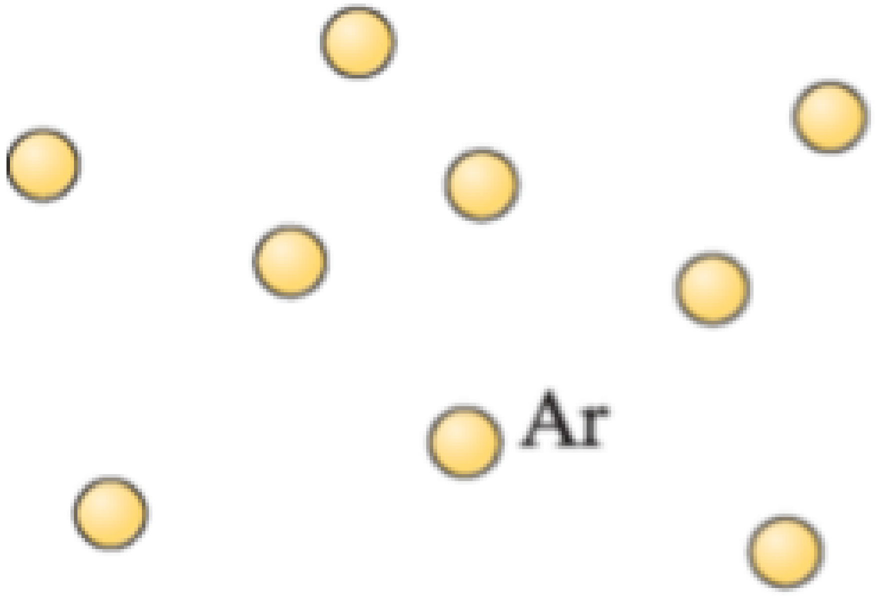
Chapter 3

Crystal Structure

Dr. Zhe Cheng

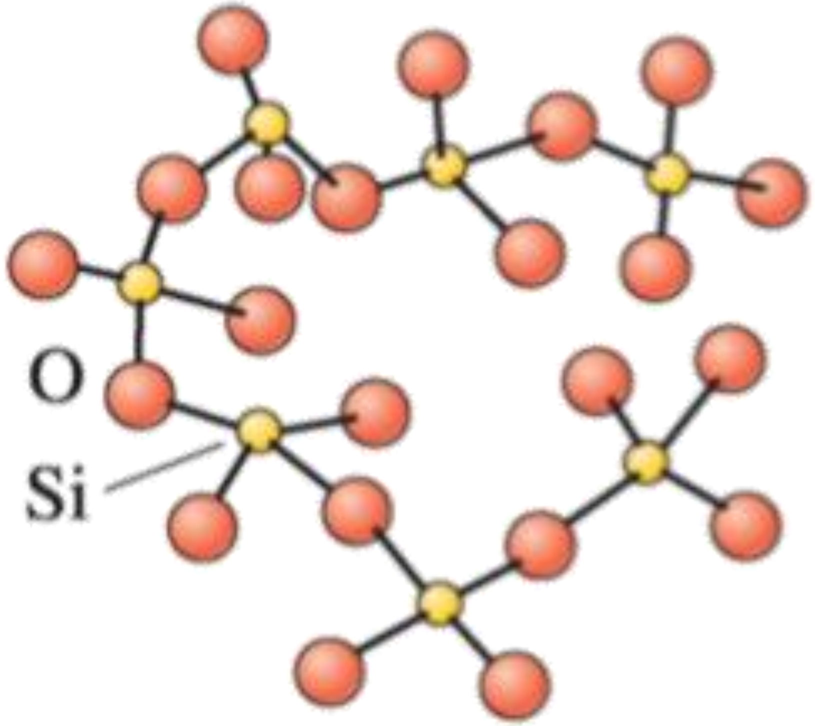
Short-Range Order vs. Long-Range Order

Complete random – NO order



Argon gas

Short-range order

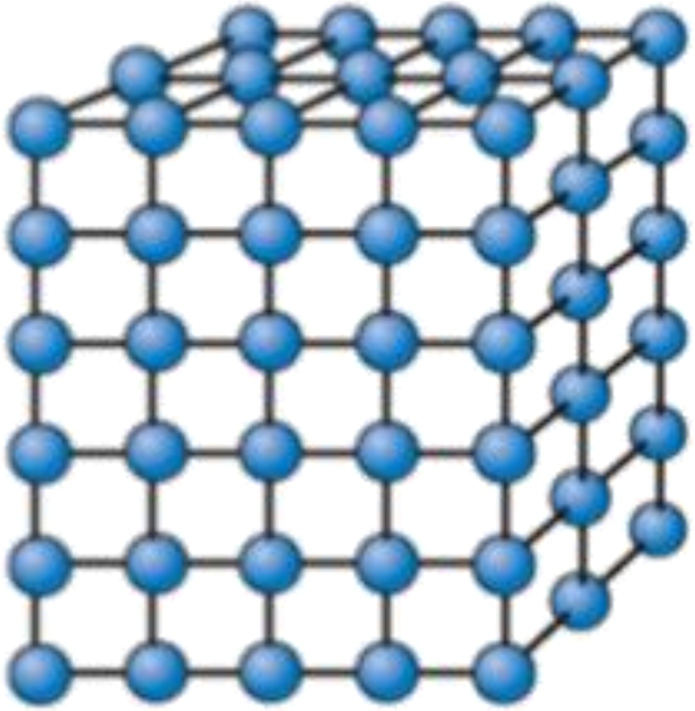


SiO_2 example

Si bonds to 4 O

O bonds to 2 Si

Long-range order



Po atom

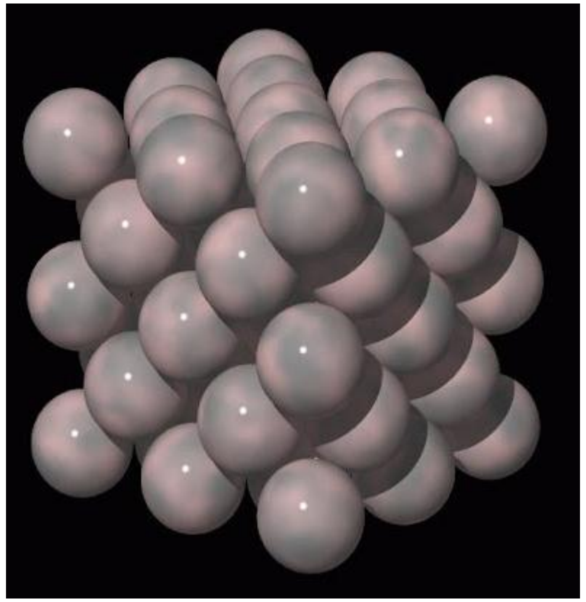
Long-range, translational symmetry

Crystalline & Amorphous Materials

- **Crystalline** Material

A pure solid material that has a long-range (up to µm, mm, or even larger) order or translational symmetry, i.e., with linearly repetitive, grid-like arrangement of atoms/ions/molecules in 3D

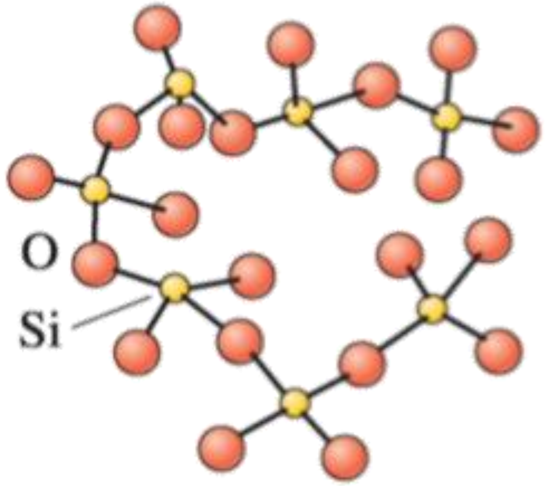
Example: common pure metals, common pure ceramics, some specially processed polymer



- **Amorphous** (Glassy) Material

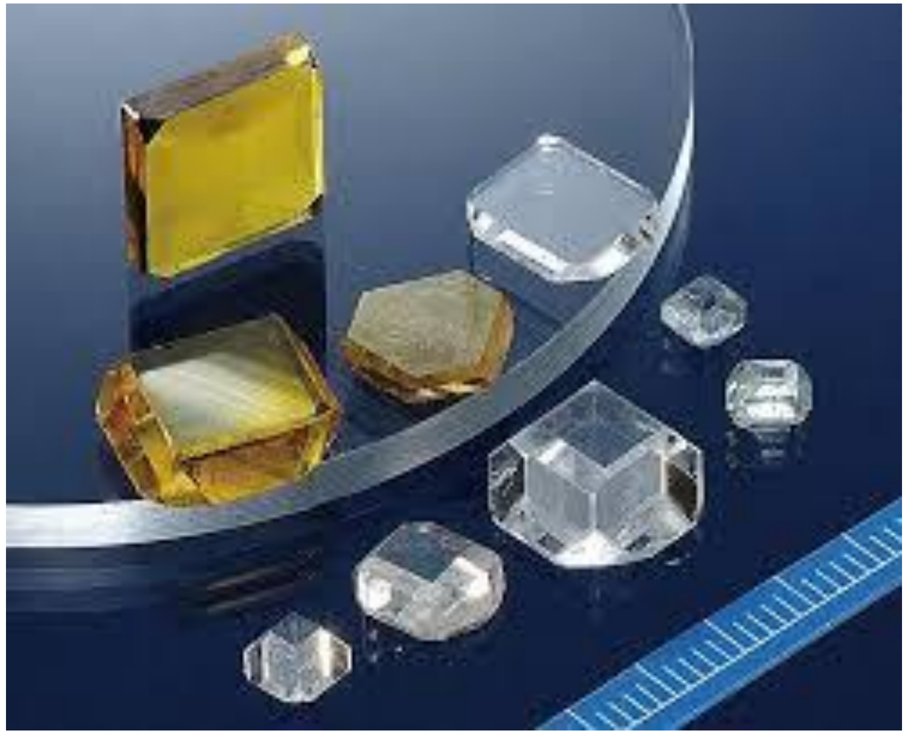
A pure solid material that has a short-range order only

