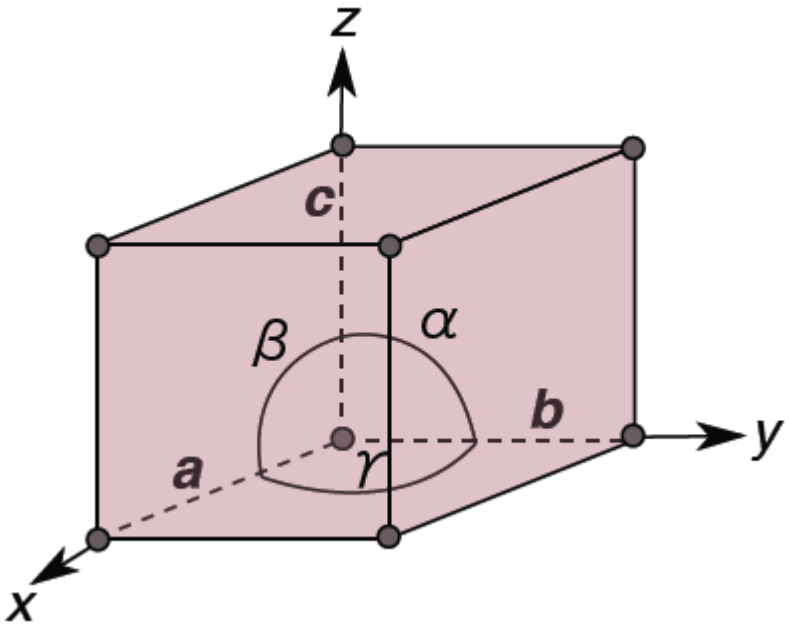


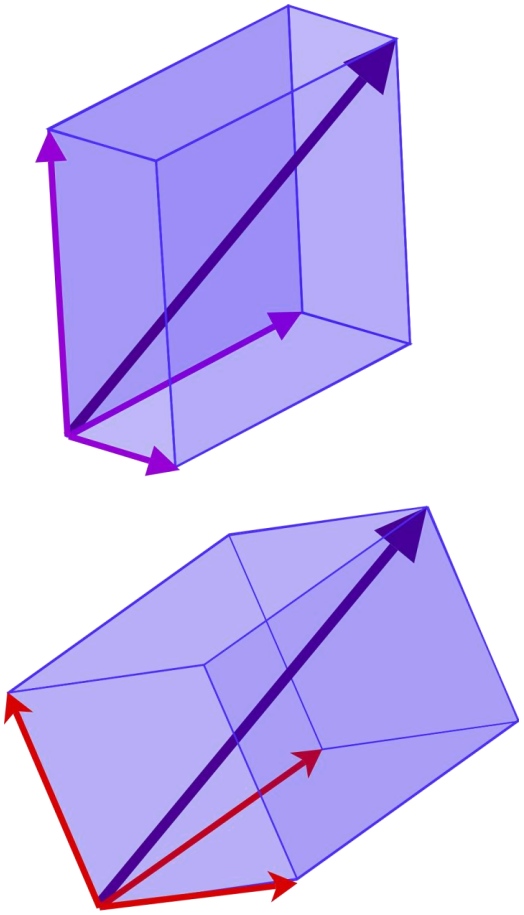


Diamond fractured along specific planes (cleavage)

