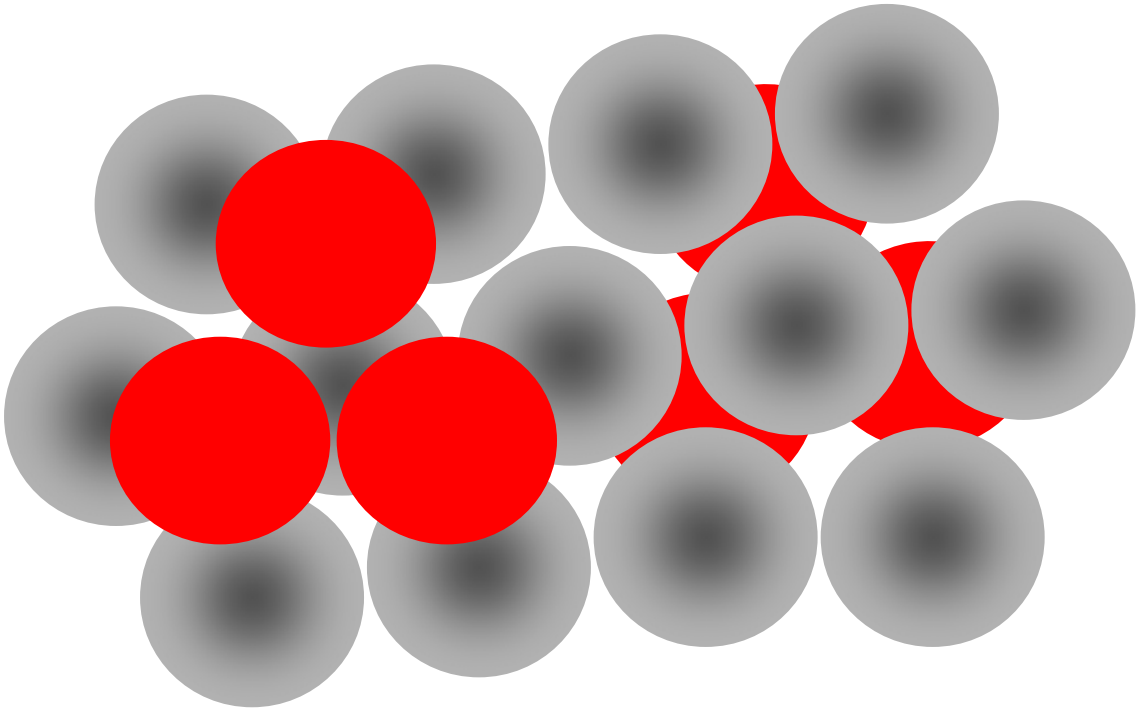
Structure

Interatomic Forces

Overview

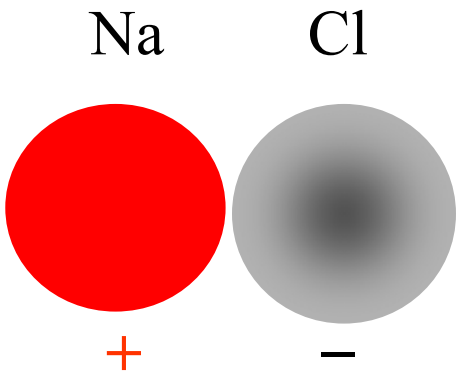
- Van der Walls (short range $V \sim 1/r^6$, weak ~0.01-0.1 eV)
- Ionic (long range, $V \sim 1/r$, strong ~5-10 eV)
- Metallic (no simple dependence, ~0.1eV)
- Covalent (no simple dependence, directional,~3 eV)
- Hydrogen (partially ionic and covalent)

Van der Waals: short range, no directional preference



Atoms arrange into close-packed structures due to lack of directional dependence of interaction. Materials with **Metallic** bonding also adopt this structure.

