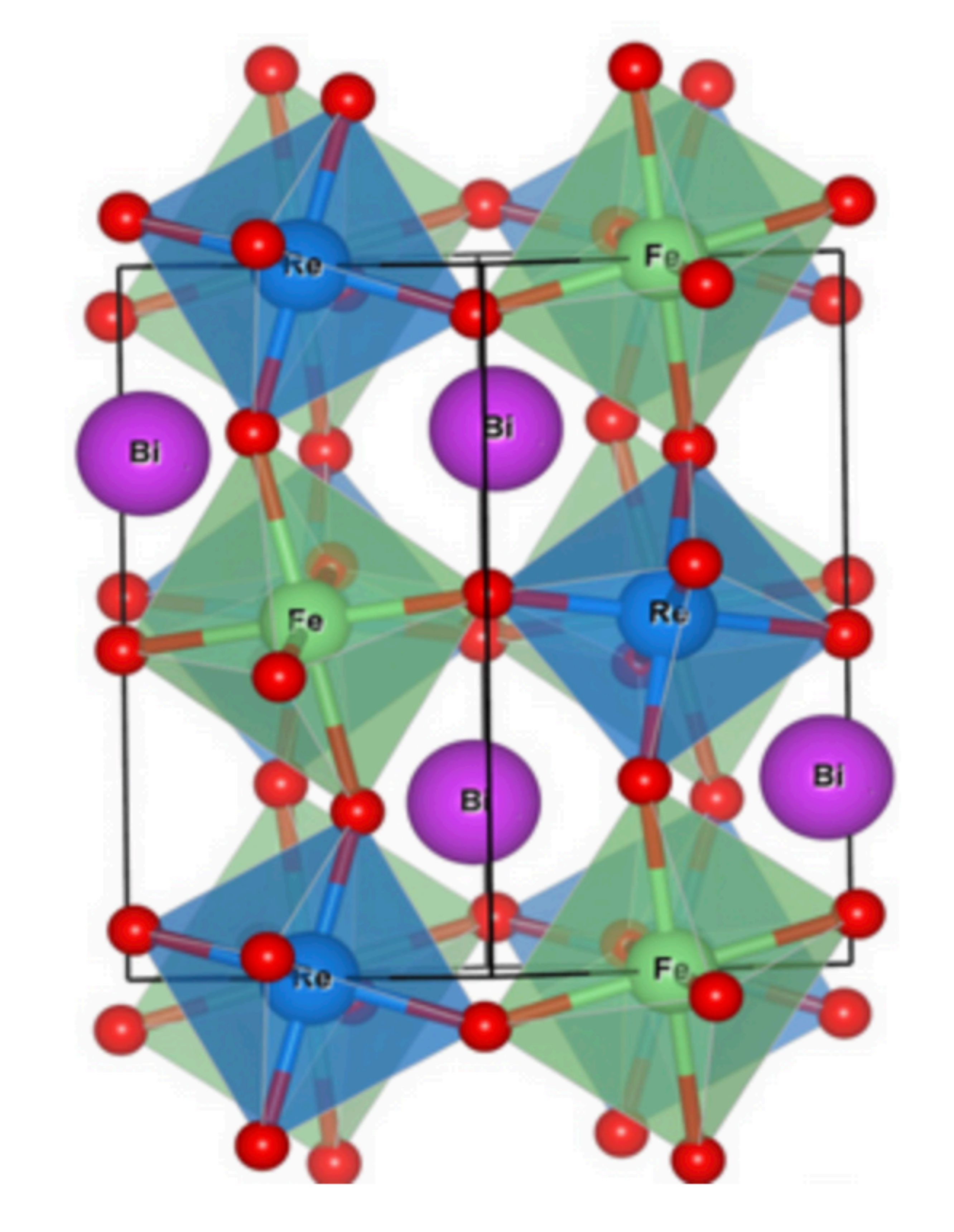

Structure of Solids - Crystal Lattices

Lecture 1

CHM 637
Chemistry & Physics of Materials

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Dept. Of Chemistry
IISER Bhopal

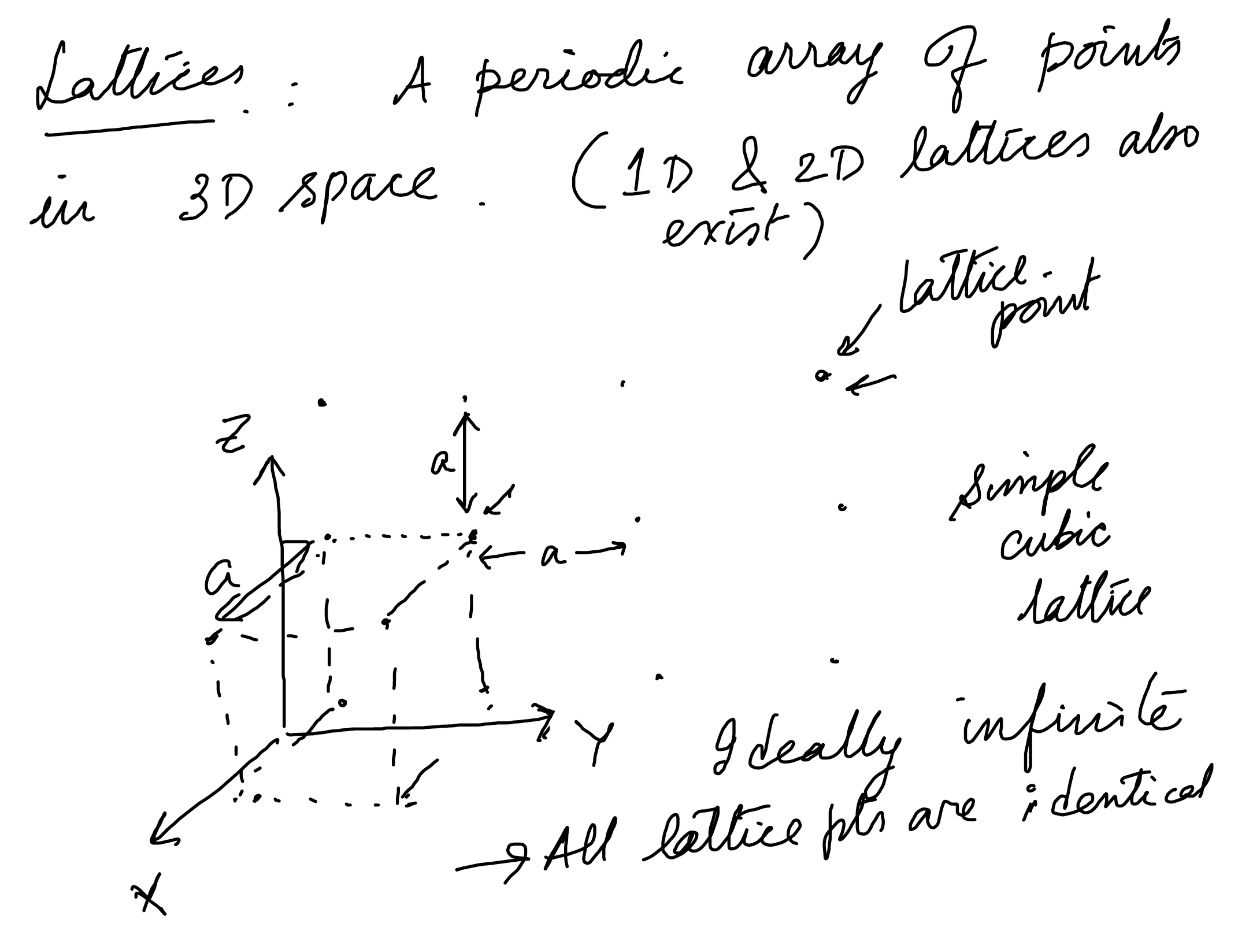
Lecture Plan

- 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

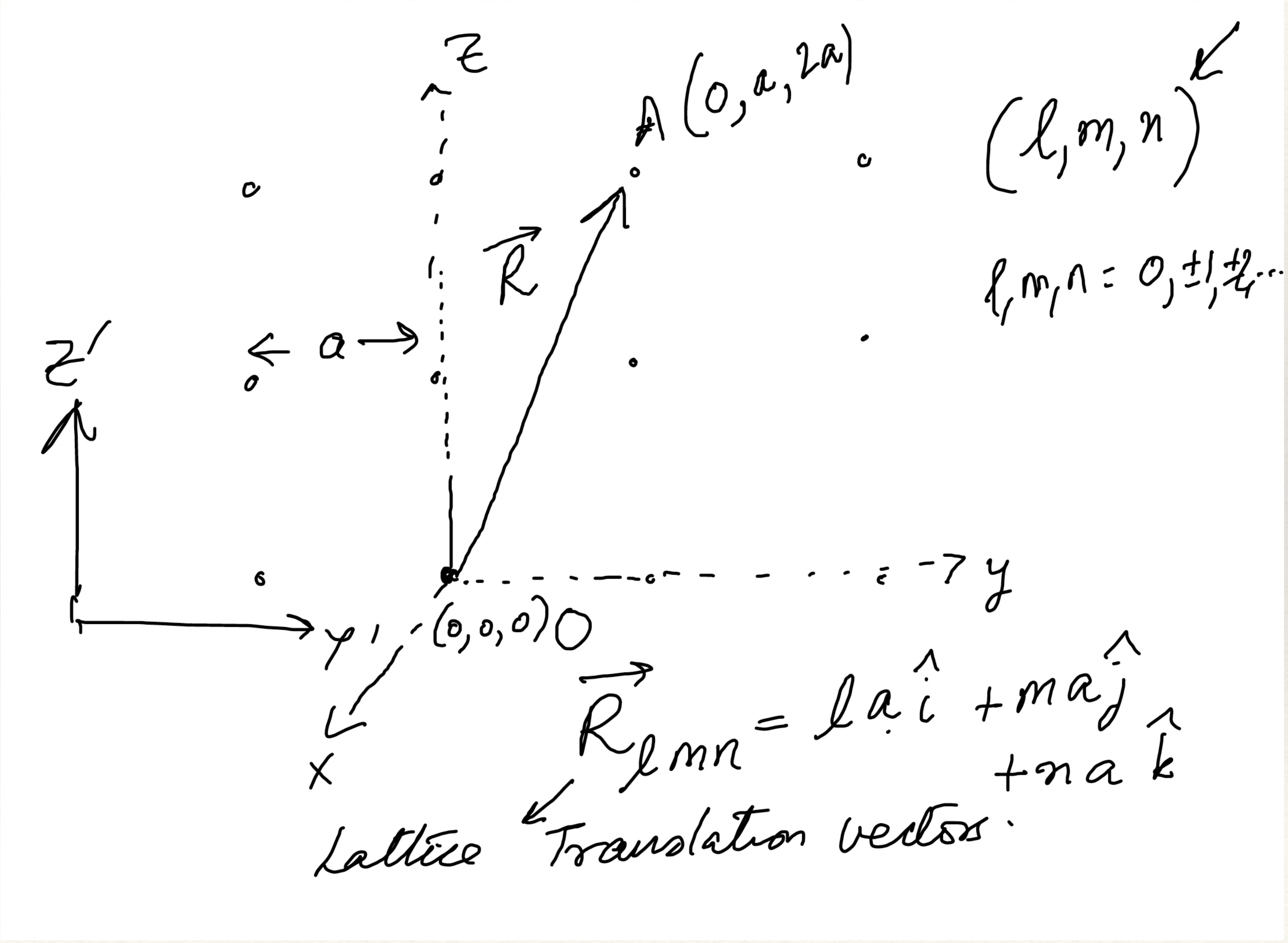
Infinite ideally but in practice bounded by the volume of the crystal.



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

$a \quad b \quad c$

Primitive Translation vectors $\leftarrow$ $\vec{a} = a\vec{u}_1, \quad \vec{b} = b\vec{u}_2, \quad \vec{c} = c\vec{u}_3$

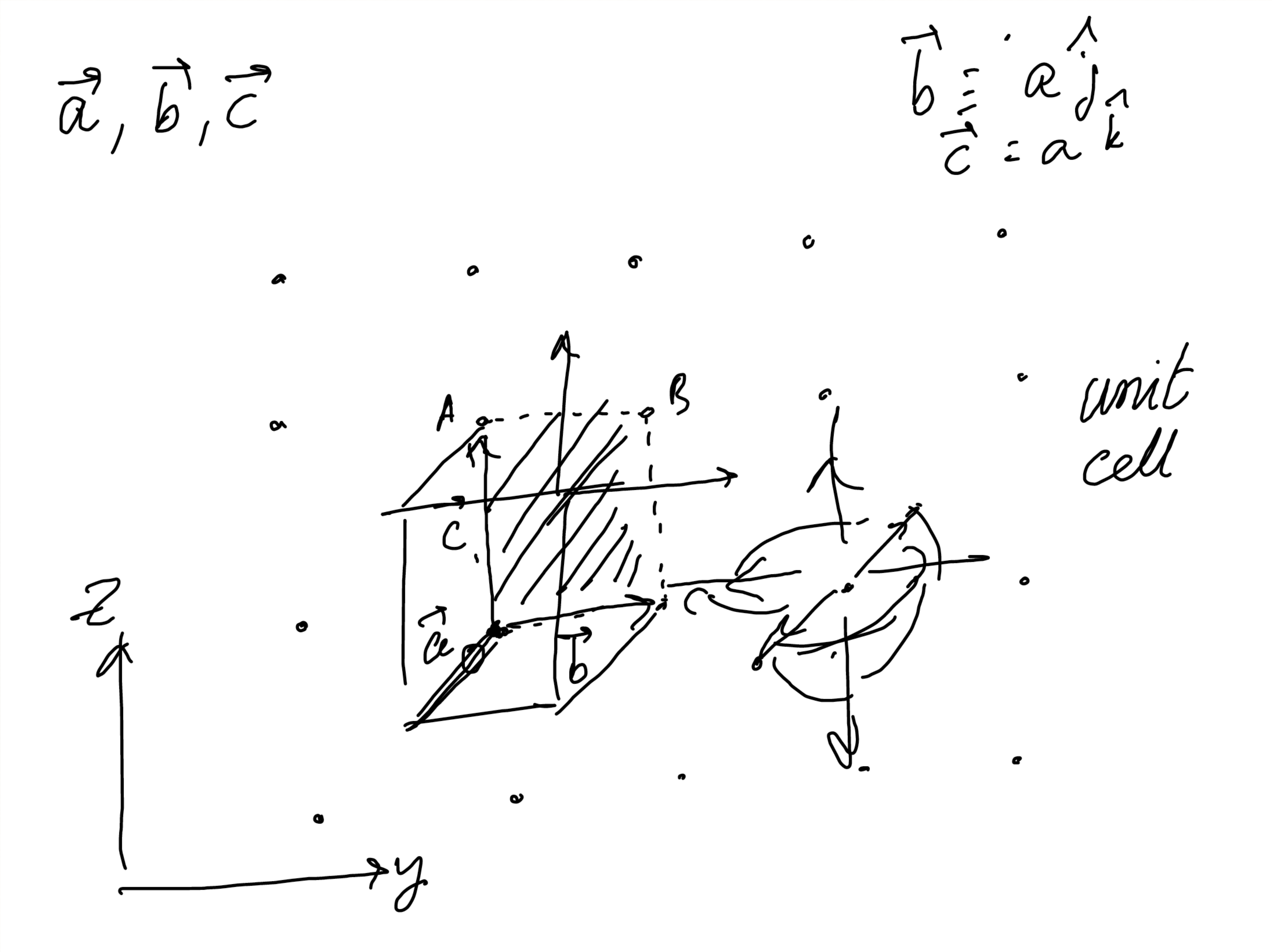
$$\vec{R}_{lmn} = l\vec{a} + m\vec{b} + n\vec{c}$$

