MATERIALS ENGINEERING

Ankush Gaurav
Assistant Professor

Mechanical Engineering Discipline

Uma Nath Singh Institute of Engineering & Technology
Veer Bahadur Singh Purvanchal University,Jaunpur,India

ankushgaurav.vbspu@gmail.com

CERAMIC CRYSTAL STRUCTURES

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- Ceramics are composed of at least two elements
- Ceramic Crystal structures are generally more complex than those for metals

Ceramic Bonding

- Mostly ionic, some covalent.
- Ionic character increases with difference in electronegativity

Material	*Percent Ionic Character*
CaF_2	89
MgO	73
$NaCl$	67
Al_2O_3	63
SiO_2	51
Si_3N_4	30
ZnS	18
SiC	12

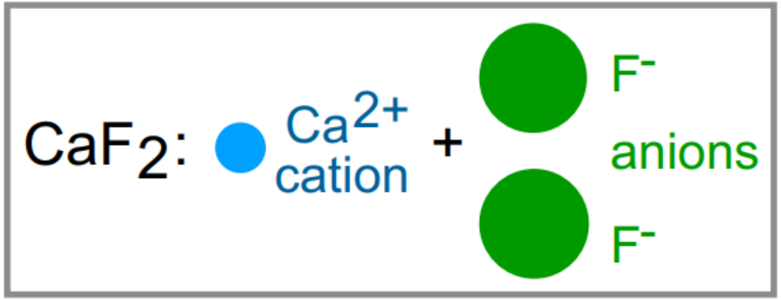
Ionic Bonding & Structure

Ceramic materials for which the atomic bonding is predominantly ionic:

- metallic ions, or **cations,** are positively charged
- **anions,** which are negatively charged

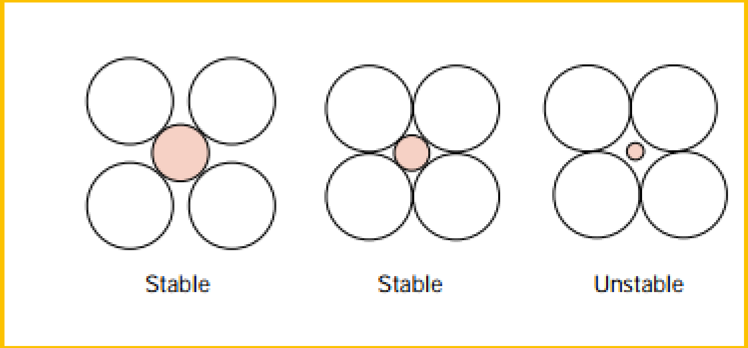
- ***Note:*** Two characteristics of the component ions in crystalline ceramic materials influence the crystal structure: **the magnitude of the electrical charge** on each of the component ions, and **the relative sizes of the cations and anions.**

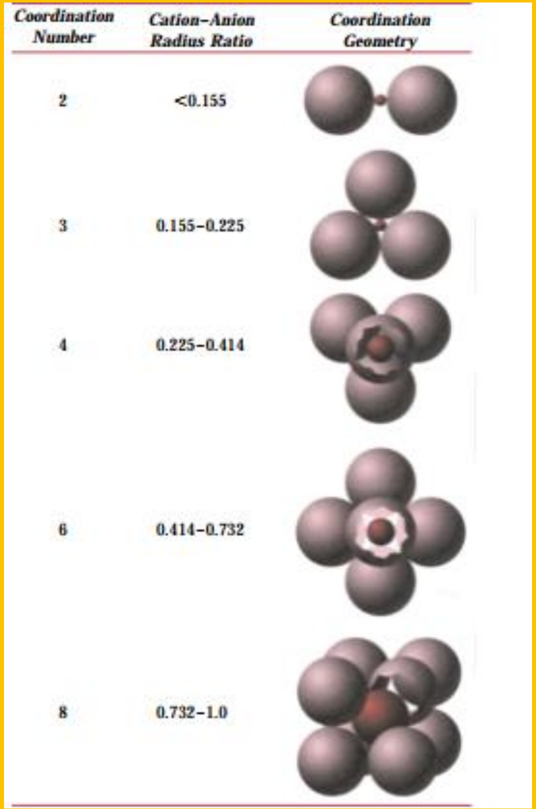
- Charge Neutrality:
  --Net charge in the structure should be zero.



