Primitive cells, Wigner-Seitz cells, and 2D lattices

4P70, Solid State Physics

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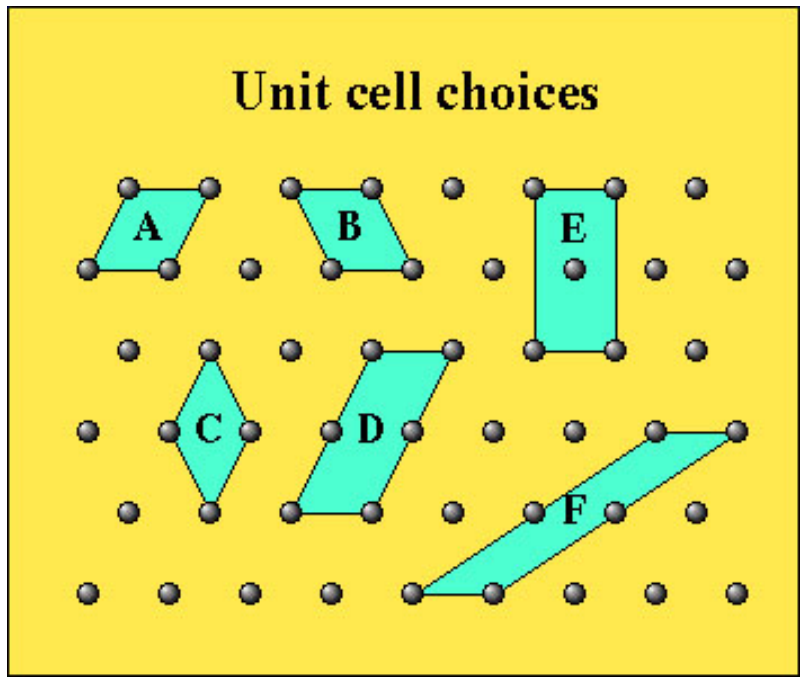
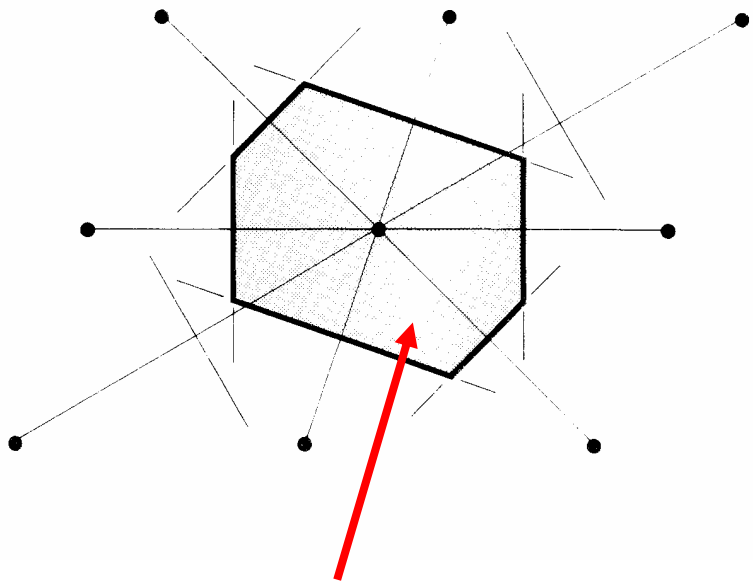
Choice of primitive cells

- Which unit cell is a good choice?
- A, B, and C are primitive unit cells. Why?
- D, E, and F are not. Why?
- Notice: the volumes of A, B, and C are the same. Also, the choice of origin is different, but it doesn't matter
- Also: There is only one lattice point in the primitive unit cells.



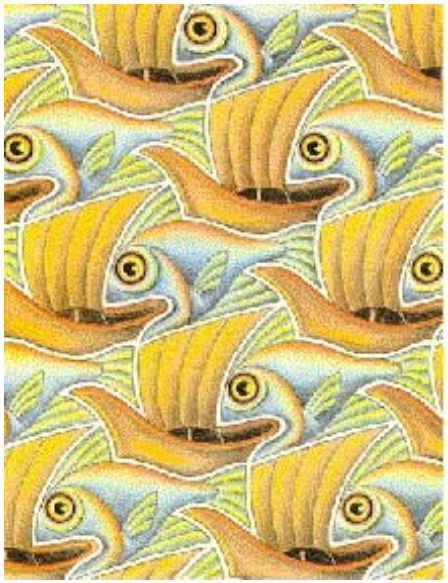
Wigner-Seitz cells

- How can we choose primitive cells?
- One algorithm is the Wigner-Seitz cell
- Steps: (1) Draw lines to connect a given lattice point to all nearby lattice points
- (2) At the midpoint and normal to these lines, draw new lines (or planes in 3D)
- (3) The smallest volume enclosed in this way is the Wigner-Seitz primitive cell

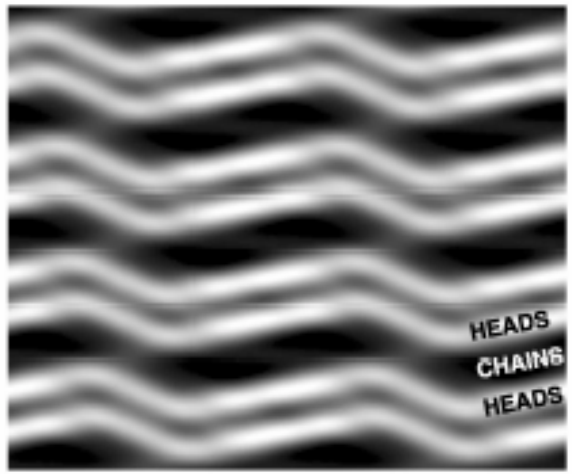


Wigner-Seitz cell

Finding Wigner-Seitz cells



(M. C. Escher)

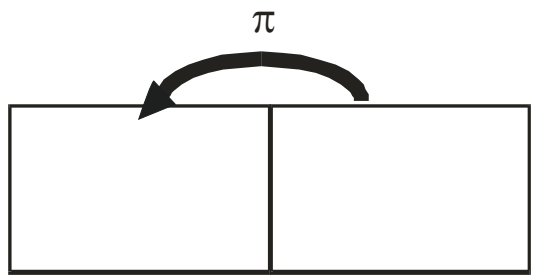


Phopholipid bilayers
(P. C. Mason *et al*, PRE, **63**, 030902 (2001))

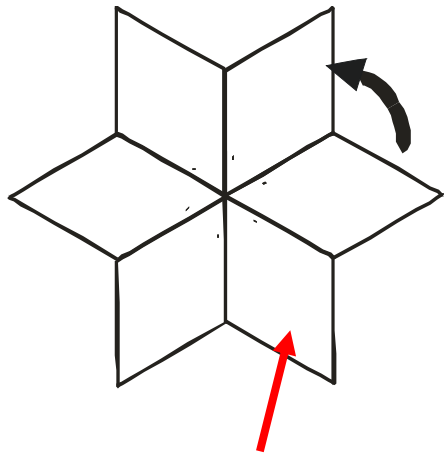
Homework: What are the Wigner-Seitz cells for these lattices?

Fundamental types of lattices

- Crystal lattices can be mapped into themselves by the lattice translations **T**, and by other symmetry operations
- Physicists use the symmetry of the unit cells to classify crystal structures and how they fill space.
- In this course, you will not have to know how this is done (this involves the use of point operations and translation operators)
- However, you do have to understand how we classify lattices
- In 2D, there are only 5 distinct lattices. These are defined by how you can rotate the cell contents (and get the same cell back), and if there are any mirror planes within the cell.
- From now on, we will call these distinct lattice types Bravais lattices.
- Unit cells made of these 5 types in 2D can fill space. All other ones cannot.



We can fill space with a rectangular lattice by 180 ° rotations (not 90° – why?)

