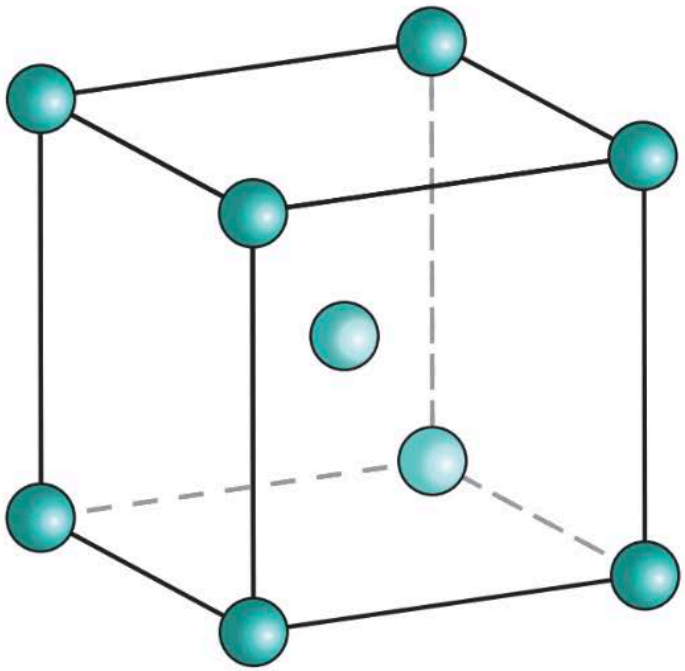
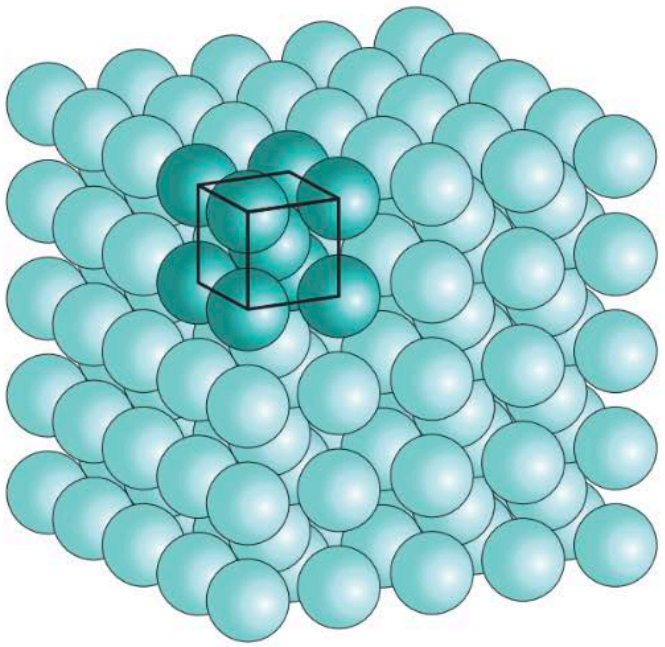
Crystalline state

Main component (atoms, molecules...) are arranged in a regular periodic arrang. in all 3D.





Crystalline state

Fluorite CaF_2

Pyrite, FeS_2

Quartz, SiO_2

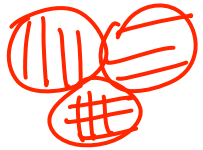
Growth facets • Inter-Planar angles • Symmetries

Crystalline state

- Some engineering applications require single crystals:

  -- diamond single crystals for abrasives

  -- turbine blades: high strength materials



- Properties of crystalline materials often related to crystal structure.