The relative sizes of the cations and anions.

- maximize the of nearest oppositely charged neighbours





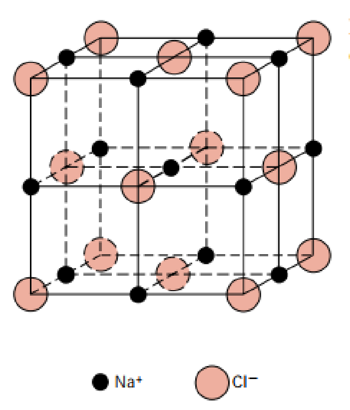
Coordination Number	Cation–Anion Radius Ratio	Coordination Geometry
2	<0.155	
3	0.155–0.225	
4	0.225–0.414	
6	0.414–0.732	
8	0.732–1.0	

AX-TYPE CRYSTAL STRUCTURES

- cations = anions

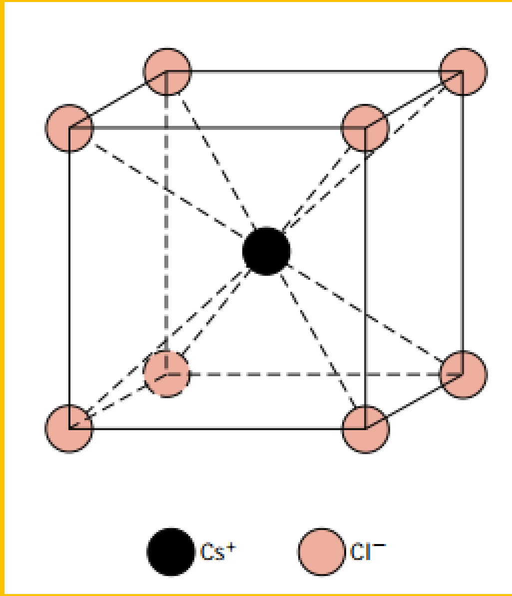
Rock Salt Structure

- Most common AX crystal structure is the *sodium chloride* (NaCl)
- The coordination number for both cations and anions is 6
- MgO, MnS, LiF, and FeO.