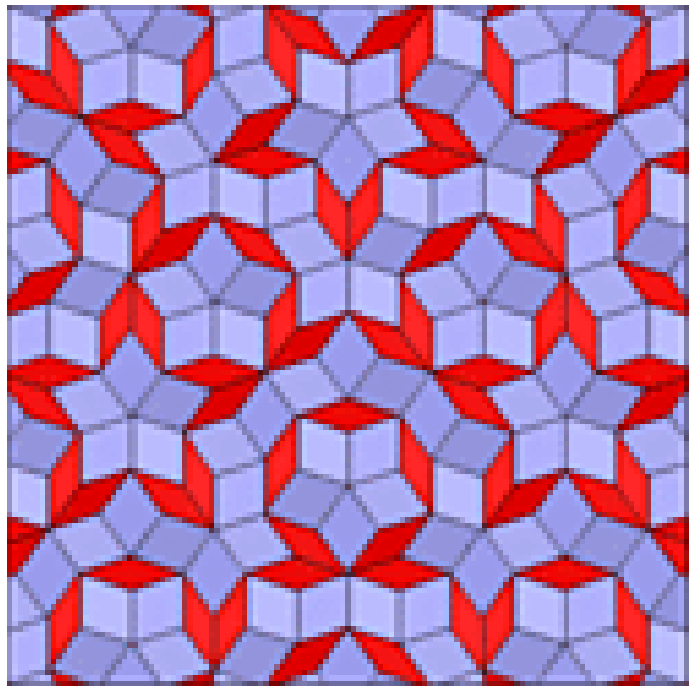


We can fill space with a hexagonal lattice by 60° rotations

Note: this is the primitive cell of a hexagonal lattice (why? See Kittel, fig 9b)

Fivefold rotations and quasicrystals

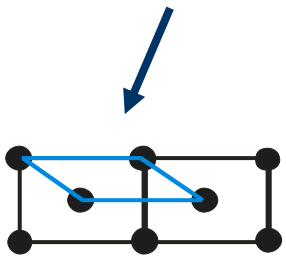
- It turns out that mathematicians discovered that you can only fill space by using rotations of unit cells by 2π, 2π/2, 2π/3, 2π/4, and 2π/6 radians (or, by 360^o, 180^o, 120^o, 90^o, and 60^0)
- But, rotations of the kind 2π/5 or 2π/7 do not fill space!
- A quasicrystal is a quasiperiodic nonrandom assembly of two types of figures (since we need two types, it is not a Bravais lattice – you cannot fill space with just one repeating unit cell)
- We will discuss these in Chapter Two



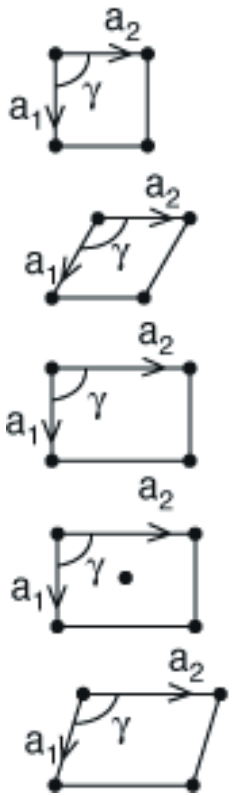
Penrose tiling in 2D

The 2D Bravais lattices

Note that this is the proper primitive cell for the centered rectangular lattice type (why? It contains only one lattice point)



(this is called a rhombus)



