UNIT-I

CRYSTAL STRUCTURES

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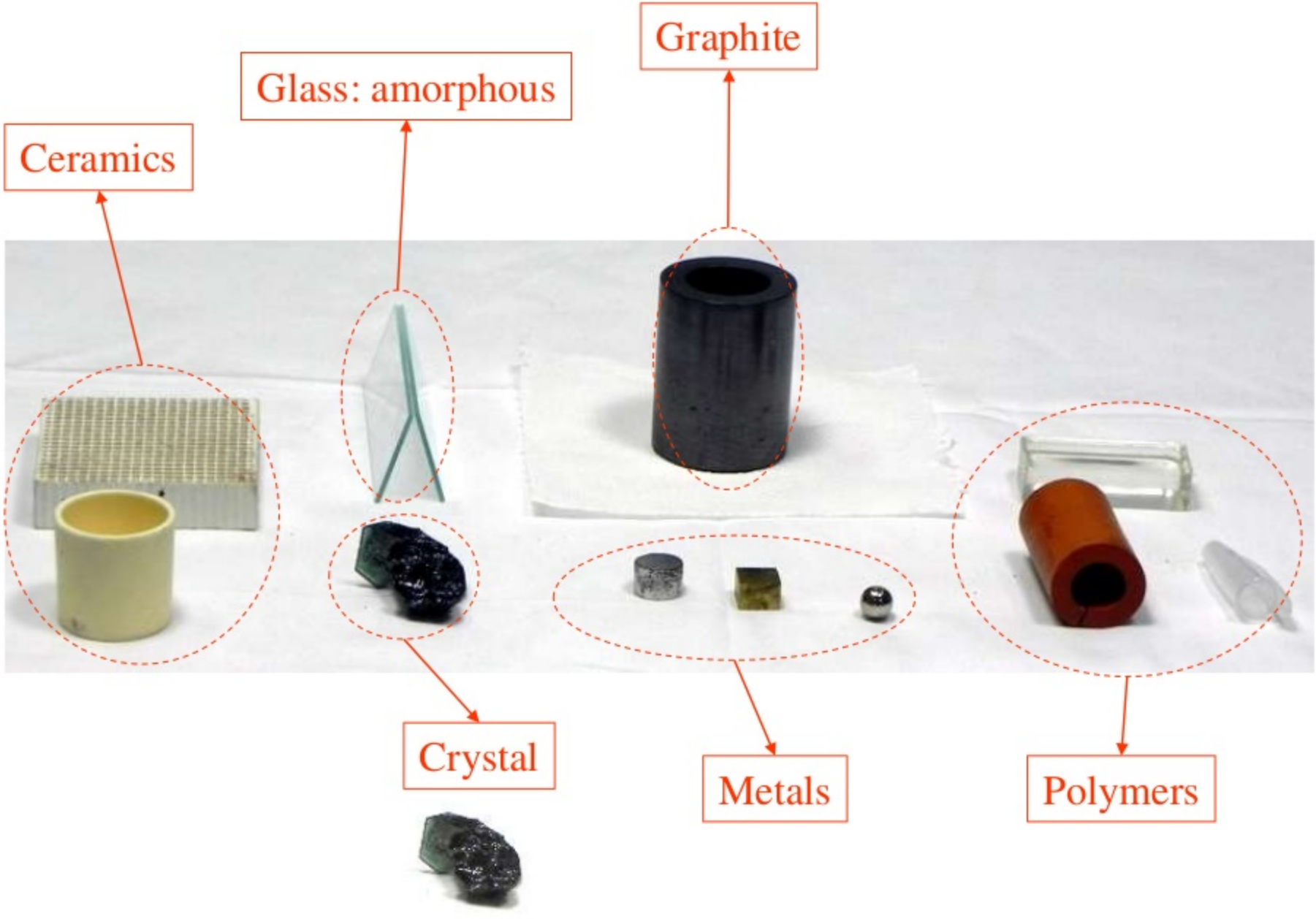
Learning objectives

- After the chapter is completed, you will be able to answer:
- Difference between crystalline and noncrystalline structures
- Different crystal systems and crystal structures
- Atomic packing factors of different cubic crystal systems
- Difference between unit cell and primitive cell
- Difference between single crystals and poly crystals

What is space lattice?