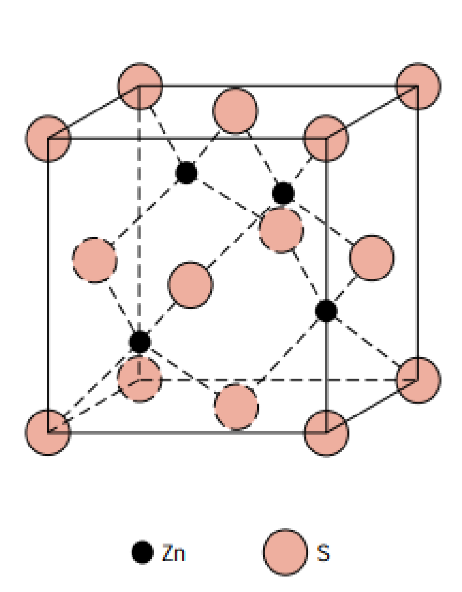
Cesium Chloride Structure

- coordination number is 8
- Not ***BCC***
- CsBr and CsI



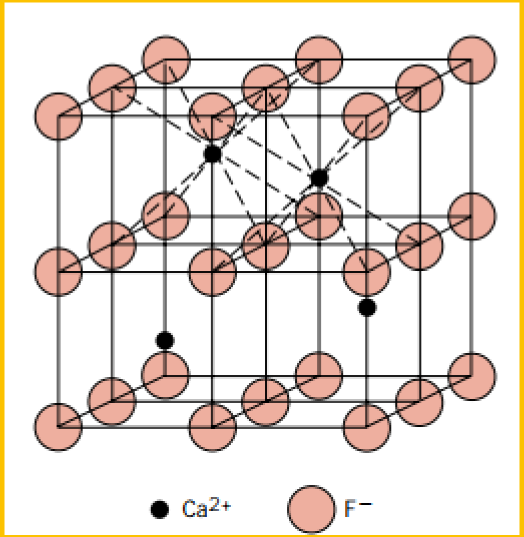
Zinc Blende Structure

- coordination number is 4
- ZnS, ZnTe, and SiC



$A_m X_p$ -TYPE CRYSTAL STRUCTURES

Cation≠Anion



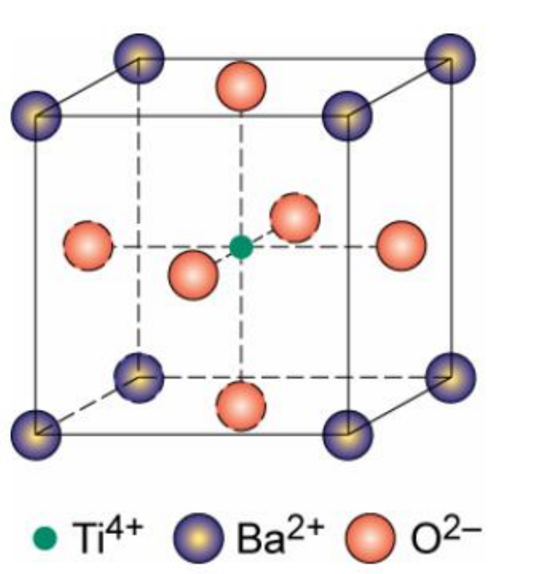
Example: CaF_2

Cation to anion size ratio is CaF_2 is about 0.8 giving co-ordination number 8

Other Example:

UO_2, PuO_2, and ThO_2

$A_mB_nX_p$-TYPE CRYSTAL STRUCTURES



Example:Barium titanate ($BaTiO_3$)

Other Example: Strontium zirconium oxide ($SrZrO_3$)

DENSITY COMPUTATIONS—CERAMICS

Number of formula units/unit cell

$$\rho = \frac{n'(\Sigma A_C + \Sigma A_A)}{V_C N_A}$$

Volume of unit cell

n' = the number of formula units[1] within the unit cell

ΣA_C = the sum of the atomic weights of all cations in the formula unit

ΣA_A = the sum of the atomic weights of all anions in the formula unit

V_C = the unit cell volume

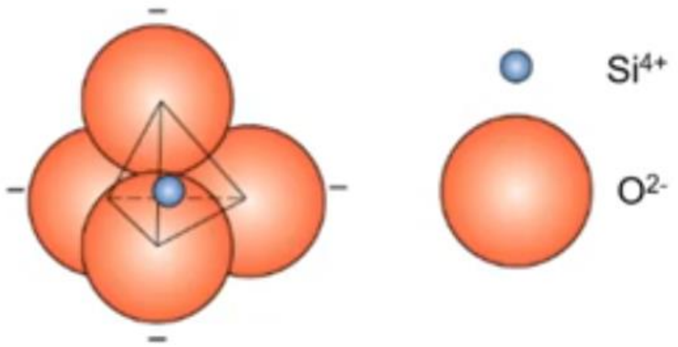
N_A = Avogadro's number, 6.023×10^{23} formula units/mol