Example: all glasses (including metallic glass), some polymers (or certain regions of polymers)



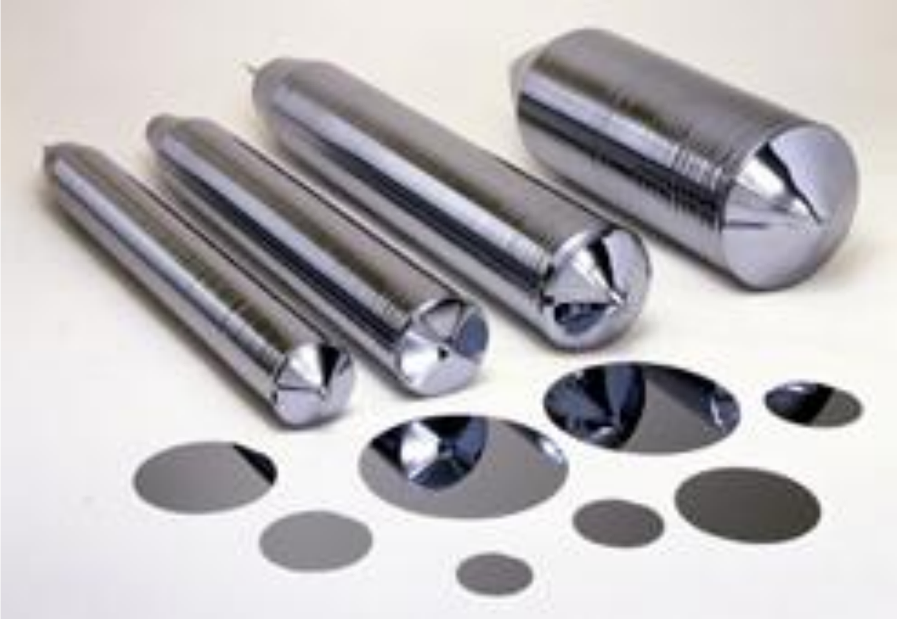
Single Crystal Materials

Periodic arrangement of atoms/molecules throughout the entire material



Single crystal **diamond** for gem, optical, cutting, abrasives applications

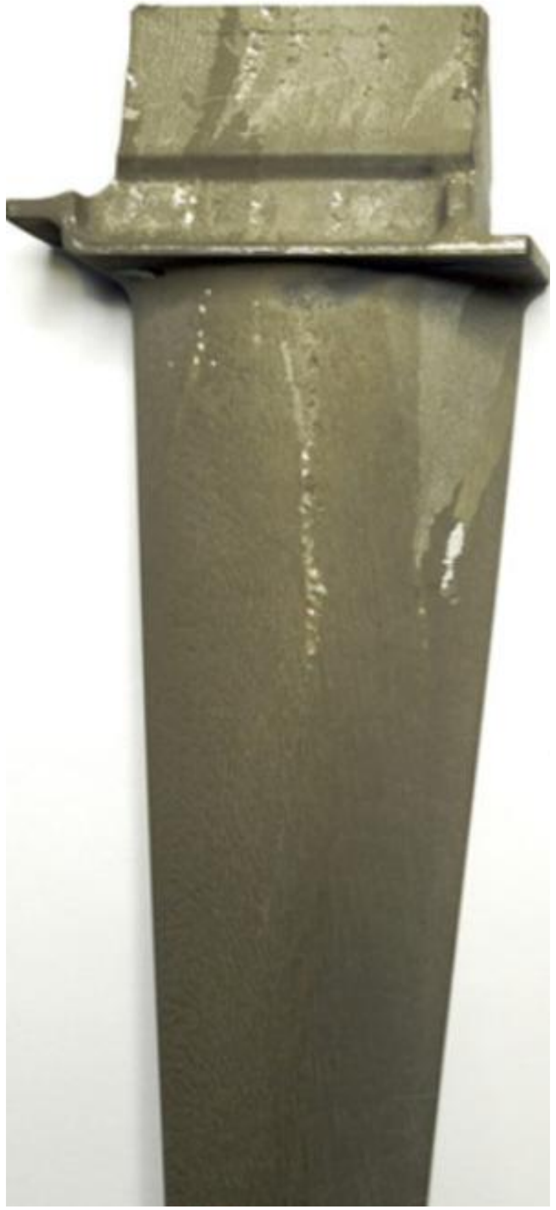
https://sumitomoelectric.com/id/dna/v16



Single crystal **silicon** for integrated circuit (IC), solar cell, and other applications

http://www.sumcosi.com/english/products/lineup.html

"Single crystal" **alloy turbine blade** for jet engines, gas turbines



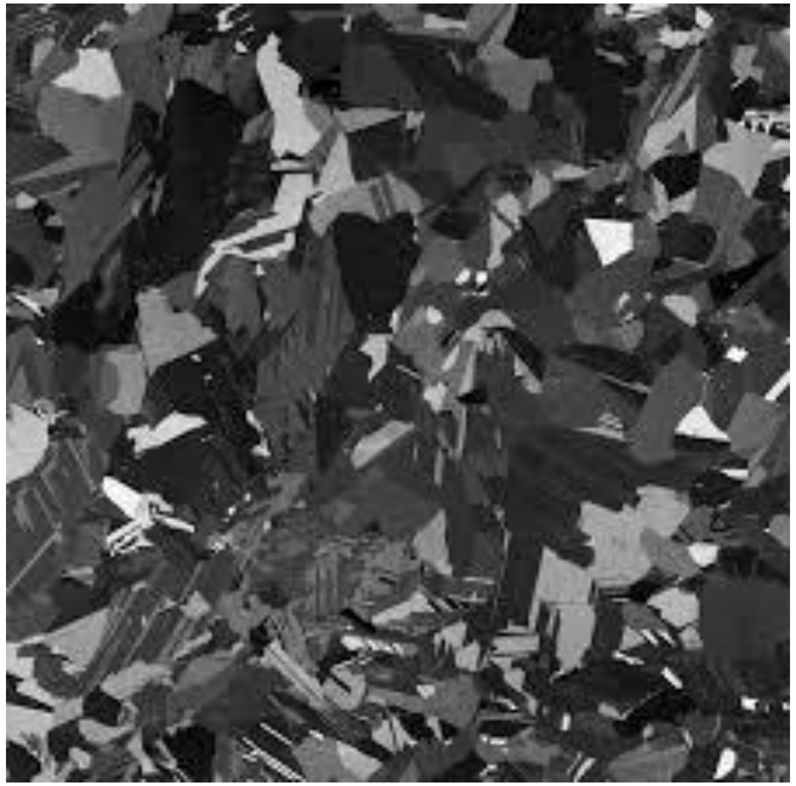
Zhang et al., Acta Materialia, v244, 118579 (2023)

Polycrystalline Materials (1)

Most engineering materials are polycrystalline, i.e., they contain many individual grains or small crystals

- Each "**grain**" is a single crystal
- “Grains” have the **same chemistry & structure**, but **different orientation**
- Grain size ranges from ~1 nm to ~1 cm

Casted poly-crystalline Si



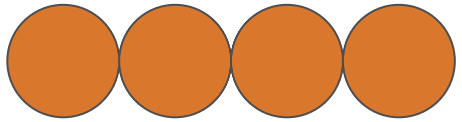
Polycrystalline Si wafer

Polycrystalline Materials (2)

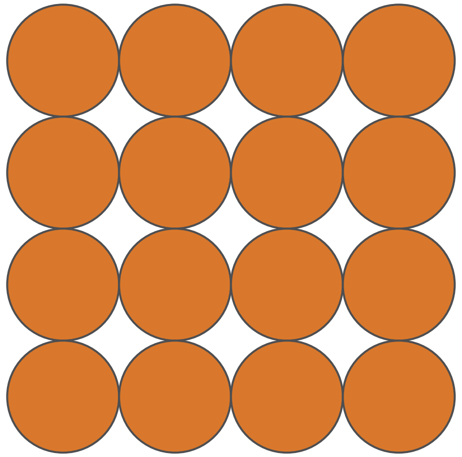
Lamp post showing polycrystalline structure

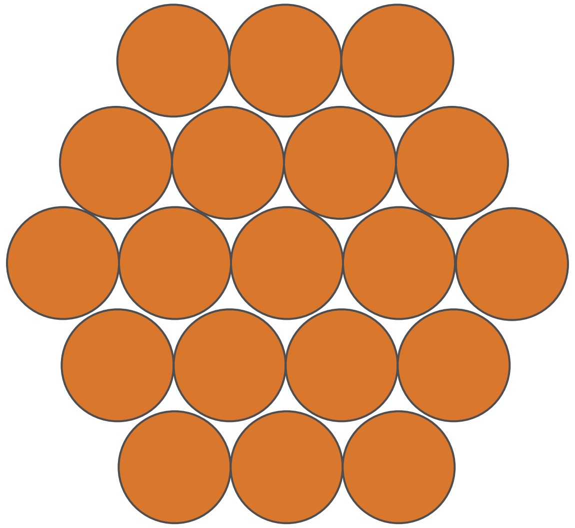
Hard Sphere Model for Crystal Structures

- Assumptions/approximations
  - Atoms are hard spheres
  - Atoms "touch" nearest neighbors
  - **Periodic** with **<u>translational</u> symmetry**
- 1D example



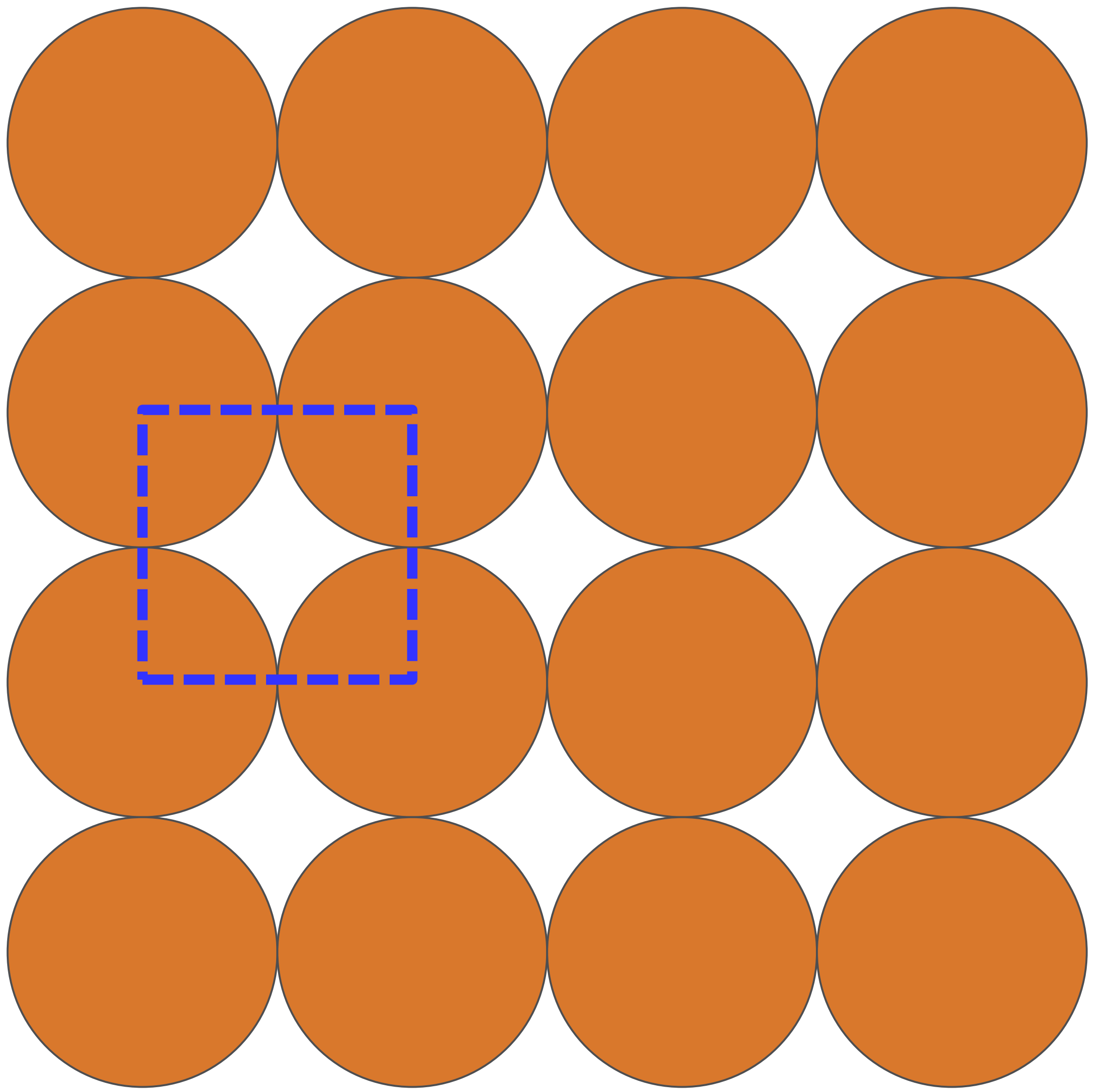
- 2D examples





Crystal Lattice, Unit Cell, & Coordination Number (CN)

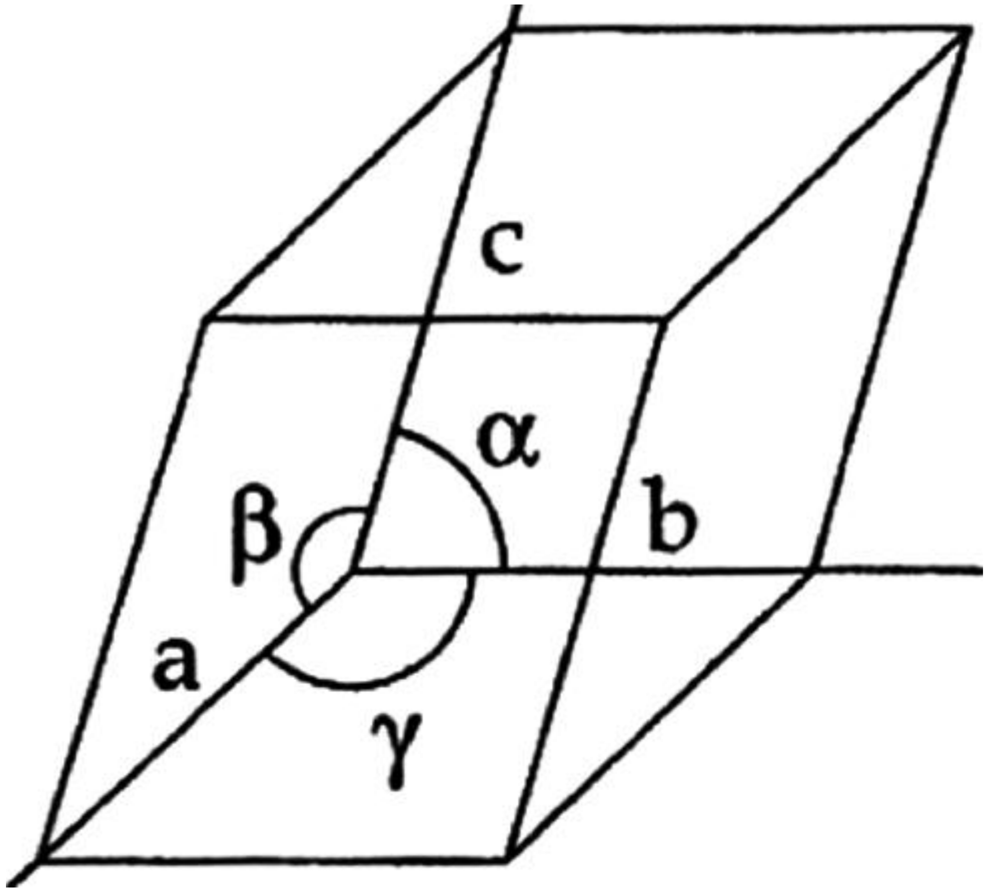
- **Lattice**: an array of points representing the geometric configuration atoms or a certain set of atoms (or molecules) in a crystal
- **Unit cell**: Smallest (simplest) repeating unit in a lattice that satisfy the followings:
  - Represent symmetry in a crystal
    - ✓ Translational
    - ✓ Rotational
    - ✓ Mirror
  - Opposite faces (for 3D)/edges are parallel
  - Each point is identical in its environment
- **Coordination Number (CN)**
  - Number of nearest (or touching) neighboring atoms for an atom within a crystal



CN = 4 for this 2D square lattice

Unit Cell Shape & 7 Crystal Systems

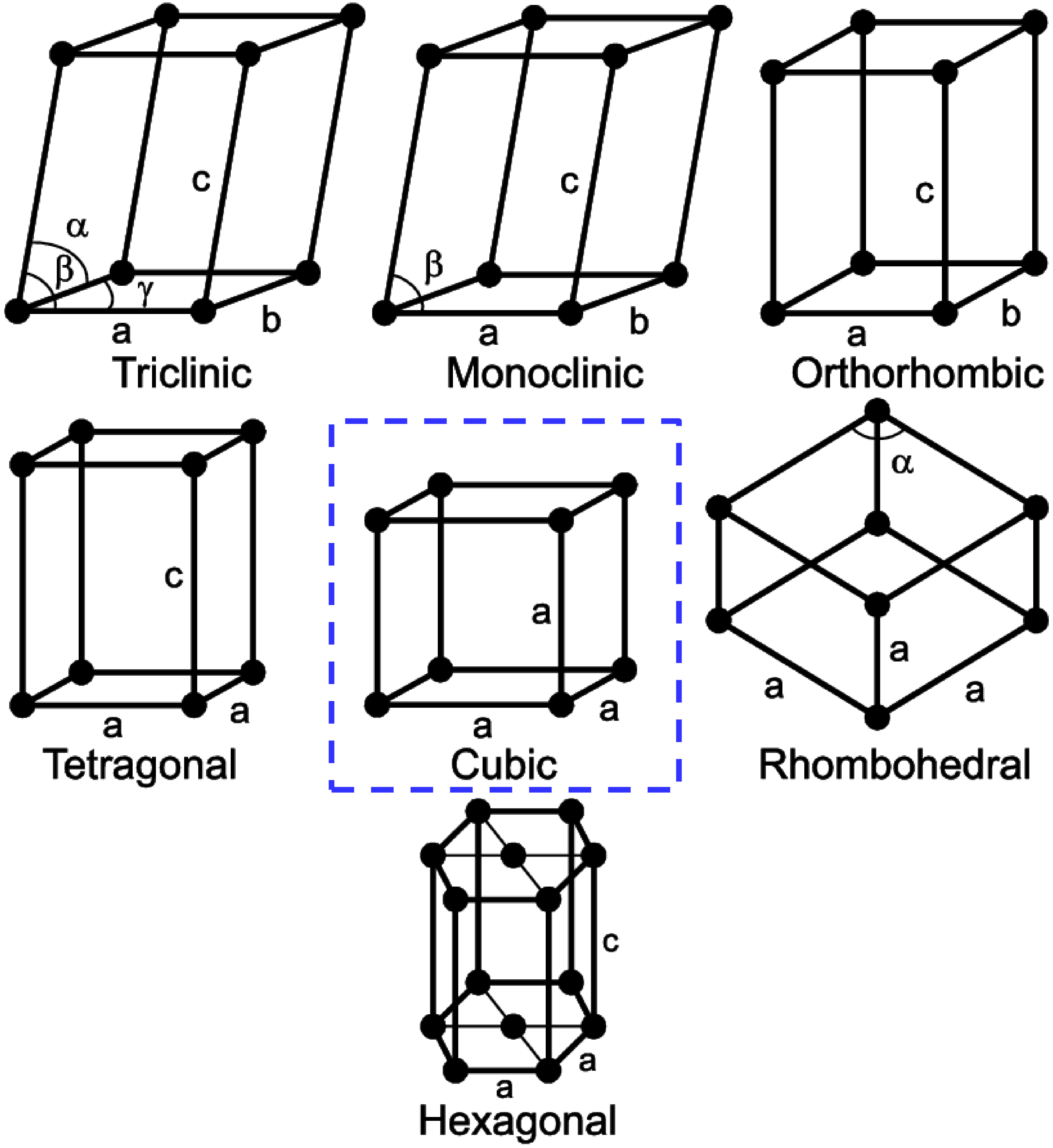
Unit cell in 3D are parallelepipeds



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

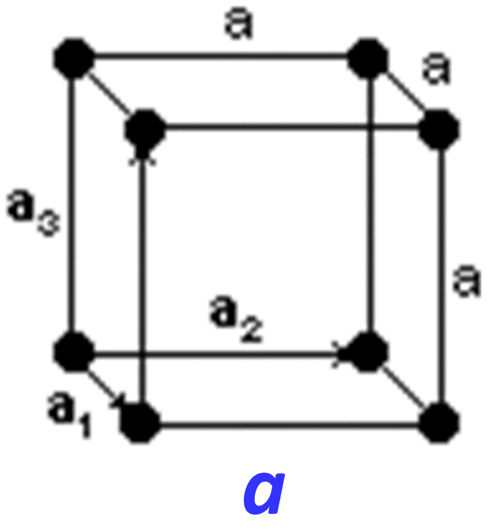
α, β, γ are **interaxial angles**

7 Crystal Systems



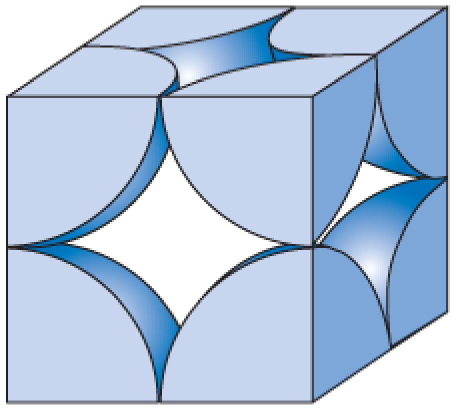
Three Cubic Lattices

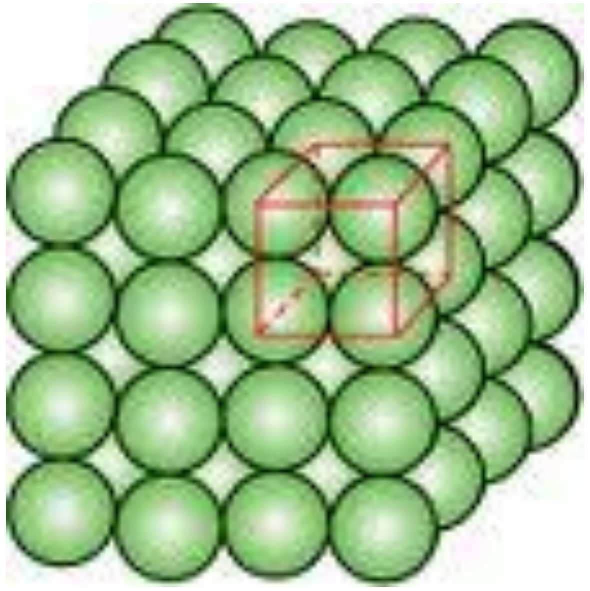
Simple cubic (SC)



a = ?R

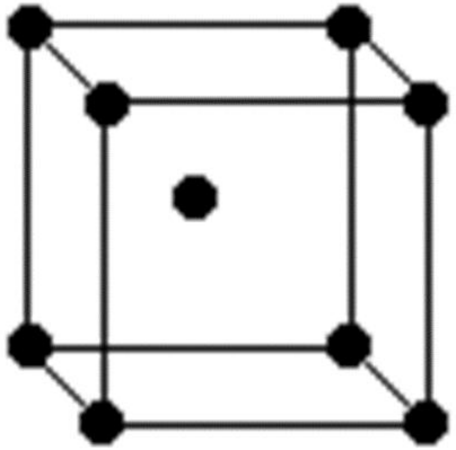
CN = ?





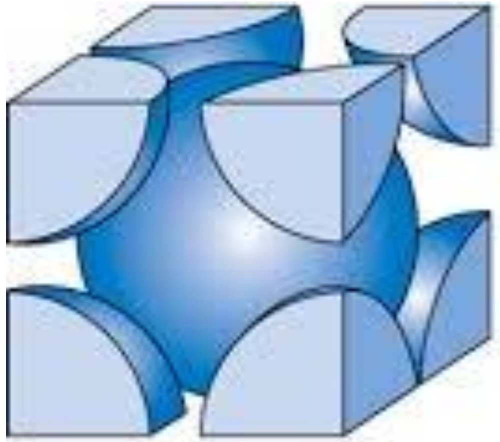
Po

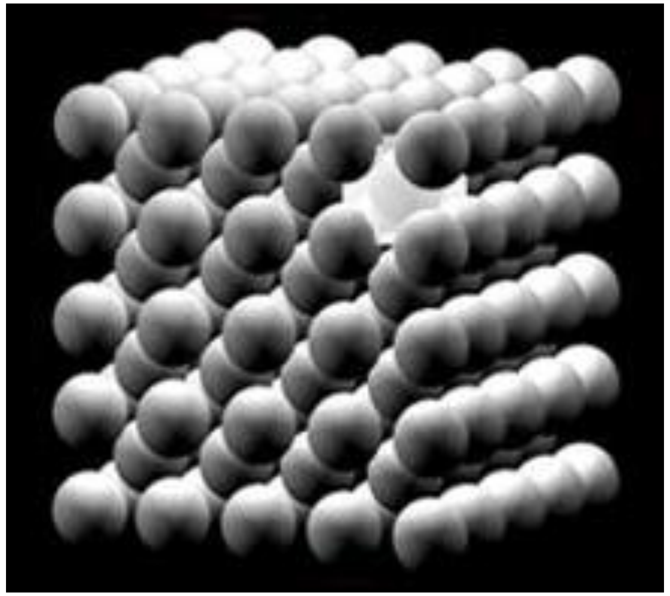
Body Centered Cubic (BCC)



a = ?R

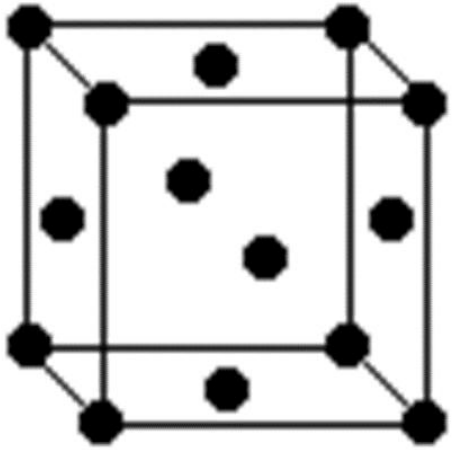
CN = ?





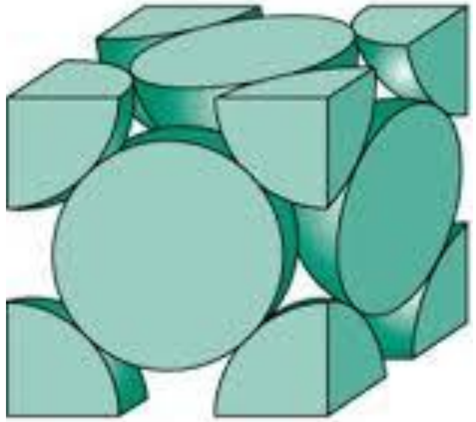
Na, K, V, Cr, Fe, Mo, W

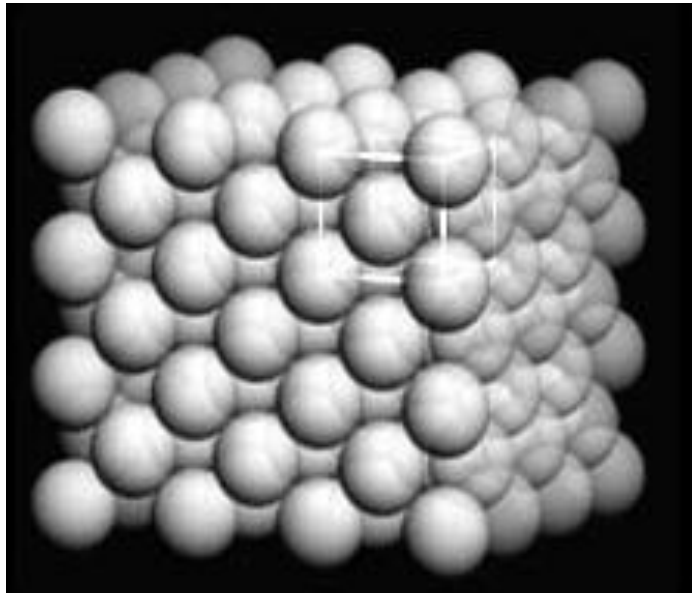
Face Centered Cubic (FCC)



a = ?R

CN = ?



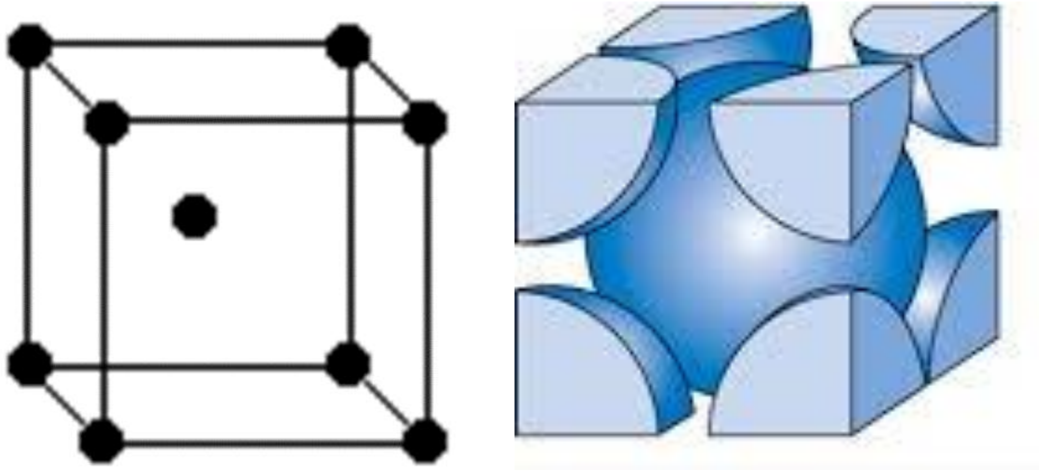


Al, Ni, Cu, Ag, Au, Pt

Estimation of Material Theoretical Density

$$Density = \frac{Mass}{Volume}$$

Iron (Fe) of BCC structure



Fe lattice constant a = 0.2866 nm

Effective number of Fe atoms WITHIN a unit cell:

$$N_{Fe} = 1 + \frac{1}{8} \times 8 = 2$$

Mass of a single Fe atom

$$m_{Fe\ atom} = \frac{55.84\ g/mol}{6.02 \times 10^{23}/mol}$$

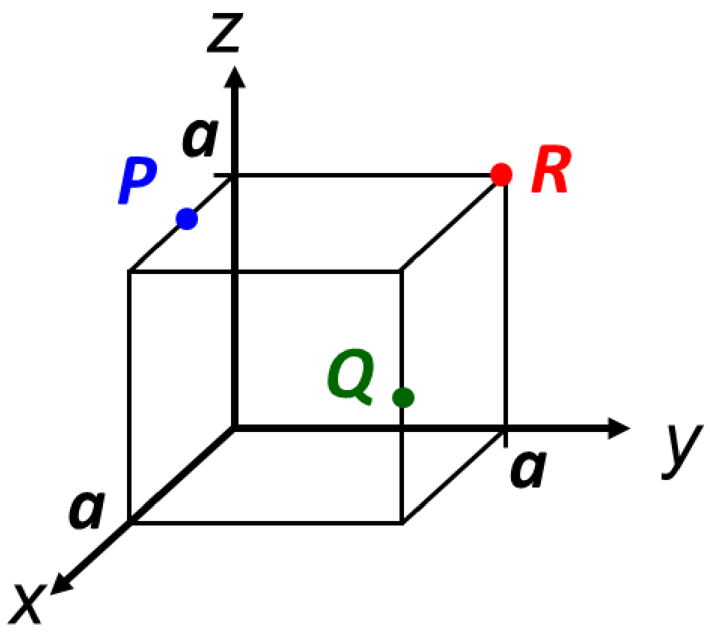
Iron (Fe) theoretical density

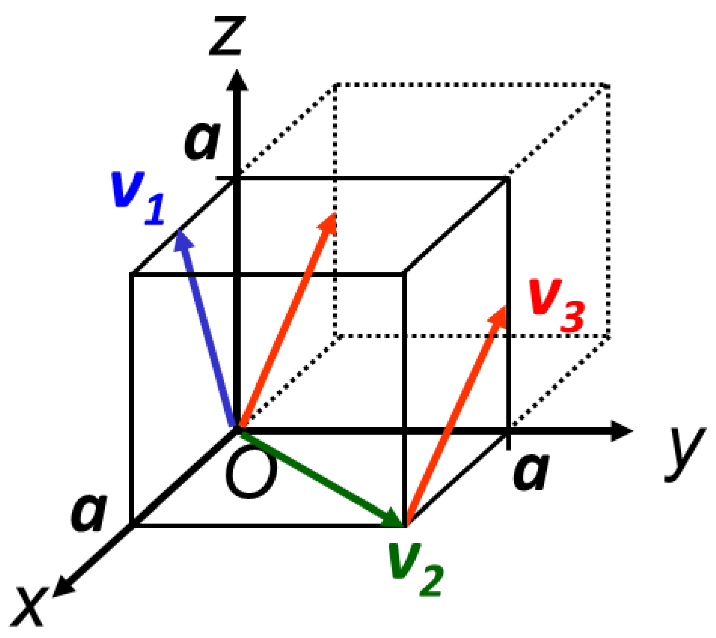
$$\rho_{Fe\_theory} = \frac{Total\ mass\ of\ Fe\ within\ a\ unit\ cell}{Volume\ of\ a\ unit\ cell} = \frac{N_{Fe} \cdot m_{Fe\ atom}}{a^3} = 7.88\ g/cm^3$$

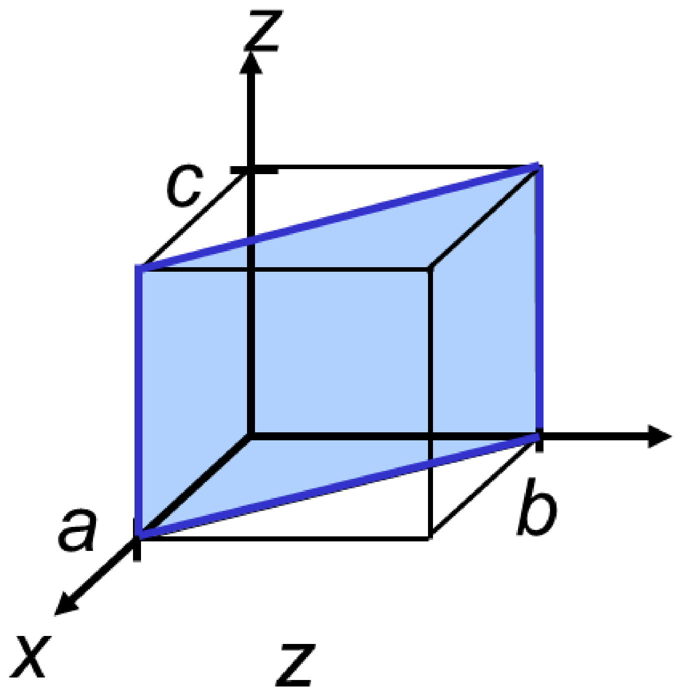
Only 0.1% error from experiment!

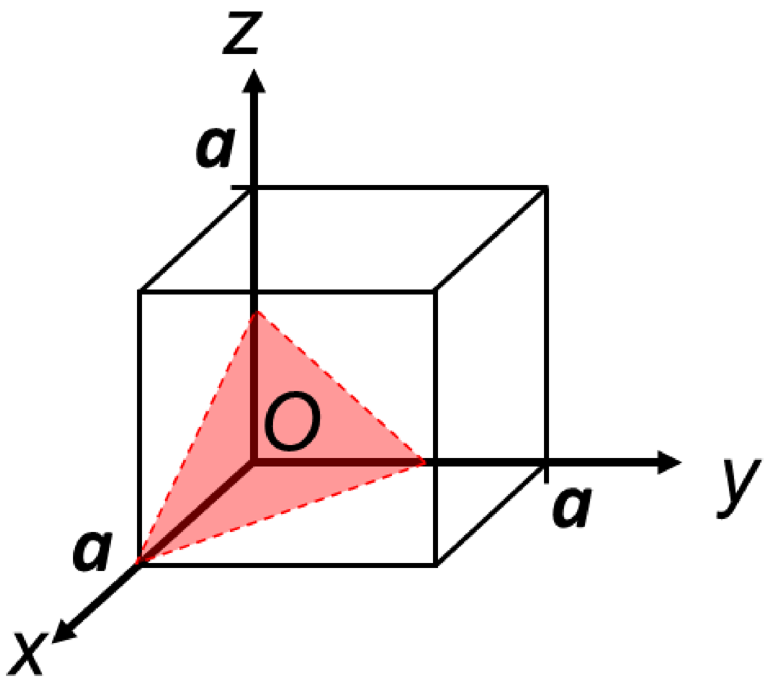
Directions & Planes in a Crystal

Points, directions, & planes in a crystal can all be <u>numerical noted</u> (NOT into details)





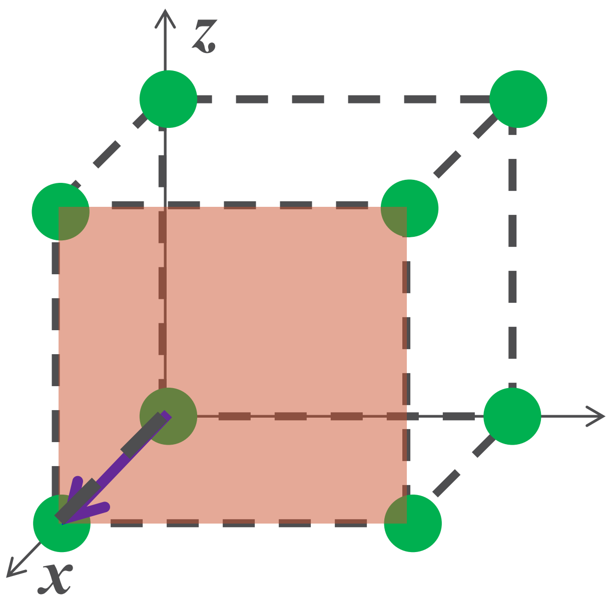




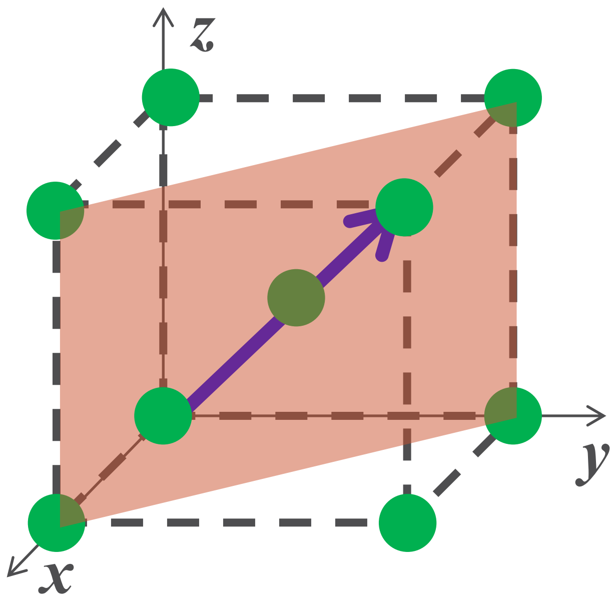
Close Packed Direction & Planes of Highest Planar Density

(Understand only - NO need to remember)

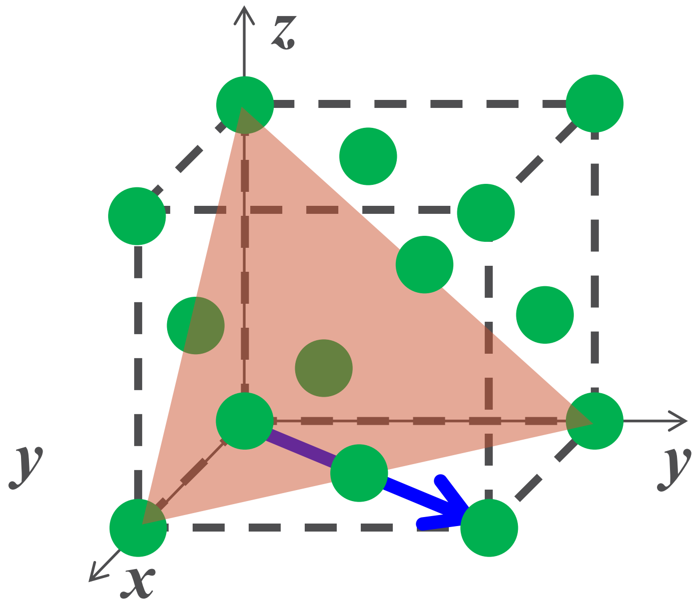
Simple Cubic



BCC



FCC



Close Packed Direction

Simple Cubic	BCC	FCC
<100>	*<111>*	*<110>*

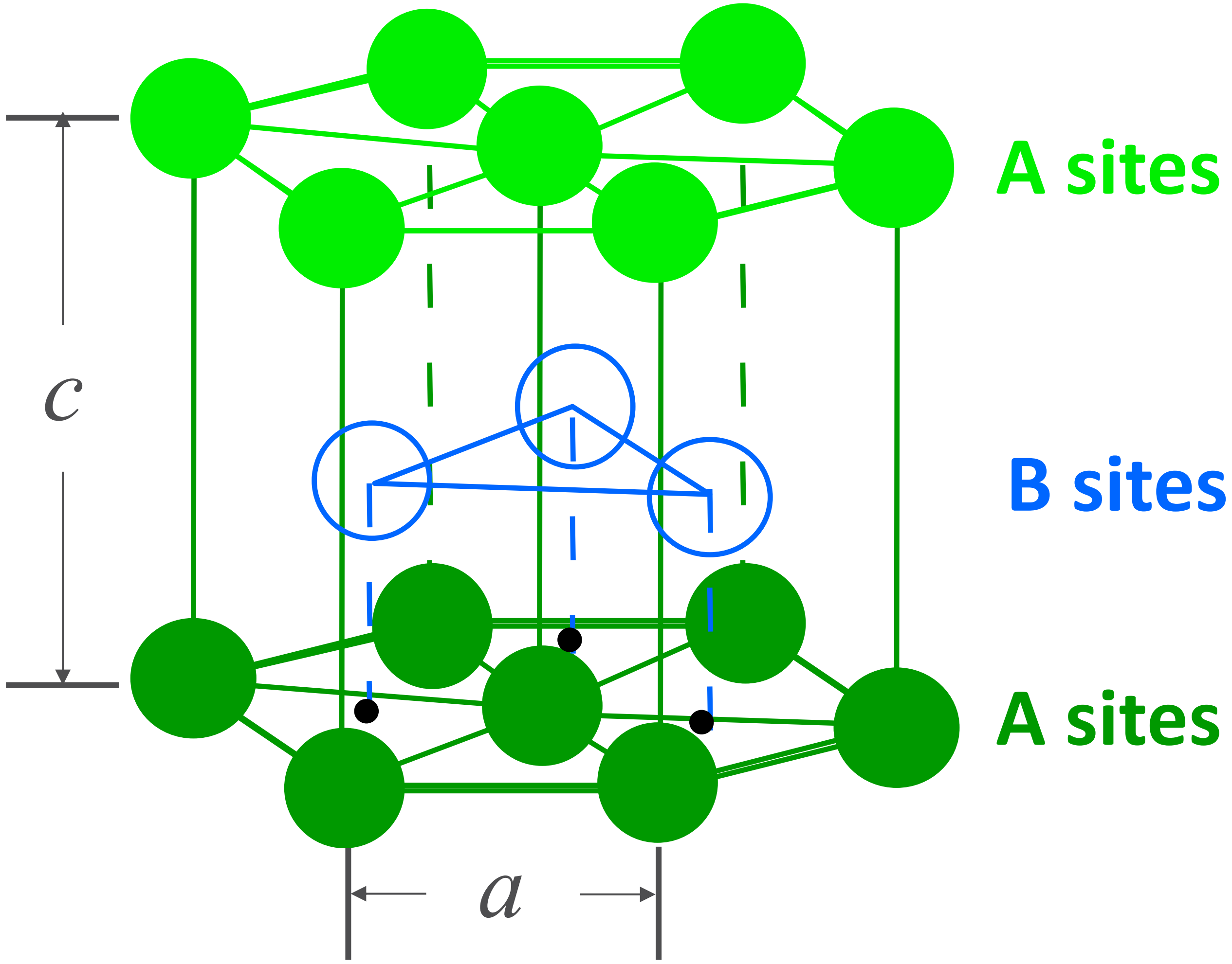
Plane with Highest Planar Density

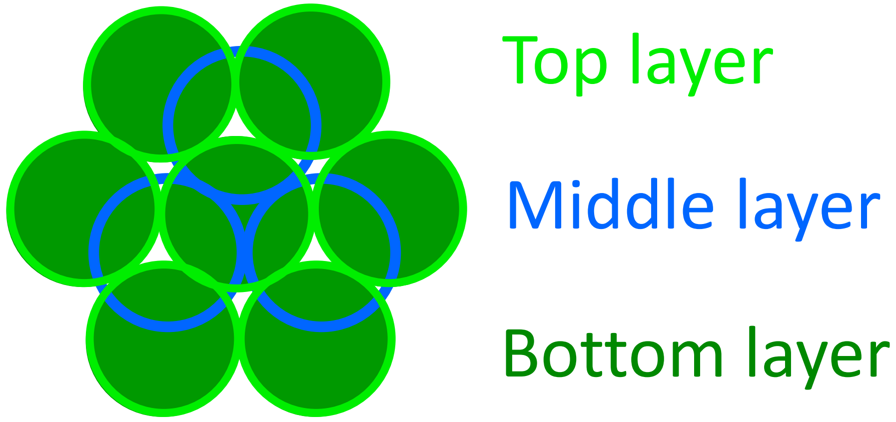
Simple Cubic	BCC	FCC
{100}	{110}	{111}

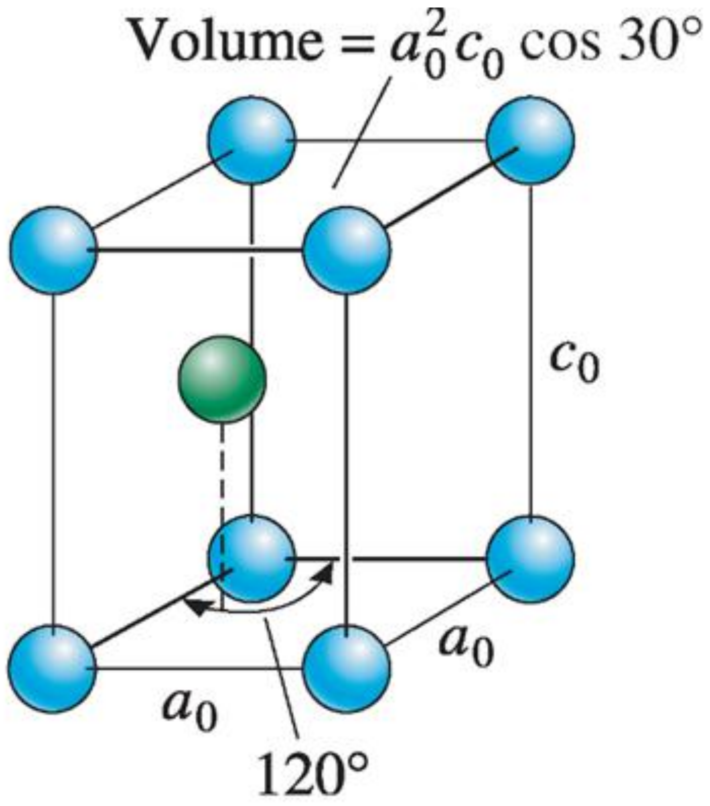
Also close packing plane

Hexagonal Close-Packed (HCP) Structure

- A different stacking sequence of atoms, different, but related to FCC
- For metals such as Mg, Ti, Zn

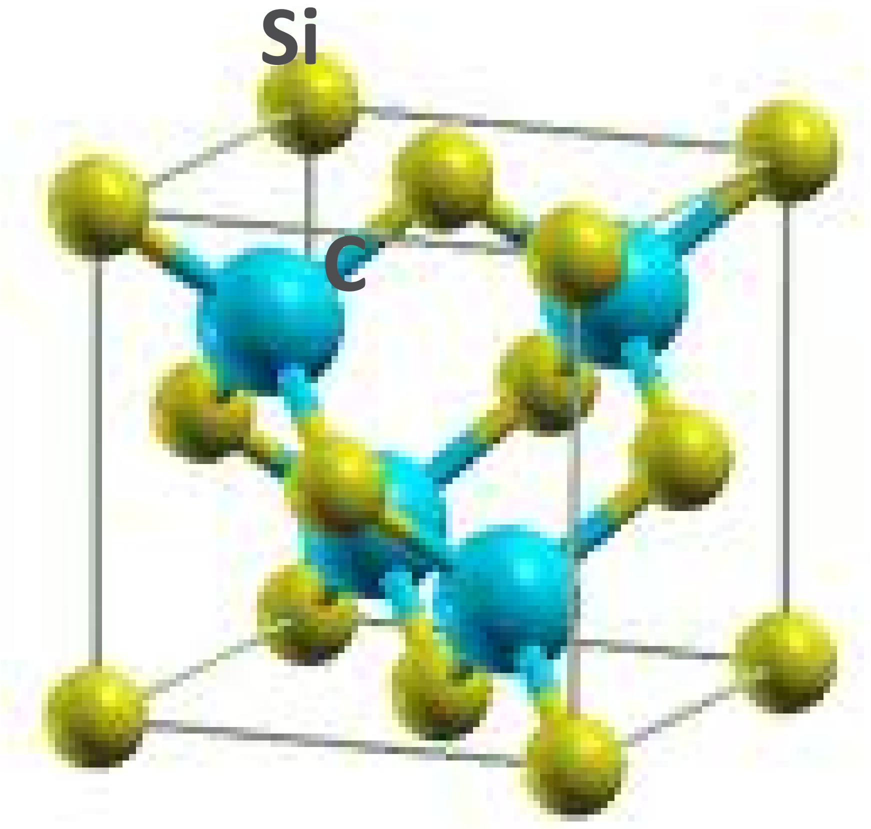




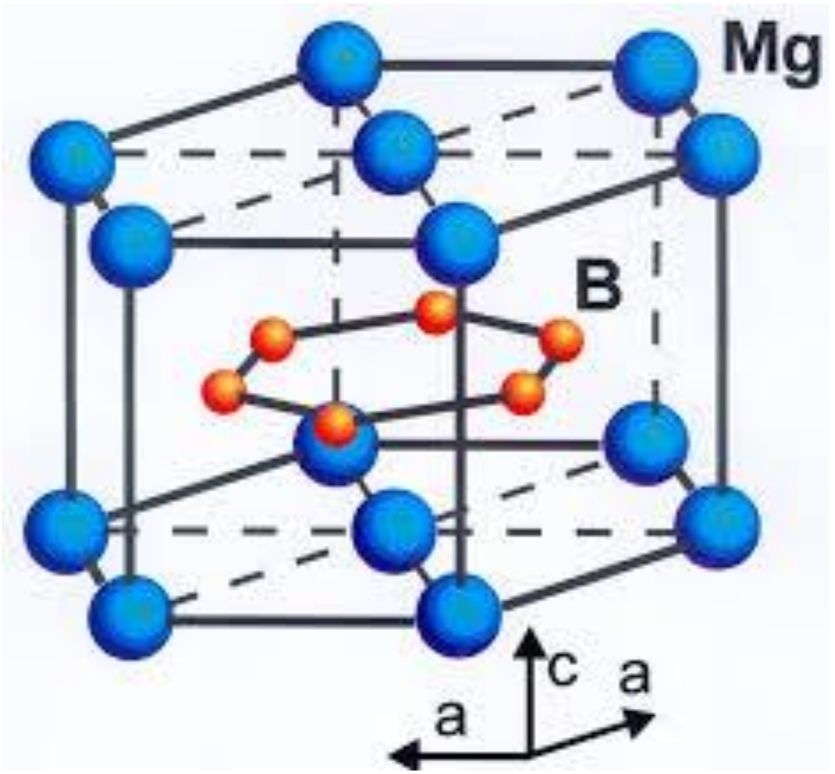


Some More Structure Examples

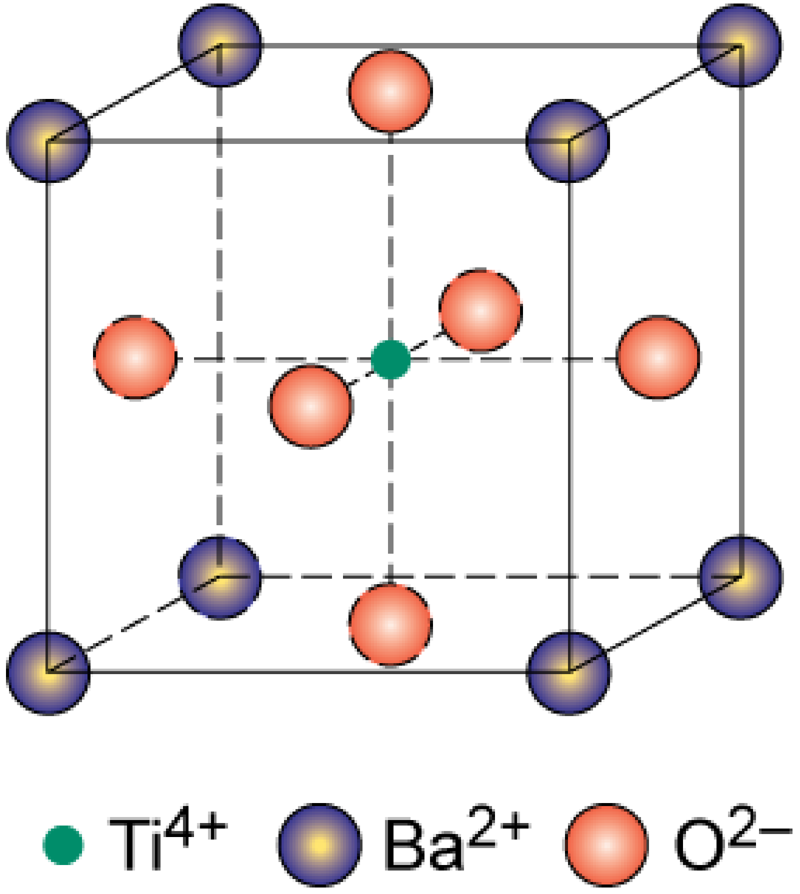
SiC



MgB_2

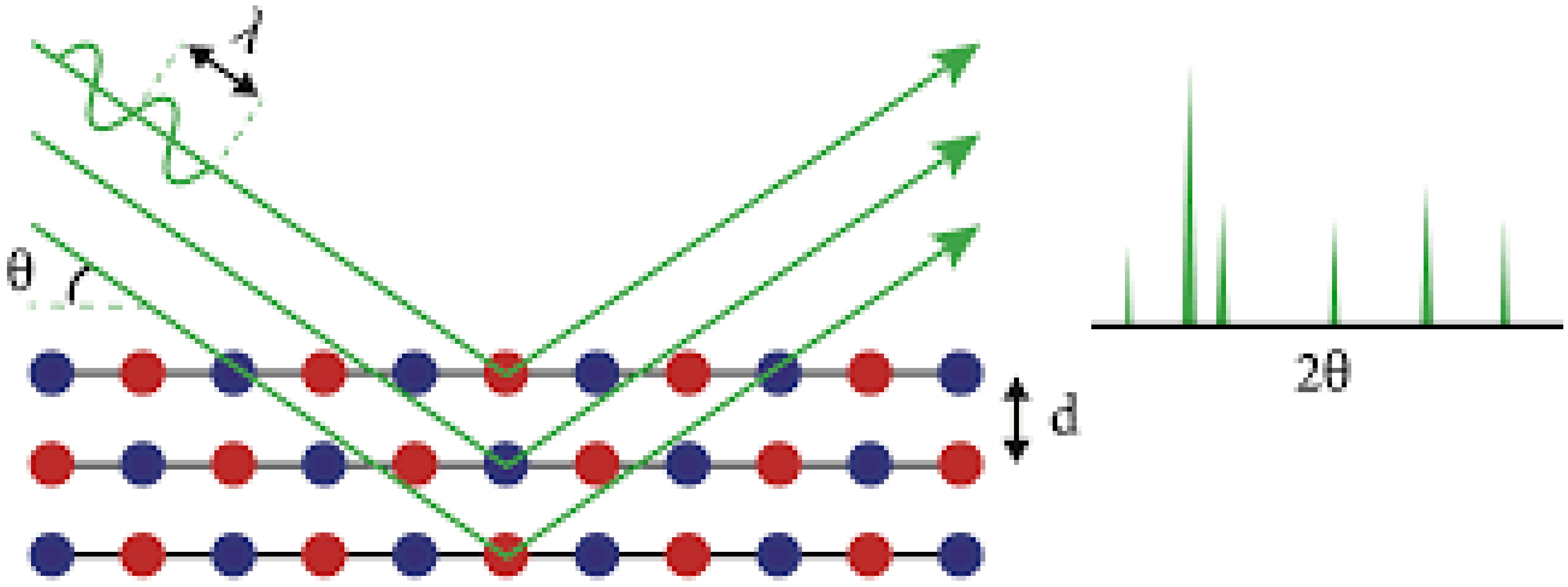


$BaTiO_3$



Crystal Structure Determination via X-Ray Diffraction

- X-ray can be used to determine a material's (either powder or bulk) crystal structure
- Wavelength (e.g., λ = 1.54 Å for Cu line), angle of the diffraction peaks, and pattern help determine crystal structure including lattice parameters and angles for a crystal



END

Homework 3.0

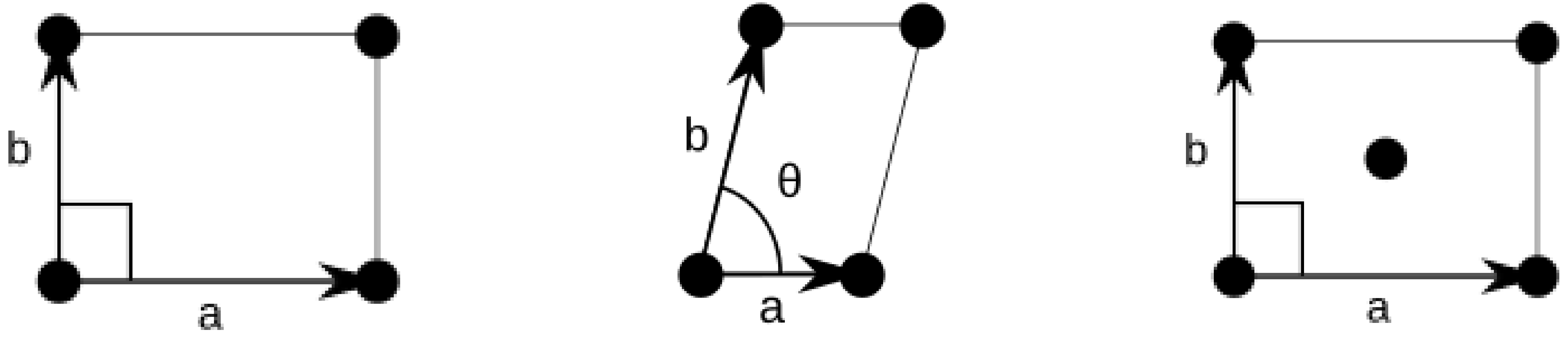
Carefully review chapter 3 lecture slides and, if time allows, read textbook sections (Askeland chapter 3.1, 3.2, 3.3, 3.4, & 3.9) and give an honor statement confirming the reading

Homework 3.1

- Ask one question you are either confused or curious about Chapter 3.
- Use AI or just search to generate the answer for your question and then provide your comment. Ideally, discuss/debate with AI to understand its strength and limitations
- **Copy & Paste from AI OK**

Homework 3.2

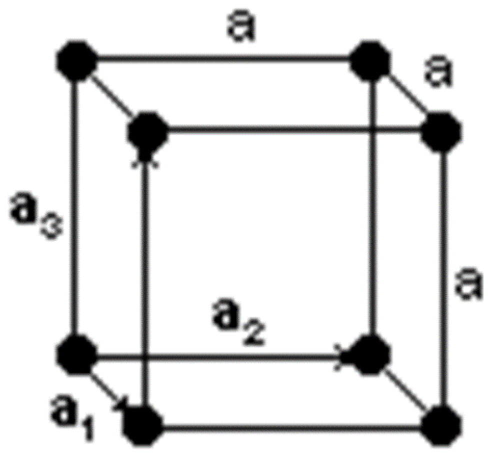
- Please identify and label the mirror planes in unit cell for the following 2D lattices (a ≠ b):

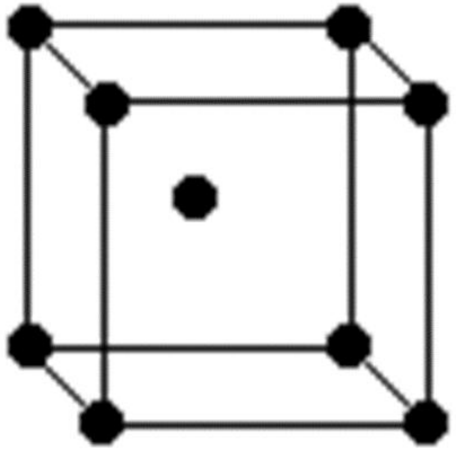


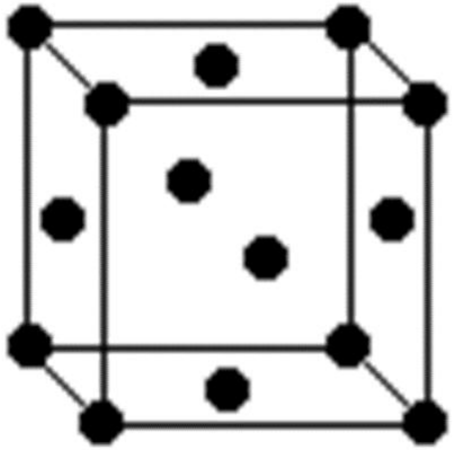
- For the above 2D unit cell, what rotational symmetry does the unit cells have? (e.g., a 6-fold rotational symmetry means a pattern rotates 60^o and would repeats itself)
- What is the coordination number (CN) for each of the above 2D lattices (**only counting the <u>nearest</u> neighbors**)? Please draw the pattern following the hard-circle (not sphere since 2D) model and give the math relationship, if applicable, between circle radius *R* and lattice constants (*a* or *b*)

Homework 3.3

Please derive the mathematical relationship between lattice parameter *a* and atom radius *R* (e.g., *a* = ?? *R*) for the three cubic lattices: simple cubic, body centered cubic, and face-centered cubic. Make sure to draw 3D/2D figures to help show the validity of your derivation





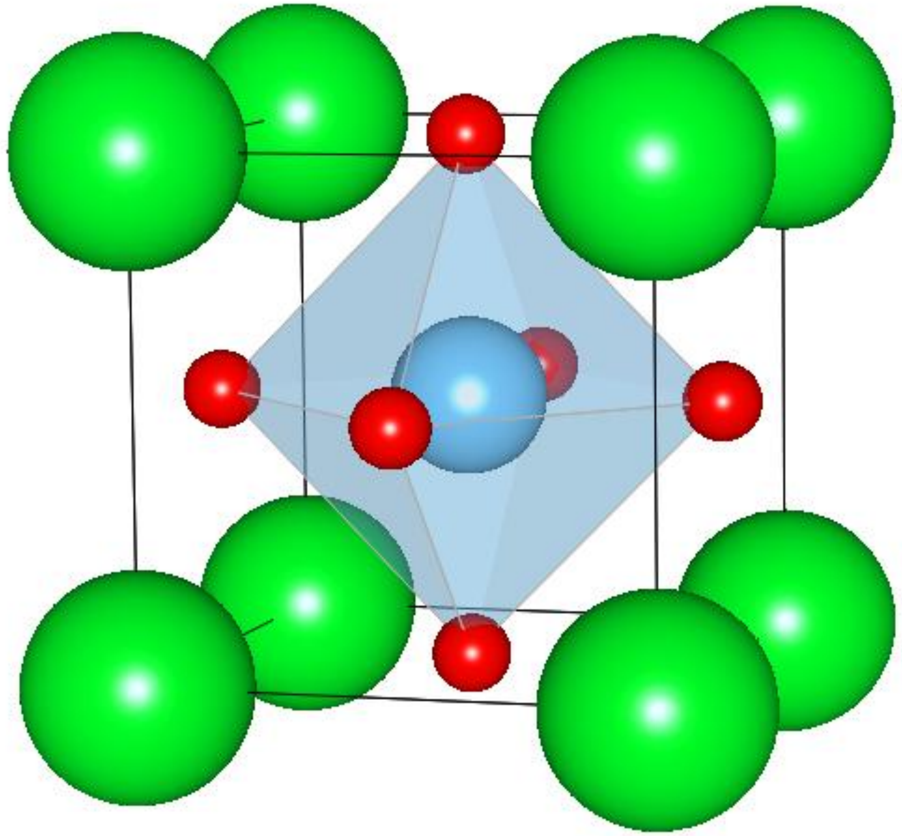


Homework 3.4

Please estimate the density for solid aluminum metal, knowing that aluminum has face-centered cubic (FCC) crystal structure with a lattice constant of 0.405 nm. Refer to periodic table for information about aluminum atomic mass.

Homework 3.5

The unit cell structure for a compound of Sr (in green large sphere), Ti (light blue medium sphere), and O (red smallest sphere) is shown below. Knowing that it is a **cubic** structure, with Sr at the corner, Ti at the cube center, while O are at the face center,



- Please give the chemical formula for the compound; be sure to explain it using the geometric information
- Please estimate the density for this material, if the lattice parameter is 0.3905 nm (refer to periodic table for atomic mass information)
- What are the length for the Sr-O bond? What about the Ti-O bond?
- What is the coordination number for Sr and Ti and why? Draw to help illustrate

Homework 3.6

Assuming the hard-sphere model for a pure element with body-centered cubic (BCC) structure, if **atomic packing factor (APF)** is defined as the ratio between volume occupied by all atoms within a unit cell to the total volume of that unit cell, i.e.,

$$APF = \frac{Volume\ for\ all\ atoms\ \boldsymbol{within}\ a\ unit\ cell}{Total\ volume\ of\ that\ unit\ cell}$$

please calculate the APF the body centered cubic structure and show your steps