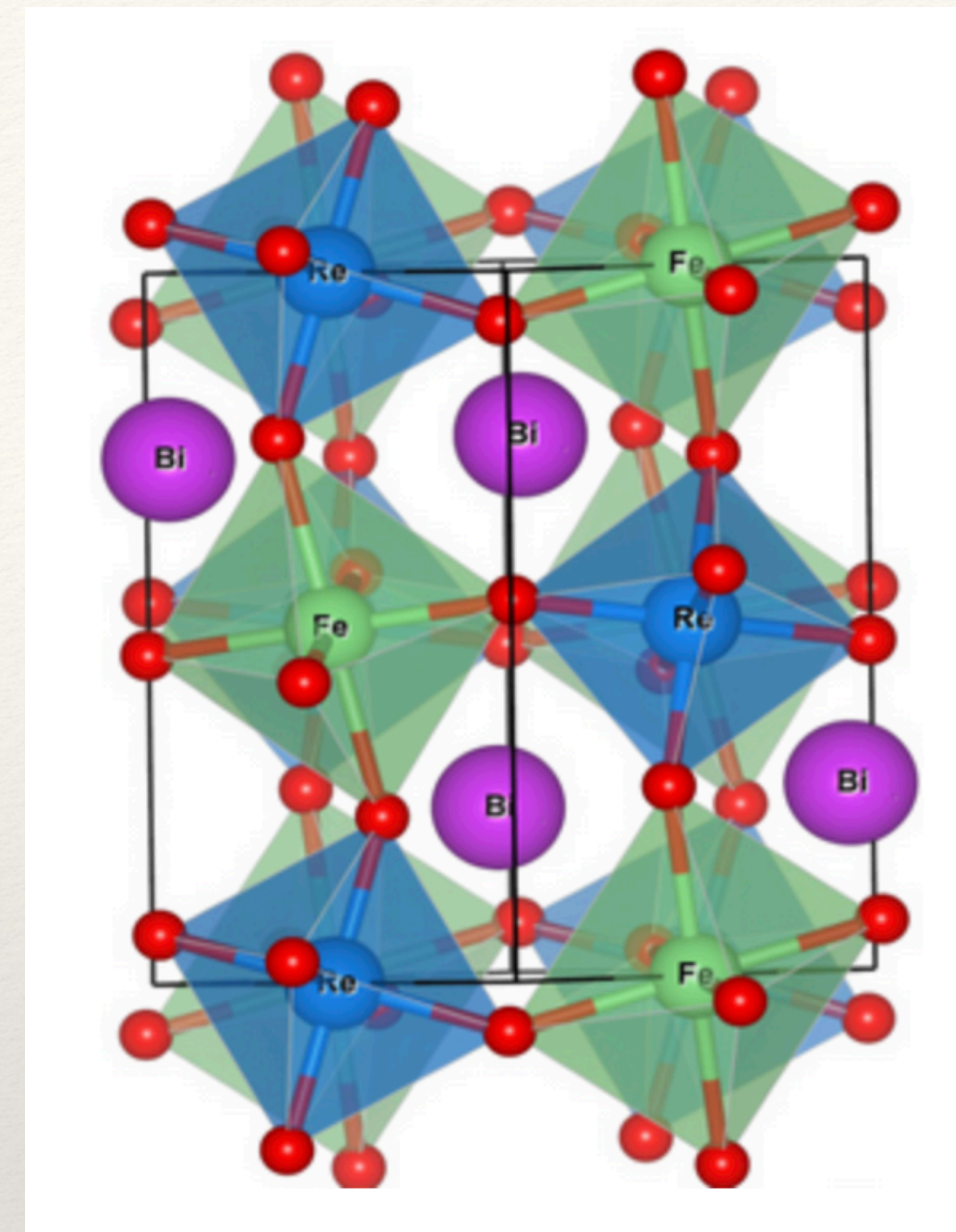


Structure of Solids - Crystal Lattices

Lecture 1

CHM 637

Chemistry & Physics of Materials



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Lecture Plan

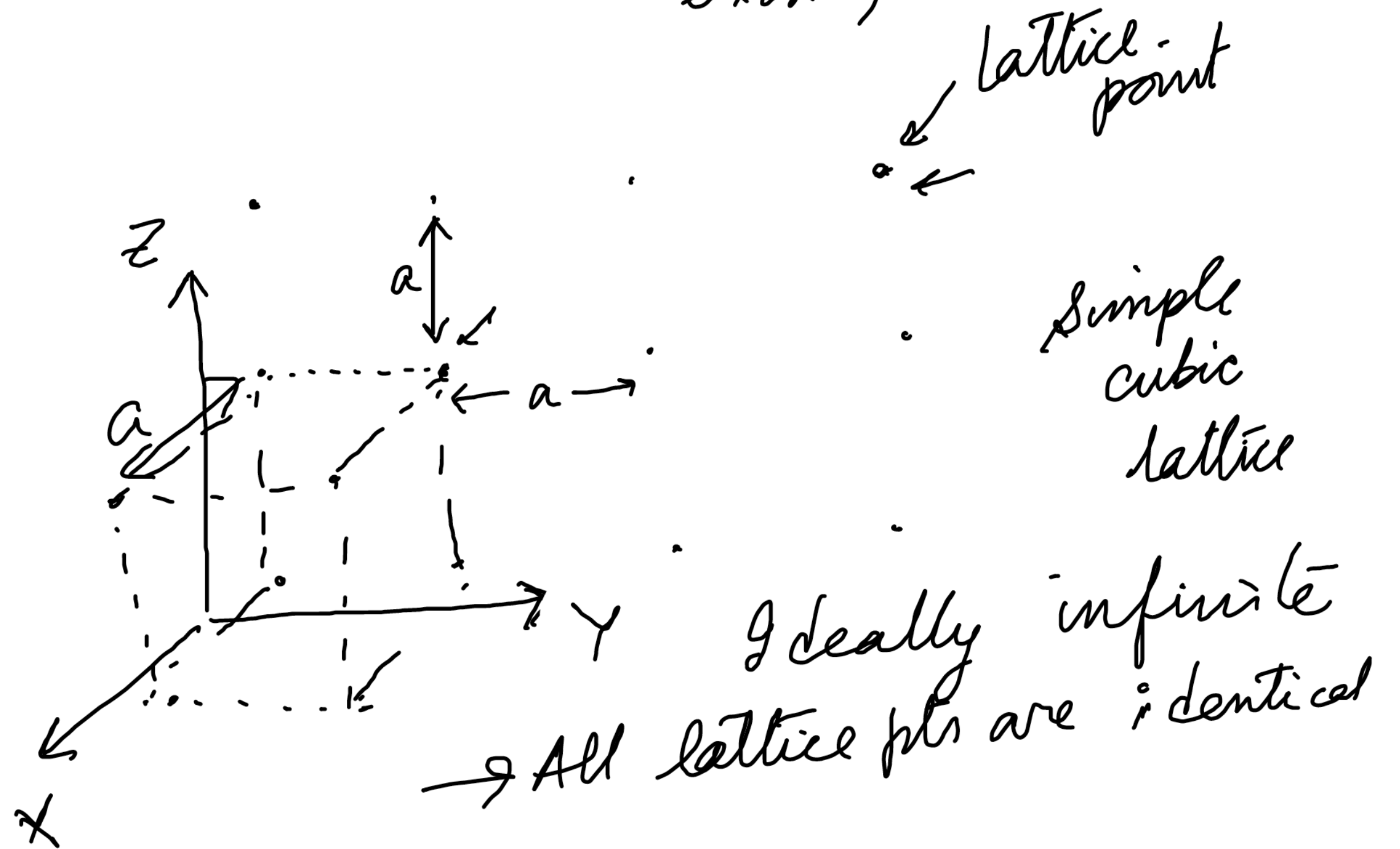
- Introduction to lattices: lattice points, unit cells, translation vectors
- Unit Cells
- Primitive and General Lattice Translation vectors
- Bravais Lattices

Introduction to lattices

Definition of a lattice

Infinite ideally but in practice bounded by the volume of the crystal.

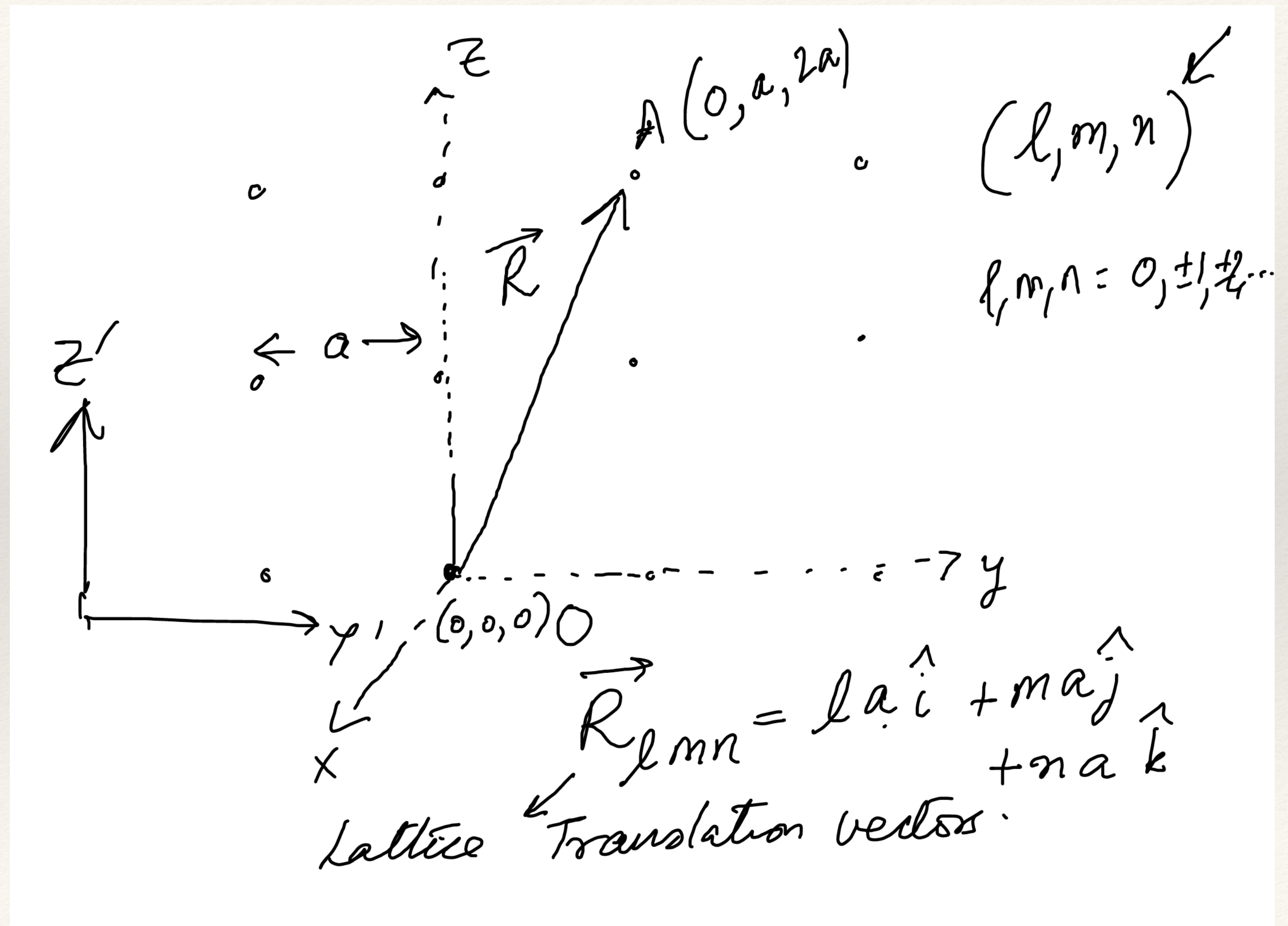
Lattices: A periodic array of points in 3D space. (1D & 2D lattices also exist)



Introduction to lattices

Traversing a lattice

Points on a (3D) lattice are connected by a triplet of integers called the **Lattice Translation Vector**.



Introduction to lattices

Translation Vectors

Primitive or fundamental translation vectors define the smallest repeating unit.

General lattice translation vectors span the entire lattice.

General lattice : $(\vec{a}, \vec{b}, \vec{c})$

$\vec{u}_1, \vec{u}_2, \vec{u}_3 \rightarrow$ unit vectors
a b c

Primitive Translation vectors $\left\{ \begin{array}{l} \vec{a} = a\vec{u}_1, \vec{b} = b\vec{u}_2, \vec{c} = c\vec{u}_3 \end{array} \right.$

