**Fundamental crystal lattice systems**

A crystal is defined as a material that has a regular arrangement of atoms, and this lecture introduces some of the vocabulary and concepts for describing this regularity.

Vocabulary:

Lattice: mathematical grid of regularly repeating **points**

Basis: group of atoms attached to these points

Primitive lattice: Set of all lattice points with position vectors $\vec{R} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ where $u_{1,2,3}$ are integers and $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are **primitive translation vectors** which can be used to construct a grid with *all* the lattice points. In the image below, $\vec{a}_1, \vec{a}_2$ and $\vec{a}_1', \vec{a}_2'$ are both primitive translation vectors, but $\vec{a}_1'', \vec{a}_2''$ are not because a linear combination of them cannot be used to construct the translation vector shown in green.
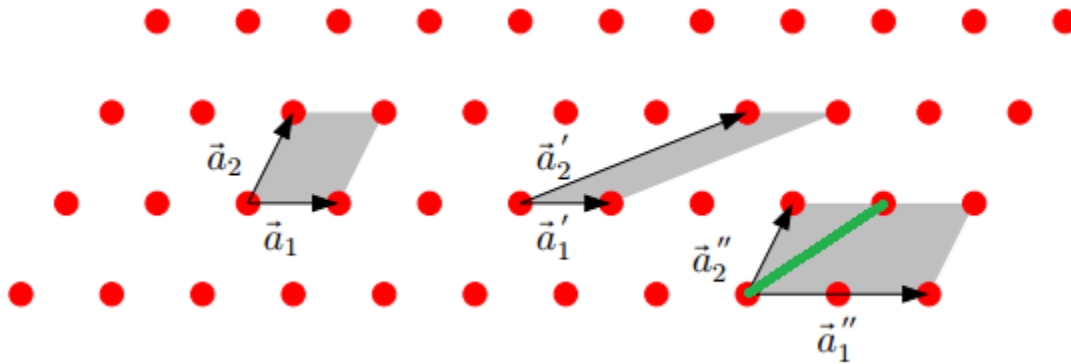
Primitive cell: the parallelepiped defined by the D primitive translation vectors in D-dimensional space. In the figure above (representing a lattice in 2 dimensions), the grey boxes bordered by , $\vec{a}_1, \vec{a}_2$ and $\vec{a}_1', \vec{a}_2'$ are two examples of primitive cells

Properties of a primitive cell:

- Only contains one lattice point (depending how the primitive cell is constructed, a given lattice point might be shared by several neighboring cells. For example, the primitive cell defined by $\vec{a}_1, \vec{a}_2$ intersects with 4 lattice points, but each of these lattice points is shared among 4 adjacent cells, giving 4*1/4 =1 point per cell)
- Can be used to tile all of space
- The volume of the primitive cell is the smallest possible volume which can be used to tile all of space and all choices for the primitive cell yield the same volume given by $V_c = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|$ in 3 dimension; in 2D $V_c = |\vec{a}_1 \times \vec{a}_2|$

How to construct a primitive cell:

- Guess + inspection

1. Can this shape I guessed be used to tile the entire lattice?
2. Does this shape contain only one lattice point?

- The **Wigner-Seitz cell** is a specific type of primitive cell constructed from a lattice given the following procedure:
  1. Pick one lattice point and draw lines to connect this to all nearby lattice points
  2. Draw perpendicular bisectors through all of these lines
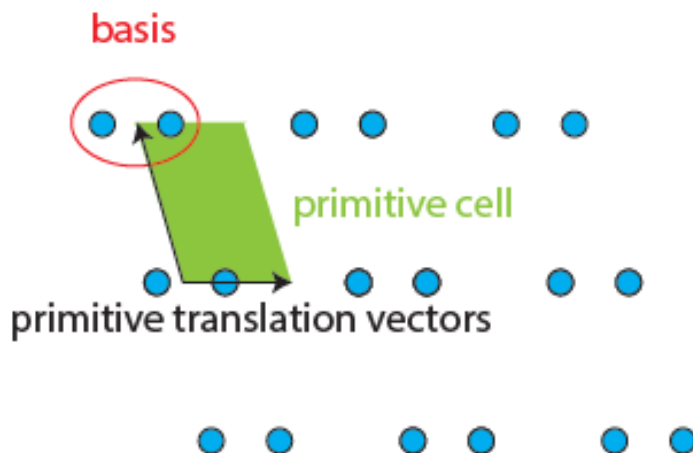 3. The shape formed from the intersection of the perpendicular bisectors is the Wigner-Seitz cell
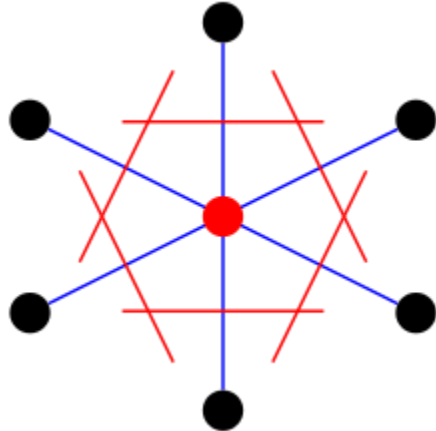
The Wigner-Seitz cell will become important in later chapters when we study the reciprocal lattice.

Unit cell: Smallest (or sometimes, most convenient) repeating unit which comprises a crystal. Consists of lattice and basis
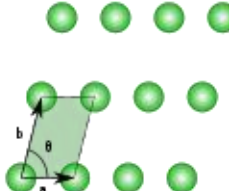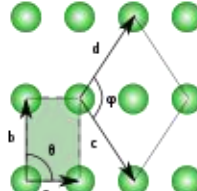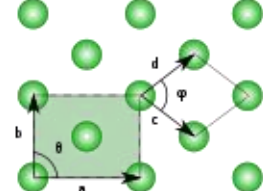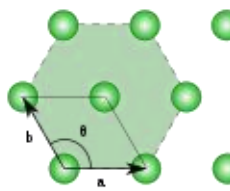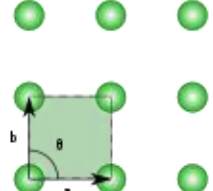
Examples:

1.
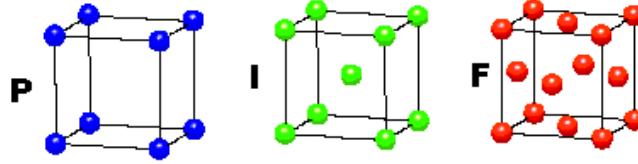

2. Honeycomb lattice
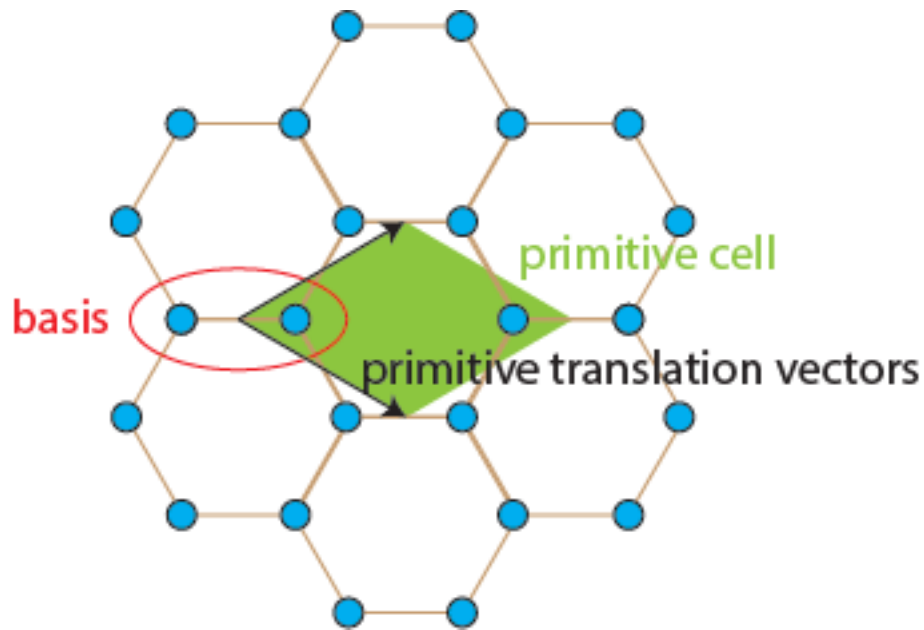
3. Body centered rectangular
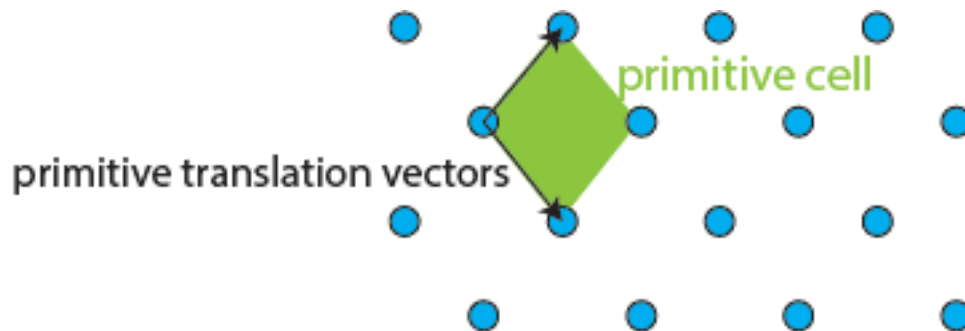
Crystal systems (lattices)

In two dimensions there are **5** special lattice types, defined by the symmetry operations which render them invariant. In 3 dimensions, there are **14** lattice types. These are referred to as Bravais lattices. All of these are primitive lattices, but sometimes they have a 'conventional' unit cell with is more convenient, but not primitive (body centered cubic, face centered cubic). On top of these Bravais lattices, there are 230 crystallographic space groups, which describe various operations one would apply to their basis atoms (e.g. translation, reflection, rotation, glide plane, etc) to produce a specific 3D crystal structure.

|a| ≠ |b|, θ ≠ 90°	|a| ≠ |b|, θ = 90° |c| = |d|, φ ≠ 90°	|a| = |b|, θ = 120°	|a| = |b|, θ = 90°
m	**o**	**h**	**t**

CUBIC

$a = b = c$
$\alpha = \beta = \gamma = 90°$

P I F

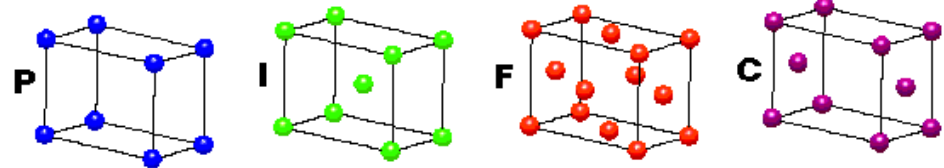**TETRAGONAL**

$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

P I

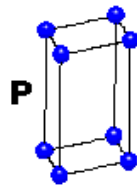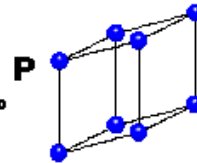**ORTHORHOMBIC**

$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$

P I F C

HEXAGONAL

$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$

P

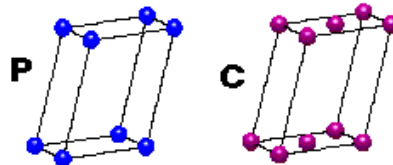**TRIGONAL**

$a = b = c$
$\alpha = \beta = \gamma \neq 90°$

P

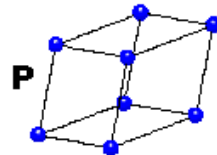**MONOCLINIC**

$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$

P C

TRICLINIC

$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

P

4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices