

Today's objectives-Structures

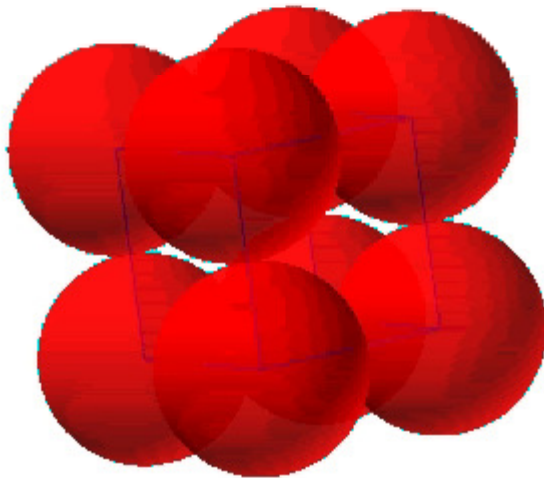
1. Basic crystal structures
2. Charge neutrality



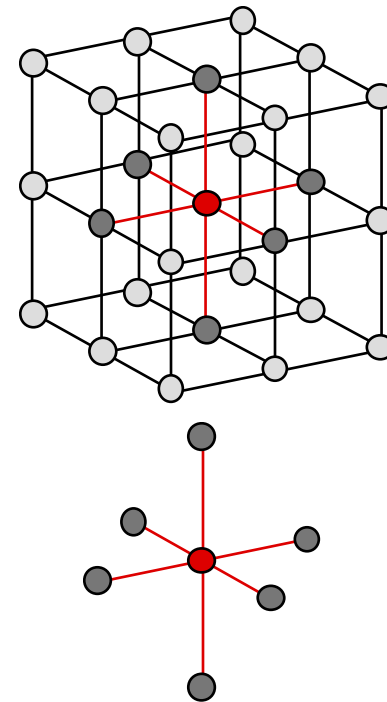
SIMPLE CUBIC STRUCTURE (SC)

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

- **Coordination # = 6**
(# nearest neighbors)



(Courtesy P.M. Anderson)

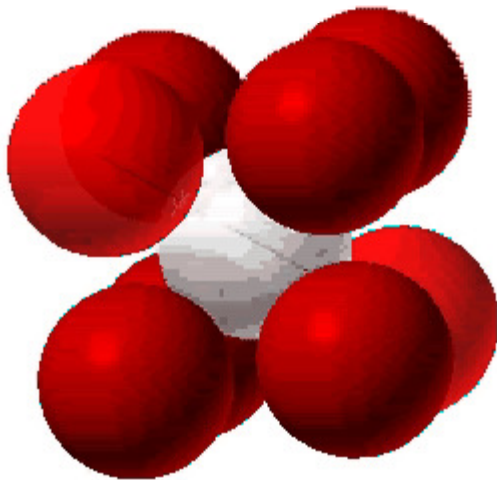


Packing factor = 0.52



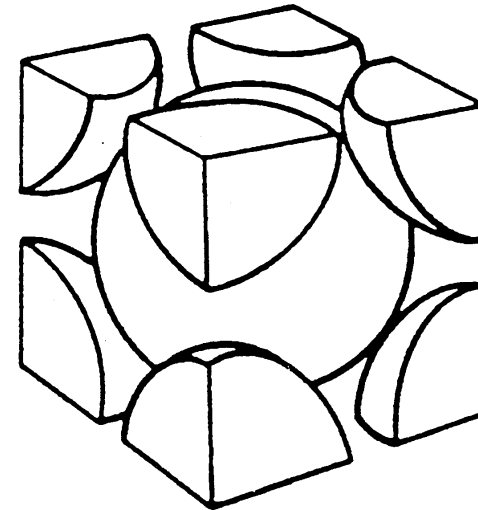
BODY CENTERED CUBIC STRUCTURE (BCC)

- **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.