$\vec{R}_{lmn} = l\vec{a} + m\vec{b} + n\vec{c}$

\downarrow Lattice translation vectors

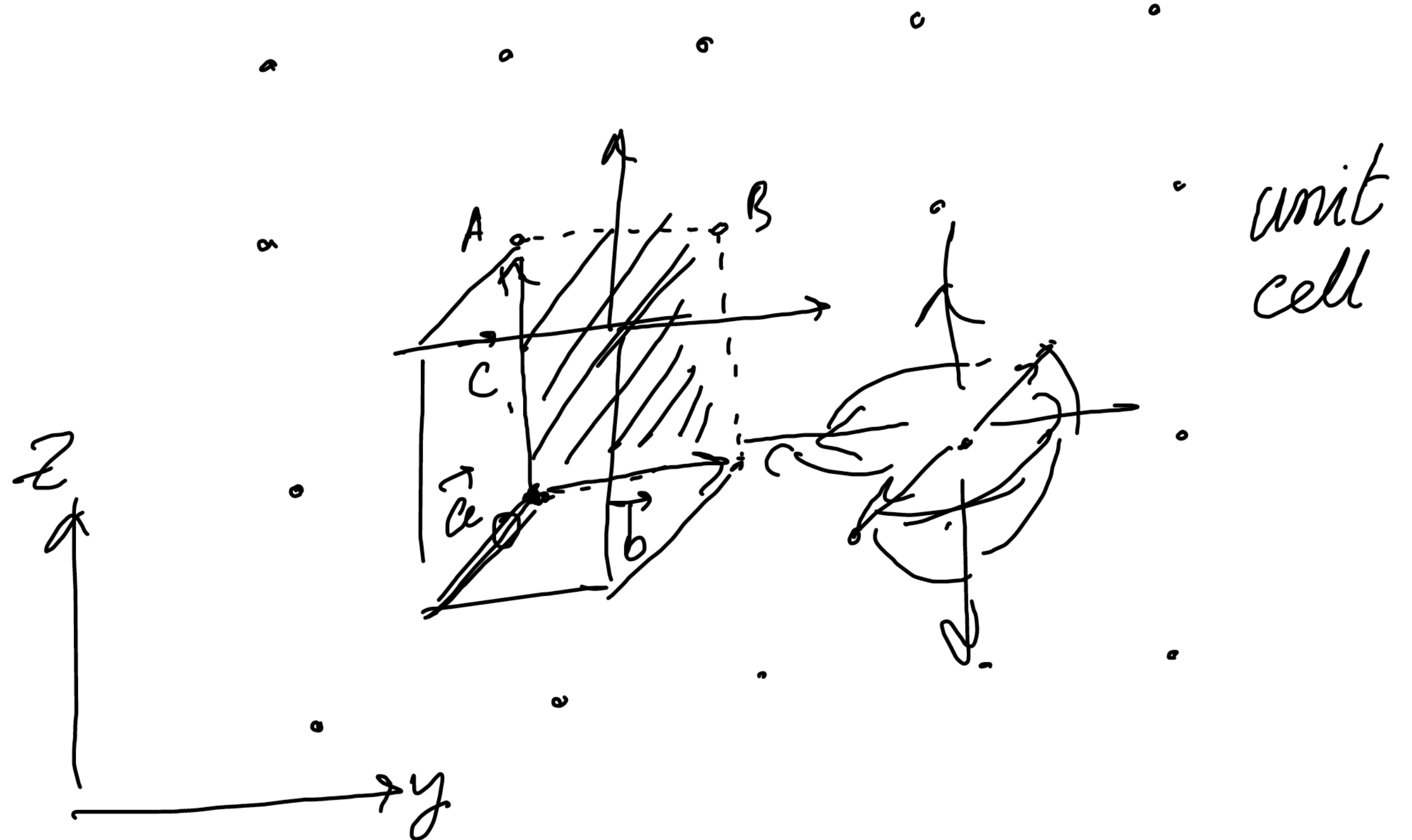
Introduction to lattices

Unit cells

Smallest volume that can be repeated to get the lattice

$$\vec{a}, \vec{b}, \vec{c}$$

$$\vec{c} = a \hat{j} + b \hat{k}$$

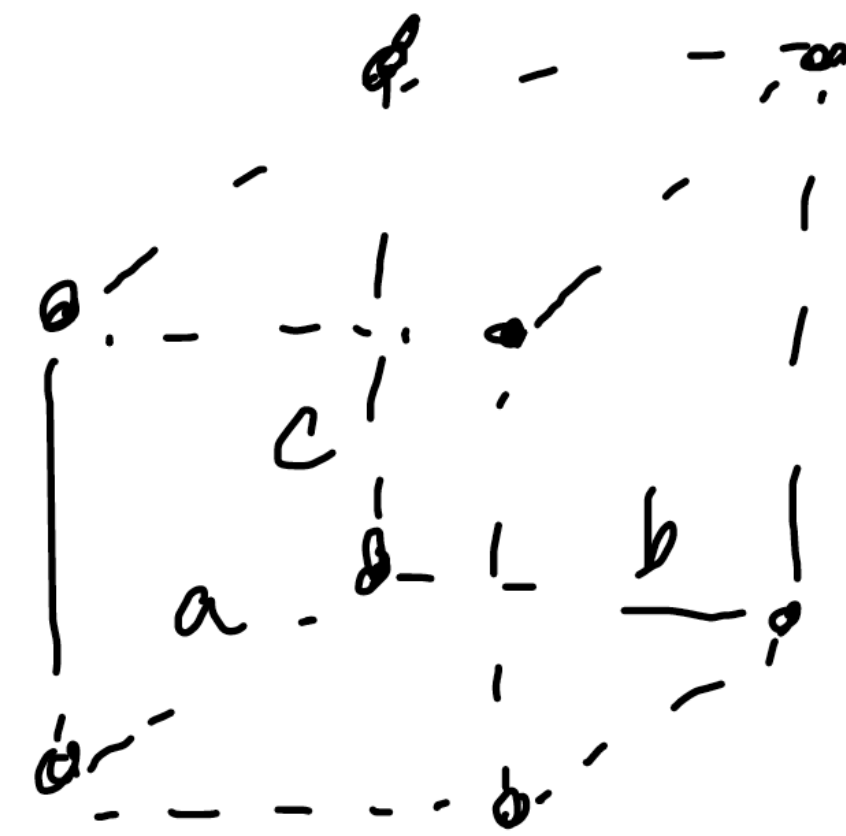


Introduction to lattices

Unit cells

Smallest volume that can be repeated to get the lattice

Primitive cells contain exactly one lattice point



Simple cubic unit cell

Each lattice point is shared by 8 unit cells.

$$\# \text{ of pts. in one unit cell} = 8 \times \frac{1}{8} = 1 \text{ lattice pt.}$$

→ Primitive unit cell.

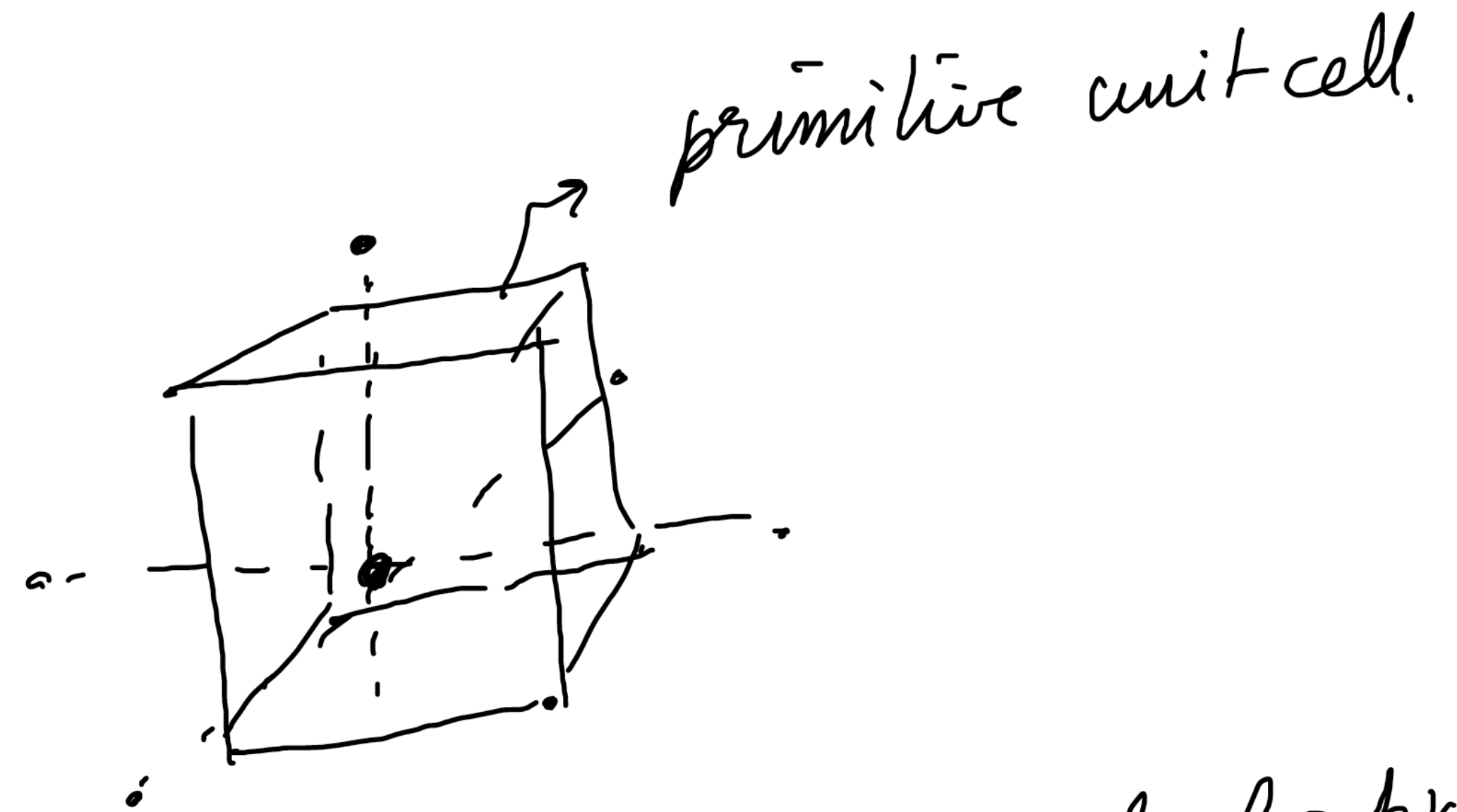
Introduction to lattices

Unit cells

Smallest volume that can be repeated to get the lattice

Conventional unit cells can contain more than one lattice point.

In some cases, they might be more convenient for description of crystal.



Conventional unit cell :- body centred cubic
face centred cubic

A hand-drawn diagram of a conventional unit cell, which is a cube with lattice points at each of the eight corners and one lattice point at the center. A vertical arrow on the right side is labeled 'a', representing the lattice constant. To the right of the diagram is the equation: $\# \text{ of pts} = 8 \times \frac{1}{8} + 1 = 2$

Up next ...

Symmetries in lattices

Bravais lattices

Introduction to lattices

Symmetries in lattices

Most important / obvious one is translation symmetry

$$\vec{r}' = \vec{r} + \vec{R}_{lmn} \quad \implies \quad P(\vec{r}') \equiv P(\vec{r})$$

Where P is any physical property of the crystal

Other symmetries include point group symmetries.

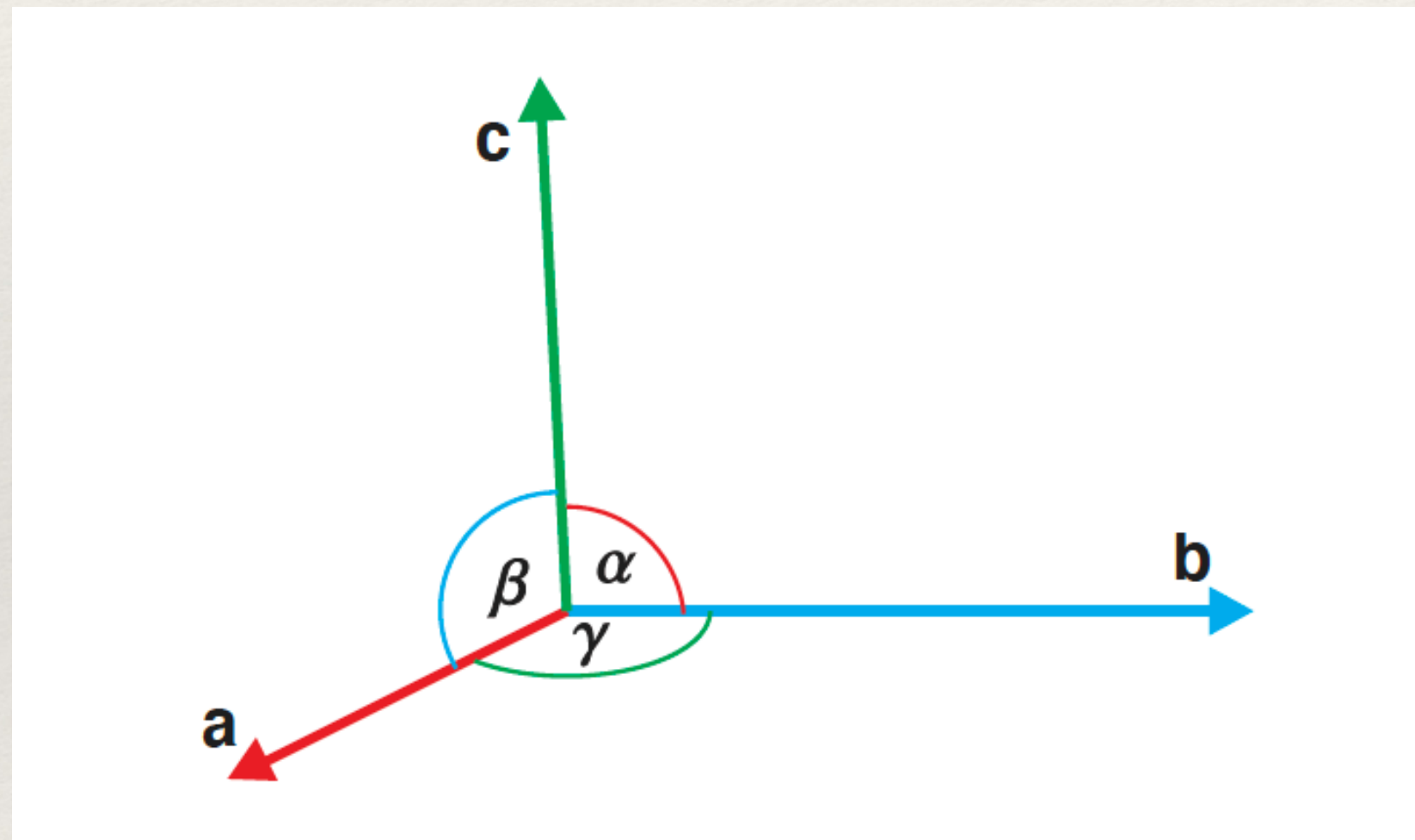
Like axes of rotation and planes of reflection

Compatibility between point and space (translation) symmetries restrict the number of types of crystals.