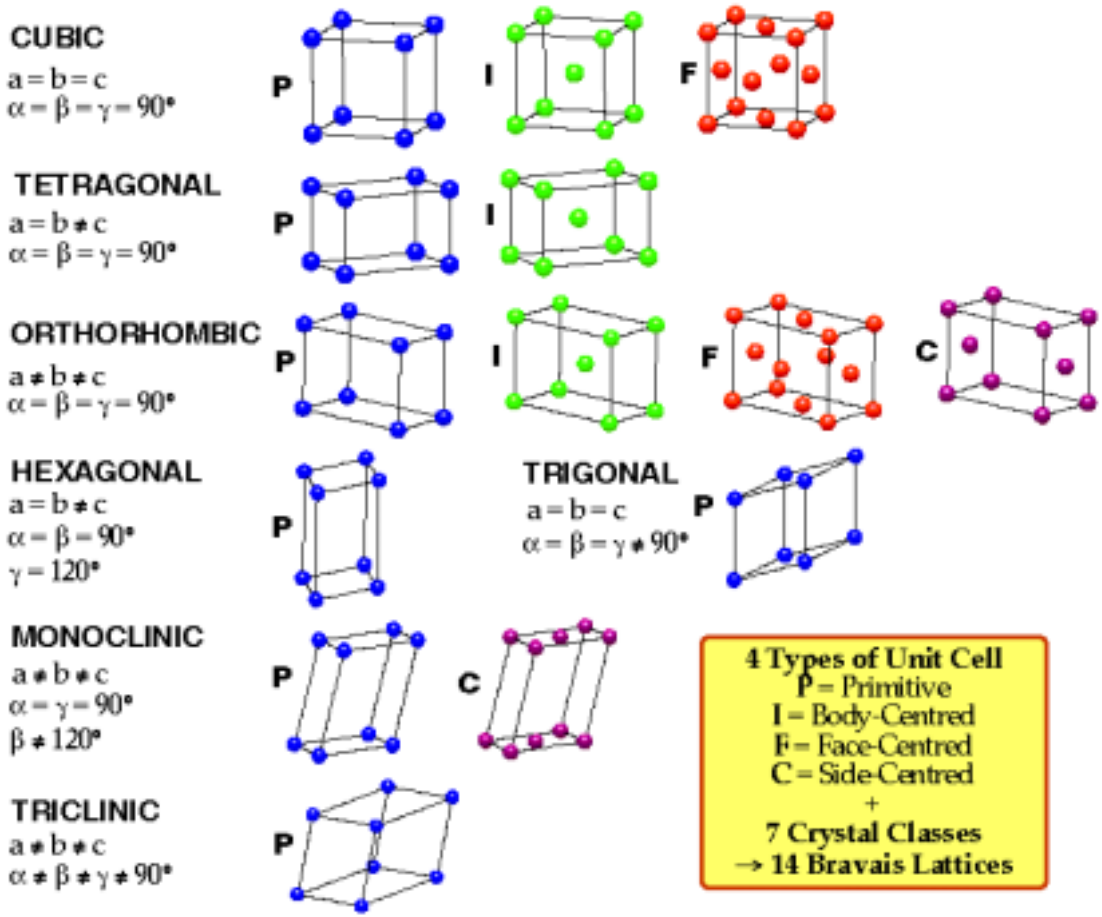
square	$a_1 = a_2$	$\gamma = 90°$
hexagonal	$a_1 = a_2$	$\gamma = 120°$
rectangular	$a_1 \neq a_2$	$\gamma = 90°$
centered rectangular	$a_1 \neq a_2$	$\gamma = 90°$
oblique	$a_1 \neq a_2$	γ π $90°, 120°$

The 3D Bravais Lattices

- In 3D, there are 7 lattice systems, which give rise to 14 bravais lattices
- The general lattice is triclinic, and all others are derived from putting restraints on the triclinic lattice
- Know the conditions of each lattice (excellent test question ☺)

Name	Number of Bravais lattices	Conditions
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = 90° \neq \gamma$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120° \neq 90°$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°, \gamma = 120°$

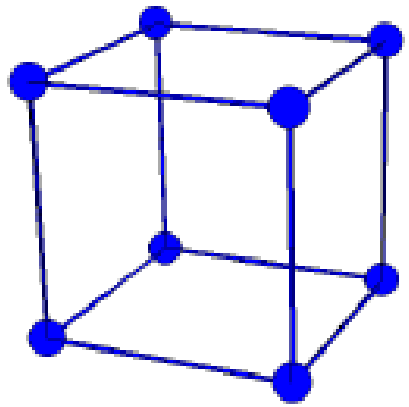
The 14 Bravais lattices in 3D



- Notice that we know have different lattice types:
- P = primitive (1 lattice point)
- I = Body-centred (2 lattice pts)
- F = Face- centred (4 lattice pts)
- C = Side-Centred (2 lattice pts)
- In this course, we will concentrate upon only a few of these types

Cubic lattices: SC, BCC and FCC

- For cubic systems, we have three bravais lattices: the simple cubic (SC), body-centred cubic (BCC) and face-centred cubic (FCC).
- The simple cubic has 1 lattice point per unit cell, with a total area of a^3
- Number of nearest neighbours: 6
- Nearest neighbour distance: a
- Number of next-nearest neighbours: 12
- Next-nearest neighbour distance: $\sqrt{2}a$ (prove this!)