SILICATE CERAMICS

Oxygen and silicon are the two most abundant elements on earth

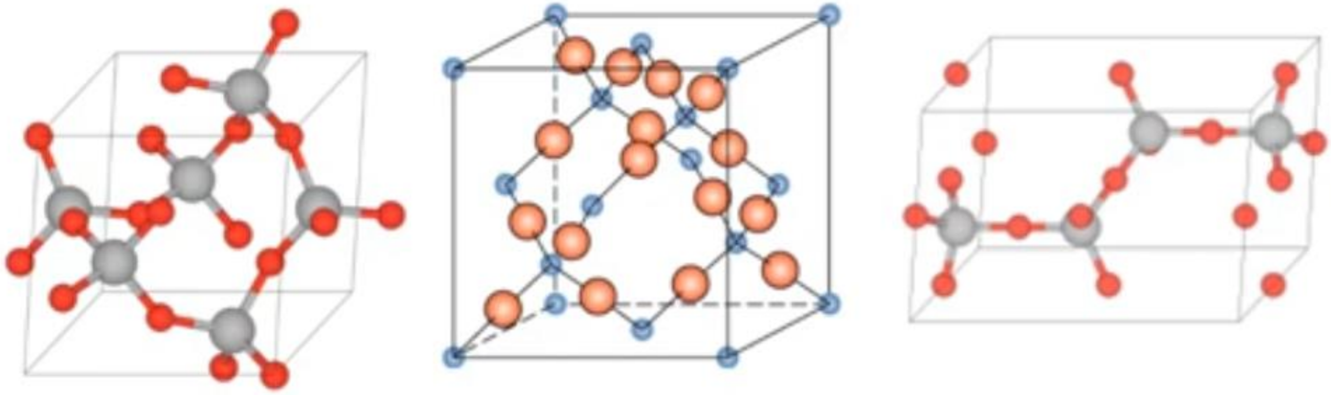
Silicates: Material comprised primarily of Si & O

- Characterized by arrangement of SiO_4^{4-} tetrahedrons



bulk of soils, rocks, clays, and sand come under the silicate classification

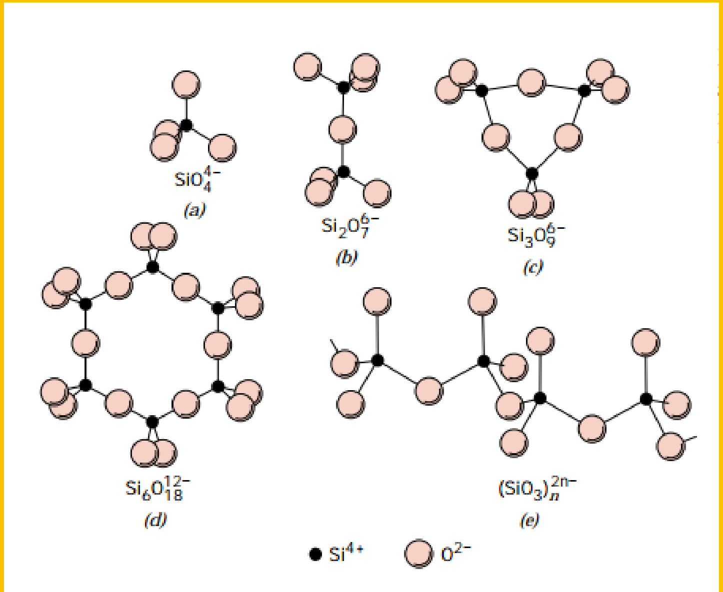
- **Silica** (SiO_2): Simplest silicate material
- 3 polymorphic crystalline structures for silica:
  - Quartz, cristobalite, tridymite
- Strong Si-O bonds → high melting temperature (1710°C)



α-quartz crystobalite β-tridymite

THE SILICATES

- Combine SiO_4^{4-} tetrahedral are shared by other tetrahedral to form some rather complex structures
  Simple Silicates



