**Crystal Structure**

Types of Solids

- **Amorphous**: Solids with considerable disorder in their structures (e.g., glass). *Amorphous*: lacks a systematic atomic arrangement.

- **Crystalline**: Solids with rigid a highly regular arrangement of their atoms. (That is, its atoms or ions, self-organized in a 3D periodic array). These can be monocrystals and polycrystals.

![Diagram of Amorphous, Crystalline, and Polycrystalline Structures]
To discuss crystalline structures it is useful to consider atoms as being hard spheres with well-defined radii. In this hard-sphere model, the shortest distance between two like atoms is one diameter.

**Lattice:** A 3-dimensional system of points that designate the positions of the components (atoms, ions, or molecules) that make up the substance.

**Unit Cell:** The smallest repeating unit of the lattice. The lattice is generated by repeating the unit cell in all three dimensions.
**Crystal Systems**

Crystallographers have shown that only **seven different types of unit cells** are necessary to create all point lattice.

- **Cubic** \( a = b = c ; \alpha = \beta = \gamma = 90 \)
- **Tetragonal** \( a = b \neq c ; \alpha = \beta = \gamma = 90 \)
- **Rhombohedral** \( a = b = c ; \alpha = \beta = \gamma \neq 90 \)
- **Hexagonal** \( a = b \neq c ; \alpha = \beta = 90, \gamma = 120 \)
- **Orthorhombic** \( a \neq b \neq c ; \alpha = \beta = \gamma = 90 \)
- **Monoclinic** \( a \neq b \neq c ; \alpha = \gamma = 90 \neq \beta \)
- **Triclinic** \( a \neq b \neq c ; \alpha \neq \gamma \neq \beta \neq 90 \)

**Bravais Lattices**

Many of the **seven crystal systems** have variations of the basic unit cell. August Bravais (1811-1863) showed that 14 standards unit cells could describe all possible lattice networks.
CUBIC
\[a = b = c\]
\[\alpha = \beta = \gamma = 90^\circ\]

TETRAGONAL
\[a = b \neq c\]
\[\alpha = \beta = \gamma = 90^\circ\]

ORTHORHOMBIC
\[a \neq b \neq c\]
\[\alpha = \beta = \gamma = 90^\circ\]

HEXAGONAL
\[a = b \neq c\]
\[\alpha = \beta = 90^\circ\]
\[\gamma = 120^\circ\]

MONOCLINIC
\[a \neq b \neq c\]
\[\alpha = \gamma = 90^\circ\]
\[\beta \neq 120^\circ\]

TRICLINIC
\[a \neq b \neq c\]
\[\alpha \neq \beta \neq \gamma \neq 90^\circ\]

4 Types of Unit Cell
\[P = \text{Primitive}\]
\[I = \text{Body-Centred}\]
\[F = \text{Face-Centred}\]
\[C = \text{Side-Centred}\]

7 Crystal Classes
\[\rightarrow 14 \text{ Bravais Lattices}\]
Principal Metallic Structures

Most elemental metals (about 90%) crystallize upon solidification into three densely packed crystal structures: body-centered cubic (BCC), face-centered cubic (FCC) and hexagonal close-packed (HCP).
## Structures of Metallic Elements

<p>| | | | | | | | | | | |</p>
<table>
<thead>
<tr>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>Li</td>
<td>Be</td>
<td>B</td>
<td>C</td>
<td>N</td>
<td>O</td>
<td>F</td>
<td>Ne</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Na</td>
<td>Mg</td>
<td>Al</td>
<td>Si</td>
<td>P</td>
<td>S</td>
<td>Cl</td>
<td>Ar</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>Ca</td>
<td>Sc</td>
<td>Ti</td>
<td>V</td>
<td>Cr</td>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
</tr>
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<td></td>
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<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Rb</td>
<td>Sr</td>
<td>Y</td>
<td>Zr</td>
<td>Nb</td>
<td>Mo</td>
<td>Tc</td>
<td>Ru</td>
<td>Rh</td>
<td>Pd</td>
<td>Ag</td>
</tr>
<tr>
<td>Cs</td>
<td>Ba</td>
<td>La</td>
<td>Hf</td>
<td>Ta</td>
<td>W</td>
<td>Re</td>
<td>Os</td>
<td>Ir</td>
<td>Pt</td>
<td>Au</td>
</tr>
<tr>
<td>Fr</td>
<td>Ra</td>
<td>Ac</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Yellow**: Primitive Cubic
- **Green**: Body Centered Cubic
- **Blue**: Cubic close packing (Face centered cubic)
- **Red**: Hexagonal close packing
<table>
<thead>
<tr>
<th>Structure</th>
<th>Metal</th>
<th>Lattice Constant</th>
<th>Atomic Radius, nm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>a, nm</td>
<td>c, nm</td>
</tr>
<tr>
<td>BCC</td>
<td>Chromium</td>
<td>0.289</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Iron</td>
<td>0.287</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Molybdenum</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Potassium</td>
<td>0.533</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Sodium</td>
<td>0.429</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Tungsten</td>
<td>0.316</td>
<td></td>
</tr>
<tr>
<td>FCC</td>
<td>Aluminum</td>
<td>0.405</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Copper</td>
<td>0.361</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Gold</td>
<td>0.408</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Nickel</td>
<td>0.352</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Silver</td>
<td>0.409</td>
<td></td>
</tr>
<tr>
<td>HCP</td>
<td>Zinc</td>
<td>0.2665</td>
<td>0.5618</td>
</tr>
<tr>
<td></td>
<td>Magnesium</td>
<td>0.3209</td>
<td>0.5209</td>
</tr>
<tr>
<td></td>
<td>Cobalt</td>
<td>0.2507</td>
<td>0.4069</td>
</tr>
<tr>
<td></td>
<td>Titanium</td>
<td>0.2950</td>
<td>0.3584</td>
</tr>
</tbody>
</table>
**SIMPLE CUBIC STRUCTURE (SC)**

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

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

- **Number of atoms per unit cell** = 1 atom
**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

\[
R = 0.5a \\
\text{close-packed directions} \\
\text{contains } 8 \times \frac{1}{8} = 1 \text{ atom/unit cell}
\]

\[
APF = \frac{\frac{4}{3} \pi (0.5a)^3}{a^3}
\]
**Body Centered Cubic (BCC)**

- Close packed directions are cube diagonals.
  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

- Coordination # = 8

  \[
  \text{Unit cell contains:} \quad 1 + 8 \times \frac{1}{8} = 2 \text{ atoms/unit cell}
  \]

  Close-packed directions:
  \[
  \text{length} = 4R = \sqrt{3}a
  \]

  \[
  \begin{align*}
  \text{APF} &= \frac{\frac{4}{3} \pi \left(\sqrt{3}a/4\right)^3}{a^3} \\
  &= \frac{2}{3} \pi \left(\sqrt{3}a/4\right)^3
  \end{align*}
  \]

- APF for a BCC = 0.68
Face Centered Cubic (FCC)

- Close packed directions are face diagonals.
  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

- Coordination # = 12
  Close-packed directions:
  \[ \text{length} = 4R = \sqrt{2}a \]

- Unit cell contains:
  \[ 6 \times \frac{1}{2} + 8 \times \frac{1}{8} = 4 \text{ atoms/unit cell} \]

- APF for a FCC = 0.74

\[ \text{APF} = \frac{4 \frac{4}{3} \pi (\sqrt{2}a/4)^3}{a^3} = 0.74 \]
Hexagonal Close-Packed (HCP)

The APF and coordination number of the HCP structure is the same as the FCC structure, that is, 0.74 and 12 respectively.

An isolated HCP unit cell has a total of 6 atoms per unit cell.

- 2 atoms shared by two cells = 1 atom per cell
- 12 atoms shared by six cells = 2 atoms per cell
- 3 atoms
Close-Packed Structures
Both the HCP and FCC crystal structures are close-packed structure. Consider the atoms as spheres:
- Place one layer of atoms (2 Dimensional solid). Layer A
- Place the next layer on top of the first. Layer B. Note that there are two possible positions for a proper stacking of layer B.
The third layer (Layer C) can be placed in also two different positions to obtain a proper stack.
(1) exactly above of atoms of Layer A (HCP) or
(2) displaced

A B A : hexagonal close packed
A B C : cubic close packed
A B C : cubic close pack
A B A : hexagonal close pack
Packing of Spheres — Part 1

A  Simple cubic
B  Body-centered cubic
**Interstitial sites**

Locations between the “‘normal’” atoms or ions in a crystal into which another - usually different - atom or ion is placed.

- **Cubic site** - An interstitial position that has a coordination number of eight. An atom or ion in the cubic site touches eight other atoms or ions.

- **Octahedral site** - An interstitial position that has a coordination number of six. An atom or ion in the octahedral site touches six other atoms or ions.

- **Tetrahedral site** - An interstitial position that has a coordination number of four. An atom or ion in the tetrahedral site touches four other atoms or ions.
Interstitial sites are important because we can derive more structures from these basic FCC, BCC, HCP structures by partially or completely different sets of these sites.
The size and number of tetrahedral and octahedral interstitial sites in the BCC, FCC, and HCP crystal structures. The sizes of the interstitial sites are given in terms of the radius ratio ($\kappa/r$) where $\kappa$ is the radius of the largest atom that can “fit” into the interstitial position and $r$ is the radius of the host atoms. The number of interstitial sites is given in terms of both the number of sites per cell and, in parentheses, the number of sites per host atom.

<table>
<thead>
<tr>
<th>Crystal structure</th>
<th>Size of tetrahedral sites</th>
<th>Size of octahedral sites</th>
<th>Number of tetrahedral sites per unit cell (per host atom)</th>
<th>Number of octahedral sites per unit cell (per host atom)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BCC</td>
<td>$\kappa/r = 0.291$</td>
<td>$\kappa/r = 0.155$</td>
<td>12 (6)</td>
<td>6 (3)</td>
</tr>
<tr>
<td>FCC</td>
<td>$\kappa/r = 0.225$</td>
<td>$\kappa/r = 0.414$</td>
<td>8 (2)</td>
<td>4 (1)</td>
</tr>
<tr>
<td>HCP</td>
<td>$\kappa/r = 0.225$</td>
<td>$\kappa/r = 0.414$</td>
<td>12 (2)</td>
<td>6 (1)</td>
</tr>
</tbody>
</table>
Density Calculations

Since the entire crystal can be generated by the repetition of the unit cell, the density of a crystalline material, \( \rho = \) the density of the unit cell = (atoms in the unit cell, \( n \)) \times (mass of an atom, \( M \)) / (the volume of the cell, \( V_c \))

Atoms in the unit cell, \( n = 2 \) (BCC); 4 (FCC); 6 (HCP)

Mass of an atom, \( M \) = Atomic weight, \( A \), in amu (or g/mol) is given in the periodic table. To translate mass from amu to grams we have to divide the atomic weight in amu by the Avogadro number \( N_A = 6.023 \times 10^{23} \) atoms/mol

The volume of the cell, \( V_c = a^3 \) (FCC and BCC)

\[ a = 2R\sqrt{2} \] (FCC);
\[ a = 4R/\sqrt{3} \] (BCC)

where \( R \) is the atomic radius.
Density Calculation

Density \( \rho \) can be calculated using the formula:

\[
\rho = \frac{nA}{V_C N_A}
\]

- \( n \): number of atoms/unit cell
- \( A \): atomic weight
- \( V_C \): volume of the unit cell
- \( N_A \): Avogadro’s number
  \( (6.023 \times 10^{23} \text{ atoms/mole}) \)

**Example** Calculate the density of copper.

\( R_{Cu} = 0.128 \text{nm}, \) Crystal structure: FCC, \( A_{Cu} = 63.5 \text{ g/mole} \)

- \( n = 4 \text{ atoms/cell}, \) \( V_C = a^3 = (2R\sqrt{2})^3 = 16\sqrt{2}R^3 \)

\[
\rho = \frac{(4)(63.5)}{[16\sqrt{2}(1.28 \times 10^8)^3 \times 6.023 \times 10^{23}]} = 8.89 \text{ g/cm}^3
\]

8.94 g/cm\(^3\) in the literature
Example

Rhodium has an atomic radius of \(0.1345\text{nm (1.345\AA)}\) and a density of \(12.41\text{g.cm}^{-3}\). Determine whether it has a BCC or FCC crystal structure. \(\text{Rh (A = 102.91g/mol)}\)

Solution

\[
\rho = \frac{nA}{V_c N_A}
\]

\(n: \text{number of atoms/unit cell} \quad A: \text{atomic weight}
\]

\[
V_c = \frac{a^3}{n} = \frac{A}{\rho N_A} = \frac{102.91\text{g.mol}^{-1}}{12.41\text{g.cm}^{-3} \times 6.023 \times 10^{23} \text{atoms.mole}^{-1}} = 1.3768 \times 10^{-23} \text{cm}^3 = 0.01376 \text{nm}^3
\]

If rhodium is BCC then \(n = 2\) and \(a^3 = \left(\frac{4r}{\sqrt{3}}\right)^3 = 12.316r^3\)

\[
a^3 = \frac{12.316 \times (0.1345\text{nm})^3}{2} = 0.0149\text{nm}^3
\]

If rhodium is FCC then \(n = 4\) and \(a^3 = \left(\frac{4r}{\sqrt{2}}\right)^3 = 22.627r^3\)

\[
a^3 = \frac{22.627 \times (0.1345\text{nm})^3}{4} = 0.01376\text{nm}^3
\]

Rhodium has a FCC structure
Linear atomic density:

\[ L_l = a = \frac{4R}{\sqrt{3}} = 2R/L_l = 0.866 \]

Planar atomic density:

\[ = 2\pi R^2/(Area \ A'D'E'B') \]
Polymorphism or Allotropy

Many elements or compounds exist in more than one crystalline form under different conditions of temperature and pressure. This phenomenon is termed \textit{polymorphism} and if the material is an elemental solid is called \textit{allotropy}.

Example: Iron (Fe – Z = 26)

- liquid above 1539 C.
- \(\delta\)-iron (BCC) between 1394 and 1539 C.
- \(\gamma\)-iron (FCC) between 912 and 1394 C.
- \(\alpha\)-iron (BCC) between -273 and 912 C.

\[
\begin{array}{c}
\alpha \text{ iron} \quad 912^\circ C & \rightarrow & \gamma \text{ iron} \quad 1400^\circ C & \rightarrow & \delta \text{ iron} \quad 1539^\circ C & \rightarrow & \text{liquid iron} \\
\text{BCC} & & \text{FCC} & & \text{BCC} & & \end{array}
\]
Another example of allotropy is carbon. Pure, solid carbon occurs in three crystalline forms – diamond, graphite; and large, hollow fullerenes. Two kinds of fullerenes are shown here: buckminsterfullerene (buckyball) and carbon nanotube.
Table 12.6  Comparison of the Properties of Diamond and Graphite

<table>
<thead>
<tr>
<th>Property</th>
<th>Graphite</th>
<th>Diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (g/cm³)</td>
<td>2.27</td>
<td>3.51</td>
</tr>
<tr>
<td>Hardness</td>
<td>&lt;1 (very soft)</td>
<td>10 (hardest)</td>
</tr>
<tr>
<td>Melting point (K)</td>
<td>4100</td>
<td>4100</td>
</tr>
<tr>
<td>Color</td>
<td>Shiny black</td>
<td>Colorless transparent</td>
</tr>
<tr>
<td>Electrical conductivity</td>
<td>High (along sheet)</td>
<td>None</td>
</tr>
<tr>
<td>$\Delta H_{\text{comb}}^0$ (kJ/mol)</td>
<td>-393.5</td>
<td>-395.4</td>
</tr>
<tr>
<td>$\Delta H_{\text{f}}^0$ (kJ/mol)</td>
<td>0 (standard state)</td>
<td>1.90</td>
</tr>
</tbody>
</table>

[Graphene image]
Crystallographic Planes and Directions

Atom Positions in Cubic Unit Cells

A cube of lattice parameter $a$ is considered to have a side equal to unity. Only the atoms with coordinates $x$, $y$ and $z$ greater than or equal to zero and less than unity belong to that specific cell.

$0 \leq x, y, z < 1$
**Directions in The Unit Cell**

For cubic crystals the crystallographic directions indices are the vector components of the direction resolved along each of the coordinate axes and reduced to the smallest integer.

**Example direction A**

a) Two points origin coordinates 0,0,0 and final position coordinates 1,1,0

b) $1,1,0 - 0,0,0 = 1,1,0$

c) No fractions to clear

d) Direction $[110]$
Example direction B
a) Two points origin coordinates 1,1,1 and final position coordinates 0,0,0
b) $0,0,0 - 1,1,1 = -1,-1,-1$
c) No fractions to clear
d) Direction $[\bar{1} \bar{1} \bar{1}]$

Example direction C
a) Two points origin coordinates $\frac{1}{2},1,0$ and final position coordinates 0,0,1
b) $0,0,1 - \frac{1}{2},1,0 = -\frac{1}{2},-1,1$
c) There are fractions to clear. Multiply times 2. $2(-\frac{1}{2},-1,1) = -1,-2,2$
d) Direction $[1 2 2]$
Notes About the Use of Miller Indices for Directions

- A direction and its negative are not identical; [100] is not equal to [bar100]. They represent the same line but opposite directions.
- A direction and its multiple are identical: [100] is the same direction as [200]. We just forgot to reduce to lowest integers.
- Certain groups of directions are equivalent; they have their particular indices primarily because of the way we construct the co-ordinates. For example, a [100] direction is equivalent to the [010] direction if we re-define the co-ordinates system. We may refer to groups of equivalent directions as directions of the same family. The special brackets < > are used to indicate this collection of directions.

Example:
The family of directions <100> consists of six equivalent directions

\[ <100> \equiv [100], [010], [001], [0\bar{1}0], [00\bar{1}], [\bar{1}00] \]
Miller Indices for Crystallographic planes in Cubic Cells

- Planes in unit cells are also defined by three integer numbers, called the Miller indices and written \((hkl)\).
- Miller’s indices can be used as a shorthand notation to identify crystallographic directions (earlier) AND planes.

Procedure for determining Miller Indices

- **locate** the origin
- **identify** the points at which the plane intercepts the \(x\), \(y\) and \(z\) coordinates as fractions of unit cell length. If the plane passes through the origin, the origin of the co-ordinate system must be moved!
- take **reciprocals** of these intercepts
- **clear fractions** but do not reduce to lowest integers
- **enclose** the resulting numbers in parentheses \((h\ k\ l)\). Again, the negative numbers should be written with a bar over the number.
Example: Miller indices for plane $A$

a) Locate the origin of coordinate.

b) Find the intercepts $x = 1$, $y = 1$, $z = 1$

c) Find the inverse $\frac{1}{x}=1$, $\frac{1}{y}=1$, $\frac{1}{z}=1$

d) No fractions to clear

e) $(1 \ 1 \ 1)$
Notes About the Use of Miller Indices for Planes

- A plane and its negative are parallel and identical.
- Planes and its multiple are parallel planes: (100) is parallel to the plane (200) and the distance between (200) planes is half of the distance between (100) planes.
Certain groups of planes are equivalent (same atom distribution); they have their particular indices primarily because of the way we construct the co-ordinates. For example, a \((100)\) planes is equivalent to the \((010)\) planes. We may refer to groups of equivalent planes as planes of the same family. The special brackets \{\} are used to indicate this collection of planes.

- In cubic systems the direction of miller indices \([h \ k \ l]\) is normal or perpendicular to the \((h \ k \ l)\) plane.
- In cubic systems, the distance \(d\) between planes \((h \ k \ l)\) is given by the formula

\[
d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}
\]

where \(a\) is the lattice constant.

**Example:**
The family of planes \(\{100\}\) consists of three equivalent planes \((100)\), \((010)\) and \((001)\)
A “family” of crystal planes contains all those planes are crystallographically equivalent.

- Planes have the same atomic packing density
- A family is designated by indices that are enclosed by braces.

- \{111\}:
  
  $(111), (1\overline{1}1), (\overline{1}11), (1\overline{1}1), (11\overline{1}), (\overline{1}11), (\overline{1}\overline{1}1), (1\overline{1}1)$
- Single Crystal
- Polycrystalline materials
- Anisotropy and isotropy

<table>
<thead>
<tr>
<th>Metal</th>
<th>[100]</th>
<th>[110]</th>
<th>[111]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>63.7</td>
<td>72.6</td>
<td>76.1</td>
</tr>
<tr>
<td>Copper</td>
<td>66.7</td>
<td>130.3</td>
<td>191.1</td>
</tr>
<tr>
<td>Iron</td>
<td>125.0</td>
<td>210.5</td>
<td>272.7</td>
</tr>
<tr>
<td>Tungsten</td>
<td>384.6</td>
<td>384.6</td>
<td>384.6</td>
</tr>
</tbody>
</table>
Two Types of Indices in the Hexagonal System

\(a_1, a_2, \text{and } c \text{ are independent, } a_3 \text{ is not!}\)

\[ a_3 = - (a_1 + a_2) \]

Miller: \((hkl)\) \hspace{1cm} (same as before)

Miller-Bravais: \((hkil) \rightarrow i = -(h+k)\)
X-Ray Spectroscopy

Visible light: 0.4-0.7m ~ 6000Å

Mo: 35KeV ~ 0.02-0.14nm

\[ E = h\nu = \frac{hc}{\lambda} \]
X-Ray Diffraction from a Crystal

- Electromagnetic radiation is wave-like:

- Waves can add constructively or destructively:
Diffraction of X-rays by Crystal Planes

Diffracted x-rays, in phase, produce a spot

Incoming x-rays

Particle layer 1

Particle layer 2

Undiffracted beam
Bragg’s Law

For constructive interference

For cubic system:

\[ n\lambda = \frac{\overline{DE} + \overline{EF}}{\overline{n}} \]

\[ n\lambda = d_{hkl} \sin \theta + d_{hkl} \sin \theta \]

\[ n\lambda = 2d_{hkl} \sin \theta \]

But no all planes diffract !!!

\[ d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \]
Figure 3.19 Schematic diagram of an x-ray diffractometer; T = x-ray source, S = specimen, C = detector, and O = the axis around which the specimen and detector rotate.

\[ \lambda = 0.1542 \text{ nm (CuK}_{\alpha}\text{-radiation)} \]
For the BCC structure the first two sets of principal diffracting planes are \{110\} and \{200\}. For the FCC structure the first two sets of principal diffracting planes are \{111\} and \{200\}.

\[
\sin^2 \theta_A = \frac{h^2_A + k^2_A + l^2_A}{h^2_B + k^2_B + l^2_B}
\]

\[
\frac{\sin^2 \theta_A}{\sin^2 \theta_B} = 0.5 \text{ (BCC)}; = 0.75 \text{ (FCC)}
\]
Ex: An element, BCC or FCC, shows diffraction peaks at $2\theta$: 40, 58, 73, 100.4 and 114.7.

Determine:

(a) Crystal structure?
(b) Lattice constant?
(c) What is the element?