$\downarrow$ Lattice translation vectors

Introduction to lattices

Unit cells

Smallest volume that can be repeated to get the lattice

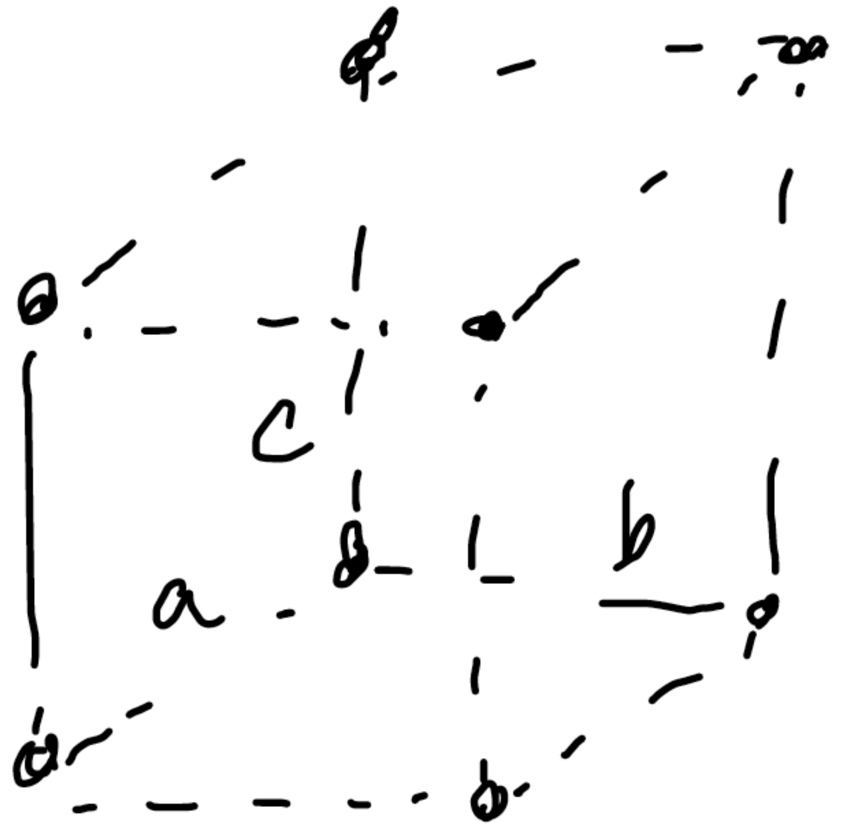


Introduction to lattices

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.

# of pts. in one unit cell $= 8 \times 1/8 = 1$ lattice pt.

→ Primitive unit cell.

