

# Summary of last lecture

- Reviewed the origin of the following bonds:
  - Ionic
  - Covalent
  - Metallic
  - van der Waals
  - Hydrogen
- and discussed the consequent properties of solids possessing these bonds
- Discussion of the origin of central-core repulsion



# Quiz on last lecture

The metallic bond has the following characteristics:

- 1) non-directional
- 2) non saturable
- 3) consists of a sea of free electrons surrounding the positive ions

Which of these characteristics contributes to the following properties of a metallic solid:

- |                         |       |
|-------------------------|-------|
| A) malleable (bendable) | (1)   |
| B) shiny surface        | (3)   |
| C) high density         | (1,2) |



# Aims of this lecture

- Introduction to crystal structure: structure = lattice + basis
- Primitive lattice vectors
- Primitive and non-primitive unit cells
- The Wigner-Seitz primitive unit cell
- Bravais lattice types in two and three dimensions



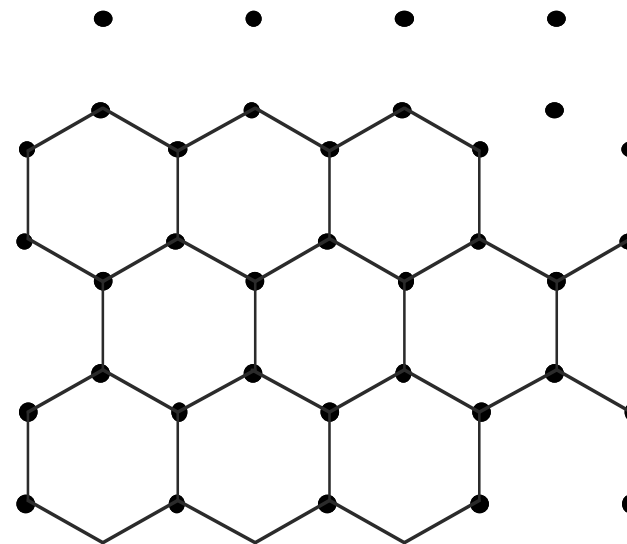
## II. Crystal Lattices

1. Concept of crystal structure as lattice plus basis. Lattice symmetries

Example: plane of graphite

Honeycomb structure

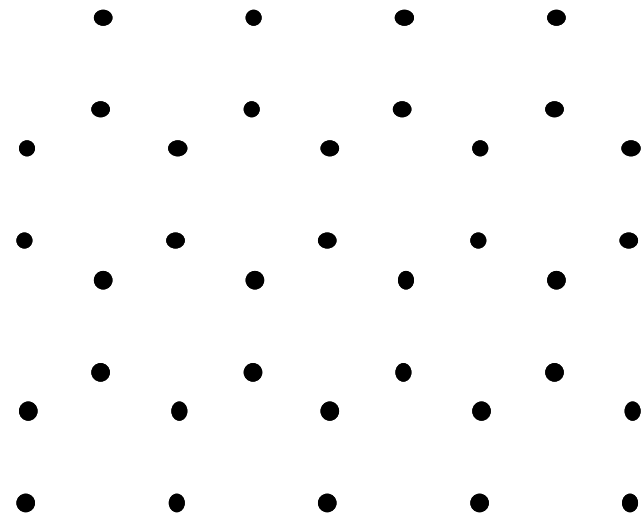
but what is the lattice?



## II. Crystal Lattices

### 1. Concept of crystal structure as lattice plus basis. Lattice symmetries

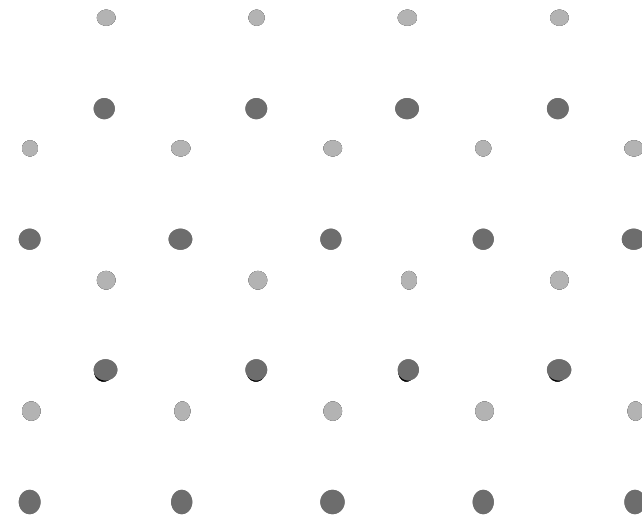
1) identify atoms in identical environments



## II. Crystal Lattices

### 1. Concept of crystal structure as lattice plus basis. Lattice symmetries

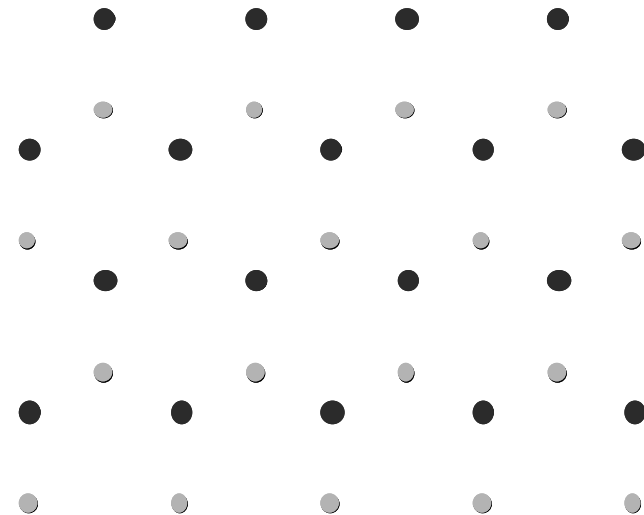
1) identify atoms in identical environments



## II. Crystal Lattices

### 1. Concept of crystal structure as lattice plus basis. Lattice symmetries

1) identify atoms in identical environments



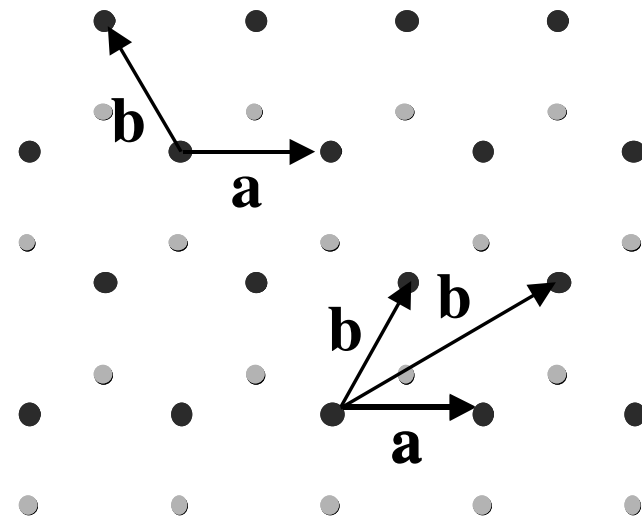
## II. Crystal Lattices

### 1. Concept of crystal structure as lattice plus basis. Lattice symmetries

- 1) identify atoms in identical environments
- 2) define coordinate axes **a** and **b**

NB not perpendicular (in this case)

choice not unique



# II. Crystal Lattices

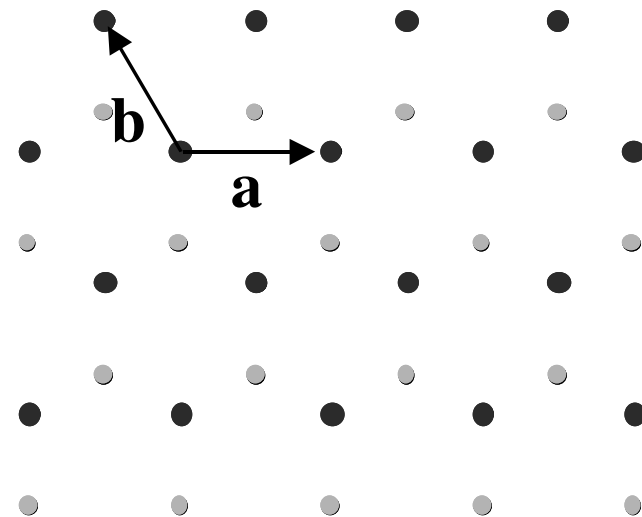
1. Concept of crystal structure as lattice plus basis

The **Lattice** is the set of points defined by:

$$\mathbf{r} = u\mathbf{a} + v\mathbf{b} \quad (u,v, \text{ integers})$$

or  $\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$   
(for three dimensions)

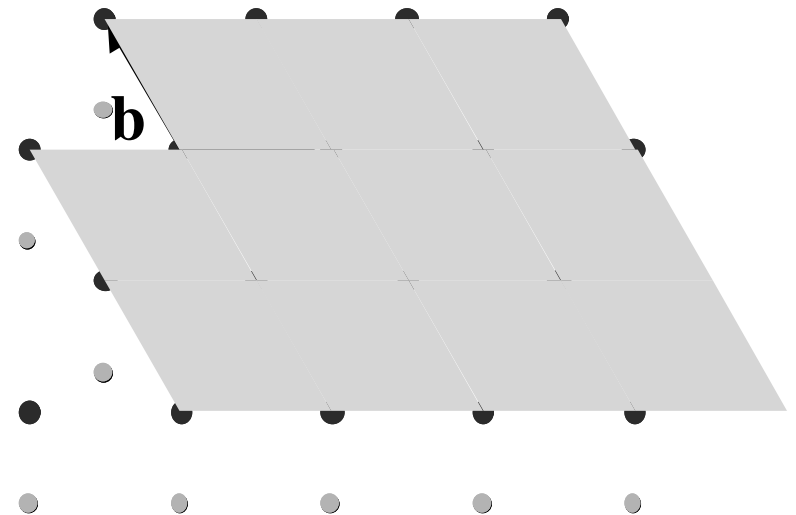
$\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$  are called the **primitive lattice vectors**



# 1. Concept of crystal structure as lattice plus basis

The region enclosed by the primitive lattice vectors is called the **primitive unit cell**.

It is the smallest area which when repeated after translating through every lattice vector  $\mathbf{r}$ , fills the whole of space



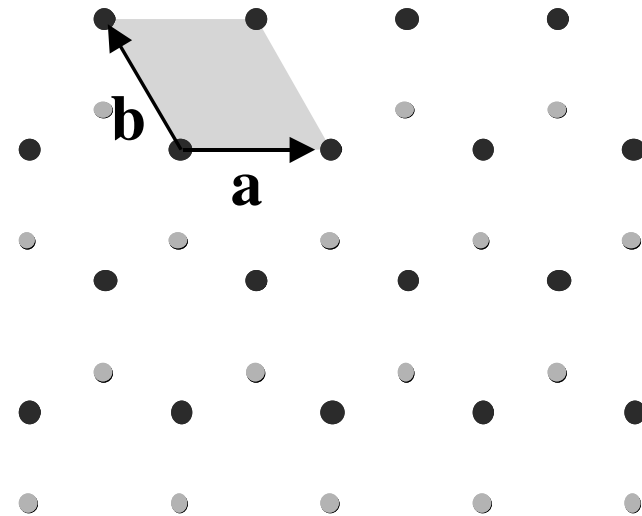
# 1. Concept of crystal structure as lattice plus basis

The region enclosed by the primitive lattice vectors is called the **primitive unit cell**.

It is the smallest area which when repeated after translating through every lattice vector  $\mathbf{r}$ , fills the whole of space

The primitive unit cell contains exactly one lattice point (in this case it shares four, with four neighbouring cells)

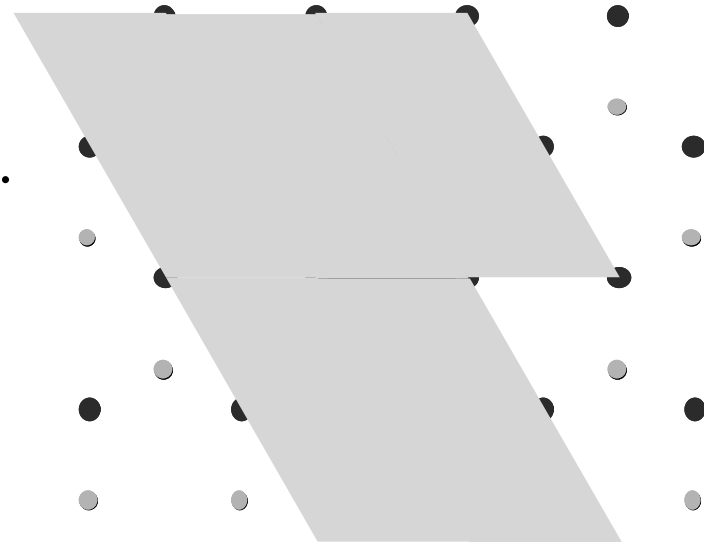
It has an area  $\mathbf{a} \times \mathbf{b}$  (in three dimensions, volume  $\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}$ )



# 1. Concept of crystal structure as lattice plus basis

It is possible to define areas which are larger than the primitive unit cell, defined by **non-primitive lattice vectors**, which will fill the whole of space when translated through those lattice vectors.

These are **non-primitive unit cells**.

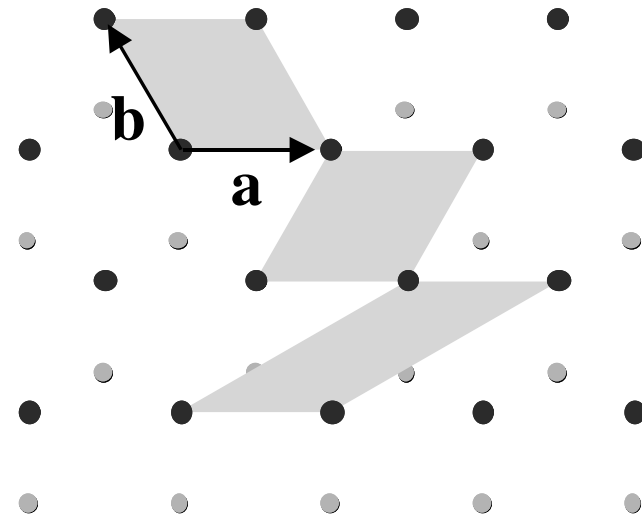


# 1. Concept of crystal structure as lattice plus basis

Unit cells are not unique:

There is often a conventional choice, called the **conventional unit cell**.

There is one particularly useful recipe for making a primitive unit cell...



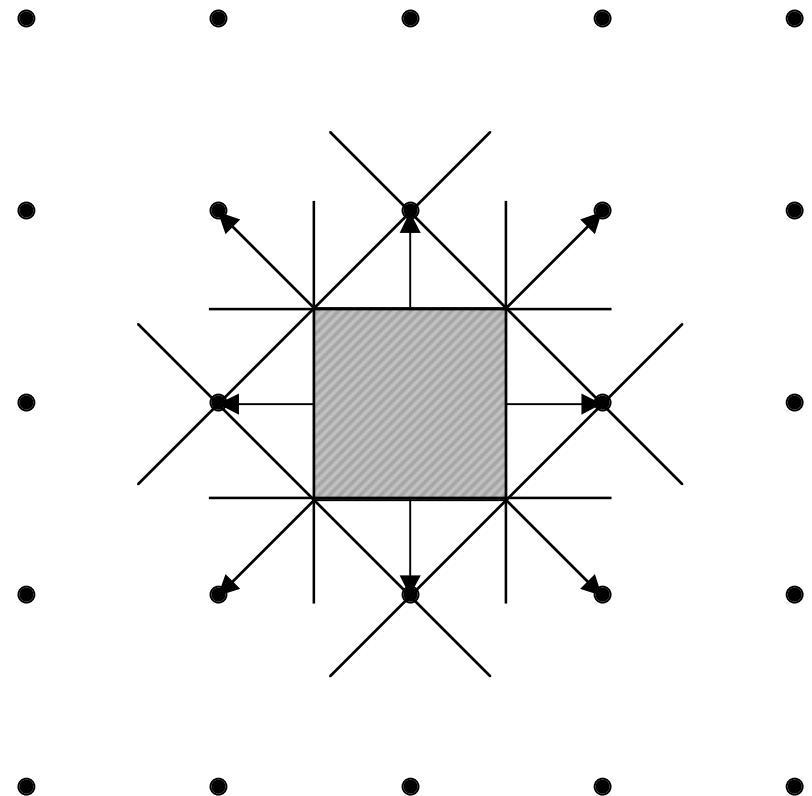
# 1. Concept of crystal structure as lattice plus basis