Mg_2SiO_4

Forsterite

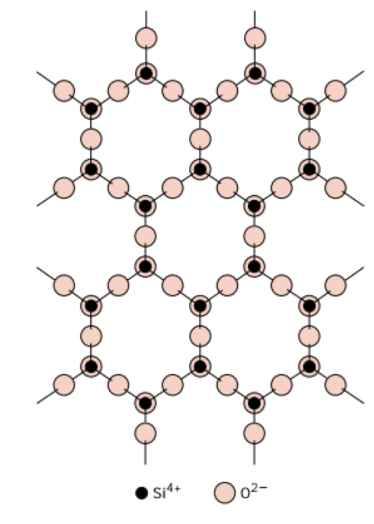
$Ca_2MgSi_2O_7$

Akermanite

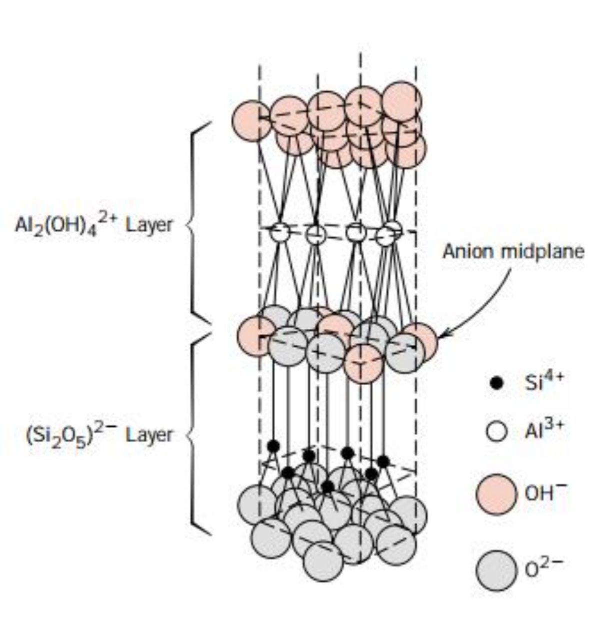
Layered Silicates

- A two-dimensional sheet or layered structure can also be produced by the sharing of three oxygen ions in e ach of the tetrahedra

$(Si_2O_5)^{2-}$



$Al_2(Si_2O_5)(OH)_4$



One of the most common clay minerals, kaolinite

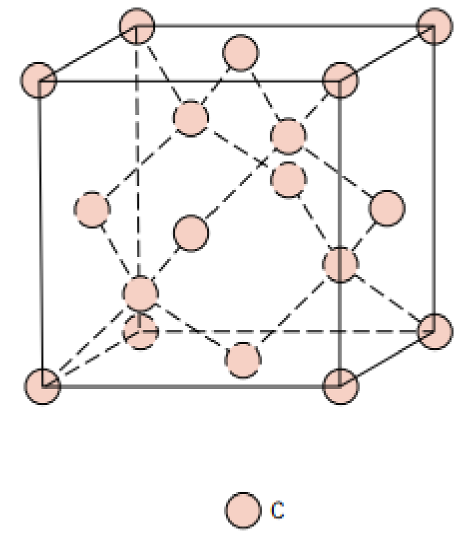
- their basic structure is characteristic of the clays and other minerals

Other example

Micas $KAl_3Si_3O_{10}(OH)_2$.
Talc $Mg_3(Si_2O_5)_2(OH)_2$

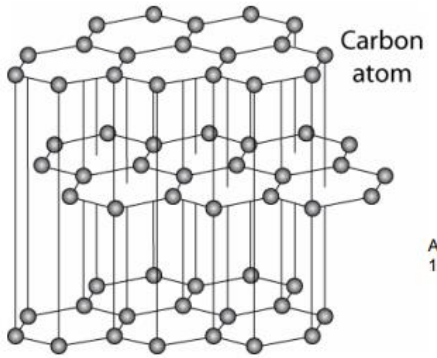
Carbon

Diamond



Graphite

- layer structure – aromatic layers



Adapted from Fig. 12.17, *Callister 7e.*

  – weak van der Waal's forces between layers
  – planes slide easily, good lubricant

Also shown by germanium, silicon

References

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- Callister - Fundamentals of Materials Science and Engineering 5e
- William D. Callister - Materials Science and Engineering. An Introduction-Wiley (2006)
- http://web.eng.fiu.edu/wangc/EGN3365-12.pdf
- https://www.youtube.com/watch?v=Wst5Ga8pHDY

Thank You