IONIC BONDING: NO DIRECTIONAL DEPENDENCE



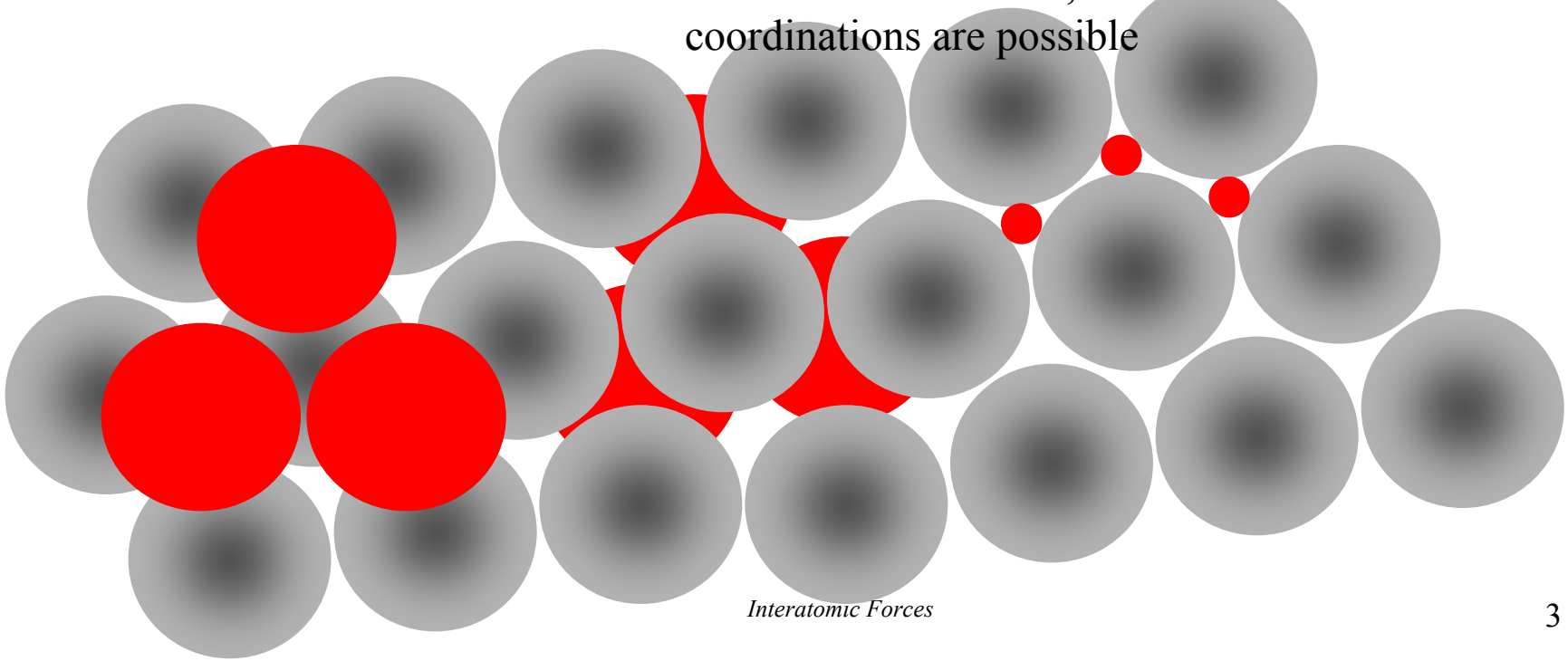
But the following must be taken into considerations to determine the structure:

a. Hetero-ionic numbers should be as high as poss2maximize electrostatic attraction

b. Like-ions must be as far ass poss2minimize repulsion

c. Local electro-neutrality must be preserved

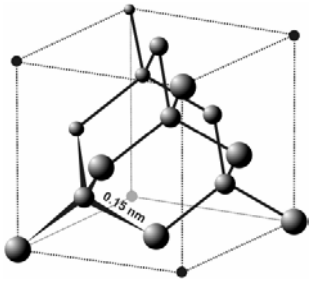
d. Size also matters here, hence 6 and 4-fold coordinations are possible



COVALENT FORCES: highly directional bonds

are forever?

Structure:



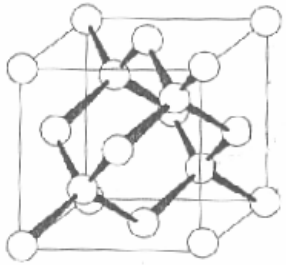
a. Determined by the bond forming direction (hybridisation)

b. Low coordination (<6)

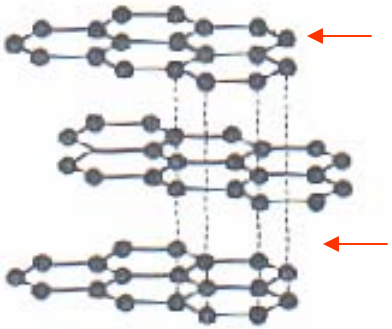
c. Low density

Carbon allotropes

Diamond



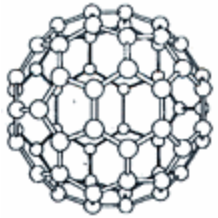
Graphite



covalent

vdW

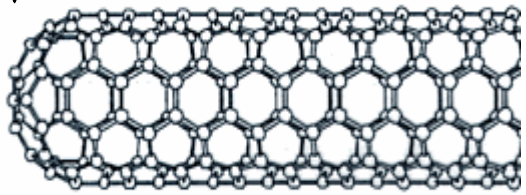
Fullerenes



d=0.7 nm

Carbon nanotubes

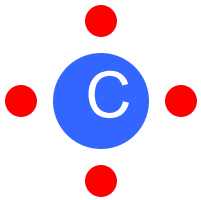
d~1.4 nm



Carbyne

≡C – C ≡ C – C ≡ C –

E.g. Carbon: covalently bonded material



4 moveable
outer electrons

IA	IIA	IIIB	IVB	VB	VI B	VII B	VIII B
H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar

Triple bond → 6 electrons → C ≡ C → 180°

Double bond → 4 electrons → C = C → 120°

Single bond → 2 electrons → C — C → 109.5°

HYDROGEN BOND: H atoms form single covalent bond to form H_2, but fully or partially ionised can form essentially ionic bonds with e.g. O (H_2O), N (NH_3) or F (HF). Bond is part (about 90%) electrostatic and part (about 10%) covalent

The water molecule: