Lecture 03

Tuesday, January 17, 2012

Cell

A [unit] cell of a Bravais lattice can be defined as non-overlapping and space-filling volume assigned to each lattice point.

For instance, a parallelepiped constructed from the three vectors $\vec{a}, \vec{b}, \vec{c}$ vectors that span the Bravais lattice is a good cell.

Wigner Seitz Cell

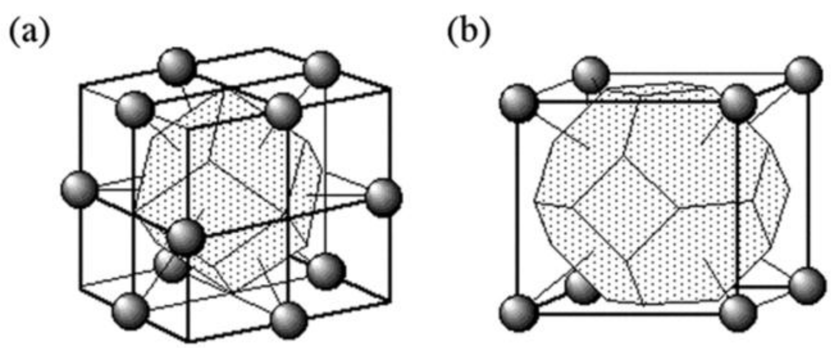
A unit cell constructed by collecting all points of space that are closer to a given lattice point than any other lattice points is called the Wigner Seitz cell.

By construction, a WS cell is an imprint of the local environment of the Bravais lattice and looks highly symmetric, revealing the full symmetry of the BL.

Operationally, a WS cell can be obtained by considering perpendicular bisector planes of all lattice translation vectors from a given lattice point. Starting from that lattice point, any points that can be connected without crossing any bisector planes form the Wigner Seitz cell around that lattice point.

Face centered cubic (fcc)
(note that the origin is shifted)

Body centered cubic (bcc)

