SOLID STATE PHYSICS

Notes by Reza'21

1. **Crystalline Solids:** Crystalline solids are materials in which the atoms, ions, or molecules are arranged in a highly ordered, repeating pattern extending in all three spatial dimensions. The regular arrangement of particles gives crystalline solids specific and characteristic shapes and properties.

2. **Amorphous or Non-crystalline Solids:** Amorphous solids lack a regular, repeating arrangement of particles at the atomic level. Instead, the atoms or molecules are arranged randomly. This results in a lack of long-range order and a characteristic absence of a well-defined melting point.

3. **Single Crystalline Materials:** Single crystalline materials are solids in which the entire sample has a consistent crystal structure with no grain boundaries. This means that the entire material is made up of a single crystal.

4. **Polycrystalline Materials/Solids:** Polycrystalline materials are composed of multiple crystalline grains, each with its own crystal structure and orientation. The grains are separated by grain boundaries, and the overall material may not have a consistent crystallographic structure.

5. **Lattice:** A lattice is a regular, repeating arrangement of points or particles in space. In the context of crystals, a lattice represents the three-dimensional arrangement of atoms, ions, or molecules.

6. **Space Lattice:** A space lattice is a three-dimensional array of lattice points that represents the arrangement of particles in a crystal.

7. **Bravais Lattice:** A Bravais lattice is an idealized lattice in which identical points are located at each lattice point, and the arrangement of lattice points is the same when viewed

from any corner of the lattice. There are 14 possible Bravais lattices in three-dimensional space.

8. **Non-Bravais Lattice:** Non-Bravais lattices do not possess the property of translational symmetry exhibited by Bravais lattices. The arrangement of lattice points is not the same when viewed from different corners.

9. **Basis or Motif:** A basis (or motif) is a group of atoms, ions, or molecules that occupy specific positions in a crystal lattice. The arrangement of these basis elements along with the lattice points forms the crystal structure.

10. **Unit Cell:** The unit cell is the smallest repeating unit in a crystal lattice that, when repeated in three dimensions, generates the entire crystal structure.

11. **Coordination Number:** The coordination number of an atom in a crystal is the number of nearest neighbor atoms to which it is bonded. In simple terms, it represents how many atoms are touching a central atom in a crystal structure.

12. **Cohesive Energy:** Cohesive energy is the energy required to completely separate a solid into its constituent atoms or molecules, thereby overcoming all intermolecular forces.

13. **Polymer:** Polymers are large molecules composed of repeating structural units called monomers. They can be both natural (like proteins and DNA) and synthetic (like plastics).

14. **Ceramic:** Ceramics are inorganic, non-metallic materials often characterized by their brittleness, high melting points, and excellent electrical and thermal insulating properties.

15. **Plasticity:** Plasticity refers to the ability of a material to undergo permanent deformation without breaking when subjected to external forces.

16. **Elasticity:** Elasticity is the ability of a material to return to its original shape and size after deformation when the applied stress is removed.

17. **Forbidden Energy Gap:** In the context of semiconductors, the forbidden energy gap (or energy band gap) is the energy range in which electron states are forbidden. Electrons in a material need a certain amount of energy to move from the valence band to the conduction band, and this energy is the band gap.

18. **Conduction Band and Valence Band:** In solid-state physics, the valence band is the range of energy levels that electrons occupy in a material at absolute zero temperature, while the conduction band is the range of energy levels that electrons can jump into when excited.

19. **Plasma States of Matter:** Plasma is a state of matter in which ionized gas particles coexist with electrons. It is characterized by high temperature and can conduct electricity due to the presence of free electrons and ions.

Q:2. Distinguish between primitive unit cell and Non-Primitive unit cell.

A primitive unit cell is the smallest repeating unit of a crystal that contains only one lattice point. A non-primitive unit cell is a unit cell that contains more than one lattice point.

Here is a table that distinguishes between primitive and non-primitive unit cells:

Characteristic	Primitive unit cell	Non-primitive unit cell
Number of lattice points	One	More than one
Size	Smallest possible	Larger than primitive unit cell
Symmetry	May or may not reflect the symmetry of the crystal	Reflects the symmetry of the crystal
Examples	Simple cubic, simple tetragonal, simple orthorhombic	Body-centered cubic, face-centered cubic, body-centered tetragonal

Primitive unit cells are often used to describe the crystal structure of a material because they are the simplest and easiest to understand. However, non-primitive unit cells are sometimes necessary to describe the symmetry of a crystal structure.

Here are some examples of primitive and non-primitive unit cells:

Primitive unit cells:
- Simple cubic: A cube with a lattice point at each corner
- Simple tetragonal: A rectangular prism with a lattice point at each corner
- Simple orthorhombic: A rectangular prism with a lattice point at each corner

Non-primitive unit cells:
- Body-centered cubic (bcc): A cube with a lattice point at each corner and one in the center of the cube
- Face-centered cubic (fcc): A cube with a lattice point at each corner and one on the center of each face
- Body-centered tetragonal (bct): A rectangular prism with a lattice point at each corner and one in the center of the prism

Which type of unit cell is used to describe a particular crystal structure depends on the material and the desired level of detail. For example, the primitive unit cell of sodium chloride (NaCl) is a simple cubic cell. However, the non-primitive unit cell of NaCl, which includes a sodium ion and a chloride ion, is more commonly used to describe the crystal structure of NaCl because it reflects the symmetry of the crystal.

Q:3. What are the differences between crystalline and amorphous solids?

Crystalline and amorphous solids are two different types of solids that differ in their atomic arrangement.

Crystalline solids have a regular, ordered arrangement of atoms. The atoms are arranged in a repeating three-dimensional pattern, called a crystal lattice. Crystalline solids have well-defined edges and faces, and they diffract X-rays. They also tend to have sharp melting points.

Amorphous solids do not have a regular, ordered arrangement of atoms. The atoms are arranged in a random or disordered way. Amorphous solids have irregular or curved surfaces, and they do not diffract X-rays. They also melt over a wide range of temperatures.

Here is a table that summarizes the key differences between crystalline and amorphous solids:

Characteristic	Crystalline solids	Amorphous solids
Atomic arrangement	Regular, ordered	Random, disordered
Crystal lattice	Yes	No
Edges and faces	Well-defined	Irregular, curved
X-ray diffraction	Yes	No
Melting point	Sharp	Wide range

Some examples of crystalline solids include:

- Salt (NaCl)
- Sugar (C12H22O11)
- Diamond (C)
- Quartz (SiO2)
- Metals (Fe, Al, Cu, etc.)

Some examples of amorphous solids include:

- Glass
- Plastic
- Rubber
- Wax
- Caramel

Crystalline and amorphous solids have different properties and applications due to their different atomic arrangements. For example, crystalline solids are generally stronger and more rigid than amorphous solids. This is because the atoms in a crystalline solid are held together in a strong, regular arrangement. Amorphous solids, on the other hand, are more malleable and ductile than crystalline solids. This is because the atoms in an amorphous solid are not held together in a strong, regular arrangement.

Crystalline solids are used in a wide variety of applications, including construction, electronics, and medicine. Amorphous solids are also used in a wide variety of applications, including packaging, insulation, and adhesives.

Q:4. What are the symbols 'P', 'I'. 'F', 'C' stand for?

In the context of crystallography, the symbols 'P', 'I', 'F', and 'C' represent different types of lattice systems:

1. **'P':** Primitive lattice or lattice with a Primitive Basis

   - In a primitive lattice, lattice points are only at the corners of the unit cell. There is only one lattice point per unit cell, and it is not shared with other unit cells.

2. **'I':** Body-Centered lattice or lattice with an Inverted Basis

   - In an I lattice, there is one lattice point at the center of the unit cell in addition to lattice points at the corners. The center point is shared by eight neighboring unit cells.

3. **'F':** Face-Centered lattice or lattice with a Face-Centered Basis

- In an F lattice, there is one lattice point at the center of each face of the unit cell, in addition to lattice points at the corners. The face-centered points are shared by adjacent unit cells.

4. **'C':** Base-Centered lattice or lattice with a Base-Centered Basis

   - In a C lattice, there is one lattice point at the center of one pair of opposite faces of the unit cell, in addition to lattice points at the corners. The base-centered points are shared by adjacent unit cells.

Bravais lattice type	Symbol
Primitive	P
Body-centered	I
Face-centered	F
Centered	C

These symbols indicate the arrangement of lattice points within a unit cell in different crystal lattice systems.

Q:5. Write down the name of seven crystal system in appropriate condition and examples.

1. **Cubic System:**

- **Condition:** All three axes are of equal length, and angles between them are 90 degrees.

   - **Examples:** Diamond, Sodium Chloride (NaCl), and Face-centered cubic metals like Copper (Cu) and Iron (Fe).

2. **Tetragonal System:**

   - **Condition:** Two axes are of equal length, and the third axis is different and perpendicular to the other two. Angles between all axes are 90 degrees.

   - **Examples:** Zirconium dioxide (ZrO_2), Rutile (TiO_2).

3. **Orthorhombic System:**

   - **Condition:** All three axes are of different lengths, and angles between them are 90 degrees.

   - **Examples:** Sulfur, Barite ($BaSO_4$), and Orthorhombic sulfur.

4. **Monoclinic System:**

   - **Condition:** All three axes are of different lengths. Two of the angles between the axes are 90 degrees, and the third angle is not 90 degrees.

   - **Examples:** Gypsum ($CaSO_4 \cdot 2H_2O$), Monoclinic sulfur.

5. **Triclinic System:**

   - **Condition:** All three axes are of different lengths, and all three angles between the axes are different (none are 90 degrees).

   - **Examples:** Microcline (a variety of feldspar), Rhodonite ($MnSiO_3$).

6. **Hexagonal System:**

   - **Condition:** Four of the axes are in the same plane and are of equal length, forming 60-degree angles with each other. The fifth axis is perpendicular to the plane of the other four.

   - **Examples:** Graphite, Quartz (SiO_2), and Close-packed structures of some metals like Magnesium (Mg).

7. **Trigonal System (Rhombohedral System):**

- **Condition:** Three axes of equal length, all intersect at equal angles (not 90 degrees). This system is often considered a subset of the hexagonal system due to similar parameters.

- **Examples:** Calcite ($CaCO_3$), Rhodochrosite ($MnCO_3$).

Crystal system	Unit cell symmetry	Examples
Triclinic	No symmetry	Microcline, plagioclase feldspar
Monoclinic	One axis of mirror symmetry	Gypsum, orthopyroxene
Orthorhombic	Three mutually perpendicular axes of mirror symmetry	Quartz, sulfur
Tetragonal	One axis of fourfold rotational symmetry	Rutile, zircon
Trigonal	One axis of threefold rotational symmetry	Calcite, corundum
Hexagonal	One axis of sixfold rotational symmetry	Beryl, graphite
Cubic	Three mutually perpendicular axes of fourfold rotational symmetry	Diamond, galena, pyrite

Q: 5. What are the Miller Indices? With example write the procedure for finding the Miller Indices. Write the importance or Uses of Miller Indices. Or, Explain the suitable diagram, how in a crystal planes are denoted the Miller Indices (hkl).

Miller indices are a set of three numbers that are used to uniquely identify a plane in a crystal structure. They are denoted by the symbols (hkl), where h, k, and l are integers.

To find the Miller indices of a plane, follow these steps:

1. Choose a unit cell for the crystal structure.

2. Find the intercepts of the plane with the three crystallographic axes. The intercepts are the points where the plane crosses the axes.

3. Take the reciprocals of the intercepts and clear the fractions. The reciprocals are the Miller indices of the plane.

For example, the Miller indices of the plane that intersects the x-axis at 1/2, the y-axis at 2, and the z-axis at infinity are (1/2, 2, 0). The infinity indicates that the plane does not intersect the z-axis.

Miller indices are important in crystallography because they can be used to:

- Identify planes in a crystal structure.

- Calculate the interplanar spacing, which is the distance between two parallel planes in a crystal structure.

- Determine the direction of diffraction peaks in X-ray diffraction data.

Miller indices are also used in many other areas of science, such as materials science, physics, and chemistry.

Here is a diagram that shows how Miller indices are used to denote planes in a crystal:
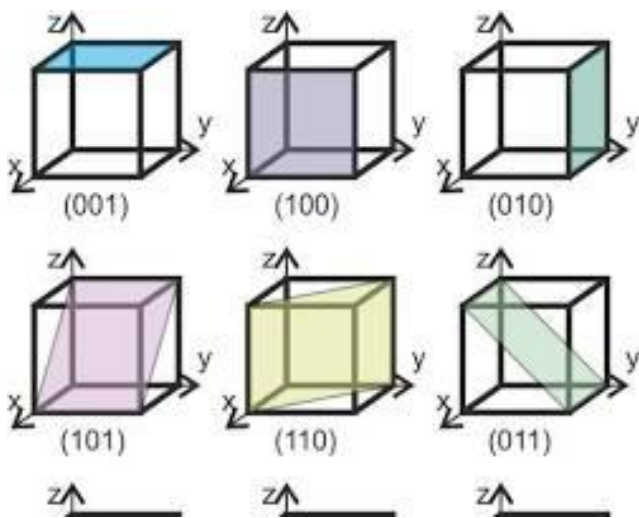
In the diagram, the plane with Miller indices (100) is the plane that intersects the x-axis at 1 and the other two axes at infinity. The plane with Miller indices (110) is the plane that intersects the x-axis at 1 and the y-axis at 1, and the z-axis at infinity.

Miller indices are a powerful tool for understanding and describing crystal structures. They are used in many different areas of science and engineering.

Q: 6(a). Define packing factor/fraction. Show that the packing factor/fraction for simple cubic structure is 0.52

Q: 6(b). Define packing factor/fraction. Show that the packing factor/fraction for body centered cubic (bcc) structure is 0.68

Or, Show that the packing factor for body centered cubic (bcc) structure/crystal is sqrt(3)π/8 .

Or, Find out the packing factor for body centered cubic (bcc) structure/crystal.

The packing factor of a crystal structure is the fraction of the unit cell volume that is occupied by atoms. It is a measure of how efficiently the atoms are packed together.

To calculate the packing factor of a crystal structure, we first need to calculate the volume of the unit cell. The volume of a unit cell can be calculated using the following formula:

```
Volume of unit cell = a^3
```

where a is the length of the unit cell edge.

Once we have calculated the volume of the unit cell, we can calculate the packing factor using the following formula:

```
Packing factor = (Volume of atoms in unit cell) / (Volume of unit cell)
```

The volume of the atoms in the unit cell can be calculated by assuming that the atoms are spheres. The volume of a sphere is calculated using the following formula:

```
Volume of sphere = (4/3)πr^3
```

where r is the radius of the sphere.

Packing factor for simple cubic structure

The simple cubic unit cell is a cube with an atom at each corner. The volume of the simple cubic unit cell is a^3.

The volume of the atoms in the simple cubic unit cell is 8(4/3)πr^3 since there are 8 atoms at the corners of the unit cell.

Therefore, the packing factor for the simple cubic structure is:

```
Packing factor = 8(4/3)πr^3 / a^3 = 0.52
```

Packing factor for body-centered cubic (bcc) structure

The bcc unit cell is a cube with an atom at each corner and one atom in the center of the cube. The volume of the bcc unit cell is a^3.

The volume of the atoms in the bcc unit cell is 9(4/3)πr^3 since there are 9 atoms in the bcc unit cell.

Therefore, the packing factor for the bcc structure is:

```
Packing factor = 9(4/3)πr^3 / a^3 = 0.68
```

Another way to calculate the packing factor for the bcc structure is to use the following formula:

```
Packing factor = sqrt(3)π / 8
```

This formula can be derived by considering the geometry of the bcc unit cell.

Packing factors are important for understanding the properties of materials. For example, materials with high packing factors are often dense and have high melting points.