Crystal Structure

CRYSTAL STRUCTURES

Lecture 2

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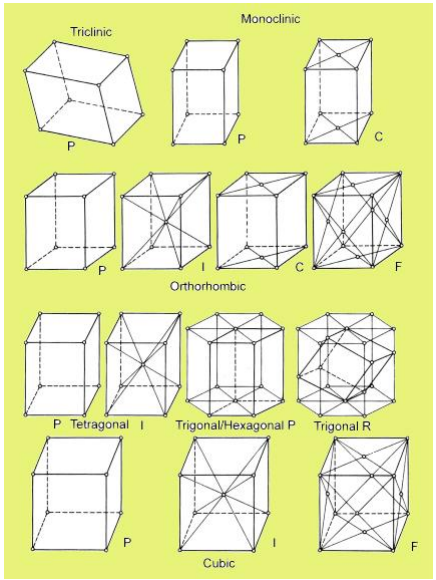
Lattice and Basis

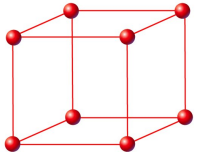
1.4.8 Fourteen Lattices in Three Dimensions



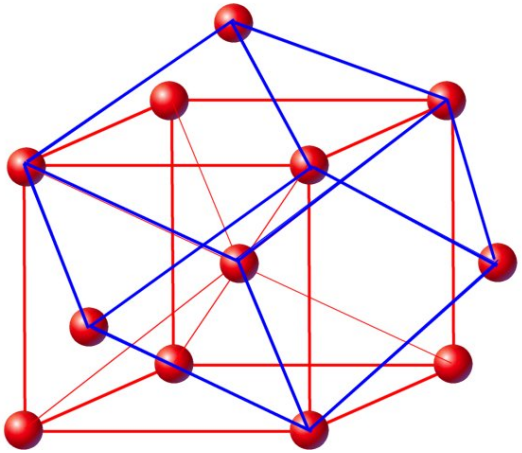
System	Type	Restrictions
Triclinic	**P**	$a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma$
Monoclinic	**P,C**	$a \neq b \neq c, \quad \alpha = \gamma = 90^\circ \neq \beta$
Orthorhmobic	**P,C,I,F**	$a \neq b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$
Tetragonal	**P,I**	$a = b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$
Cubic	**P,I,F**[1]	$a = b = c, \quad \alpha = \beta = \gamma = 90^\circ$
Trigonal	**P**	$a = b = c, \quad \alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
Hexagonal	**P**	$a = b \neq c, \quad \alpha = \beta = 90^\circ, \ \gamma = 120^\circ$

No need to learn details except for cubic, basic ideas of hexagonal.

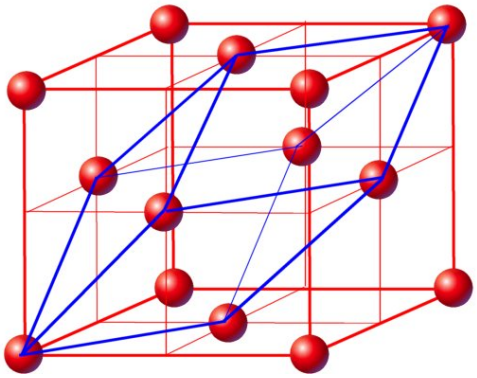
1.4.9 Cubic Unit Cells



Primitive Unit Cells of cubic system Simple cubic: cube containing one lattice point (or 8 corner points each shared among 8 cubes: $8 \times \frac{1}{8} = 1$).
Body centred cubic: 2 points in cubic cell



Rhombohedral primitive cell of body centred cubic system.
Face centred cubic: 4 points in cubic cell (8 corner points shared 8 ways, 6 face points shared 2 ways: $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$.



Rhombohedral primitive cell of face centred cubic system.
We will work with non-primitive, conventional cubic cells.

1.4.10 Length Scale

Typical interatomic distance: a few Ångstroms, say 0.25 nm.

1.4.11 Cell Volume

If the primitive lattice vectors are $\underline{a}$, $\underline{b}$ and $\underline{c}$, the cell volume is $|\underline{a}.\underline{b}\times\underline{c}|$. The lengths of the lattice vectors, $a = |\underline{a}|$ etc., are called the *lattice parameters*. For cubic crystals, $a = b = c$, so cell volume is a^3.