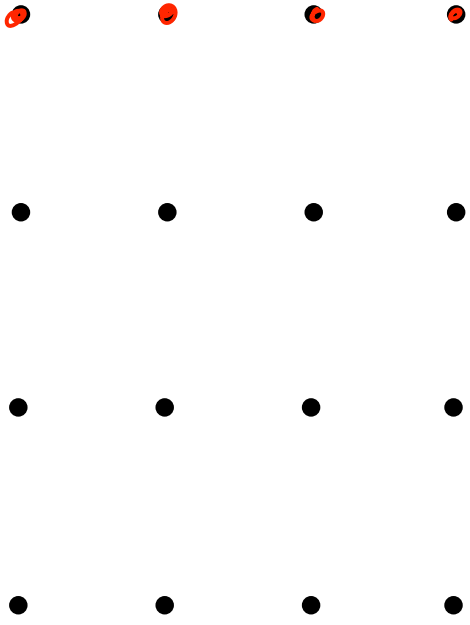
  -- electrical conductors and semiconductors: copper, silicon…

- Understanding the crystalline descriptors is essential ➔ ***crystallography*** is a theory of ***spatially periodic, long-range ordered patterns***.

Translational symmetry

1

Lattice (3D)
Net (2D)



+

2

Motif

➔

crystal

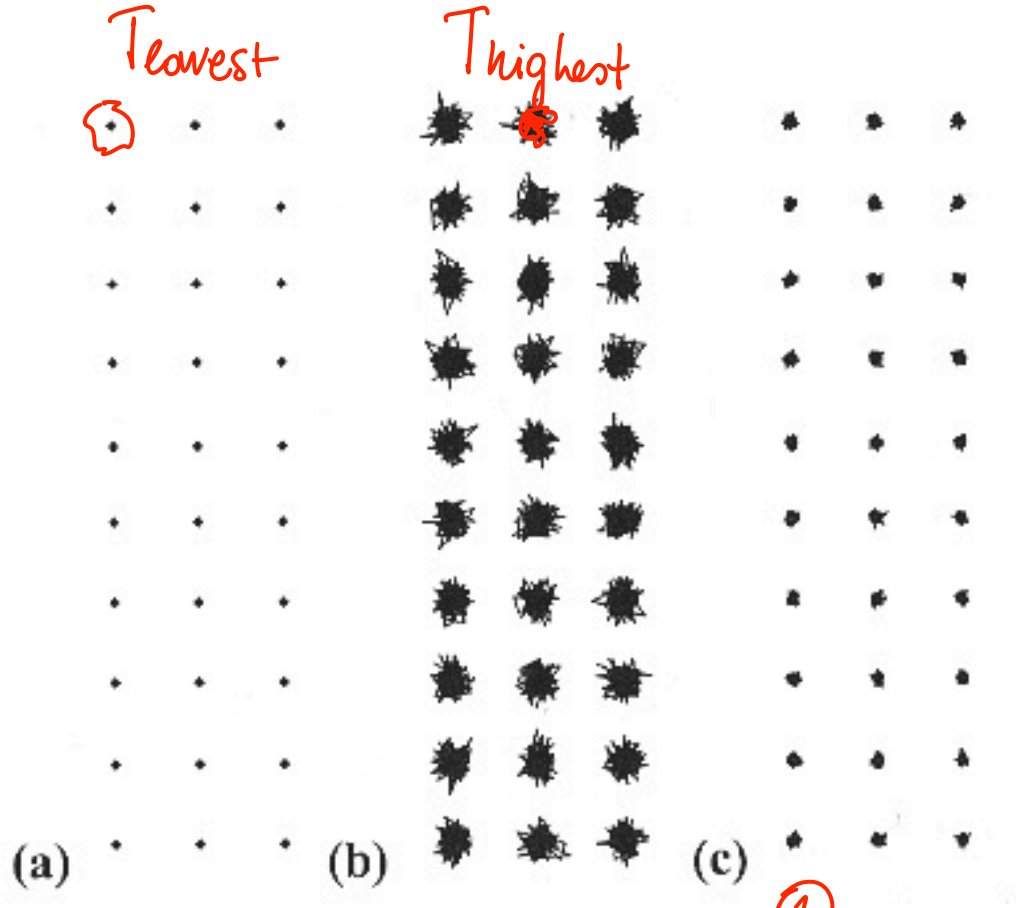
Structure

crystal = lattice + motif

Translational symmetry

= atom

- "Real" position at finite temperatures?
- Position confined by other surrounding atoms



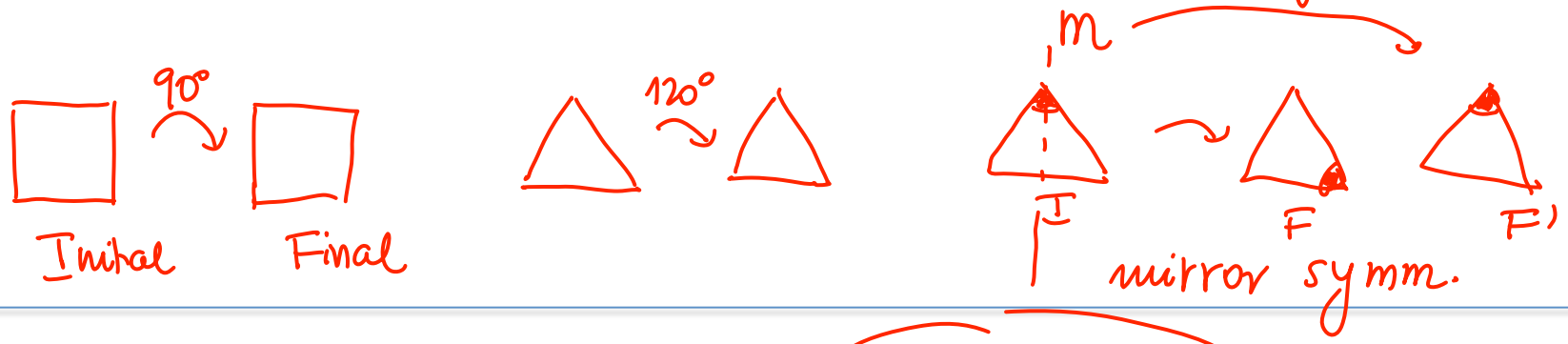
Time-invariant, 3D arrang. of atoms or molecules (1) on a lattice (2)

MOTIF

Crystallography in 2 dimensions

Symmetry operations

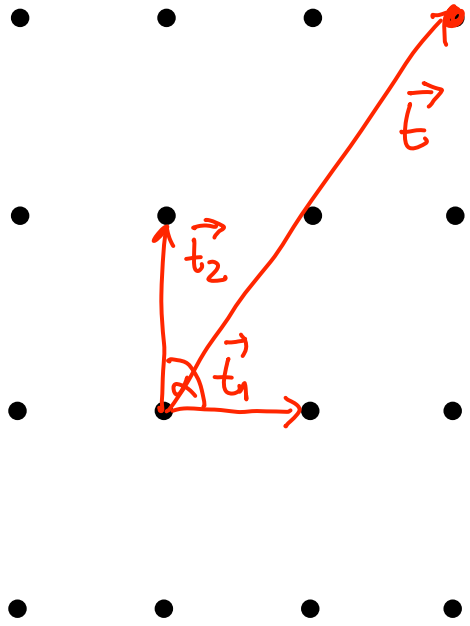
Operation from initial → final state such that the initial & final patterns cannot be distinguished.



Translational symmetry – all crystals have it!

Surroundings viewed from an arbitrary position (origin) is identical to the surroundings viewed from a point separated by a vector $\vec{t}$.

Crystallography in 2 dimensions



descriptors

$|\vec{t}_1| = a$

$|\vec{t}_2| = b$

} lattice paramet.

$\measuredangle(\vec{t}_1, \vec{t}_2) = \alpha$

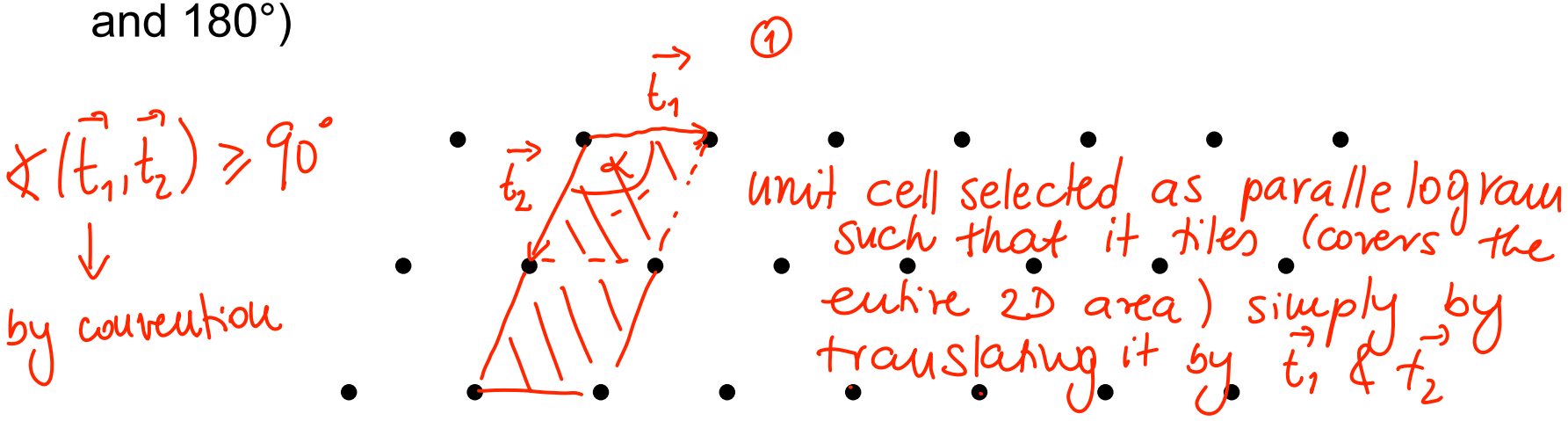
$\vec{t} = p \cdot \vec{t}_1 + q \vec{t}_2$

p & q integers

- define lattice points through translation symmetry operations
- any 2-dimensional lattice can be described in terms of nonparallel translation vectors – **basis vectors** $\mathbf{t_1}$ and $\mathbf{t_2}$
- the repeat distance: **lattice constant**
- this results in a **lattice:** a periodic array of points in space

