625-102 GEOLOGY

Lecture 2

Atomic Structures of Minerals

Melbourne Earth Sciences

Mineral properties controlled by:

RECAP OF LECTURE 1

- Chemical composition
  - - the chemical elements that are present
- Atomic structure
  - How the atoms are arranged
- These two features
  control all the physical properties of minerals

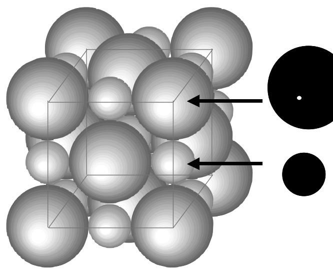
Earth Materials

Ionic Bonding

- Most minerals behave mostly as ionic solids
- Ionic bonds are formed by the attraction of oppositely charged ions
- The ions behave like uniformly charged spheres
- Size measured by the Ionic Radius
- Ionic radius is useful in predicting how ions are packed together
- eg NaCl, Halite

Earth Materials

Halite Structure (NaCl)



Cl^-
Ionic Radius 1.81Å

Na^+
Ionic Radius 0.97Å

Note: each ion is surrounded by 6 others

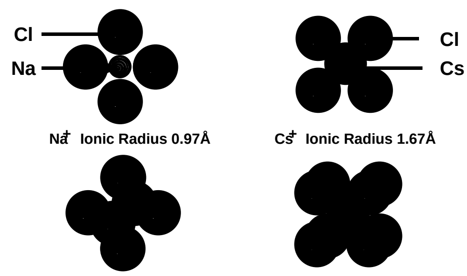
Earth Materials

Coordination Number

- Coordination Number
  - The number of Anions (-ve) around each Cation (+ve)
  - Controlled by the ionic radii of the cations and anions
- Ionic Radii
  - Sodium (Na^+) 0.97 Å
  - Chlorine (Cl^-) 1.81 Å
  - Caesium (Cs^+) 1.67 Å

Earth Materials

Sodium Chloride | Caesium Chloride

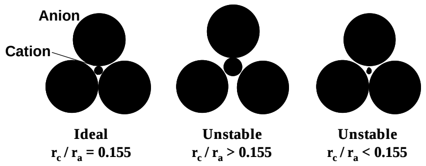


→ 6-fold Coordination | → 8-fold Coordination

Earth Materials

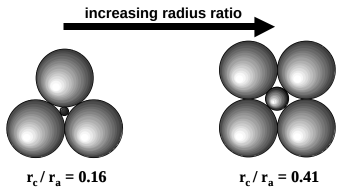
Radius Ratio 1

- Coordination depends on the ratio of ionic radii
- Radius Ratio = Cation radius / Anion radius
- Determines the packing denisty of the ions
- eg For a coordination number of 3

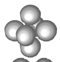
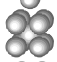
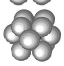


Radius Ratio 2

- Coordination number increases with increasing radius ratio
- eg for ions arranged in one plane



Coordination No. and Radius Ratio

Coord. No.	Min. Rad. Ratio	Arrangement	Shape
CN = 3	0.155	Triangle	
CN = 4	0.225	Tetrahedron	
CN=6	0.414	Octahedron	
CN=8	0.732	Cube	
CN=12	1.0	Dodecahedron	

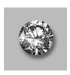
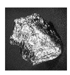
Polymorphism

- Polymorphism is where the same chemical compound occurs in two or more atomic structures
- Literally means 'many shapes'
- Some examples are
  - diamond and graphite (C)
  - calcite and aragonite ($CaCO_3$)
  - andalusite, kyanite and sillimanite (Al_2SiO_5)
- Polymorphs have different physical properties
- Polymorphs form under different physical conditions to each other

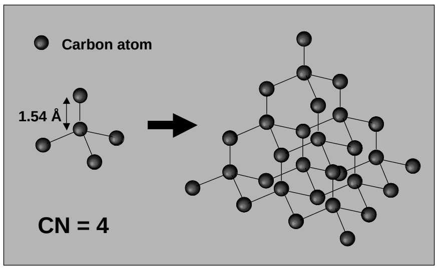
ARAGONITE - $CaCO_3$
Orthorhombic
H = 3.5-4
D = 2.9+
Cleavage: one plane

CALCITE - $CaCO_3$
Trigonal
H = 3
D = 2.7
Cleavage: three planes

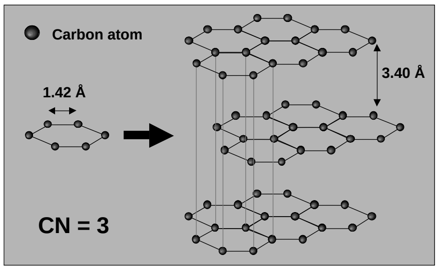
Polymorphs of Carbon

	Diamond	Graphite
Crystal System	Cubic	Hexagonal
Crystal form	Octahedron	Hexagonal flakes
Cleavage	Yes, octahedral	Yes, basal, like mica
Hardness	Hardest substance	one of softest known
Colour	Mainly colourless	Black
Density	3.50	2.2
		

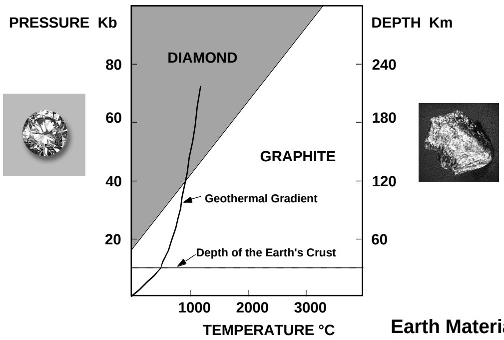
Diamond Structure



Graphite Structure



Carbon Stability Fields



Isomorphism

- Isomorphism is where two minerals can have different compositions but the same structure
- Literally means ‘same shape’
- Isomorphs have the same proportions of ions that are approximately the same size
- Examples are the Olivine minerals
  - Forsterite Mg_2SiO_4
  - Fayalite Fe_2SiO_4
  - Continuous variation between these minerals
  - These pure compositions are called end-members
  - General formula for Olivine group is $(Mg,Fe)_2 SiO_4$

Ionic Substitution

- Isomorphism occurs by substitution of ions
- In Olivine, Fe^{2+} can substitute for Mg^{2+} because:
  - the ionic radii are very similar: Fe = 0.66, Mg = 0.74 Å
  - the charges are the same
- Also called “Solid-Solution”
  - analogous to liquid solution
- Ionic Substitution is common in minerals
- Can occur wherever:
  - different ions have similar ionic size
  - charge balance in the lattice can be maintained

Olivine

$(Fe,Mg)_2SiO_4$

REFERENCES

- Hamblin & Christiansen (9ed), Chapter 3, p.55-66
- Skinner and Porter, Chapter 3, p. 48-49
- Clark and Cook, Chapter 6c, p. 128-129