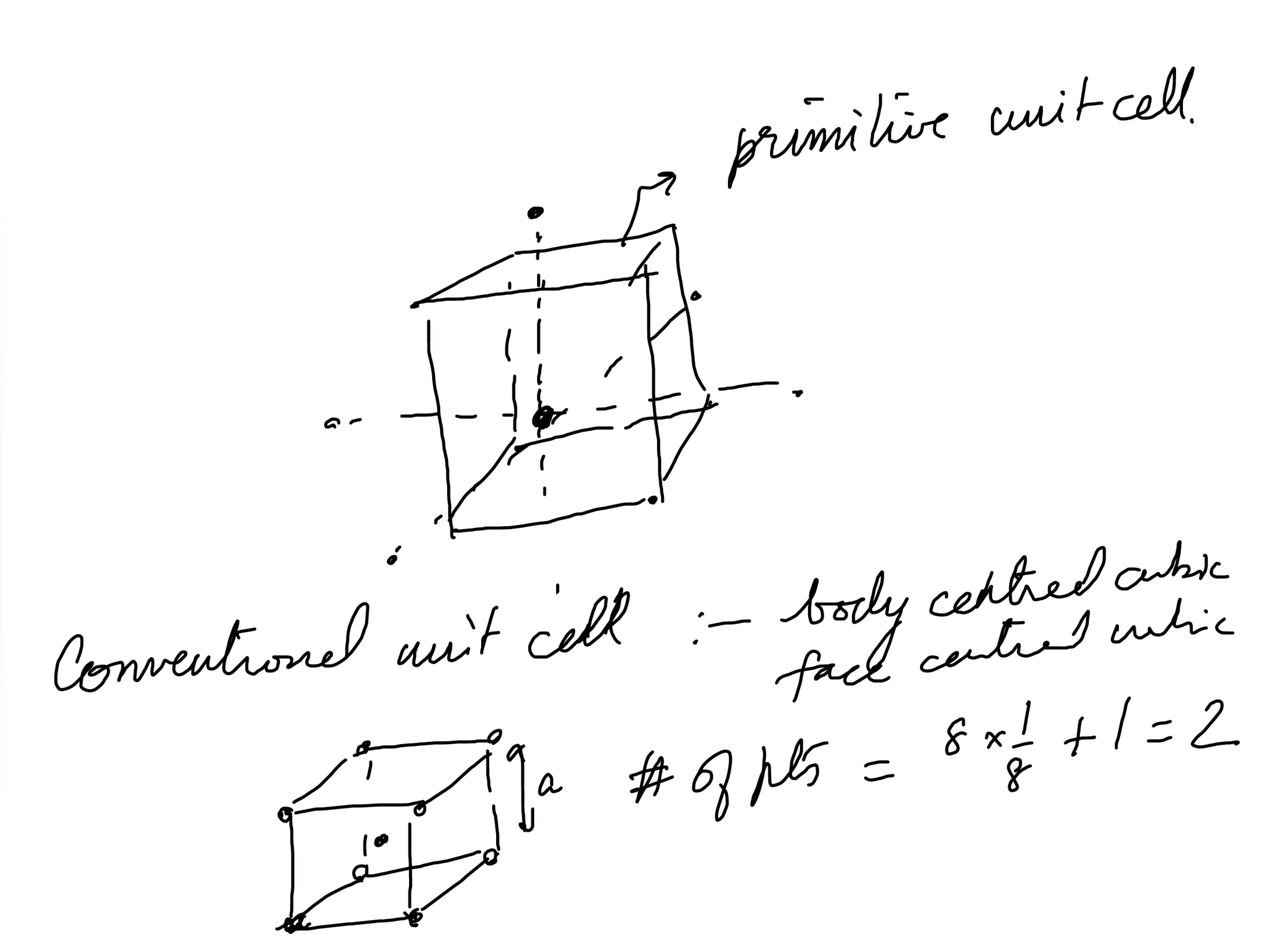
Introduction to lattices

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.



Up next …

Symmetries in lattices

Bravais lattices

Introduction to lattices

Symmetries in lattices

Most important/obvious one is translation symmetry

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

Where P is any physical property of the crystal

Other symmetries include point group symmetries.

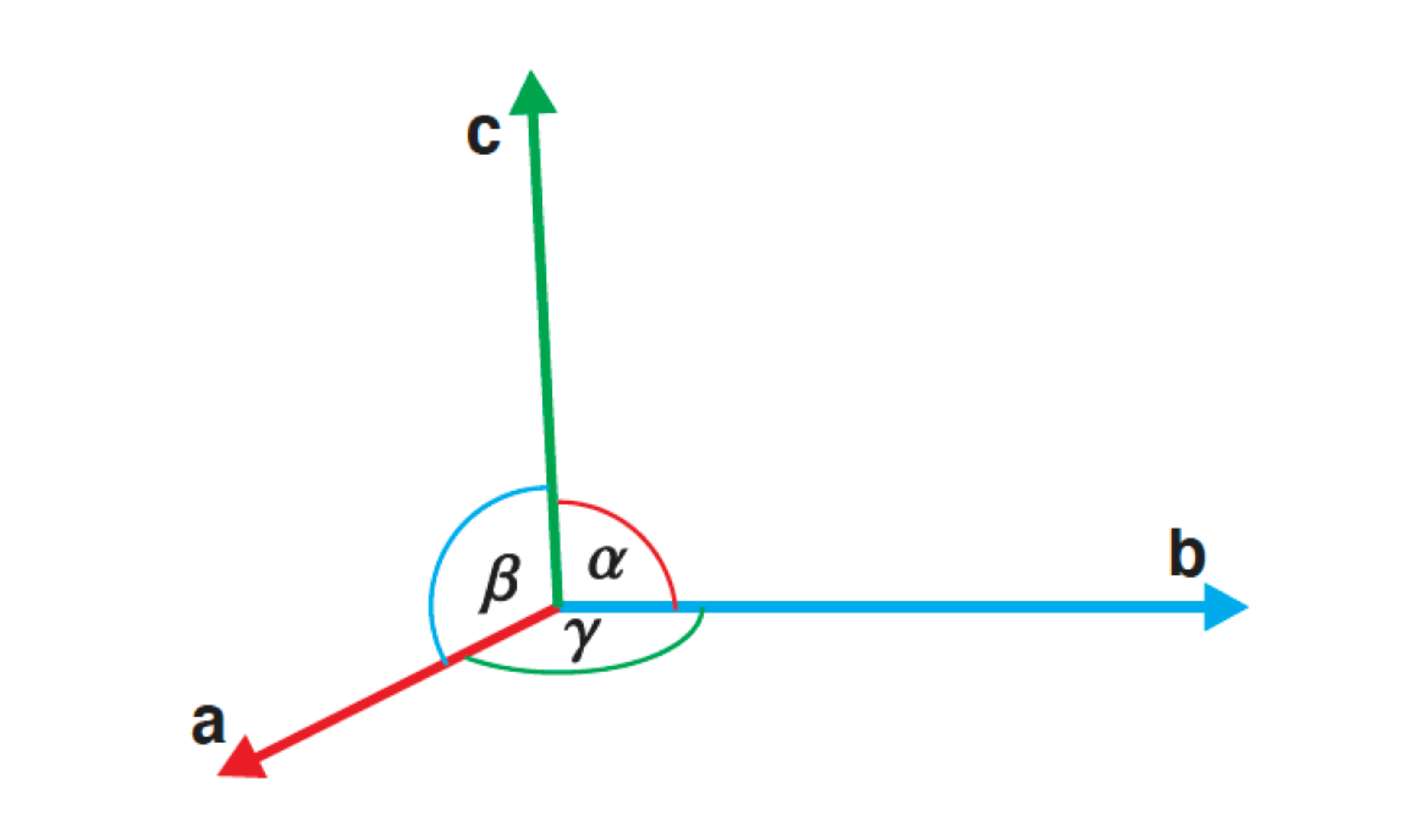
Like axes of rotation and planes of reflection