Simple cubic lattice

Packing fraction = (atomic volume)/ (bravais unit cell volume)

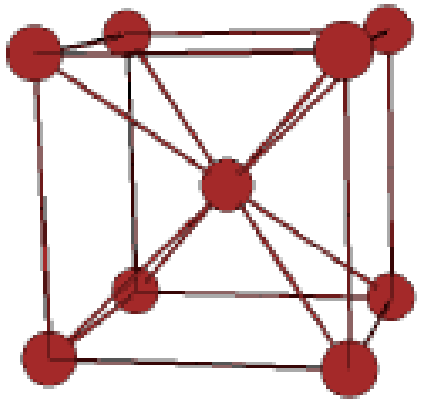
$$\frac{(4/3)\pi(a/2)^3}{(a^3)}$$

$$= \pi / 6$$

The Body-Centred Cubic Lattice

(Li (at room temp.), Na, K, V, Cr, Fe, Rb, Nb, Mo, Cs, Ba, Eu, Ta)

Body-Centred Cubic Lattice (BCC)



Packing fraction = (atomic volume)/ (bravais unit cell volume)

$$\frac{(4/3)\pi(\sqrt{3}a/4)^3}{(a^3/2)}$$

$$= \sqrt{3}\pi / 8$$

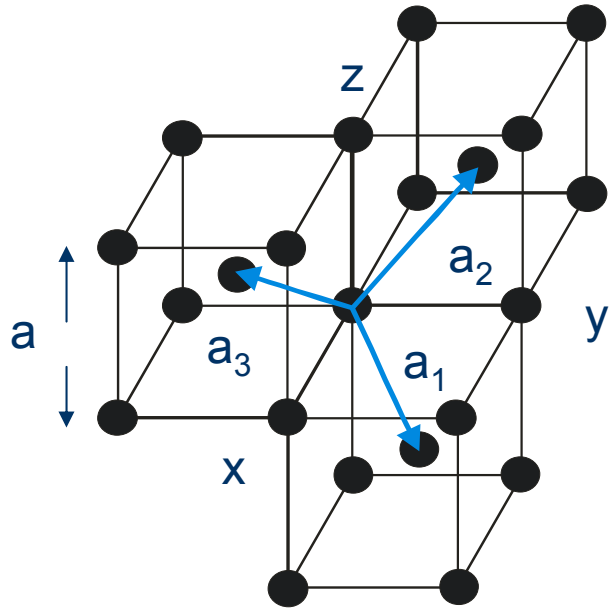
- The body-centred cubic lattice has 2 lattice points per unit cell, with a total primitive cell volume of $a^3/2$
- Number of nearest neighbours: 8
- Nearest neighbour distance: $\sqrt{3}\ a/2 = 0.866\ a$ (prove this!)
- Number of next-nearest neighbours: 6 (where are these?)
- Next-nearest neighbour distance: a (prove this!)

The Body-Centred Cubic Lattice

- The primitive cell of the BCC lattice is defined by the translation vectors:

$$\vec{a}_1 = \tfrac{1}{2}\, a\, (\vec{x} + \vec{y} - \vec{z})$$
$$\vec{a}_2 = \tfrac{1}{2}\, a\, (-\vec{x} + \vec{y} + \vec{z})$$
$$\vec{a}_3 = \tfrac{1}{2}\, a\, (\vec{x} - \vec{y} + \vec{z})$$

where $\vec{x}$, $\vec{y}$, and $\vec{z}$ are the Cartesian unit vectors. These translation vectors connect the lattice pt at the origin to the points at the body centres (and make a rhombohedron)



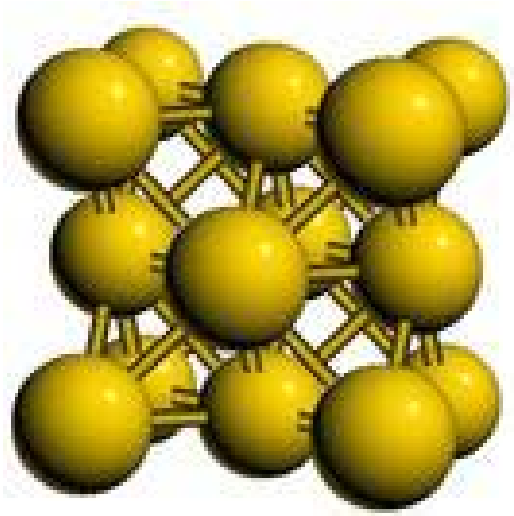
See figure 11 in Kittel for a picture of the primitive cell in more detail

The angle between adjacent edges is 109.3°

The Face-Centred Cubic Lattice

(Al, Cu, Ni, Sr, Rh, Pd, Ag, Ce, Tb, Ir, Pt, Au, Pb, Th)

- The face-centred cubic lattice has 4 lattice points per unit cell, with a total primitive cell volume of $a^3/4$
- Number of nearest neighbours: 12
- Nearest neighbour distance: $a/\sqrt{2} = 0.707\ a$ (prove this!)
- Number of next-nearest neighbours: 6 (where are these?)
- Next-nearest neighbour distance: a (prove this!)