1.4.12 The basis

So far we have been in the realm of abstract mathematics – now we need to attach the motif, the pattern itself, the atoms, to the lattice. The *basis* is the arrangement of atoms associated with each lattice point. Sometimes there is only one atom per lattice point – a *monatomic* lattice – but often there are more. Mathematically, this association of one copy of something with every point is a *convolution*.

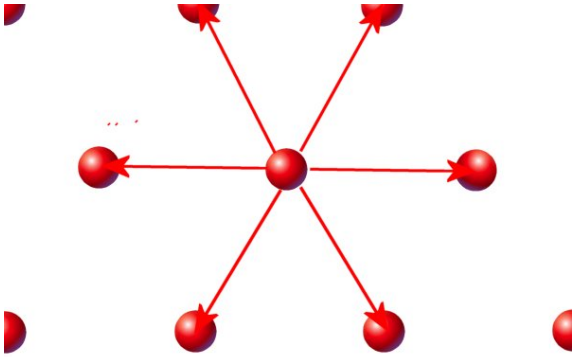
1.4.13 Monatomic crystals

Some elements crystallize in forms with only one atom per unti cell:

- **copper – face-centred cubic**
- **iron (at low temperatures) – body-centred cubic**
- **polonium – simple cubic**

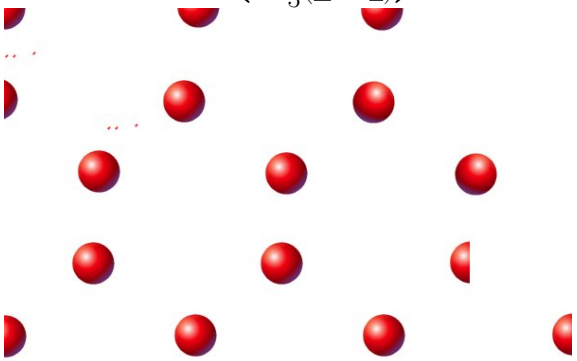
1.5 Planar Hexagonal

Each lattice point is hexagonally coordinated (six neighbours at equal distances)

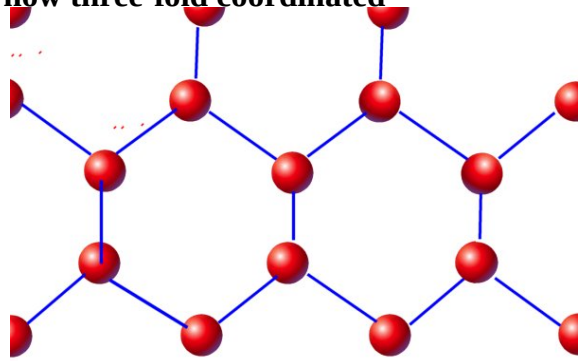


No atom forms bonds in quite that way.

Add another atom in each cell (at $\frac{1}{3}(\underline{a}+\underline{b})$).