- Space lattice is the distribution of points in 3D in such a way that every point has identical surroundings, i.e., it is an infinite array of points in three dimensions in which every point has surroundings identical to every other point in the array.

Common materials: *with various 'viewpoints'*



Common materials: *examples*

- Metals and alloys ➢ Cu, Ni, Fe, NiAl (intermetallic compound), Brass (Cu-Zn alloys)
- Ceramics (usually oxides, nitrides, carbides) ➢ Alumina (Al_2O_3), Zirconia (Zr_2O_3)
- Polymers (thermoplasts, thermosets) (Elastomers)➢ Polythene, Polyvinyl chloride, Polypropylene

Based on Electrical Conduction

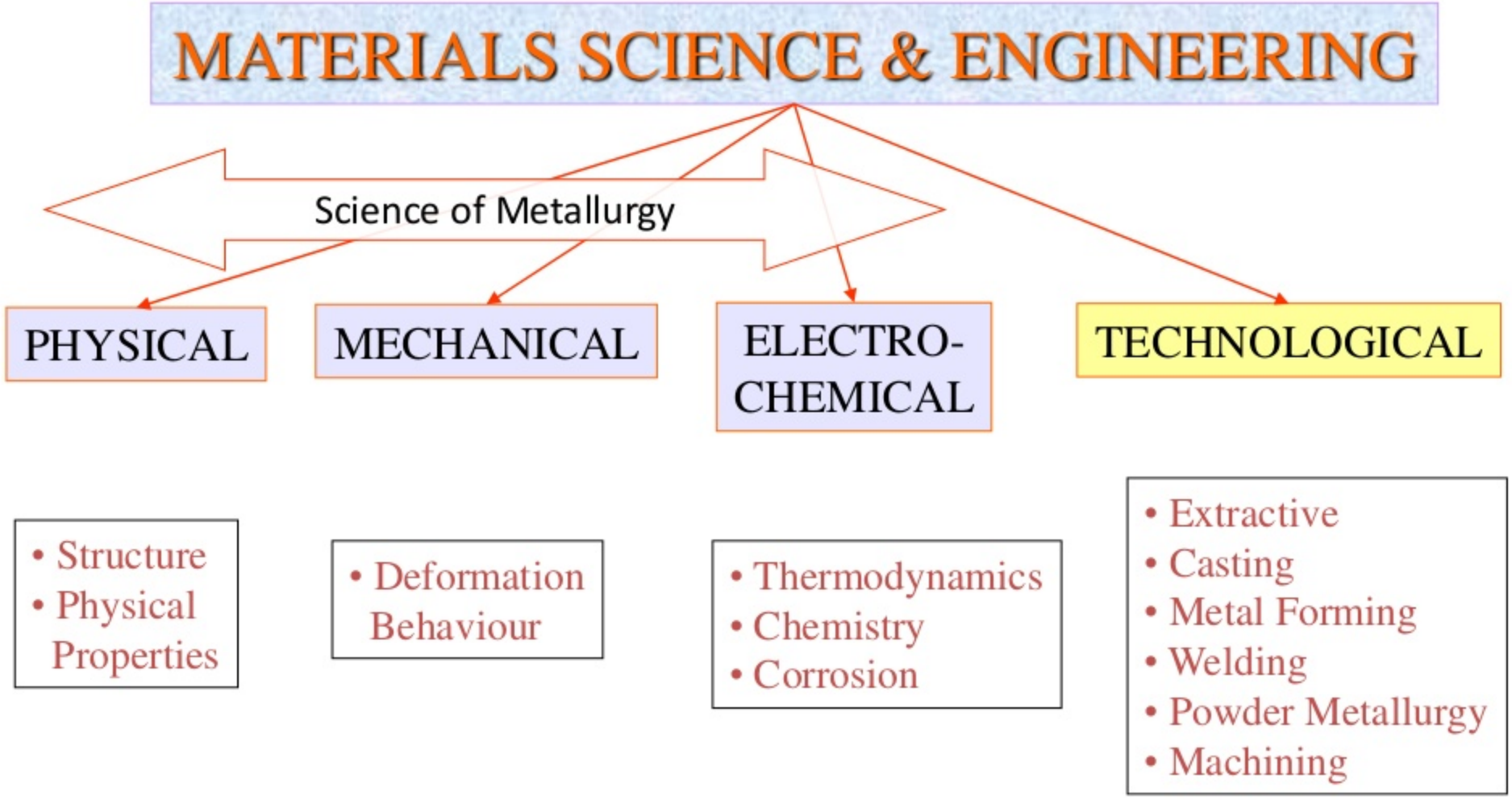
- Conductors ➢ Cu, Al, NiAl
- Semiconductors ➢ Ge, Si, GaAs
- Insulators ➢ Alumina, Polythene*

Based on Ductility

- Ductile ➢ Metals, Alloys
- Brittle ➢ Ceramics, Inorganic Glasses, Ge, Si

** some special polymers could be conducting*

- The broad scientific and technological segments of Materials Science are shown in the diagram below.
- To gain a comprehensive understanding of materials science, all these aspects have to be studied.



Definition 1

Crystal = Lattice + Motif

Motif or **Basis**:
typically an atom or a group of atoms associated with each lattice point

Lattice ➤ the underlying periodicity of the crystal
Basis ➤ Entity associated with each lattice points

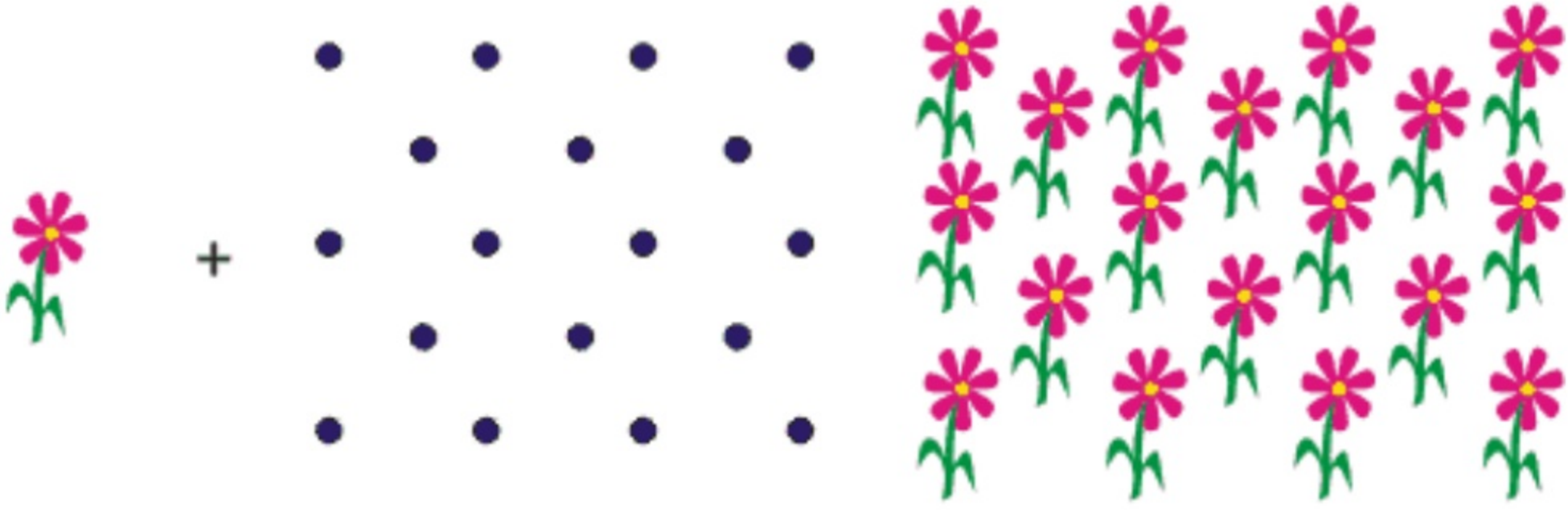
Lattice ➤ how to repeat
Motif ➤ what to repeat

Lattice

Translationally periodic arrangement of points

Crystal

Translationally periodic arrangement of motifs



Basis Lattice = Crystal

Space Lattice

A lattice is also called a Space Lattice

An array of points such that every point has *identical surroundings*

- **In Euclidean space ⇒ infinite array**
- **We can have 1D, 2D or 3D arrays (lattices)**

or

Translationally periodic arrangement of points in space is called a lattice

Unit cell: A unit cell is the sub-division of the space lattice that still retains the overall characteristics of the space lattice.

Primitive cell: the smallest possible unit cell of a lattice, having lattice points at each of its eight vertices only.

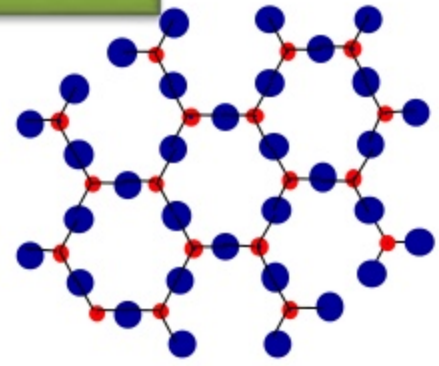
A primitive cell is a minimum volume cell corresponding to a single lattice point of a structure with translational symmetry in 2 dimensions, 3 dimensions, or other dimensions.

A lattice can be characterized by the geometry of its *primitive cell*.

Materials and Packing

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
  -many ceramics
  -some polymers

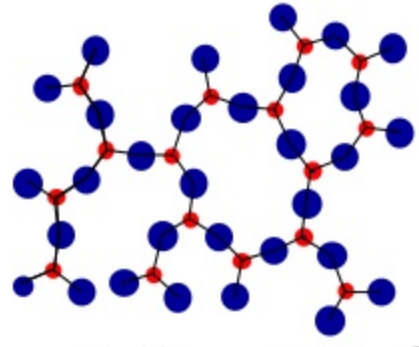


crystalline SiO_2 (Quartz)

• Si ● Oxygen

Non-crystalline materials...

- atoms have no periodic packing
- occurs for: -complex structures
  -rapid cooling

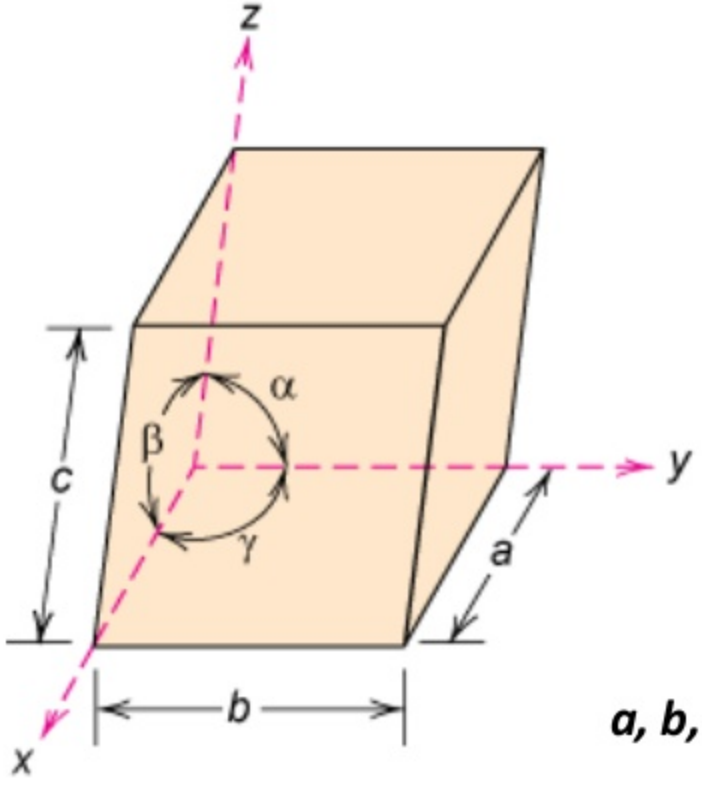


"Amorphous" = Noncrystalline

noncrystalline SiO_2 (Glass)

Crystal Systems

Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.



7 crystal systems

14 crystal lattices

***a, b,* and *c* are the lattice constants**

The Unite Cell is the smallest group of atom showing the characteristic lattice structure of a particular metal.
It is the building block of a single crystal.
A single crystal can have many unit cells.