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)	$a = b = c$; $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$
Tetragonal	$a = b \neq c$; $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$
Orthorhombic	$a \neq b \neq c$; $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$
Monoclinic	$a \neq b \neq c$; $\alpha = 90°$, $\beta \neq 90°$, $\gamma = 90°$
Triclinic	$a \neq b \neq c$; $\alpha \neq 90°$, $\beta \neq 90°$, $\gamma \neq 90°$
Hexagonal	$a = b \neq c$; $\alpha = 90°$, $\beta = 90°$, $\gamma = 120°$
Rhombohedral*	$a = b = c$; $\alpha = \beta = \gamma \neq 90°$ $a' = b' \neq c'$; $\alpha' = 90°$, $\beta' = 90°$, $\gamma' = 120°$

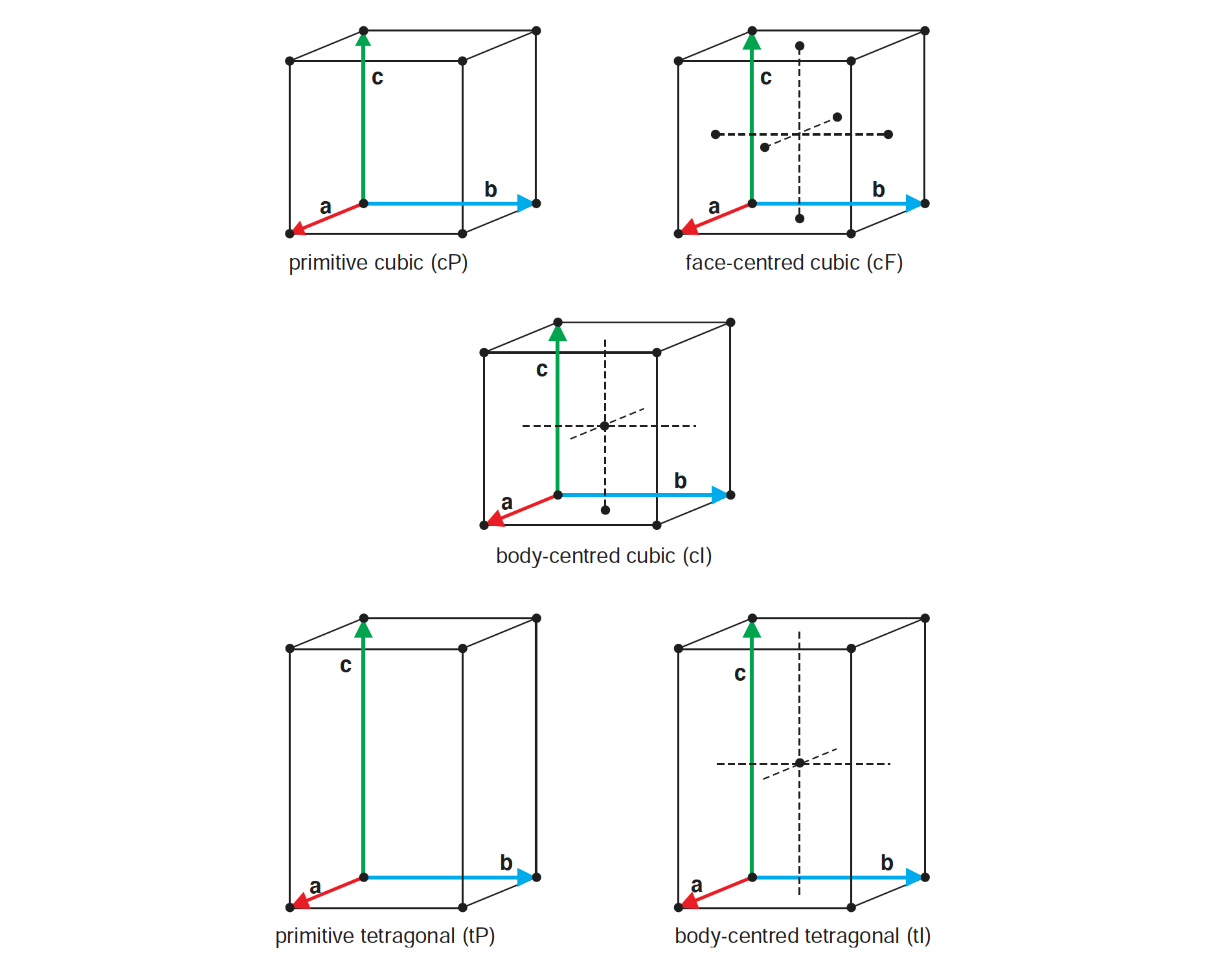
*Rhombohedral unit cells are often specified in terms of a bigger hexagonal unit cell.