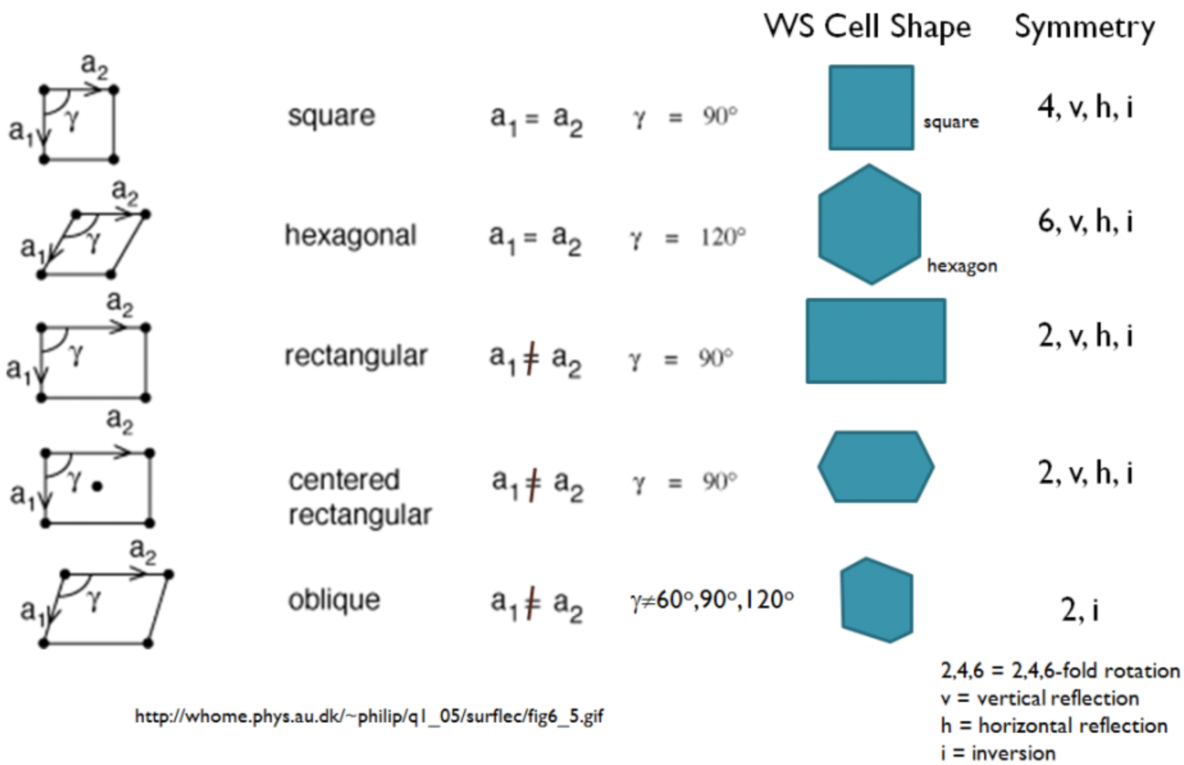


rhombic dodecahedron   truncated octahedron

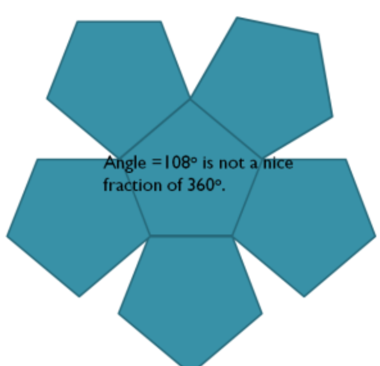
http://journals.iucr.org/j/issues/2003/04/00/ks7313/ks7313fig6.html

Classification of BL

In 2D, there are 5 possible kinds of BL. They are listed here. Note that by symmetry alone, one can conclude that the reciprocal of a square/hexagonal/oblique BL is another square/hexagonal/oblique BL.



Why not (regular) pentagon?



There is NO 5-fold (or 10-fold) lattice/crystal.

In 3D, there are 14 BLs (see page 9 of text). Given a BL, how symmetric the basis is defines the actual symmetry of the crystal. Thus, one talks about "space group" of a crystal, according to the symmetry. There are 230 space groups corresponding to all symmetries possible for 3D crystals. This is the subject of crystallography. For your information on crystallography, check out

- Crystal Group
  e.g. http://img.chem.ucl.ac.uk/sgp/mainmenu.htm
- Real crystal struct. data base (real compounds)
  e.g. http://icsd.ill.fr/icsd/index.html

Reciprocal Lattice

For a given BL spanned by $\vec{a}, \vec{b}, \vec{c}$, its reciprocal is a BL spanned by $\vec{a}^*, \vec{b}^*, \vec{c}^*$, which are defined by

$$\vec{a}^* \cdot \vec{a} = \vec{b}^* \cdot \vec{b} = \vec{c}^* \cdot \vec{c} = 2\pi$$

$$\vec{a}^* \cdot \vec{b} = \vec{a}^* \cdot \vec{c} = \vec{b}^* \cdot \vec{a} = \vec{b}^* \cdot \vec{c} = \vec{c}^* \cdot \vec{a} = \vec{c}^* \cdot \vec{b} = 0$$

A general D-dimensional case with spanning vectors $\vec{a}_i$ $(i = 1..D)$, we have

$$\vec{a}_i{}^* \cdot \vec{a}_j = 2\pi\delta_{ij}$$

One can show (homework) that the volume of the cell of the original BL, V, and the volume of the cell of the reciprocal BL, V^*, satisfies

$$V^* V = (2\pi)^D$$

In 2D, for example, the product of the area of the unit cell in real space and the area of the unit cell in the reciprocal space would be $4\pi^2$.

The above definition of the reciprocal BL is good enough to calculate it given a BL.

Note that the reciprocal of the reciprocal BL is the original BL. Since the above definition is symmetric w.r.t. $\vec{a}_i$ and $\vec{a}_i^*$, this is obvious.

In 3D, more explicit expressions can be obtained for computing $\vec{a}^*, \vec{b}^*, \vec{c}^*$.

$$\vec{a}^* = 2\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})}, \qquad \vec{b}^* = 2\pi \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})}, \qquad \vec{c}^* = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot (\vec{a} \times \vec{b})}$$

$$V = \vec{a} \cdot (\vec{b} \times \vec{c}) = \vec{b} \cdot (\vec{c} \times \vec{a}) = \vec{c} \cdot (\vec{a} \times \vec{b})$$

Some properties of the reciprocal lattice:

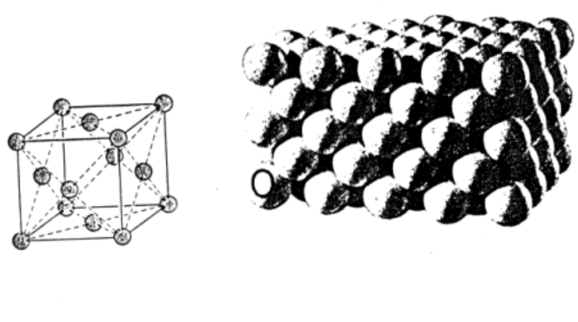
- The reciprocal is a BL also.

- Its reciprocal is the original BL (proved above).
- The reciprocal BL as the same symmetry as the original BL. (Two different views of the same thing -- the crystal with the basis replaced by a sphere.)
- $V^*V = (2\pi)^D$ (V, V^*: unit cell volumes)
- Dense if the original BL is sparse and vice versa ($V^*V = (2\pi)^D$).