The Wigner-Seitz unit cell:

Choose a lattice point, and draw lattice vectors from it to its neighbours

Draw the perpendicular bisectors of these vectors

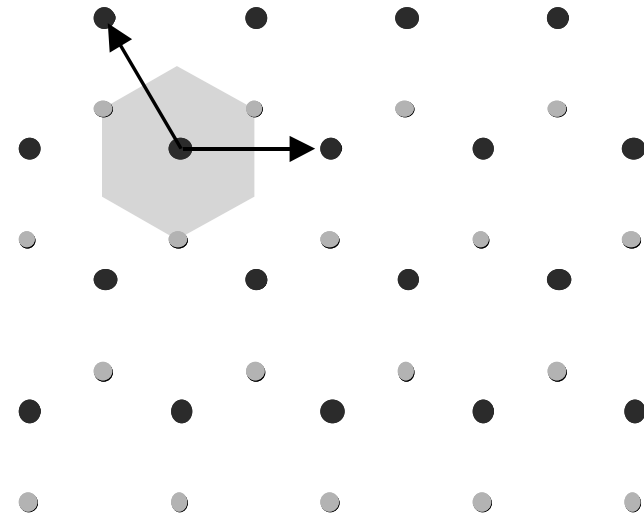
The Wigner-Seitz primitive unit cell is the region around the lattice point, enclosed by the bisectors



# 1. Concept of crystal structure as lattice plus basis

So the Wigner-Seitz cell of the triangular lattice that we have been dealing with is:

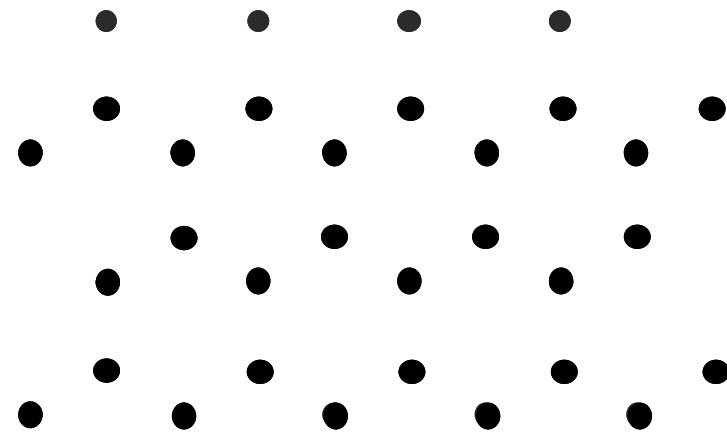
Can also think of it as the region of space closer to the chosen lattice point than to any other



# 1. Concept of crystal structure as lattice plus basis

A **crystal structure** is formed by placing a collection of atoms, called a **basis**, at each point of the **lattice**.

So the crystal structure of a plane of graphite consists of:



A triangular lattice...

with a basis of two carbon atoms

one at the origin and one at  $\mathbf{r} = \frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}$

a basis of C(0,0) C(2/3,1/3) (using "fractional coordinates")



# 1. Lattice symmetries

A **Bravais lattice** is an infinite array of points which looks the same from whichever of the points it is observed.