Unit Cell Directions and Planes

Directions and planes given in terms of basis vectors



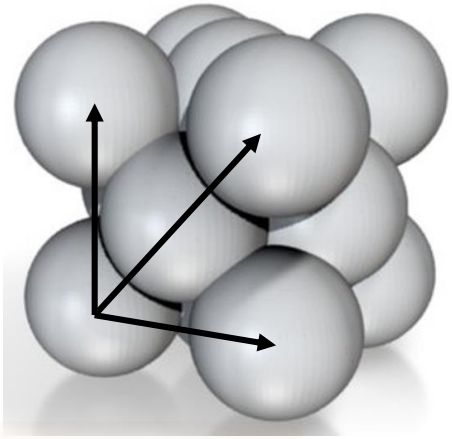


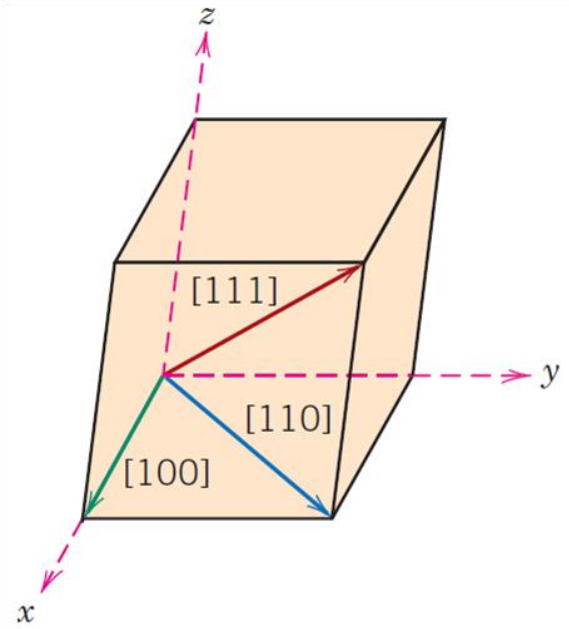
For the cubic systems this matches Cartesian – more complex for hexagonal but we ignore that here

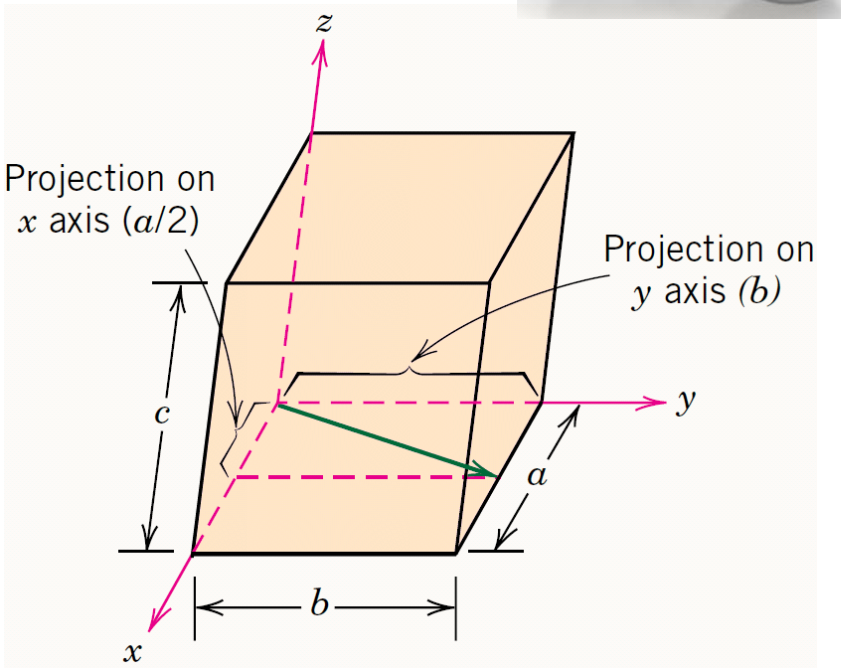
Directions

Directions join lattice points (atoms)

Simply vectors with weird notation *e.g.* [111]





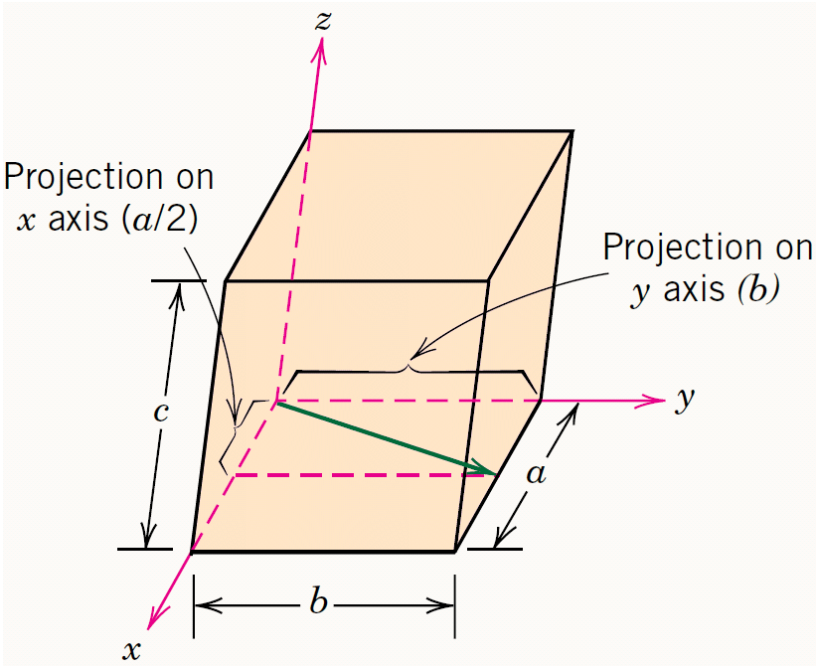


	x	y	z
Projections	a/2	b	0c
Projections (in terms of a, b, c)	½	1	0
Reduction*	1	2	0
Enclosure		[120]	