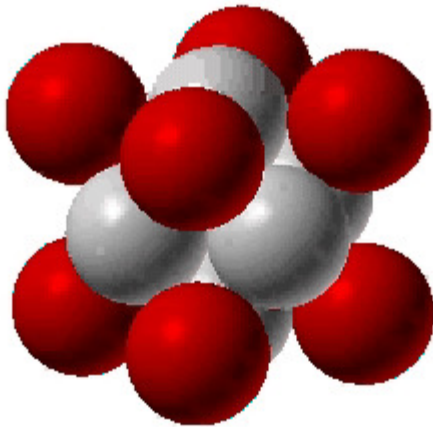
Packing factor = 0.68



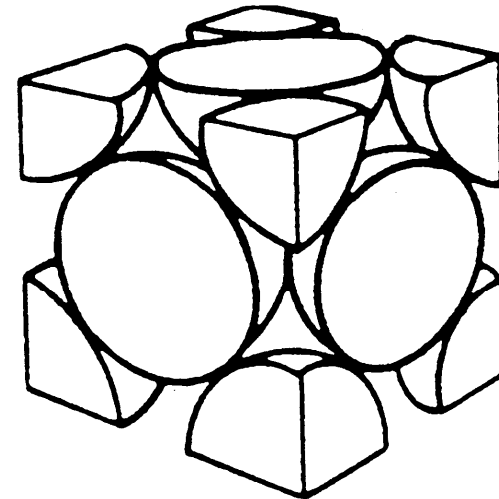
FACE CENTERED CUBIC STRUCTURE (FCC)

- **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.