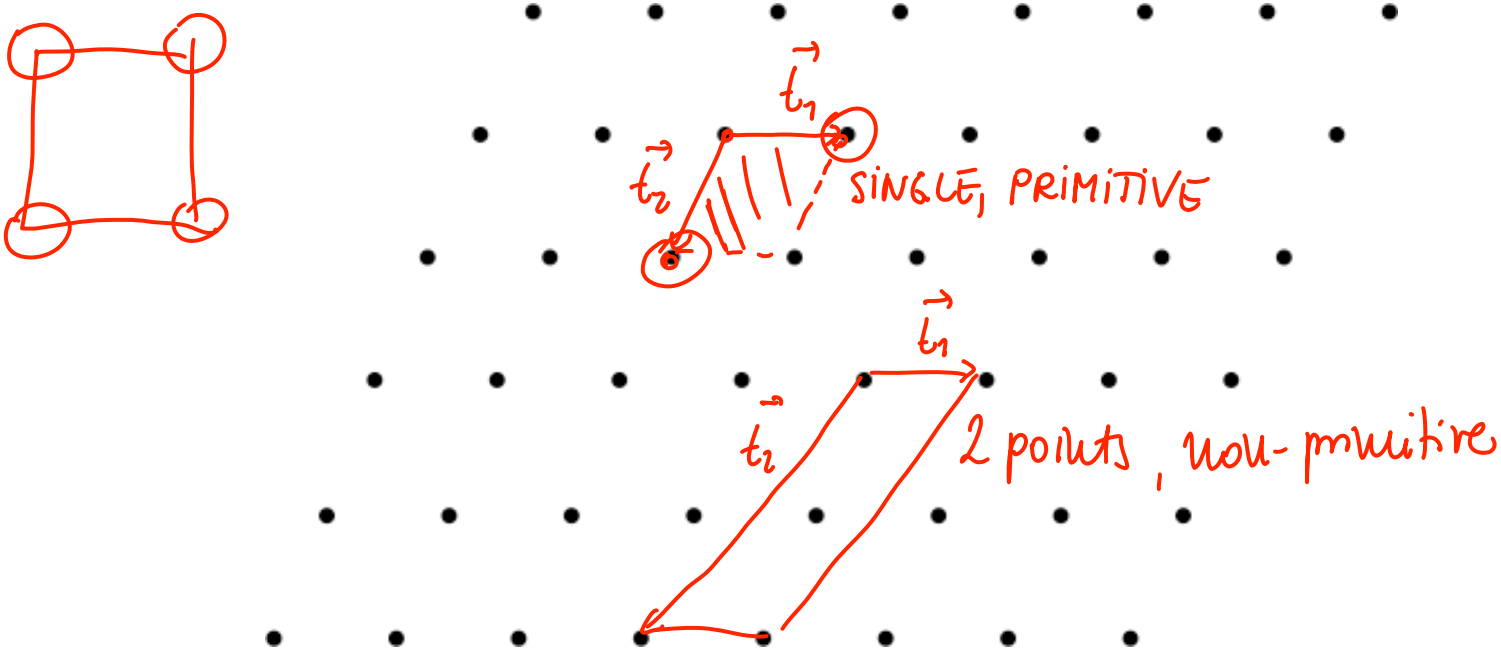
Crystallography in 2 dimensions

- Note that the choice of basis vectors is not unique for a given structure
- By convention, $\mathbf{t}_1$ is the shortest lattice translation
- $\mathbf{t}_2$ is next-to-shortest (and the angle between $\mathbf{t}_1$ and $\mathbf{t}_2$ is between 90° and 180°)



Primitive cell

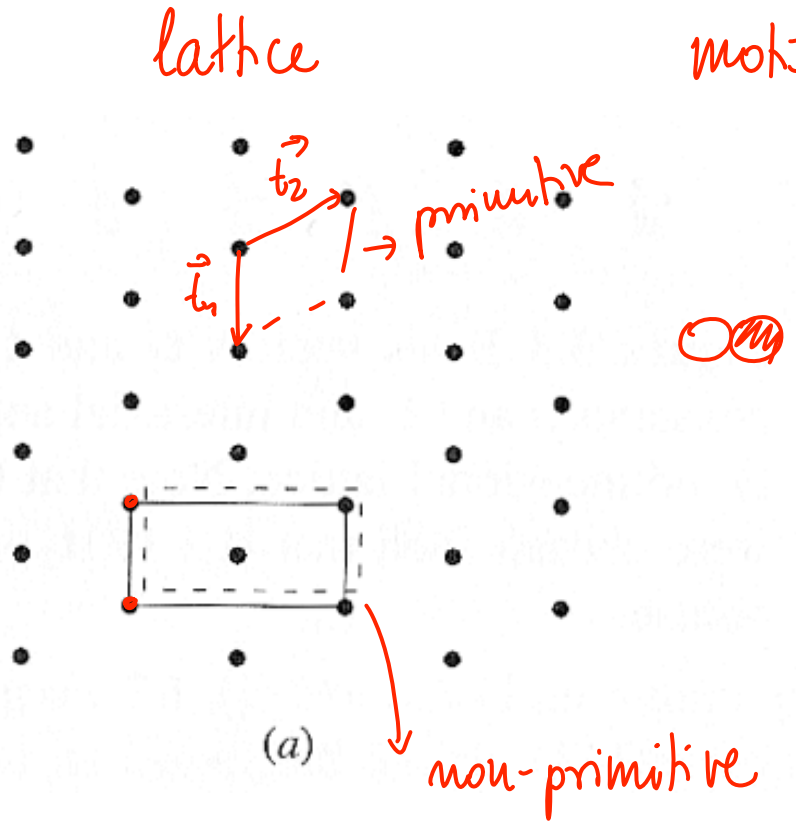
- Because basis vector selection is arbitrary, several parallelogram cell types can be distinguished
- **Primitive cells**: contain a single lattice point
- **Multiple cells** (non-primitive): contain more than one lattice point