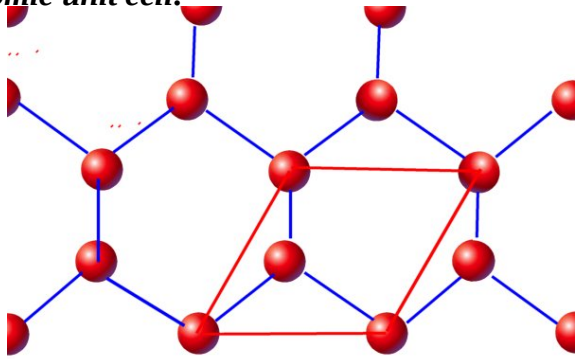


Each atom is now three-fold coordinated



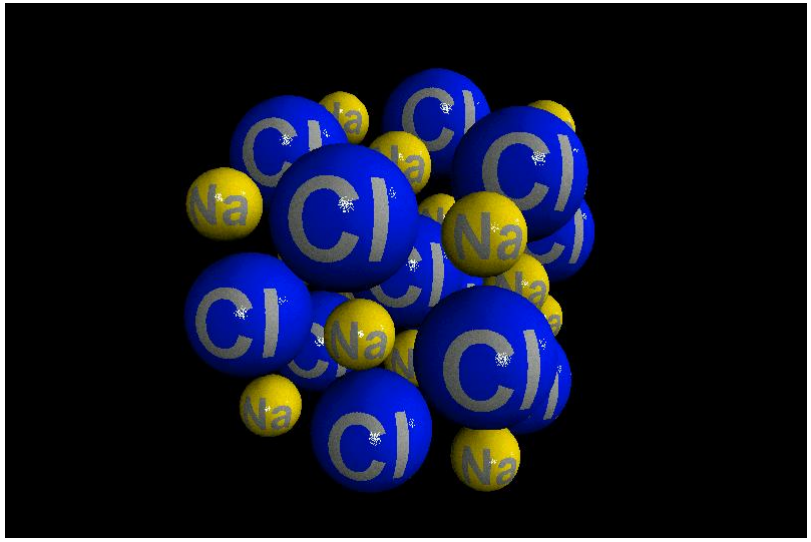
as in one of the planes of graphite.

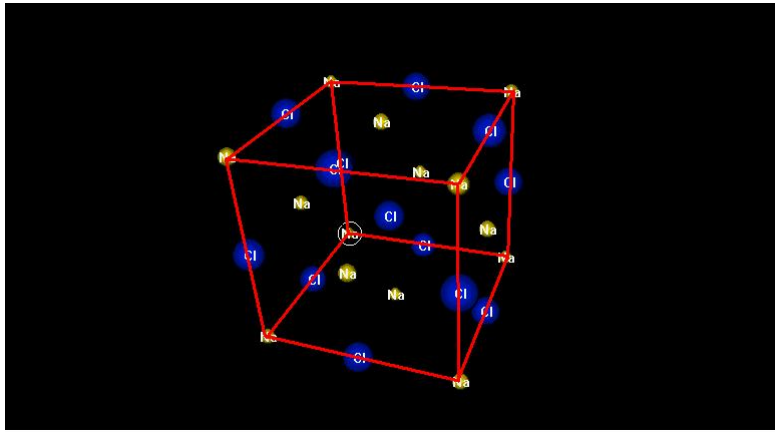
This is a *diatomic unit cell*.