Taken from *Understanding Solids: The Science of Materials*, R. J. D. Tilley, 2nd Endition, Wiley

Introduction to lattices

Types of crystals

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



Introduction to lattices

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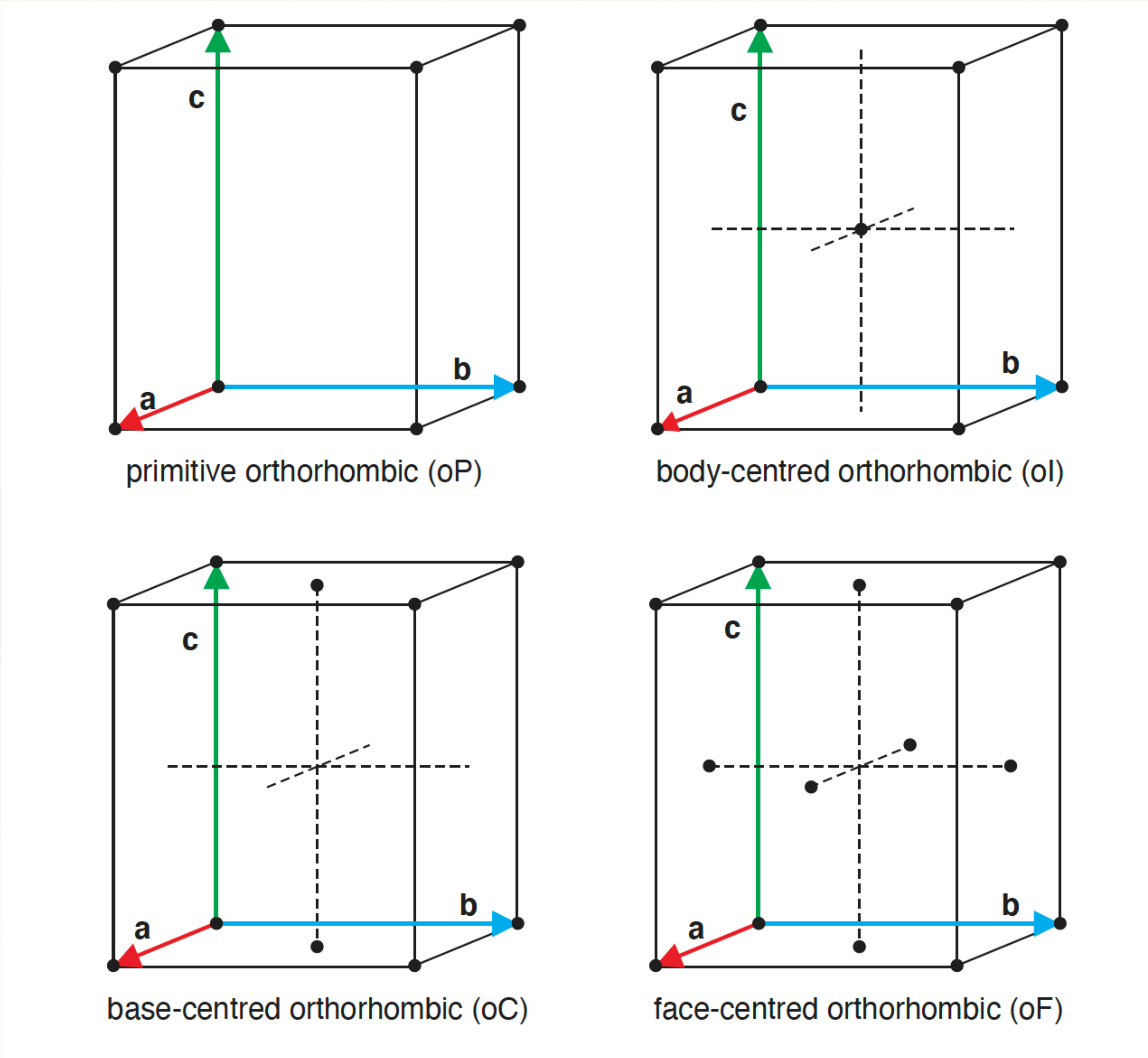