Introduction to lattices

Types of crystals

Unit cell parameters



7 Unit Cell Types

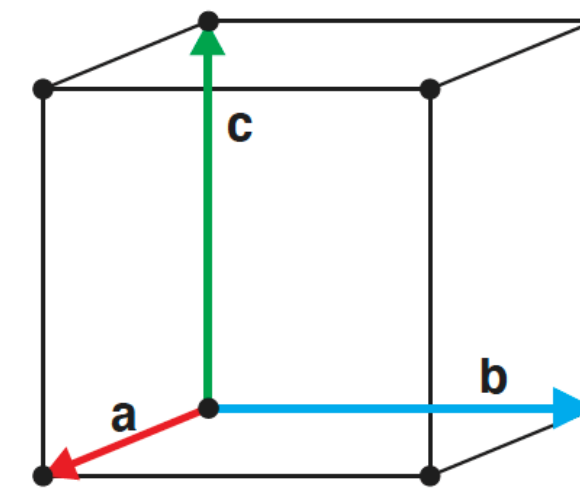
System	Unit cell parameters
Cubic (isomorphic)	$a = b = c; \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$
Tetragonal	$a = b \neq c; \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$
Orthorhombic	$a \neq b \neq c; \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$
Monoclinic	$a \neq b \neq c; \alpha = 90^\circ, \beta \neq 90^\circ, \gamma = 90^\circ$
Triclinic	$a \neq b \neq c; \alpha \neq 90^\circ, \beta \neq 90^\circ, \gamma \neq 90^\circ$
Hexagonal	$a = b \neq c; \alpha = 90^\circ, \beta = 90^\circ, \gamma = 120^\circ$
Rhombohedral*	$a = b = c; \alpha = \beta = \gamma \neq 90^\circ$ $a' = b' \neq c'; \alpha' = 90^\circ, \beta' = 90^\circ,$ $\gamma' = 120^\circ$

*Rhombohedral unit cells are often specified in terms of a bigger hexagonal unit cell.

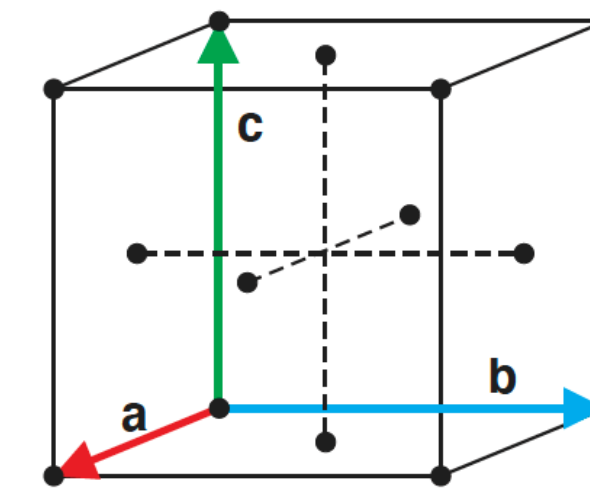
Introduction to lattices

Types of crystals

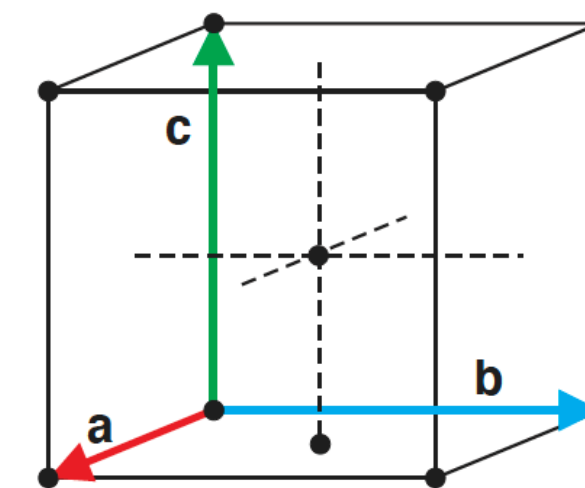
The 7 unit cell types give rise to 14 types of basic lattices called Bravais lattices.



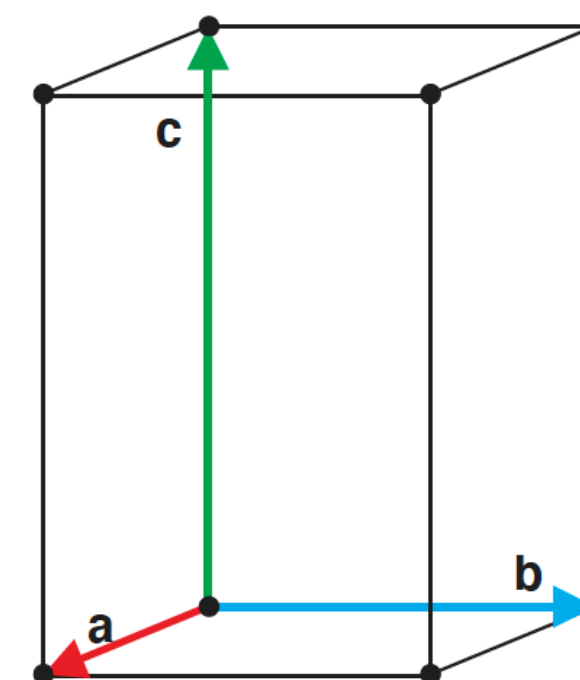
primitive cubic (cP)



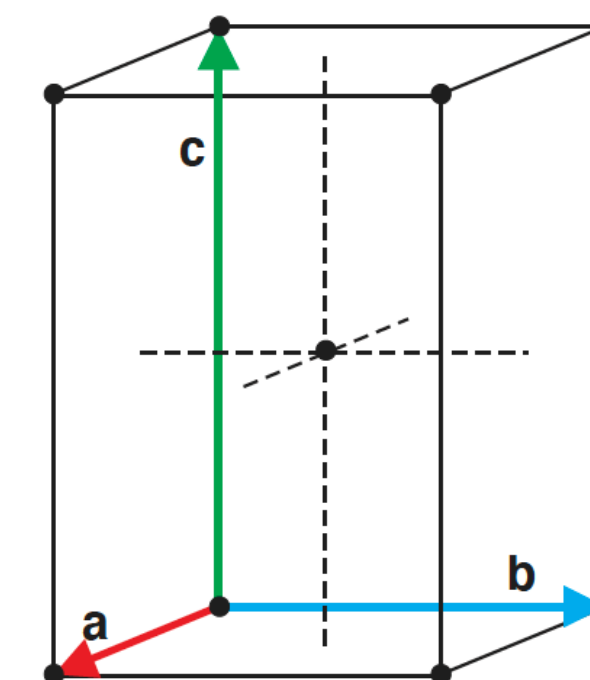
face-centred cubic (cF)



body-centred cubic (cI)



primitive tetragonal (tP)