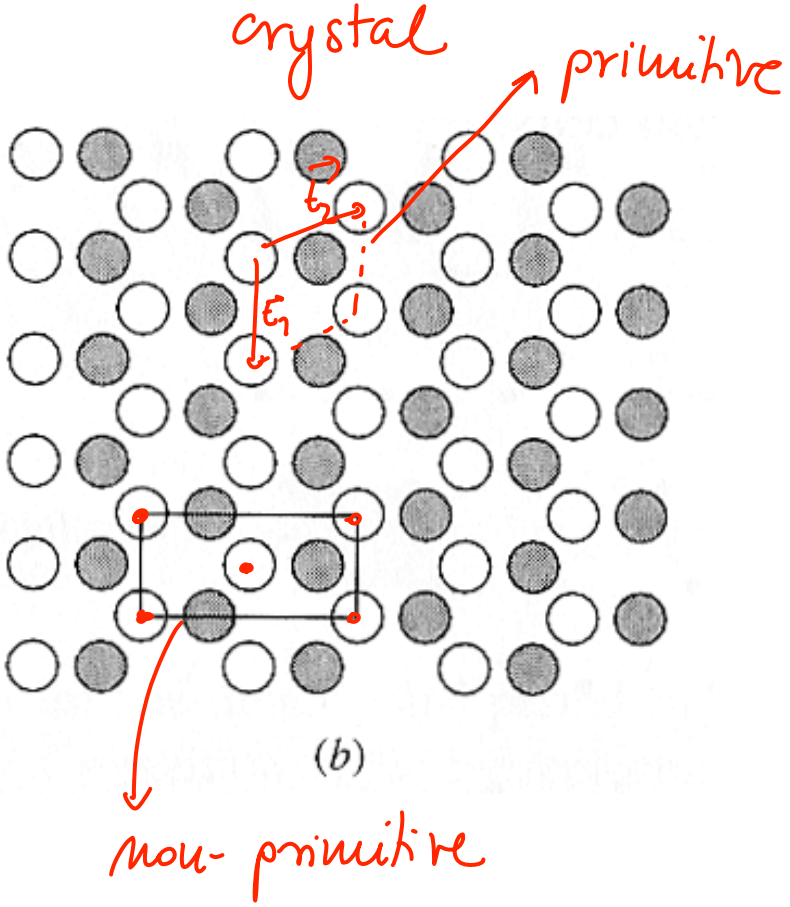


$$2 \cdot \frac{1}{6} + 2 \cdot \frac{2}{6} = 1$$

Number of atoms in a primitive cell

Primitive and non-primitive cell



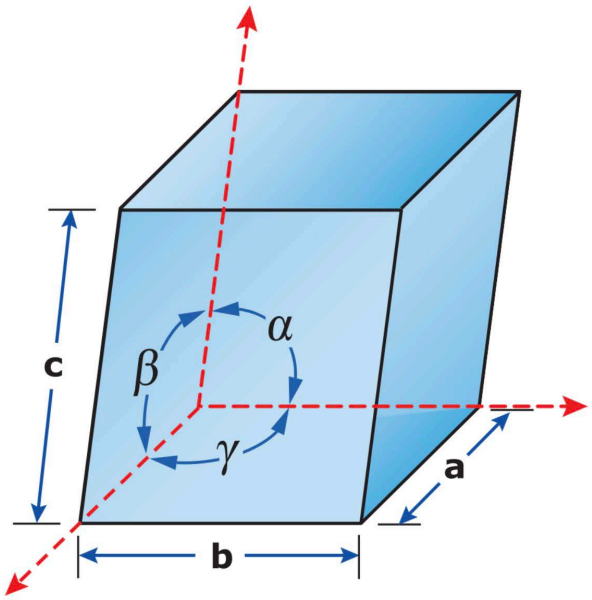


1

Number of objects/motifs in a primitive cell

Crystallography in 3 dimensions

- In three dimensions, a lattice is specified by a set of three noncolinear, noncoplanar basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$
- Because it is periodic, a lattice is infinite in extent.
- The set of all lattice points may be represented $\{p\mathbf{a}_1+q\mathbf{a}_2+r\mathbf{a}_3\}$, where p, q, and r are integers.