All lattices therefore possess the property of **translational symmetry**:

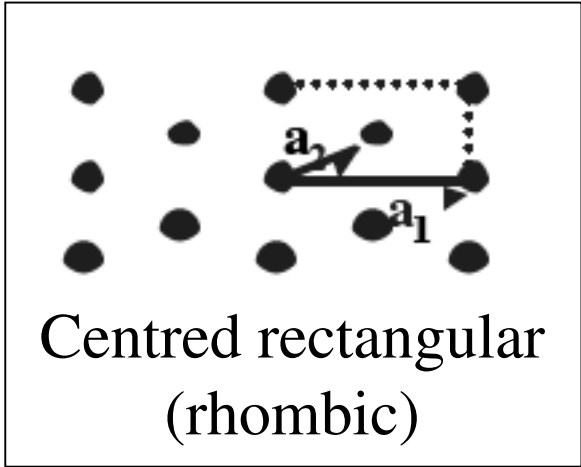
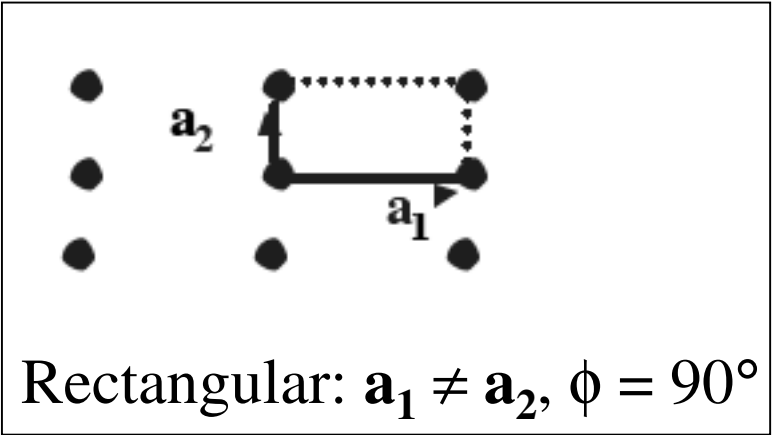
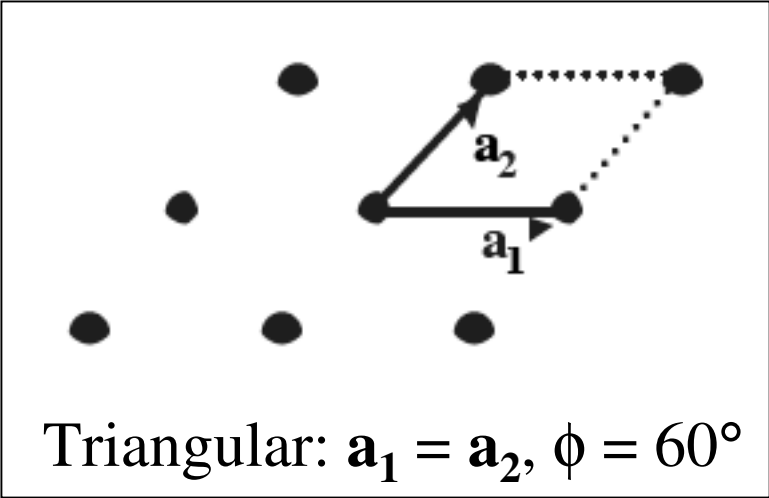
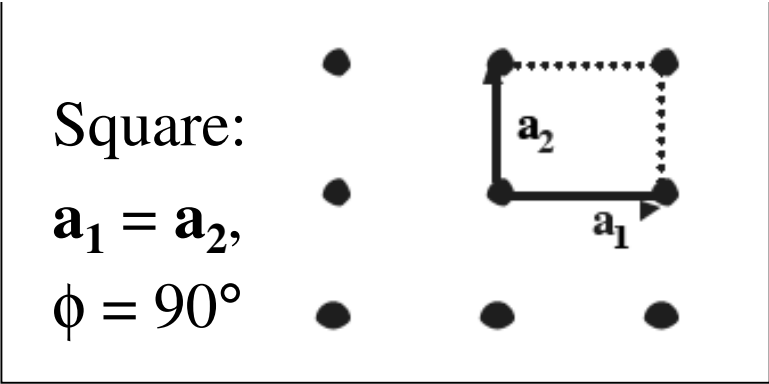
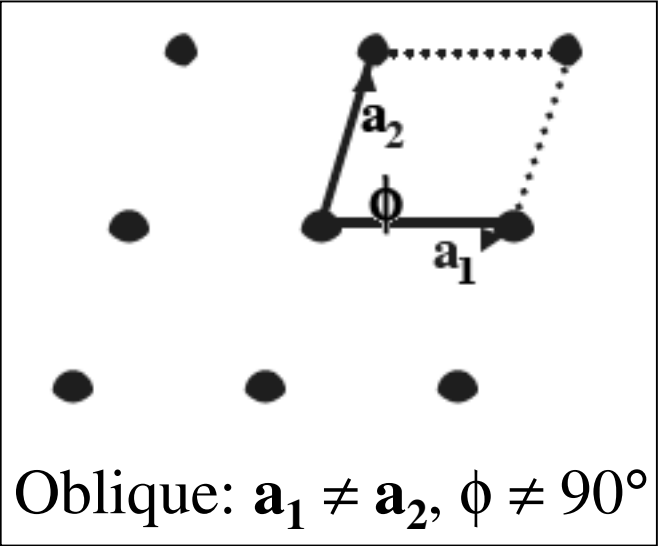
the lattice transforms into itself (i.e. remains the same) when moved through integer numbers of lattice vectors