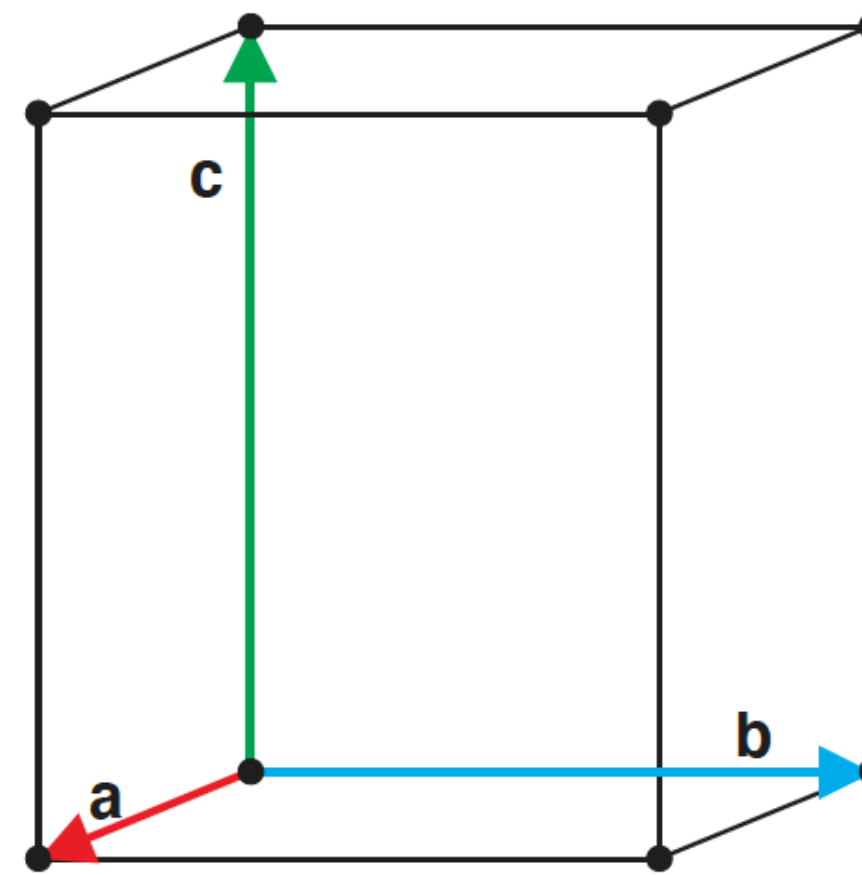


body-centred tetragonal (tI)

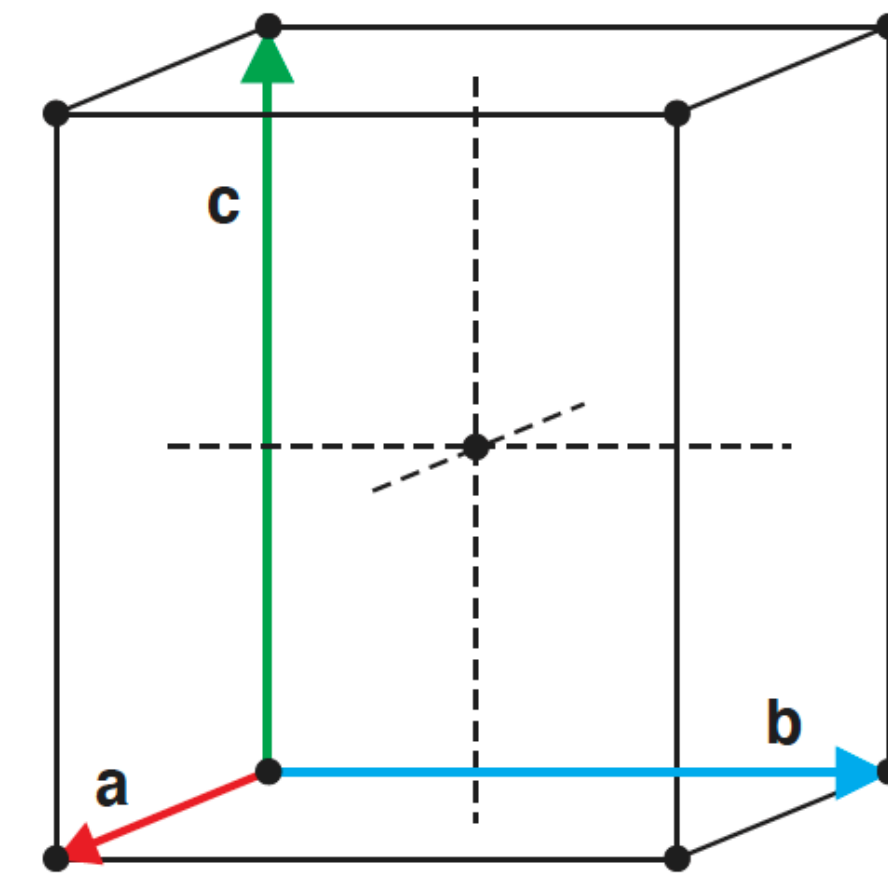
Introduction to lattices

Types of crystals

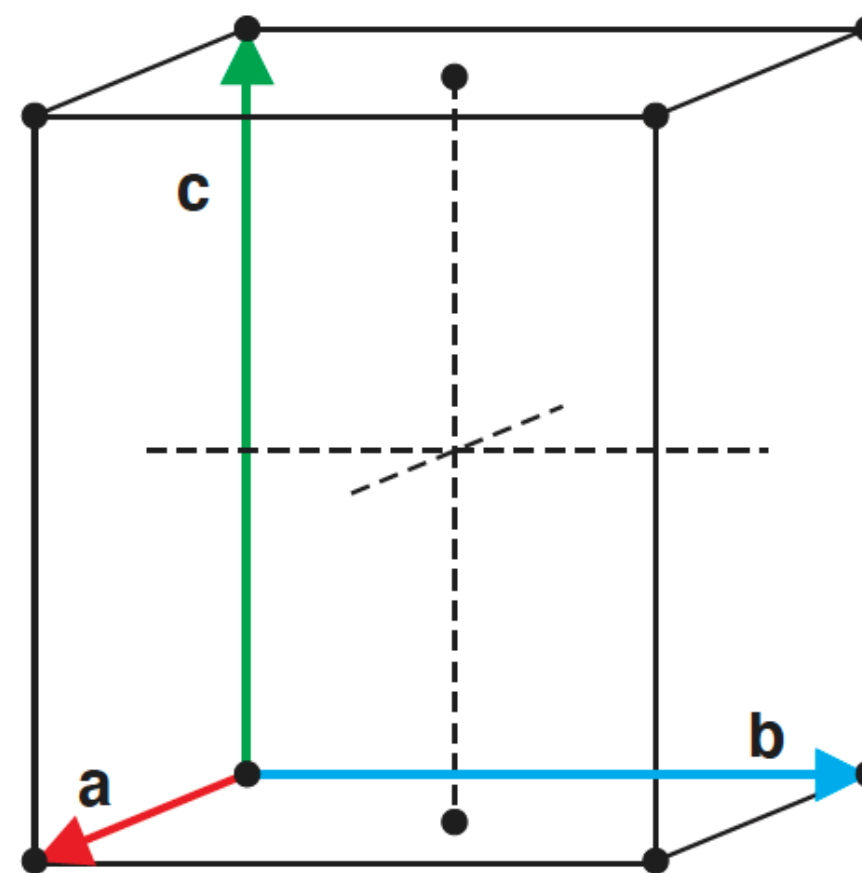
The 7 unit cell types give rise to 14 types of basic lattices called **Bravais lattices**.



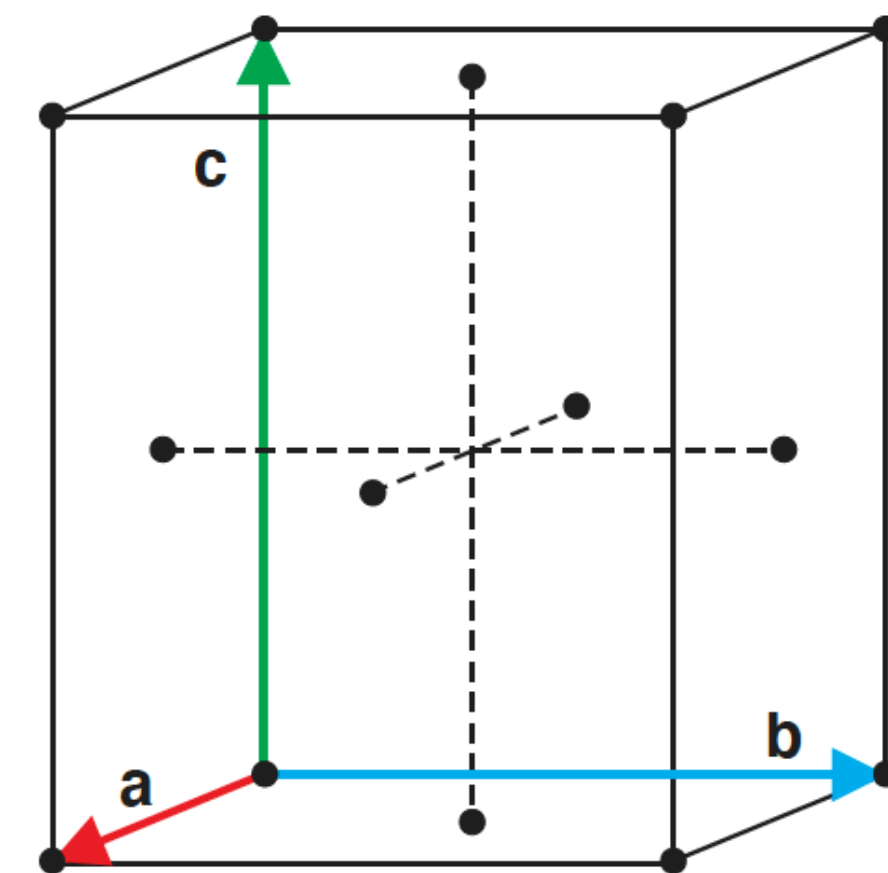
primitive orthorhombic (oP)



body-centred orthorhombic (oI)



base-centred orthorhombic (oC)

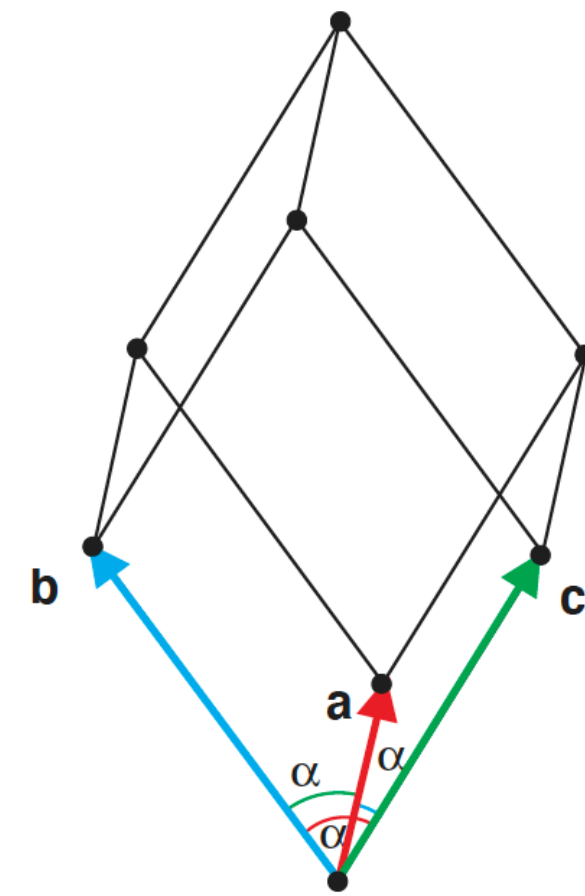


face-centred orthorhombic (oF)

