PHYS485
Materials Physics

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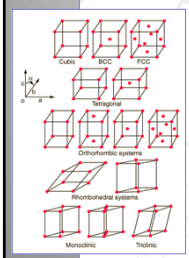
Bravais Lattices

The Fourteen Bravais Lattices

The ways in which we can specify the lattice points in space and keep translational symmetry is limited. In 1848, Auguste Bravais demonstrated that there are in fact only fourteen possible point lattices and no more. For his efforts, the term Bravais lattice is often used in place of point lattice.



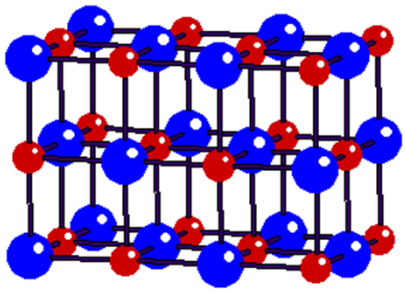
System	Number of Lattices	Lattice Symbol	Restriction on crystal cell angle
Cubic	3	P or sc, I or bcc,F or fcc	a=b=c α =β =γ=90°
Tetragonal	2	P, I	a=b≠c α=β =γ=90°
Orthorhombic	4	P, C, I, F	a≠b≠ c α=β =γ=90°
Monoclinic	2	F, C	a≠b≠ c α=β=90 °≠β
Triclinic	1	P	a≠b≠ c α≠β≠γ
Trigonal	1	R	a=b=c α=β =γ <120° ,≠90°
Hexagonal	1	P	a=b≠c α =β =90° γ=120°

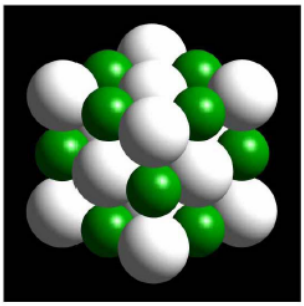
Table 1. Seven crystal systems make up fourteen Bravais lattice types in three dimensions.

P - Primitive: simple unit cell
F - Face-centred: additional point in the centre of each face
I - Body-centred: additional point in the centre of the cell
C - Centred: additional point in the centre of each end
R - Rhombohedral: Hexagonal class only

NaCl Structure

- Most alkali halides (group 1)
- Most oxides alkaline earths (group 2)
- Many nitrides, carbides, hydrides (*e.g.* ZrN, TiC, NaH)





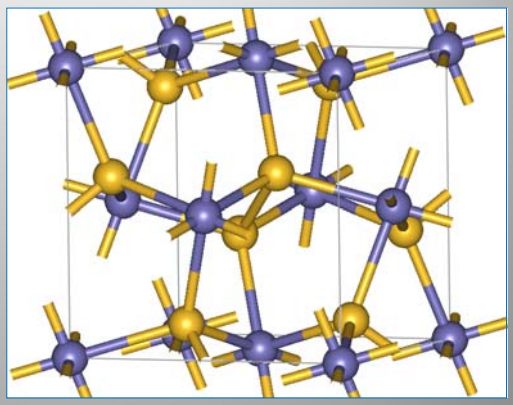
Face Centered Cubic Bravais Lattice
Two atoms (one Na, one Cl) per basis
In the conventional cubic lattice there are eight atoms per basis.

Ex. What are these eight atoms' positions?

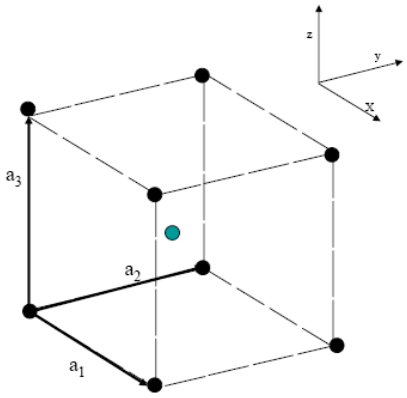
http://www.phys.psu.edu/~ralbert/phys412/chapter1.pdf

FeS_2 - pyrite

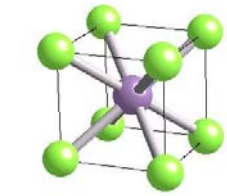
- Fe atoms occupy FCC sites
- 2 S atoms within cubic unit cell

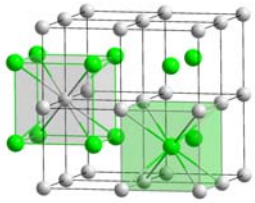


CsCl Structure



Simple Cubic Bravais Lattice
Two atoms per basis

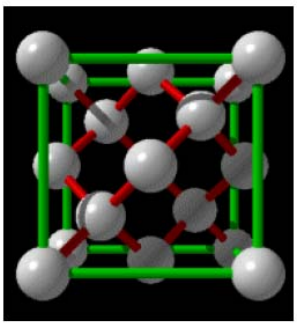


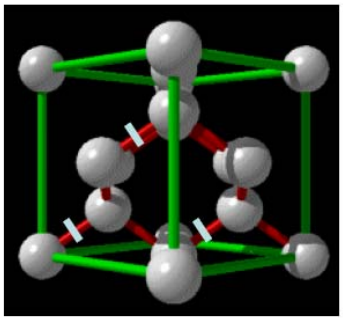


From http://www.ilpi.com/inorganic/structures/cscl/index.html

http://www.phys.psu.edu/~ralbert/phys412/chapter1.pdf

Diamond crystal structure





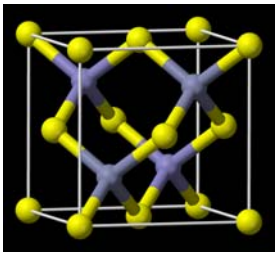
Face Centered Cubic Bravais Lattice
Two identical atoms per basis
Ex. What are the basis atoms' positions? How does the diamond structure differ from the NaCl structure?

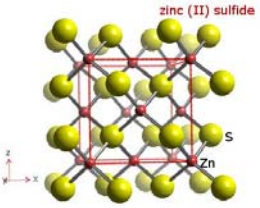
Note also ZnS (zinc blende) structure!

Zinc Sulfide (ZnS) Structure

- Mineral: sphalerite (zinc blende); chief ore of Zn
- Zn in FCC configuration with S tetrahedron within, S atoms at (1/4, 1/41/4), (3/4, 3/4,1/4), (1/4,3/4,3/4), & (3/4,1/4,3/4)

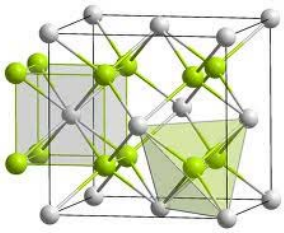
Ex: Cu(F,Cl,Br,I), AgI, Zn(S,Se,Te), Ga(P,As), Hg(S,Se,Te)

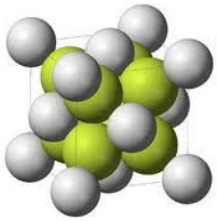




Fluorite (CaF_2) Structure

- FCC Ca^{2+} with F^- in all "tetrahedral holes"
- **4**CaF_2 in unit cell

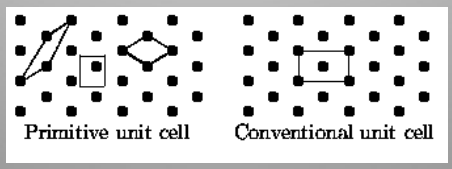




• Fluorides of large divalent cations, chlorides of Sr, Ba
• Oxides of large quadrivalent cations (Zr, Hf, Ce, Th, U)

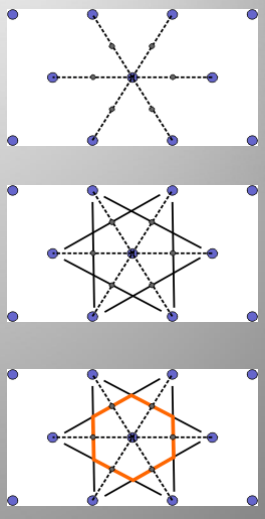
Unit Cells

- Unit cells are volumes that fill up space completely, no overlap
- A *primitive unit cell* contains exactly one Bravais lattice point; atoms in it can be used as basis to construct Xtal
- A *unit cell* can contain more than one lattice point; a *conventional unit cell* has been selected for each Bravais lattice

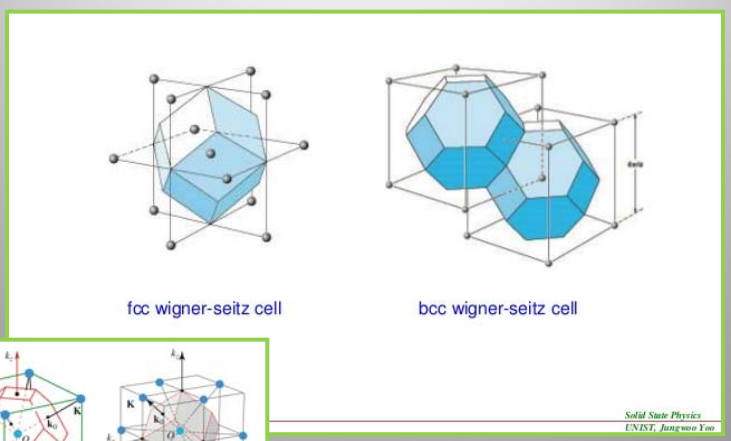


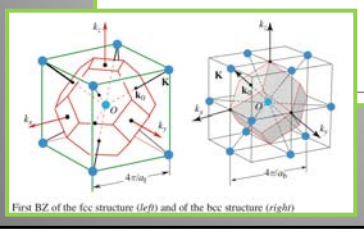
The Wigner-Seitz Cell

- Select a lattice point and draw construction lines to the nearest neighboring points.
- Draw lines that perpendicularly bisect the construction lines
- The smallest enclosed area represents the Wigner-Seitz cell. Here shown in orange.

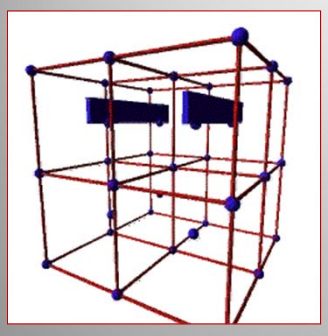


Wigner-Seitz cells

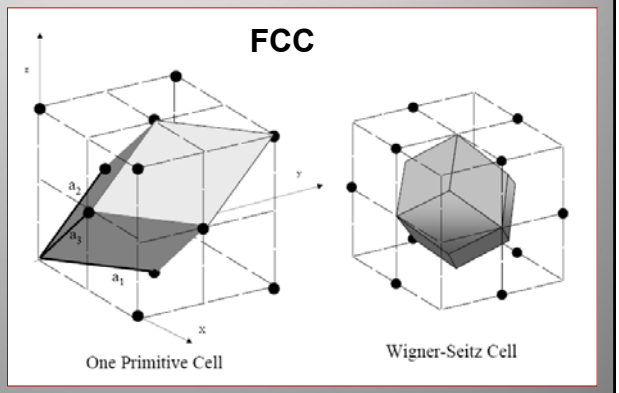




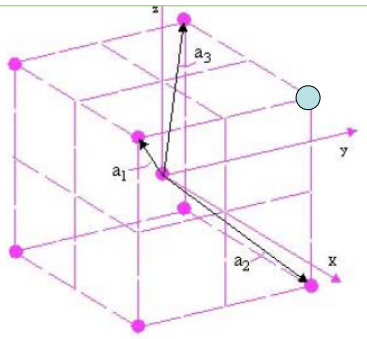
Wigner-Seitz cells



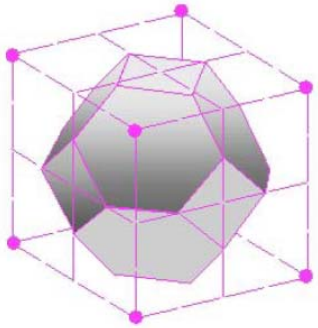
rhombic dodecahedron



BCC Structure



Body Centered Cubic Lattice



Wigner-Seitz Cell for
Body Centered Cubic Lattice

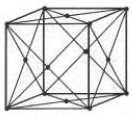
$$\vec{a}_1 = \frac{a}{2}(-\hat{i} + \hat{j} + \hat{k}), \quad \vec{a}_2 = \frac{a}{2}(\hat{i} - \hat{j} + \hat{k}), \quad \vec{a}_3 = \frac{a}{2}(\hat{i} + \hat{j} - \hat{k})$$

FCC Structure

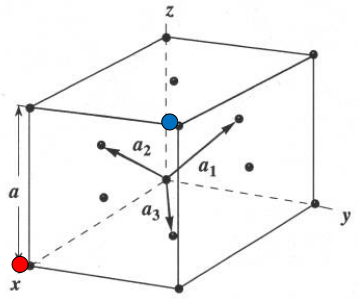
- Again, write down the primitive lattice vectors in terms of the Cartesian unit vectors!

$$\vec{a}_1 = \frac{a}{2}(\hat{j} + \hat{k}), \quad \vec{a}_2 = \frac{a}{2}(\hat{i} + \hat{k}), \quad \vec{a}_3 = \frac{a}{2}(\hat{i} + \hat{j})$$

- Indicate the positions of the red and blue atoms using this basis set.



fcc lattice



Directions, Planes, & Miller Indices

- Directions can be given by vectors in terms of the basis vectors [xyz]
- Perpendicular to these vectors are planes that are described by Miller indices (xyz)

- EX: Miller indices for simple cubic symmetry