Packing fraction = (atomic volume)/ (bravais unit cell volume)

$= \sqrt{2}\pi / 6$

(do this on your own)

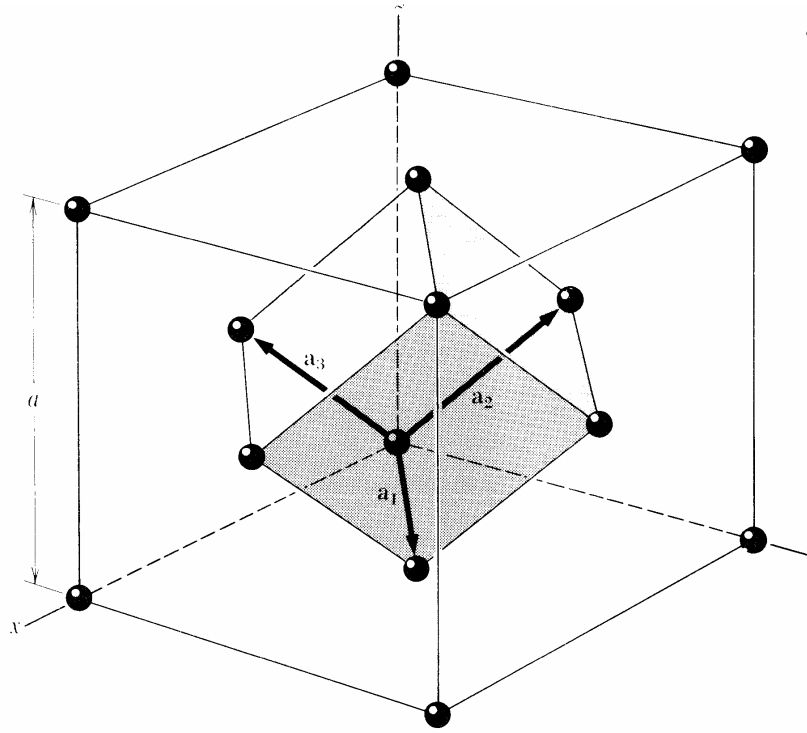
The Face-Centred Cubic Lattice

- The primitive cell of the FCC lattice is defined by the translation vectors:

$$\vec{a}_1 = \tfrac{1}{2} a (\vec{x} + \vec{y})$$
$$\vec{a}_2 = \tfrac{1}{2} a (\vec{y} + \vec{z})$$
$$\vec{a}_3 = \tfrac{1}{2} a (\vec{z} + \vec{x})$$

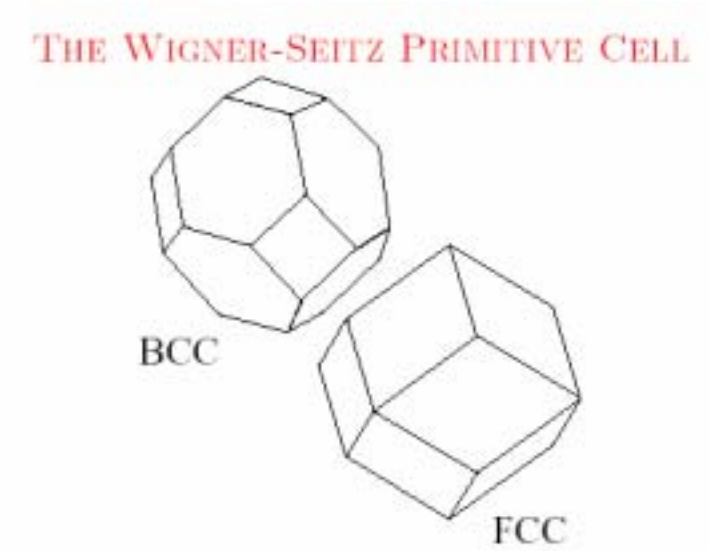
where $\vec{x}$, $\vec{y}$, and $\vec{z}$ are the Cartesian unit vectors. These translation vectors connect the lattice pt at the origin to the points at the face centres.

The angles between the axes are 60°



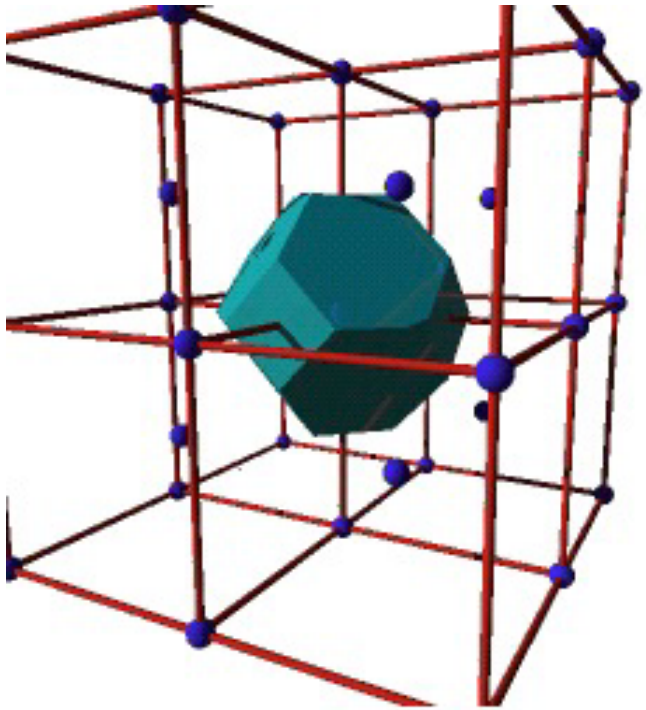
Wigner-Seitz cells for BCC, FCC lattices

- Note: You can also construct Wigner-Seitz cells for the FCC and BCC lattices. These look a bit strange, but they will be useful when we look at reciprocal space in the next chapter.
- These are made by taking the lines to the nearest and next-nearest neighbour points, and bisecting them with planes. The resulting figure is the Wigner-Seitz cell (which have the same volumes as the primitive cells we made above)

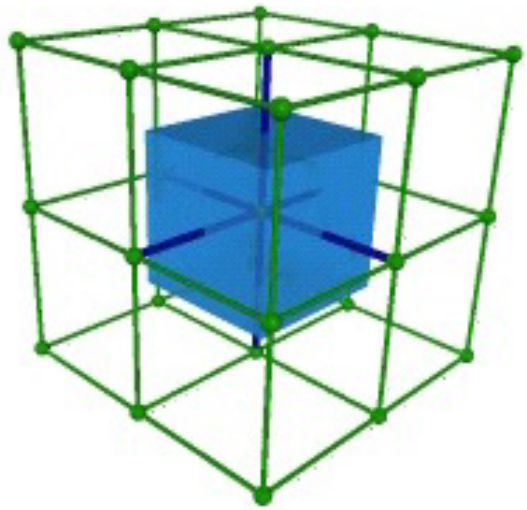


Wigner-Seitz cells for BCC and FCC 3D lattices

Wigner-Seitz cells



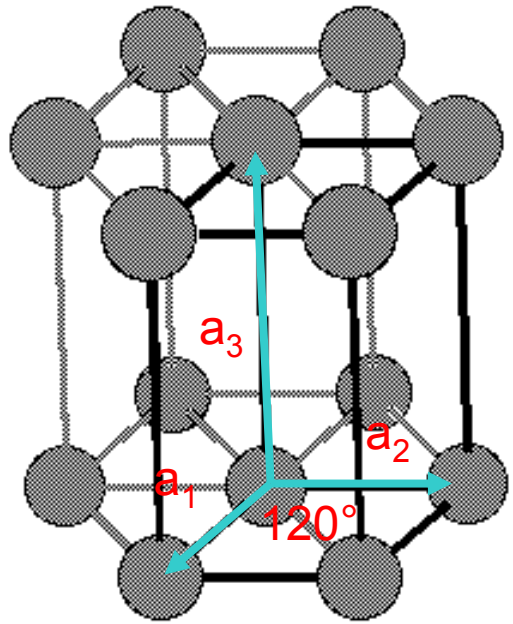
BCC lattice



Simple cubic lattice

Hexagonal unit cell

- The primitive cell in a hexagonal system is a right prism based on a rhombus with an included angle of 120°
- Note here that $a_1 = a_2 \neq a_3$
- Later, we will look at the hexagonal close-packed structure, which is this structure with a basis (and is related to the fcc structure).



(primitive cell is in bold)