

625-102 GEOLOGY



Lecture 2

Atomic Structures of Minerals

Melbourne Earth Sciences

Mineral properties controlled by:

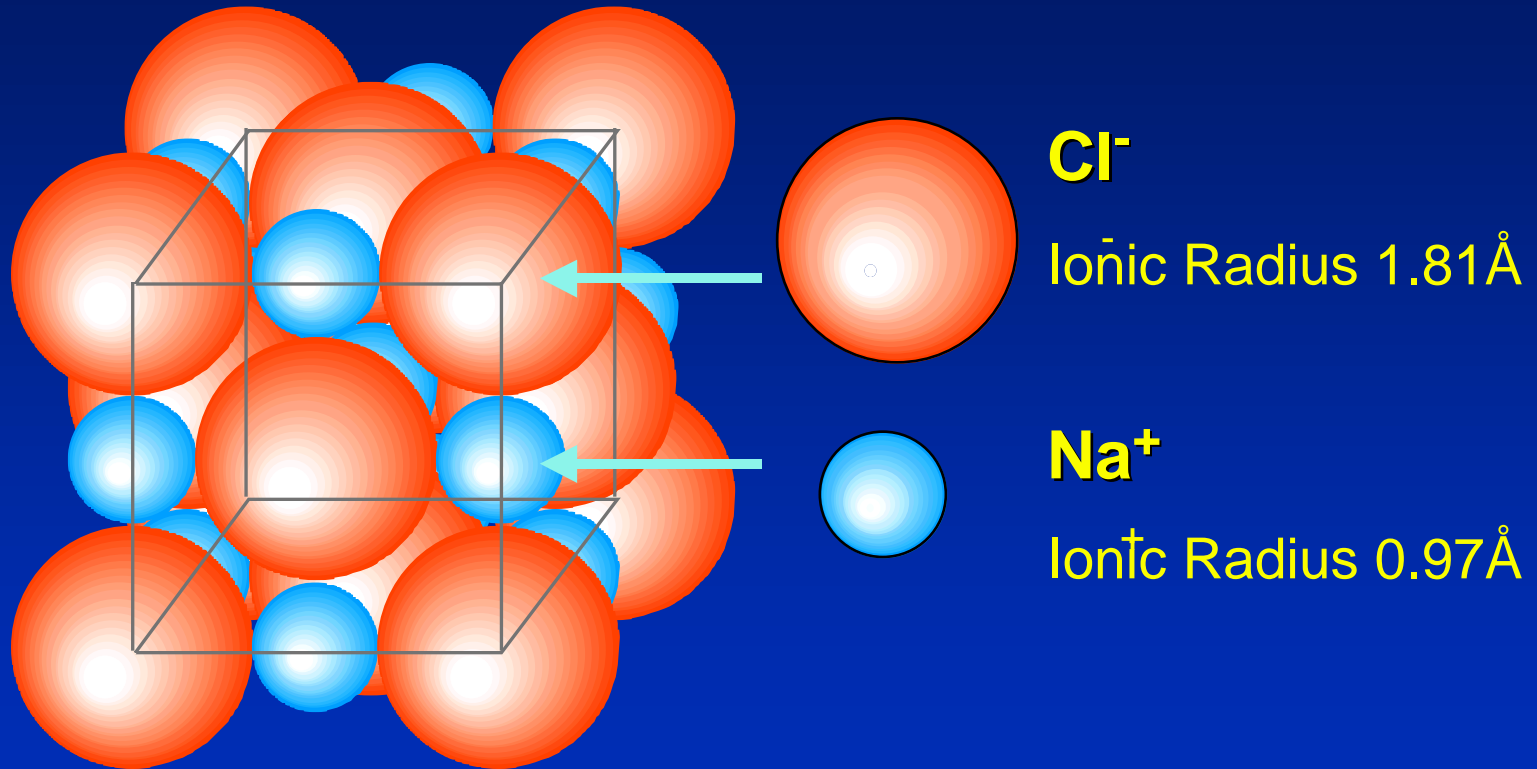
RECAP OF LECTURE 1

- **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

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

Halite Structure (NaCl)