Crystal systems

Cubic	Three equal axes, mutually perpendicular $a=b=c \quad \alpha=\beta=\gamma=90^\circ$
Tetragonal	Three perpendicular axes, only two equal $a=b\neq c \quad \alpha=\beta=\gamma=90^\circ$
Hexagonal	Three equal coplanar axes at 120° and a fourth unequal axis perpendicular to their plane $a=b\neq c \quad \alpha=\beta=90^\circ \quad \gamma=120^\circ$
Rhombohedral	Three equal axes, not at right angles $a=b=c \quad \alpha=\beta=\gamma\neq90^\circ$
Orthorhombic	Three unequal axes, all perpendicular $a\neq b\neq c \quad \alpha=\beta=\gamma=90^\circ$
Monoclinic	Three unequal axes, one of which is perpendicular to the other two $a\neq b\neq c \quad \alpha=\gamma=90^\circ\neq\beta$
Triclinic	Three unequal axes, no two of which are perpendicular $a\neq b\neq c \quad \alpha\neq\beta\neq\gamma\neq90^\circ$

Some engineering applications require single crystals:

--diamond single crystals for abrasives

--turbine blades

What is coordination number?

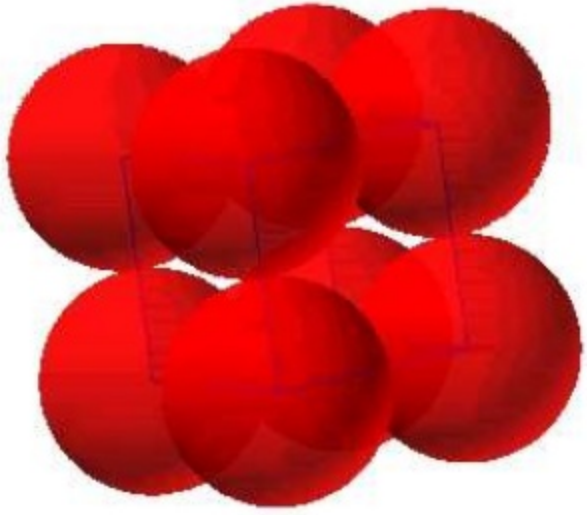
- *The **coordination number** of a central atom in a crystal is the number of its nearest neighbours.*

What is lattice parameter?

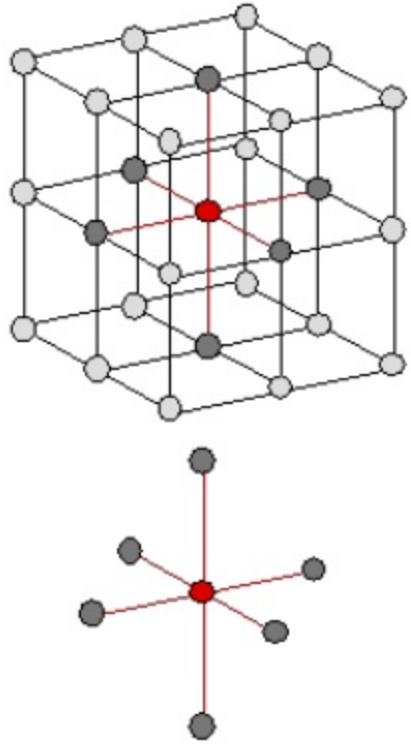
- *The **lattice constant**, or **lattice parameter**, refers to the physical dimension of unit cells in a crystal **lattice**.*
- ***Lattices** in three dimensions generally have three **lattice constants**, referred to as a, b, and c.*

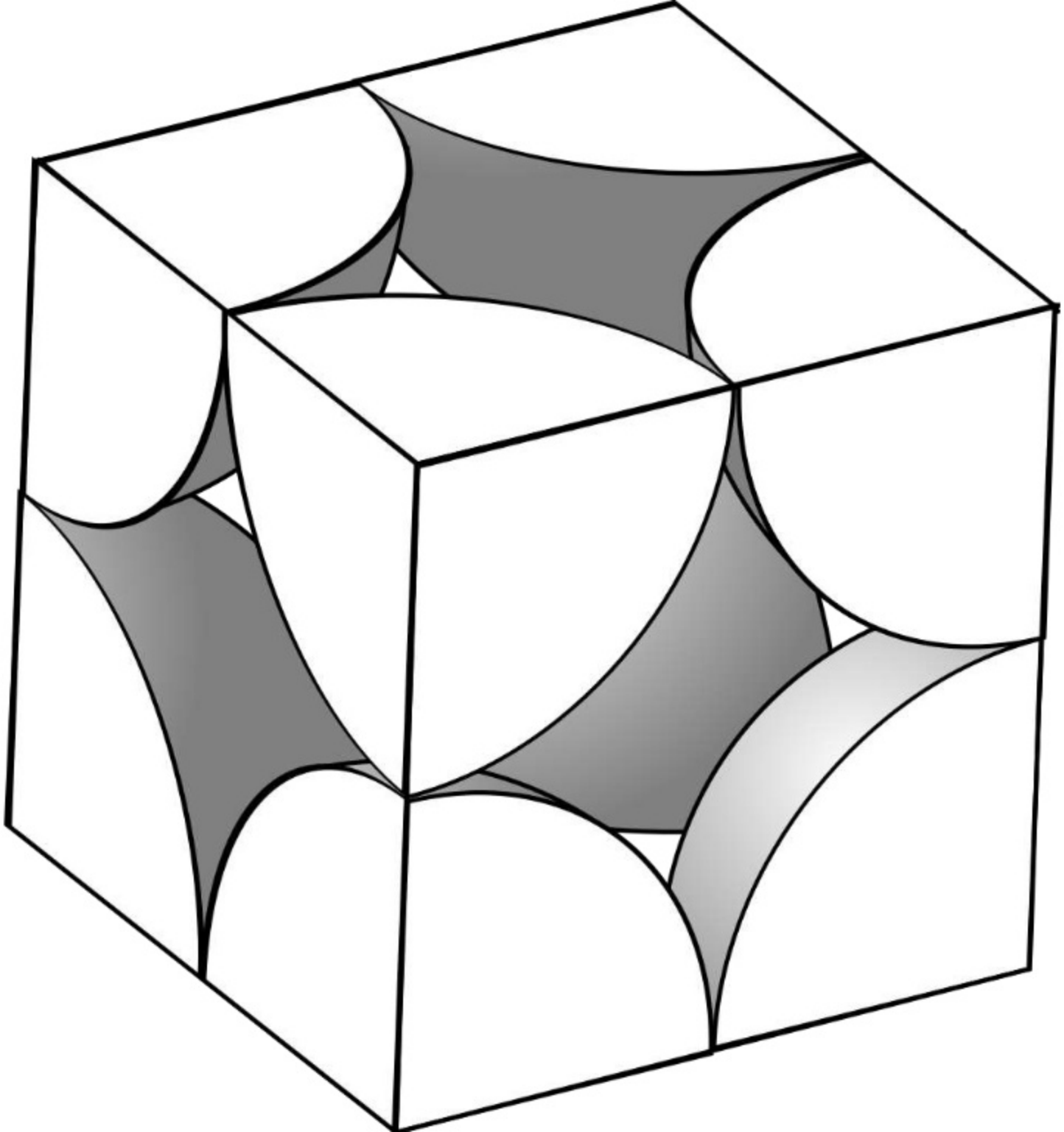
Simple Cubic Structure (SC)