* Reduction is accompanied by a multiplication by 2 (common factor) to reduce to lowest integer

Directions

Drawing directions just works in reverse



	x	y	z
Enclosure		[120]	
Reduction	1	2	0
Projections (in terms of a, b, c)	½	1	0
Projections	a/2	b	0c

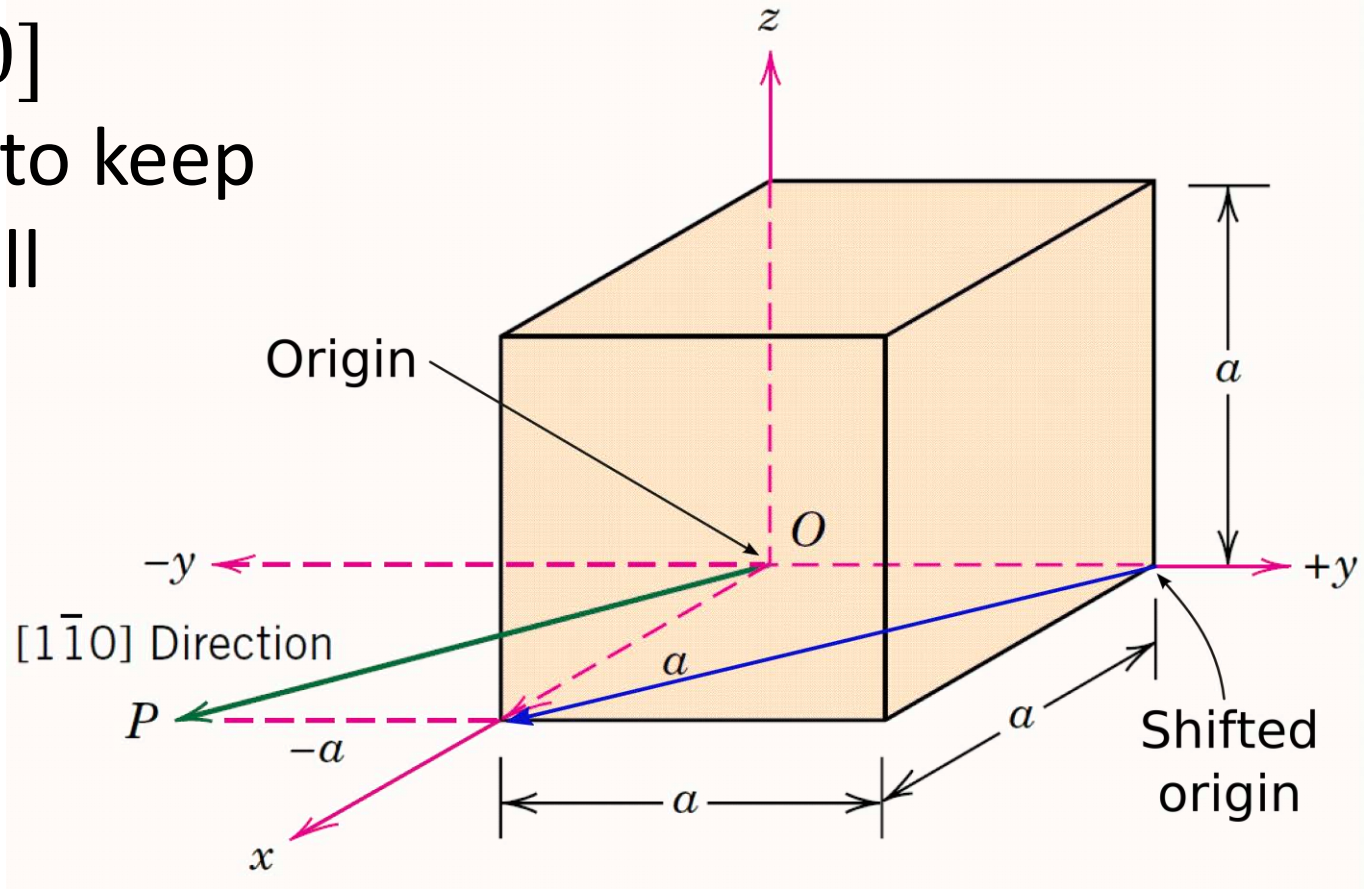
Directions

Negative directions use bar:

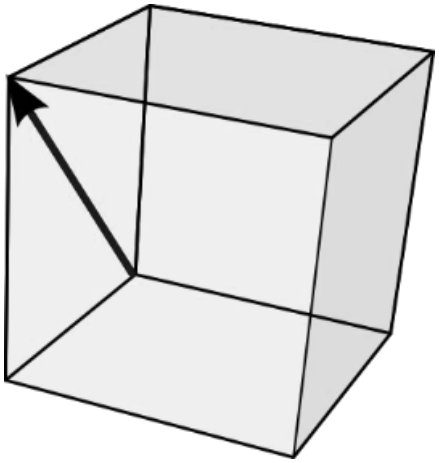
$[1\bar{1}0]$

Shift origin to keep vector in cell

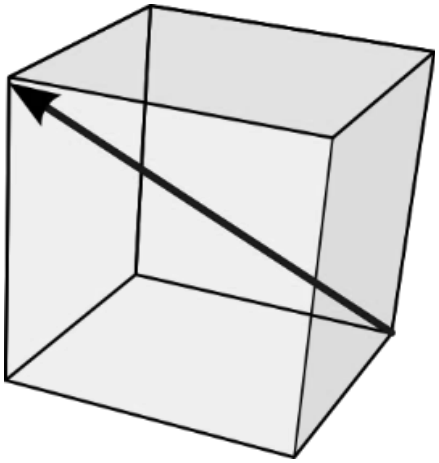
These two vectors are identical!