There are various types of lattice, distinguished by the other symmetries (rotations, reflections) that they possess.



## 2. 2D and 3D lattices

Five distinct 2D lattices:



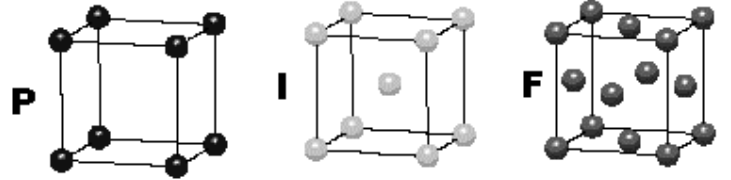
## 2. 2D and 3D lattices

...and 14 distinct  
3D lattices:

### CUBIC

$$a = b = c$$

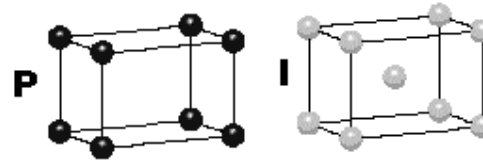
$$\alpha = \beta = \gamma = 90^\circ$$



### TETRAGONAL

$$a = b \neq c$$

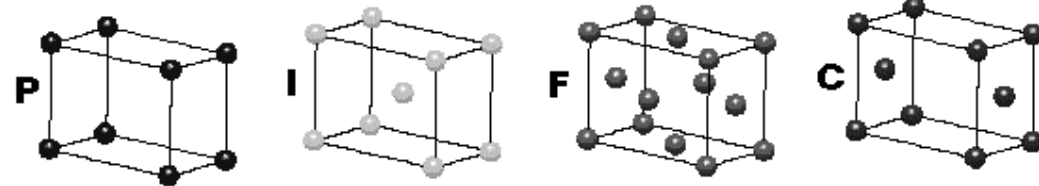
$$\alpha = \beta = \gamma = 90^\circ$$



### ORTHORHOMBIC

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

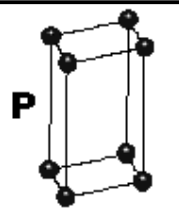


### HEXAGONAL

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

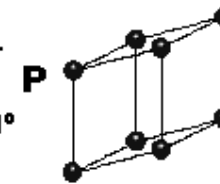
$$\gamma = 120^\circ$$



### TRIGONAL

$$a = b = c$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

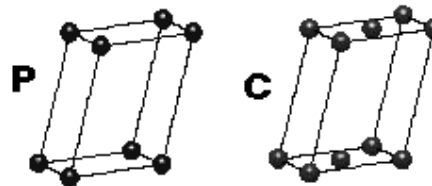


### MONOCLINIC

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ$$

$$\beta \neq 120^\circ$$



### TRICLINIC

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

+

7 Crystal Classes

→ 14 Bravais Lattices