Packing factor = 0.74



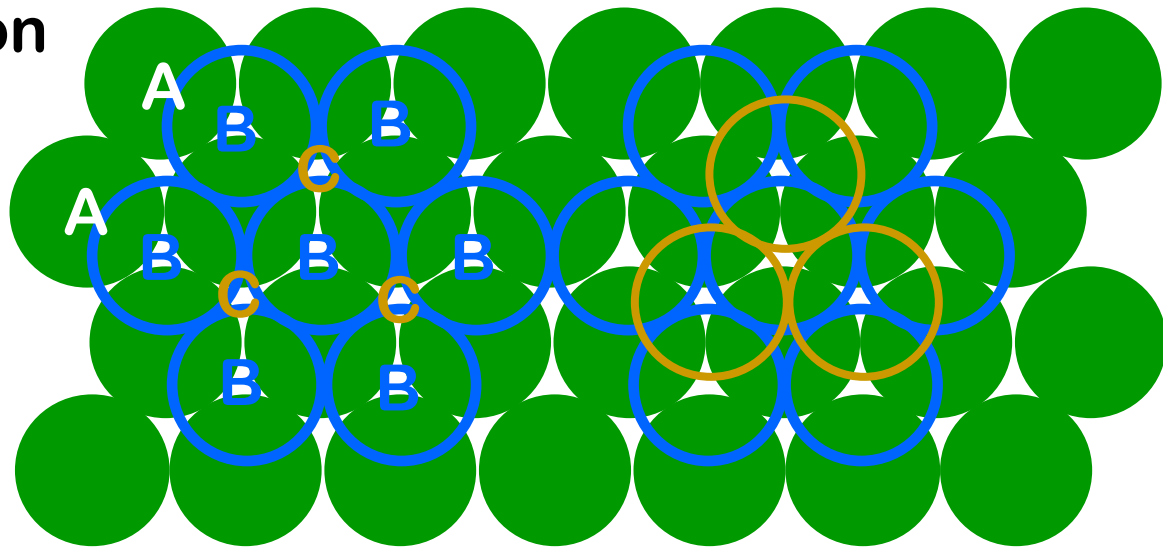
FCC STACKING SEQUENCE

- ABCABC... Stacking Sequence
- 2D Projection

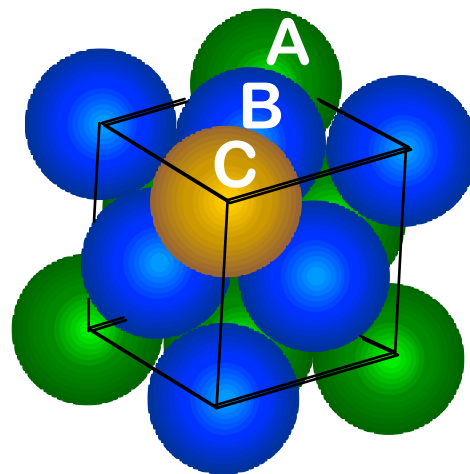
A sites

B sites

C sites

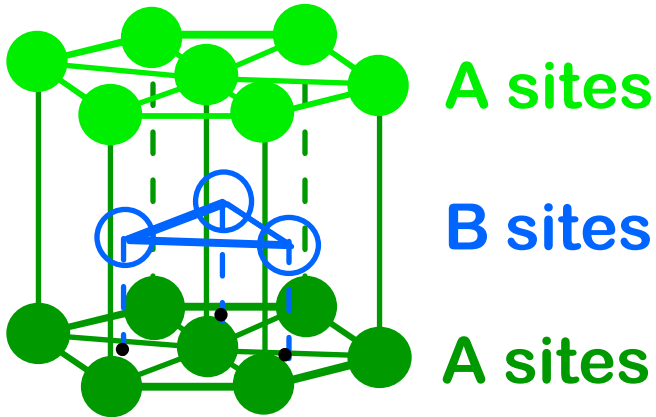


- FCC Unit Cell



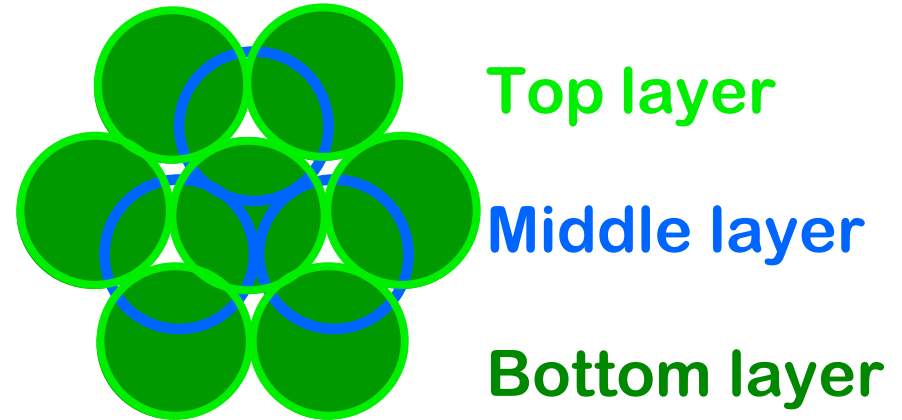
HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3,
Callister 6e.

- 2D Projection



- Coordination # = 12
- APF = 0.74

CERAMIC BONDING

- **Bonding:**
 - Mostly ionic, some covalent.
 - % ionic character increases with difference in electronegativity.
- **Large vs small ionic bond character:**

IA												IIIA				IVA		VA		VIA		VIIA		0
H 2.1												B 2.0	C 2.5	N 3.0	O 3.5	F 4.0			He -					
Li 1.0	Be 1.5											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0			Ne -					
Na 0.9	Mg 1.2											VIII								Ar -				
K 0.8	Ca 1.0	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.8	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8			Kr -						
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5			Xe -					
Cs 0.7	Ba 0.9	La-Lu 1.1-1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2			Rn -					
Fr 0.7	Ra 0.9	80-100 Ac-No 1.1-1.7																						

CaF₂: large (arrow from Ca to F)

SiC: small (arrows from Si and C)

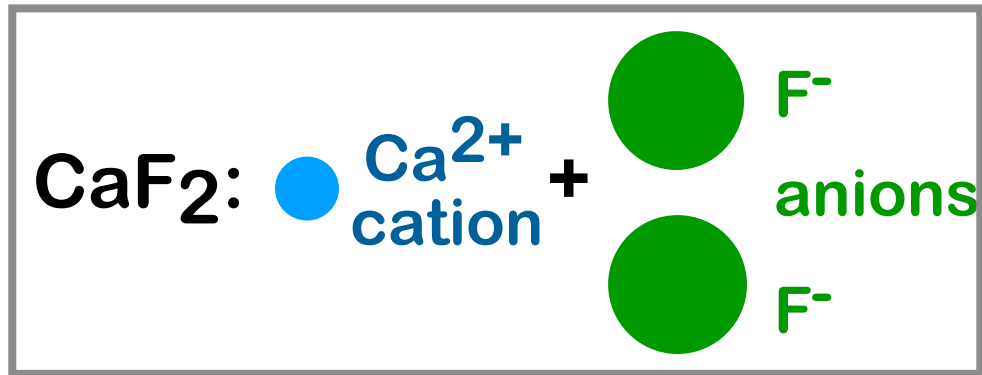
Table of Electronegativities

Adapted from Fig. 2.7, *Callister 6e*. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.)



Rules for Ionic Structures

- **Rule 1: Charge Neutrality:**
 - Net charge in the structure should be zero.



--General form: $A_m X_p$

m, p determined by charge neutrality

Examples: K_mCl_p , Mg_mO_p , Na_mS_p , Li_mP_p , Si_mN_p

- What is the charge on:

K Mg Na Li Si

- What is the charge on:

Cl O S P N

- What are the formulas for:

KCl MgO NaS LiP SiN

8 Elements in Ceramics and Glasses

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr



SUMMARY

- Ceramic materials have both covalent & ionic bonding.
- Structures must maintain:
 - charge neutrality

Reading for next class

Chapter sections: 12.5 + 3.7-10