Note: each ion is surrounded by 6 others

Coordination Number

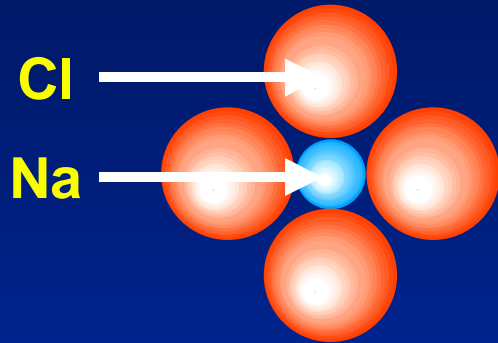
- **Coordination Number**

- The **number of Anions (-ve) around each Cation (+ve)**
- **Controlled by the ionic radii** of the cations and anions

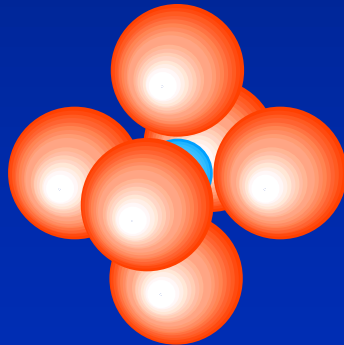
- **Ionic Radii**

- Sodium (Na^+) 0.97 Å
- Chlorine (Cl^-) 1.81 Å