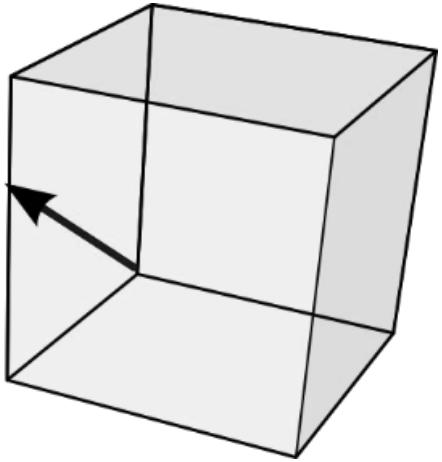
Examples



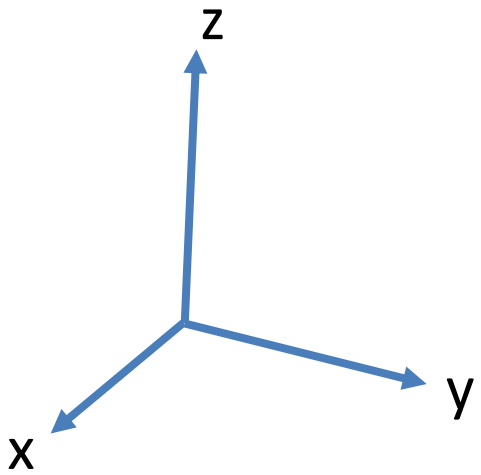
$[101]$



$[1\bar{1}1]$



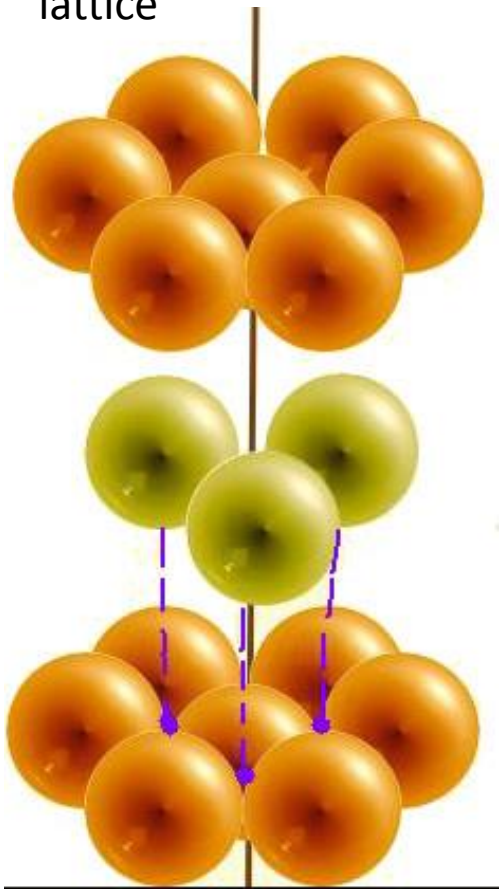
$[201]$

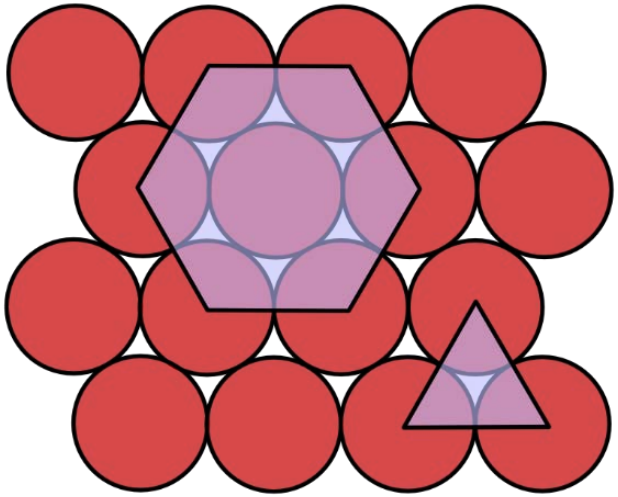


These are common directions in the cell

Planes

HCP (Hexagonal Close Packing) – obtained by stacking hexagonal lattice



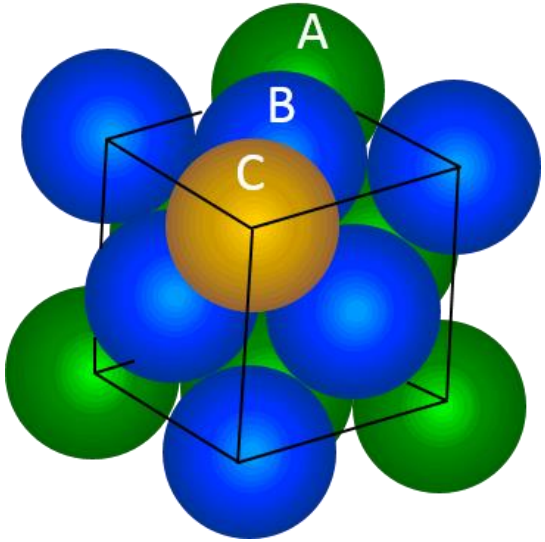


Hexagonal lattice
Closest packed 2D structure

Face Centred Cubic (FCC) – obtained by stacking square lattice or hexagonal lattice

From last lecture

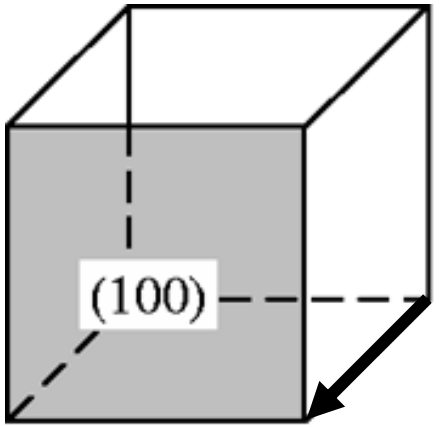
Unit cell constructed from planes – 2D arrays of periodic atoms

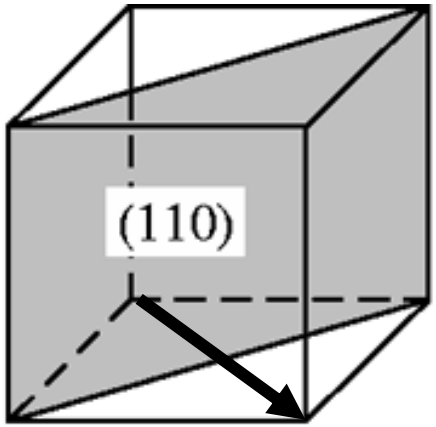


Planes

- Direction of plane normal
  - Read off intercepts of plane with axes in terms of *a*, *b*, *c*
  - Take reciprocals of intercepts
  - Reduce to smallest integer values
  - Enclose in parentheses, no commas

(hkl)





Next

- We now have basic language for talking about crystals
- Use this to understand mechanical behaviour
  - Fracture
  - Plastic slip
  - Strengthening mechanisms
  - Estimating strength