$|\vec{a}_1| = a$
$|\vec{a}_2| = b$
$|\vec{a}_3| = c$

Lattice constants or lattice parameters

By convention, the interaxial angles (angles between the basis vectors) are designated as:

$\alpha = \sphericalangle(\vec{a}_2, \vec{a}_3)$
$\beta = \sphericalangle(\vec{a}_3, \vec{a}_1)$
$\gamma = \sphericalangle(\vec{a}_1, \vec{a}_2)$

The volume V of the primitive cell is given by the triple product:

$$V = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = |\vec{a}_2 \cdot \vec{a}_3 \times \vec{a}_1| = |\vec{a}_3 \cdot \vec{a}_1 \times \vec{a}_2|$$

Unit cell

• Most crystalline materials have special symmetry such as rotational symmetry axes and glide planes (to be defined in future lectures) that in turn can have an important influence on crystal properties.
• Crystallographic convention dictates that unit cells for various crystal lattices be chosen so as to contain important symmetry elements of the crystal structure.
• Important: unit cell can be primitive (contain one atom) or non-primitive (contains more than one atom)

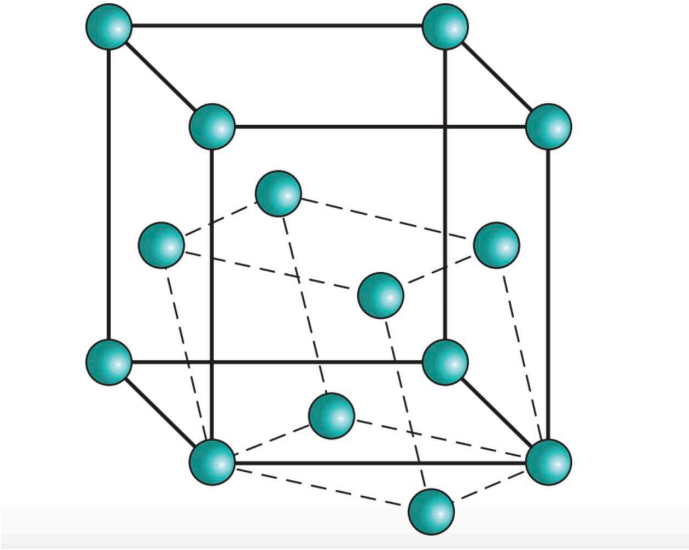
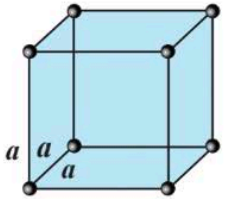
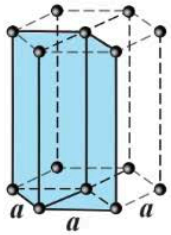
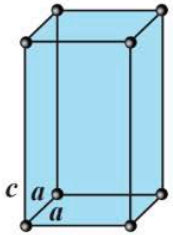
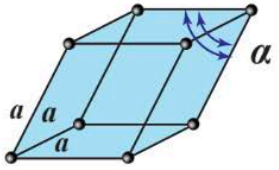
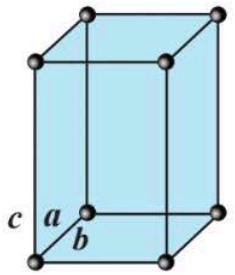
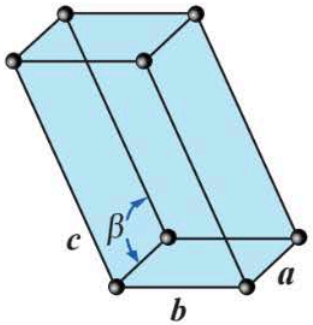


Figure 1: A portion of a face-centered cubic (f.c.c.) lattice. The conventional unit cell is shown by the solid lines. It contains four lattice points per cell. The dashed lines outline a primitive cell for the same lattice, containing only a single lattice point.

7 crystal systems

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°,\ \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	

7 crystal systems

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$