Introduction to lattices

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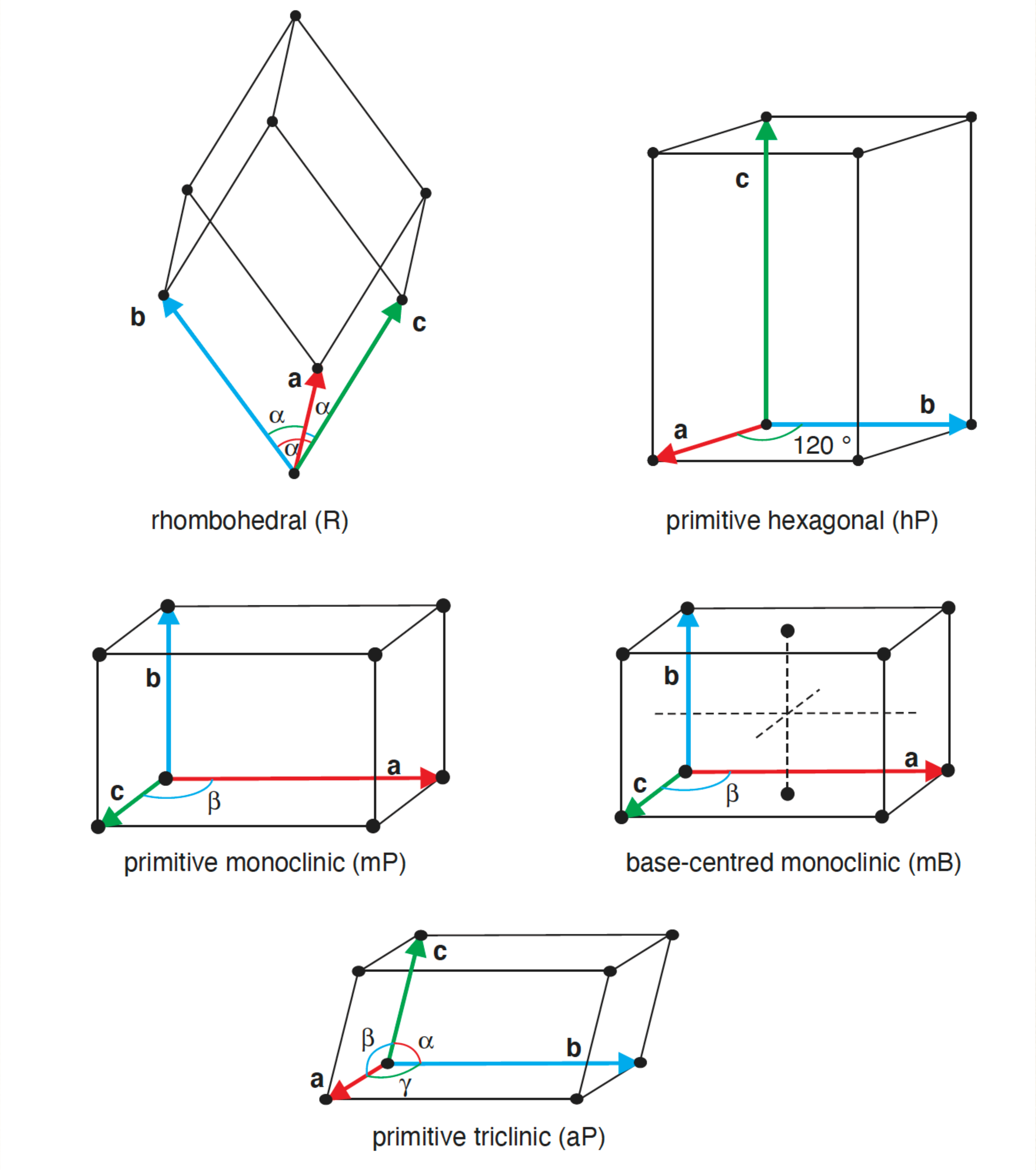


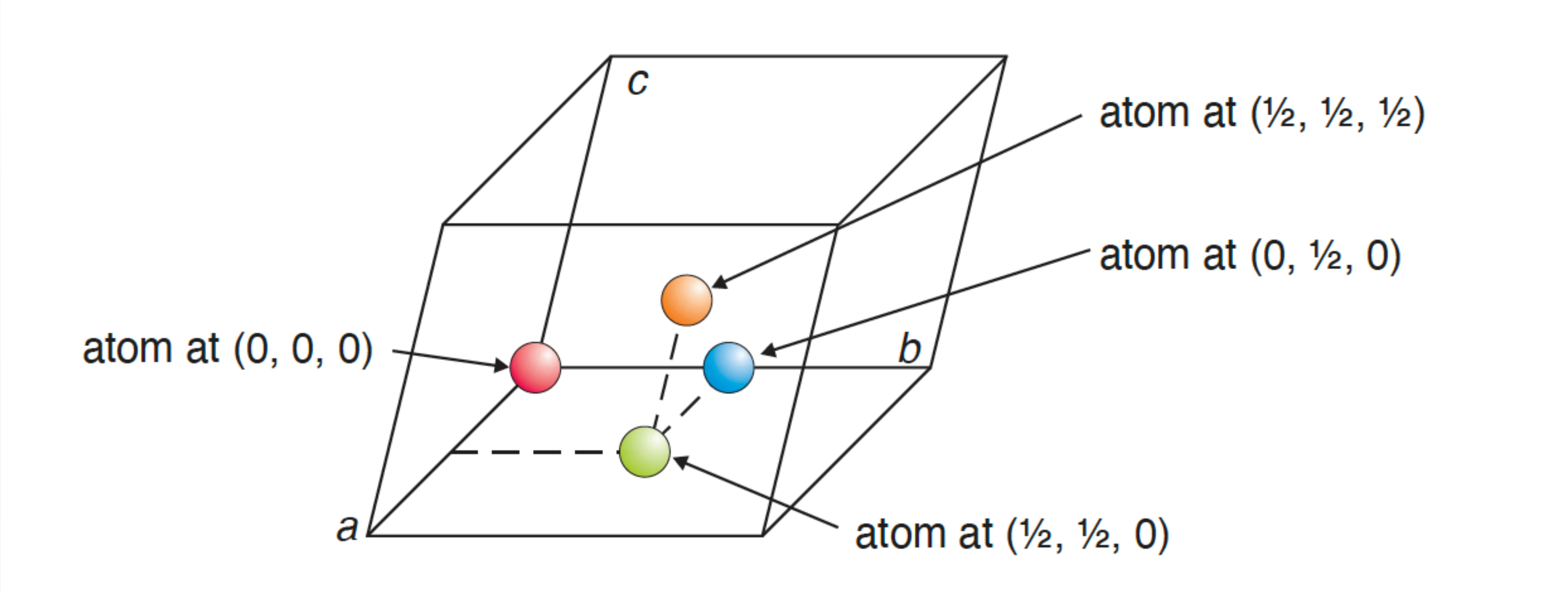
Introduction to lattices

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.