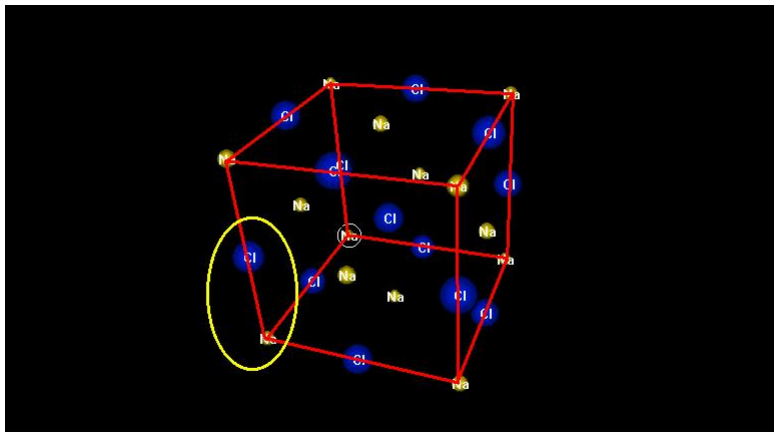


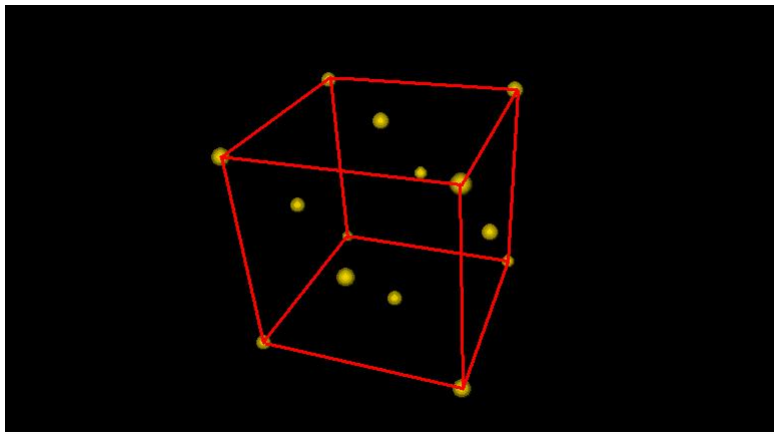
1.6 Cubic crystals

1.6.1 Sodium Chloride





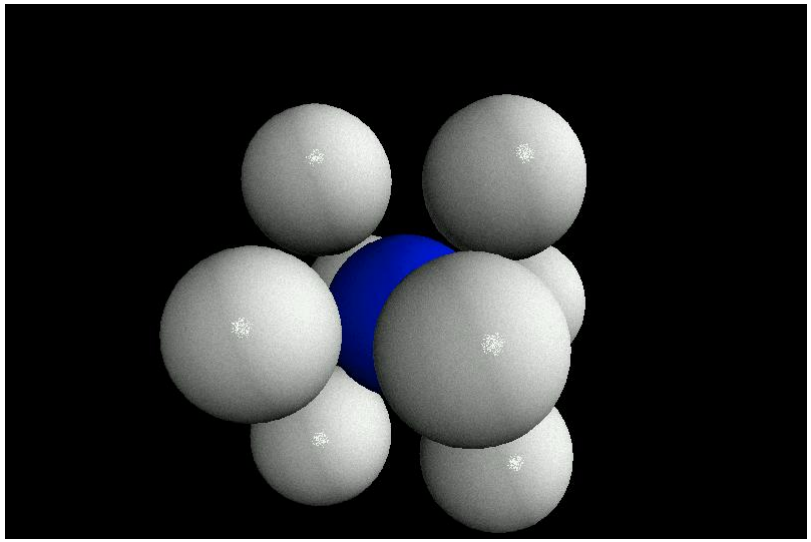


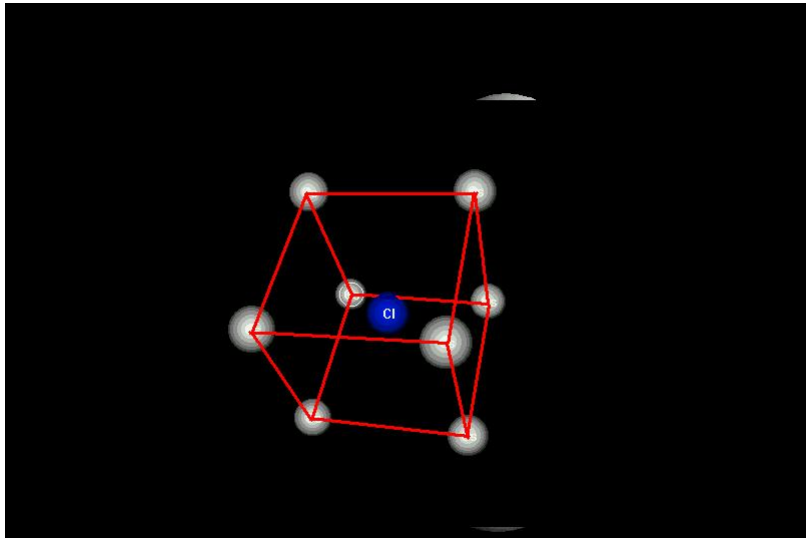


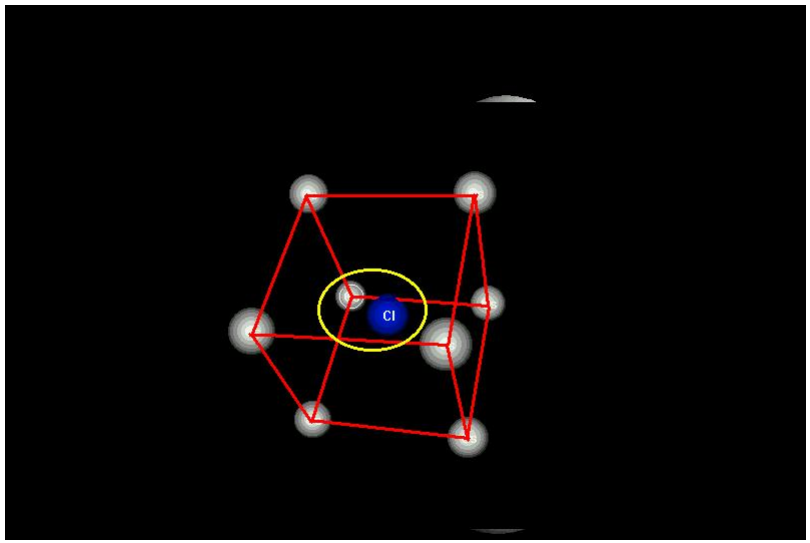
NaCl is a face-centred cubic structure. That is:

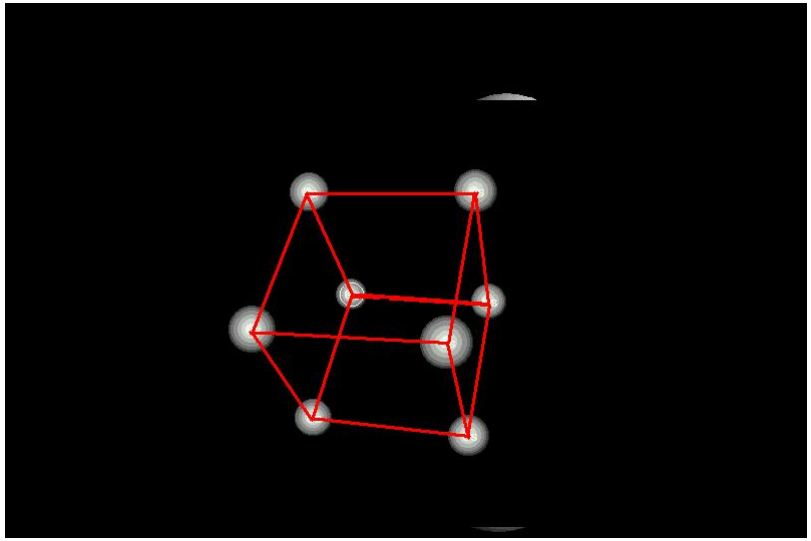
- **look at the structure**
- **identify the repeat unit**
- **focus on one atom in the repeat unit**
- **the lattice is revealed by the pattern of that atom**

1.6.2 Caesium Chloride









CsCl is a simple cubic structure.

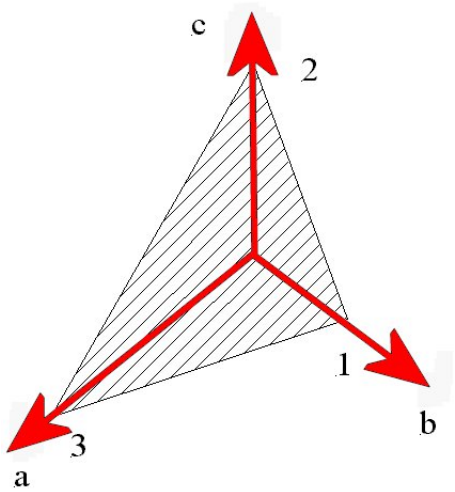
1.7 Planes, Lines etc

1.7.1 Miller Indices

To index a plane

- **find where the plane cuts the axes (at A, B, C)**
- **express the intercepts as $u\ a$, $v\ b$, $w\ c$**
- **reduce the *reciprocals* to the simplest set of integers h, k, l**
- **the plane is then the (hkl) plane.**
- **conventionally, choose h, k and l with common factors removed**
- **note if intercept is at infinity, corresponding index is 0.**
- **note convention: round brackets**
- **note convention: negative values are quoted with a bar over.**

Example:



Intercepts: 3a, 1b, 2c
Reciprocals 1/3, 1, 1/2
Miller Indices (2,6,3)

Families of planes:
the indices (hkl) may refer to a single plane, or to a set of parallel planes. The (100) planes are a set of planes perpendicular to the x-axis, a distance a apart. The (200) planes are a set of planes perpendicular to the x-axis, a distance $a/2$ apart.

1.7.2 Directions

Square bracket notation $[hkl]$. For cubic systems only, $[hkl]$ direction is perpendicular to (hkl) plane.

1.7.3 Symmetry-related sets

Of directions: $\langle hkl \rangle$
Of planes: $\{hkl\}$**.**

1.7.4 Spacing between planes

In a cubic system with lattice parameter (unit cell side) a, the (hkl) planes are separated by

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$

Think about the geometry, and thus the proof of this, before the next lecture.