- Caesium (Cs^+) 1.67 Å

Sodium Chloride

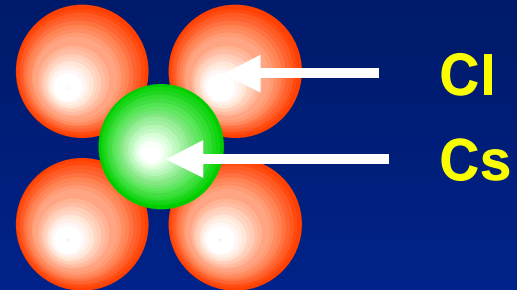


Na^+ Ionic Radius 0.97\AA

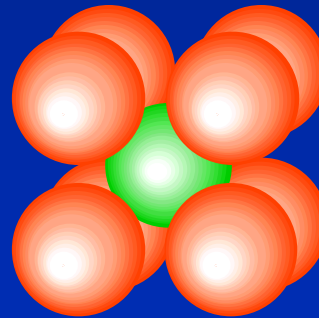


➔ 6-fold Coordination

Caesium Chloride



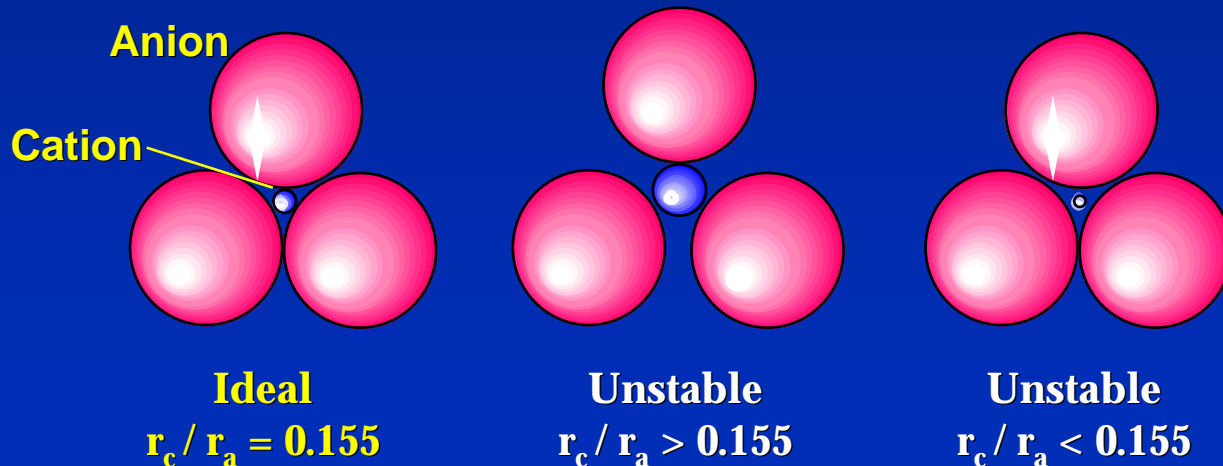
Cs^+ Ionic Radius 1.67\AA



➔ 8-fold Coordination

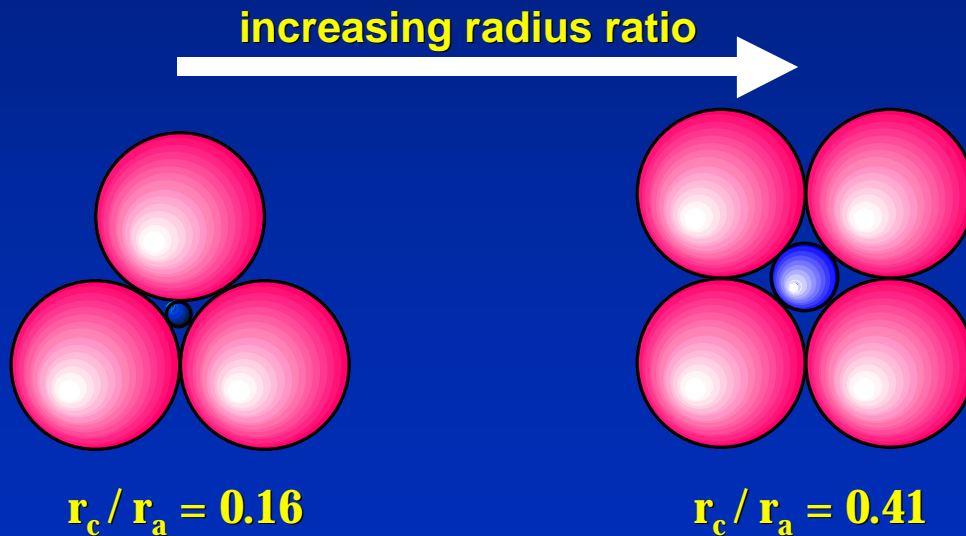
Radius Ratio 1

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

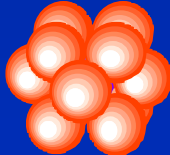


Radius Ratio 2

- 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

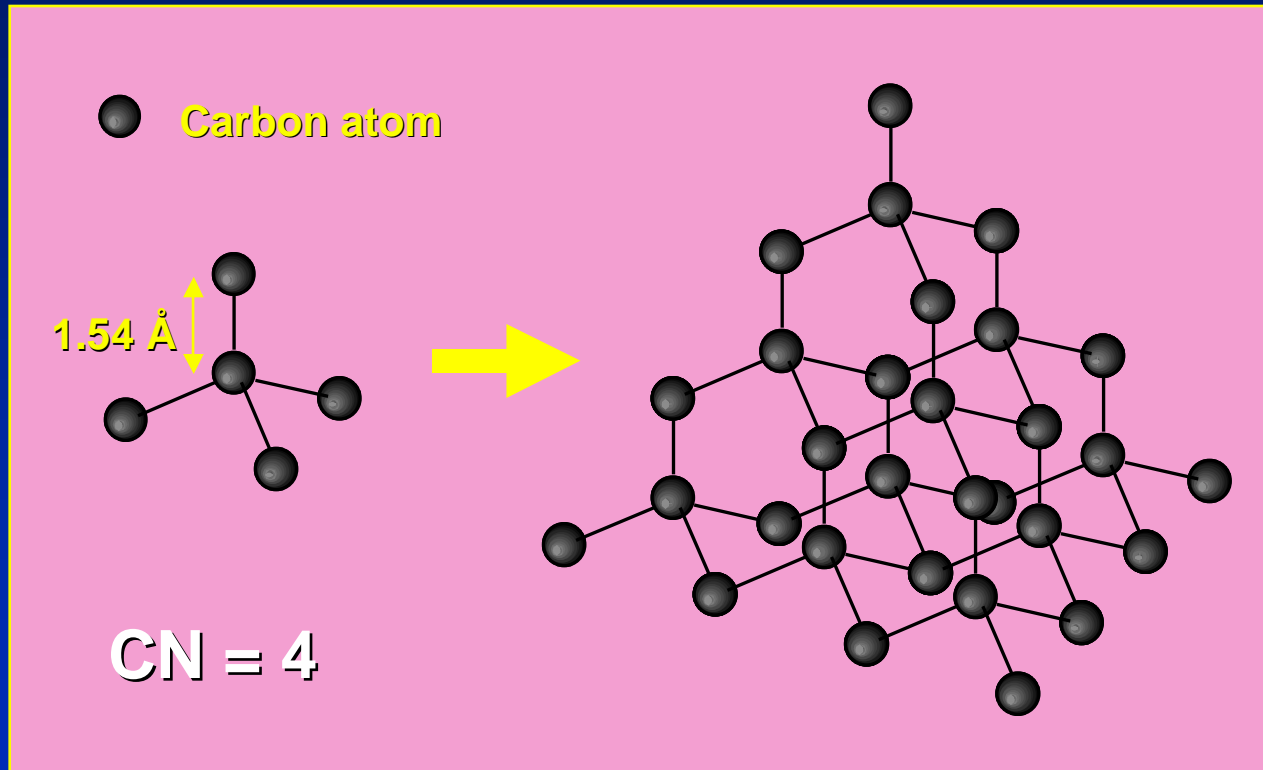
Density

3.50

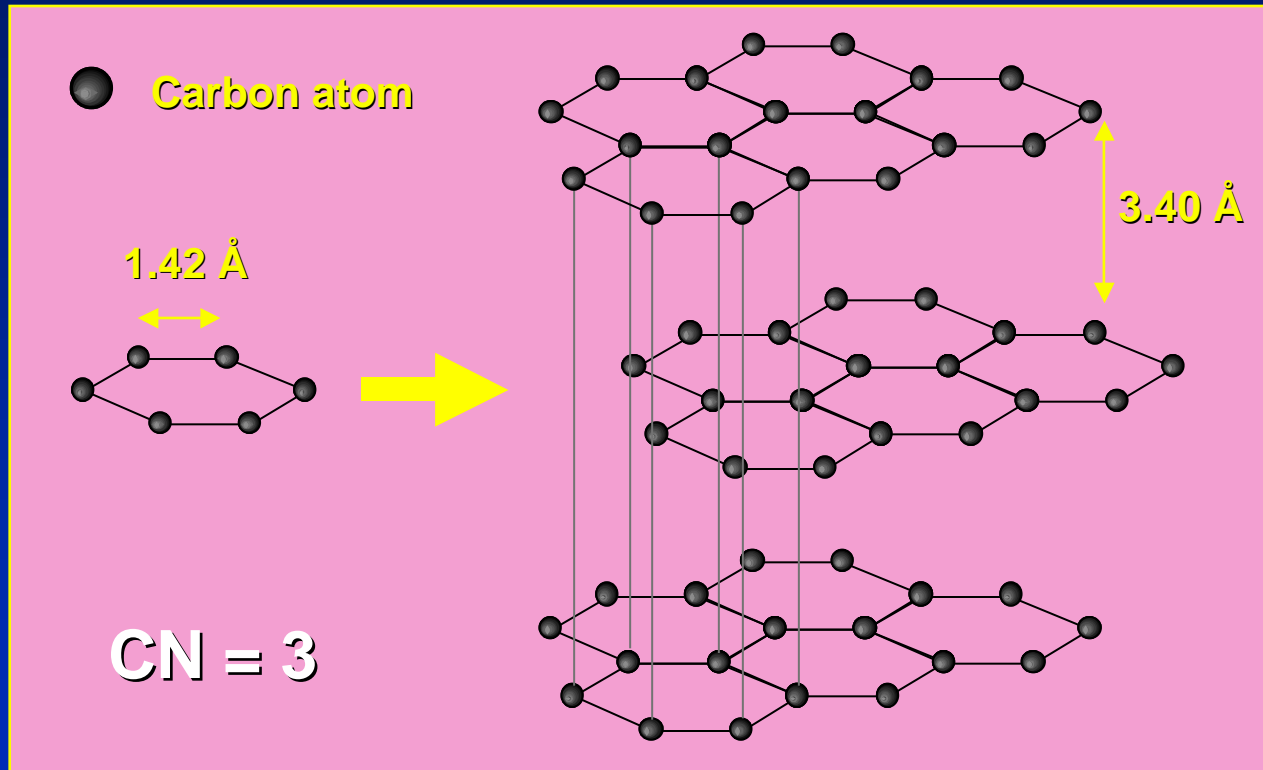
2.2



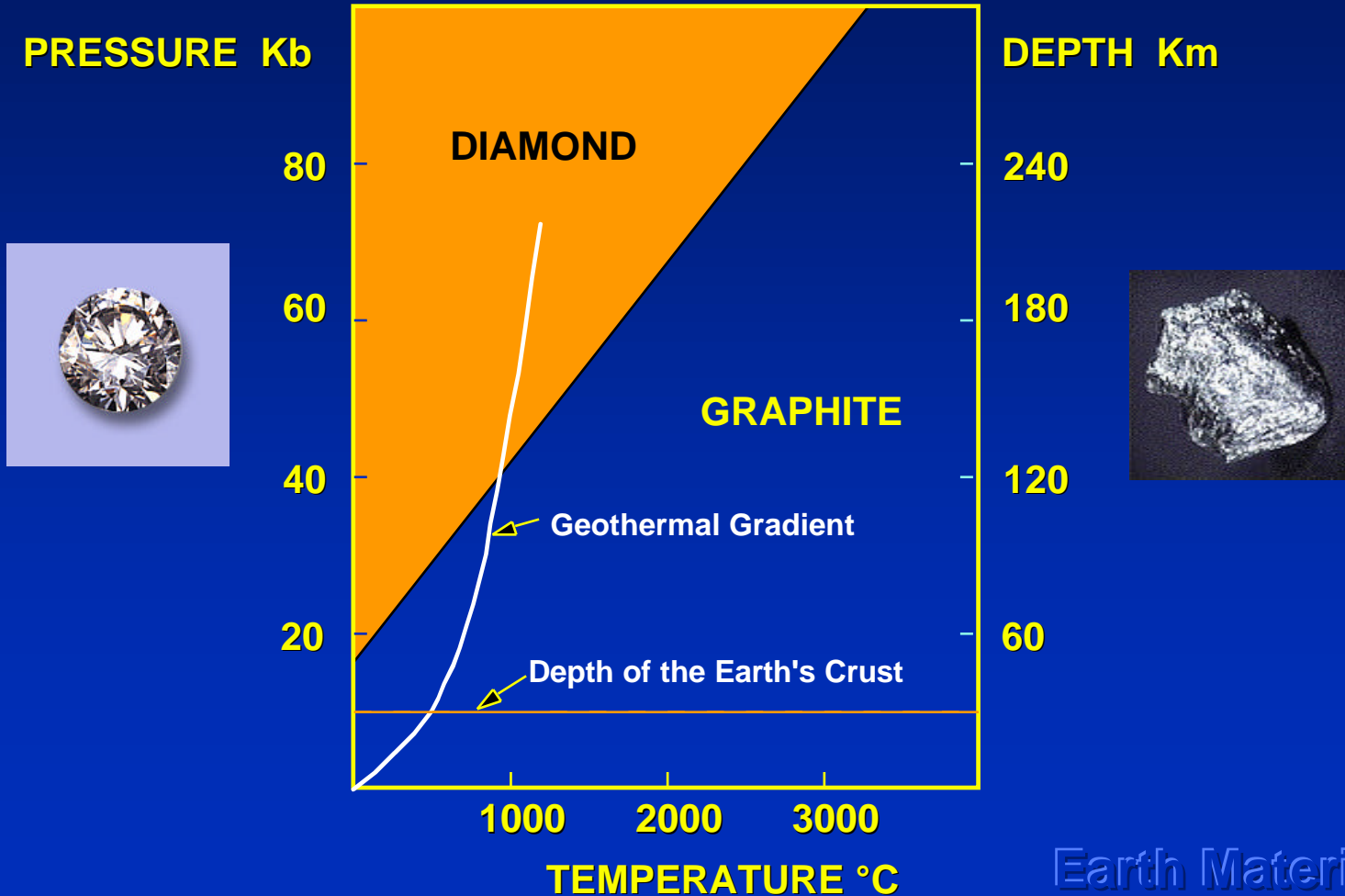
Diamond Structure



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 $(\text{Mg,Fe})_2 \text{SiO}_4$

Ionic Substitution

- **Isomorphism** occurs by **substitution of ions**
- In Olivine, Fe^{2+} can substitute for Mg^{2+} because:
 - the **ionic radii are very similar**: $\text{Fe} = 0.66$, $\text{Mg} = 0.74 \text{ \AA}$
 - 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



REFERENCES

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