Some crystal structures

Inert Gas Elements
He, Ne, Ar, Kr, Xe

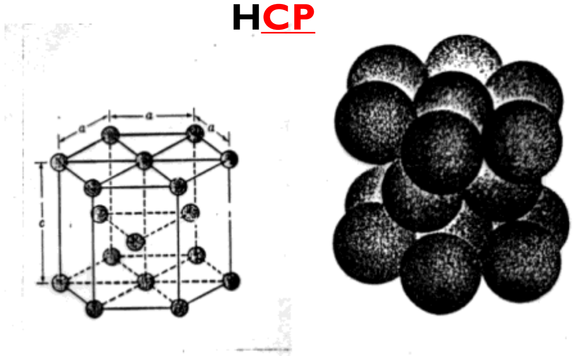
FCC (CCP)



Face Centered Cubic Lattice

Inert Gas Elements
He

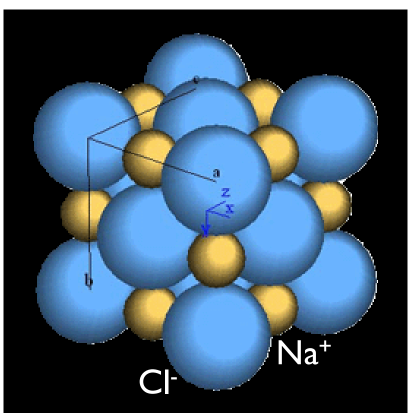
HCP



Hexagonal Lattices

http://www.ae.iitm.ac.in/~sriram/as401/materials

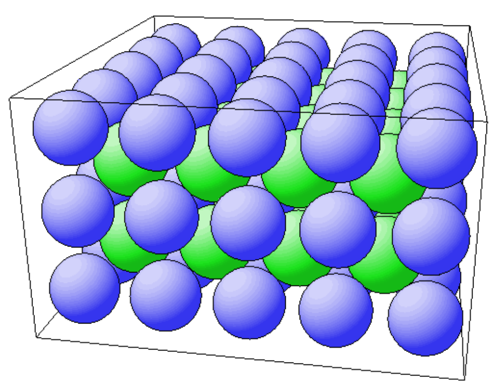
- NaCl



http://www.matsci.ucdavis.edu/MatSciLT/ENG-45L/images/CaRlne.gif

Cl^- bigger than Na^+, by a factor of 2
Looks like close packing of bigger ions
fcc with two atom basis

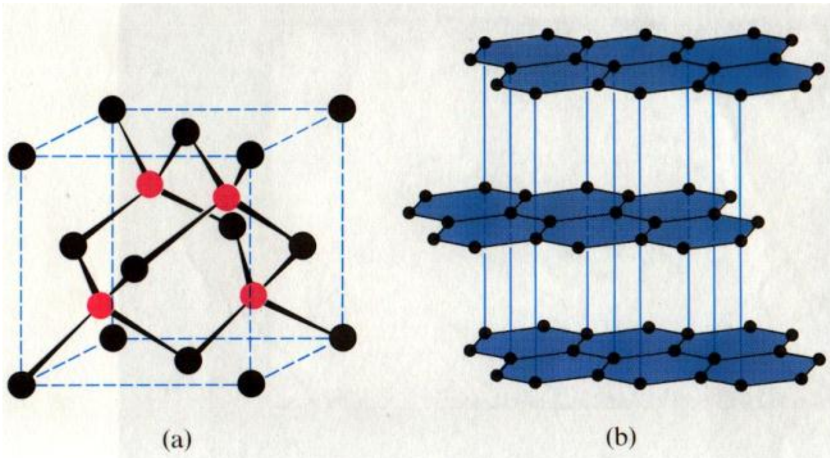
- CsCl

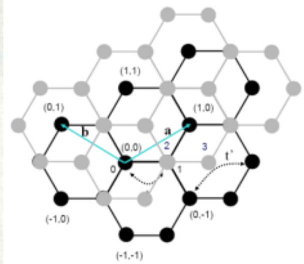


http://www.cmmp.ucl.ac.uk/~ijf/3c25/CsCl.gif

sc (simple cubic) with two atom basis

- Diamond
- Graphite





Top view
Gray=top
Black=next layer

http://library.tedankara.k12.tr/chemistry/vol2/allotropy/h76.jpg

fcc with two atom basis
000 and ¼, ¼, ¼
ZnS, Si, Ge, GaAs
sp3 covalent bonding

Hexagonal with four atom basis
sp2 bonding
Weak inter-plane bonding ("Van der Waals")
More stable than diamond!