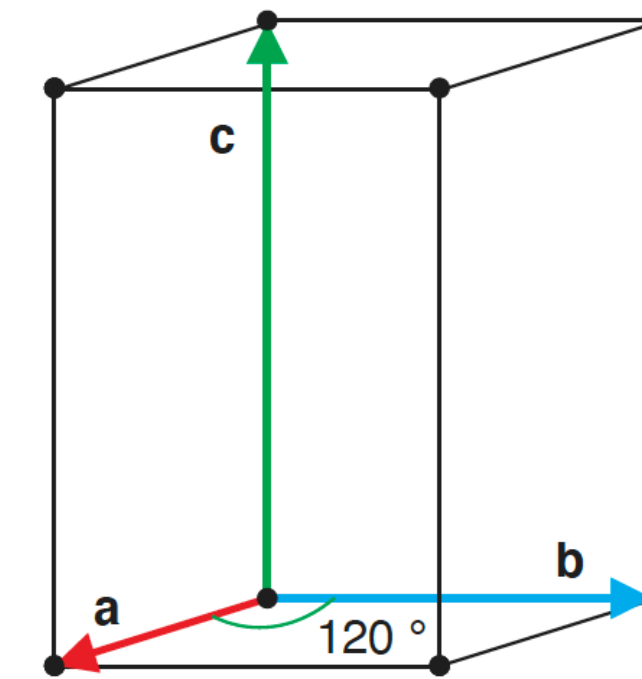
Introduction to lattices

Types of crystals

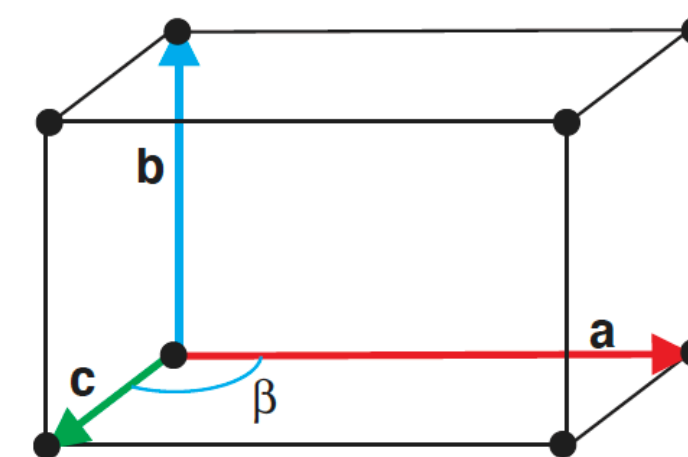
The 7 unit cell types give rise to 14 types of basic lattices called **Bravais lattices**.



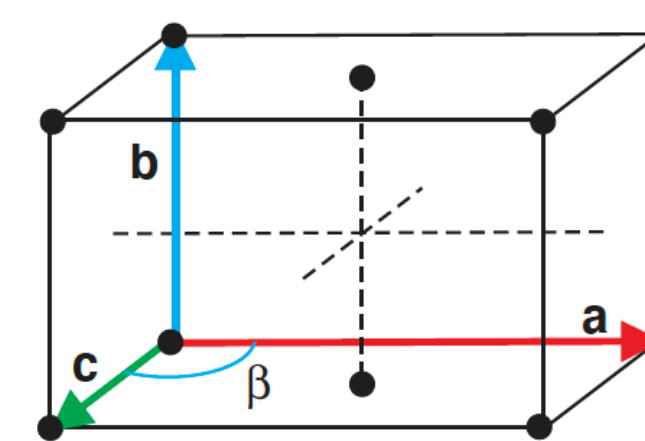
rhombohedral (R)



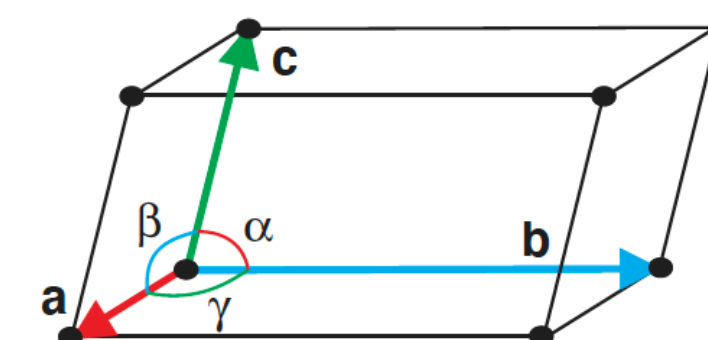
primitive hexagonal (hP)



primitive monoclinic (mP)



base-centred monoclinic (mB)



primitive triclinic (aP)

Introduction to lattices

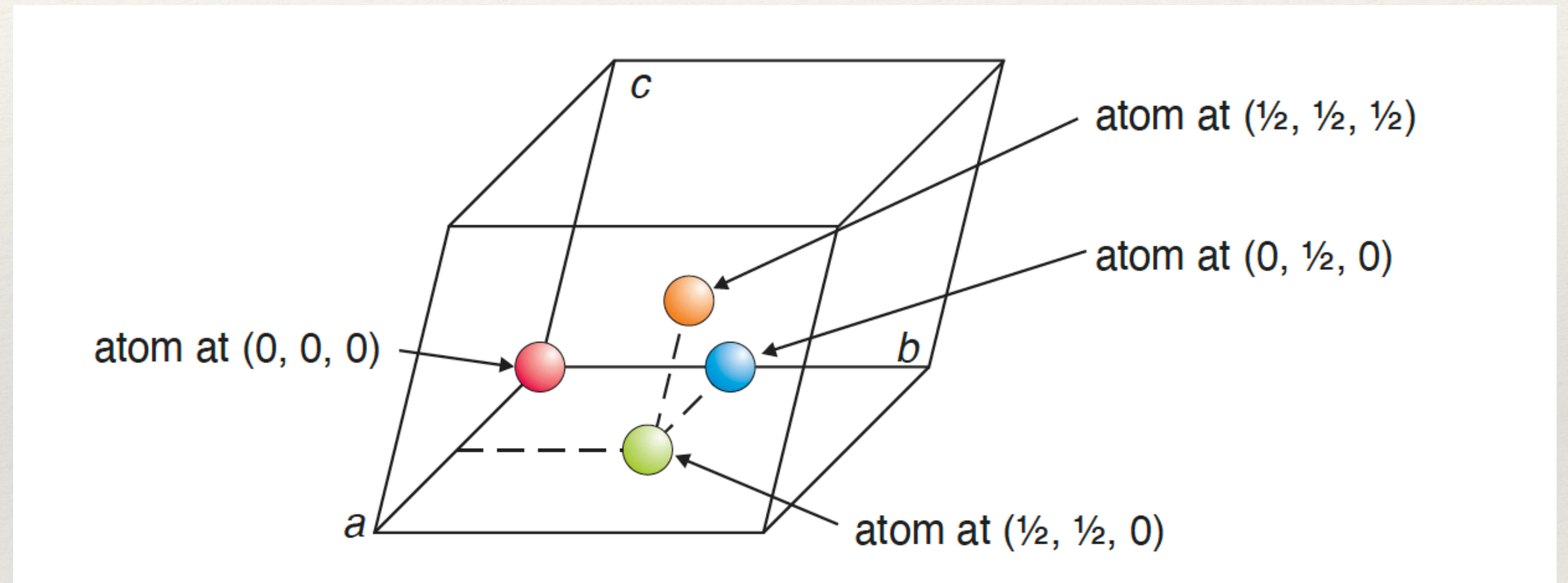
Constituents of a unit cell

Each lattice point is associated with one or a group of atoms - *motif* or *basis*.

The motif repeats in space as per the periodicity of the lattice and generates the crystal.

Thus,

Crystal = lattice + basis / motif



Coordinates of atoms in the basis are conventionally specified in fractions of the primitive translation vectors.