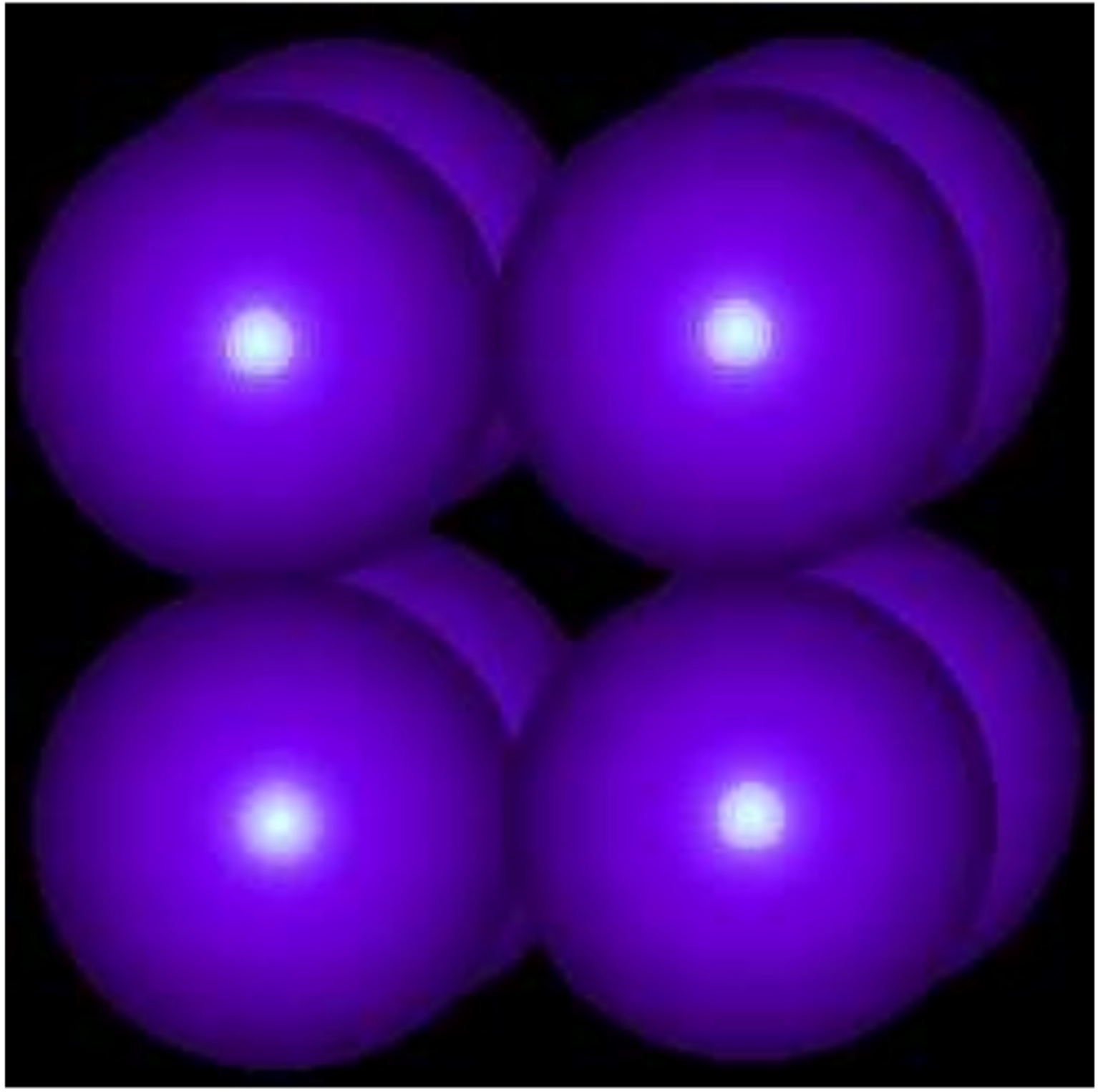
- **Rare due to low packing density (only Po has this structure)**
- **Close-packed directions are cube edges.**



- **Coordination # = 6**
  (# nearest neighbors)





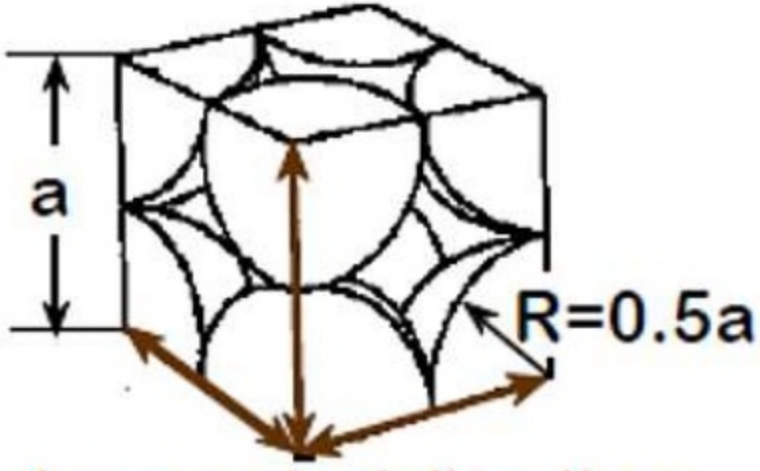


Atomic Packing Factor (APF)

$$APF = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains 8 x 1/8 =
1 atom/unit cell

$$APF = \frac{\frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}}}{\frac{\text{volume}}{\text{unit cell}}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$