

Phy-322 Assignment

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 - Questions
 - Answers
 - * 1. Give all possible definitions of Crystal that you know.
 - * 2. Give two definitions of amorphous materials.
 - * 3. Give three definitions of a lattice.
 - * 4. Give two definitions of Bravais lattice.
 - * 5. Define what is meant by basic/basis cell.
 - * 6. List two definitions of the primitive unit cell.
 - * 7. Draw the basic vector that represents the primitive unit cell in the following 3D order
 - * 8. Give full atomic coordinates of NaCl structure.
 - * 10. Calculate the atomic packing fraction of
 - Hexagonal-Closed Packed structure
 - Packing Fraction

Questions

1. Give all possible definitions of Crystal that you know.
2. Give two definitions of amorphous materials.
3. Give three definitions of a lattice.
4. Give two definitions of Bravais lattice.
5. Define what is meant by basic/basis cell.
6. List two definitions of the primitive unit cell.
7. Draw the basic vector that represents the primitive unit cell in the following 3D order
 - Body-Centered Cubic (BCC)
 - Face-Centered Cubic (FCC)
 - Hexagonal-Closed Packed (HCP)
8. Give full atomic coordinates of NaCl structure.
9. Derive the atomic coordinates of the HCP structure other than the method used in class.
10. Calculate the atomic packing fraction of
 - Hexagonal Crystal lattice
 - Hexagonal-Closed Packed structure
11. Given the basic vector of Body-Centered Cubic lattice in real space with the expression.

$$a_1 = \frac{a}{2}x + \frac{a}{2}y - \frac{a}{2}z$$
$$a_2 = -\frac{a}{2}x + \frac{a}{2}y + \frac{a}{2}z$$

$$a_3 = \frac{a}{2}x - \frac{a}{2}y + \frac{a}{2}z$$

- Determine the reciprocal lattice vectors.
- Draw the diagram of the Body-Centered System, showing the appropriate primitive basis vectors.

Answers

1. Give all possible definitions of Crystal that you know.

- A crystal or crystalline solid is a solid material whose constituents (such as atoms, molecules, or ions) are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions.
- A crystal is a solid material in which atoms, ions and molecules are arranged in regularly repeating pattern that extends in all three spatial dimensions,
- A crystal is any solid crystalline substance, and thus has a regular and ordered internal arrangement of atoms, ions or molecules.
- A crystal is a solid substance that is composed of atoms, ions, and molecules that are arranged in a regular geometric pattern. In general, “crystal” is used to describe materials that have a regular repeating and symmetrical atomic structure

Reference Open AI Chat GPT-3

2. Give two definitions of amorphous materials.

- An amorphous material is a solid material that lacks long-range order in its atomic structure.
- A solid in which the constituent particles do possess a regular three-dimensional arrangement.
- An amorphous material can also be defined as a solid that has a somewhat random internal arrangement of atoms, ions and molecules, which gives them a glassy appearance. Examples of amorphous solids include glass, plastics, and many types of rubber.

Reference Open AI Chat GPT-3

3. Give three definitions of a lattice.

- A lattice is a regularly repeating arrangement of points in three-dimensional space, that is usually occupied by atoms, ions or molecules.
- A lattice can also be defined as a three-dimensional array of points that form a regular and repeating pattern. *Reference Open AI Chat GPT-3*
- A set of mathematical points to which the crystal is attached.

Reference Solid State Physics Kittel

4. Give two definitions of Bravais lattice.

- A Bravais Lattice is an array of discrete points that look the same in all directions and orientations that look the same in all directions.

Reference *byjus.com*

- A Bravais Lattice is the basic building block from which all crystals can be constructed. **Reference** *libretexts.org*

5. Define what is meant by basic/basis cell.

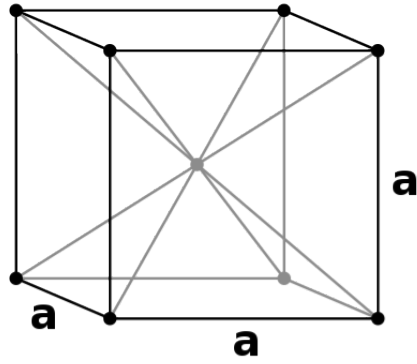
A basic cell or basis cell is the smallest unit cell that can be used to construct the entire crystal lattice without gaps or overlaps. It is a three-dimensional structure that is repeated in a crystal lattice to create the overall crystal structure. The basic cell is characterized by the lengths of its sides and the angles between them, and it is used to define the fundamental geometry of the crystal lattice. The arrangement of atoms within the basic cell determines the overall properties of the crystal, such as its hardness, electrical conductivity, and thermal conductivity.

6. List two definitions of the primitive unit cell.

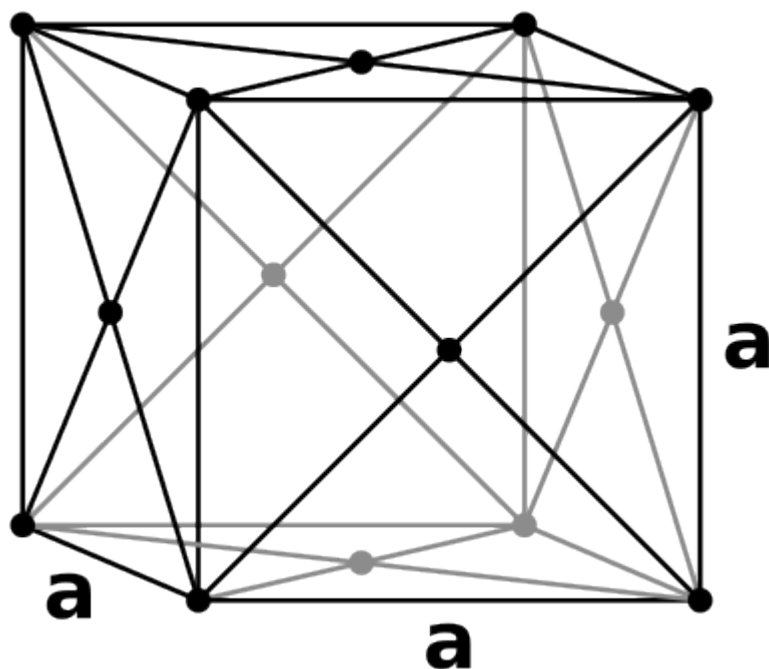
- A primitive unit cell is a basic building block of a crystal lattice. It is the smallest unit cell that can be used to construct the entire crystal lattice without gaps or overlaps.
- A primitive unit cell is a three-dimensional structure that is repeated in a crystal lattice to create the overall crystal structure. It is the smallest unit cell that can be used to construct the entire crystal lattice without gaps or overlaps, and it is characterized by the lengths of its sides and the angles between them. **Reference** *Open AI Chat GPT-3*

7. Draw the basic vector that represents the primitive unit cell in the following 3D order

- Body-Centered Cubic (BCC)



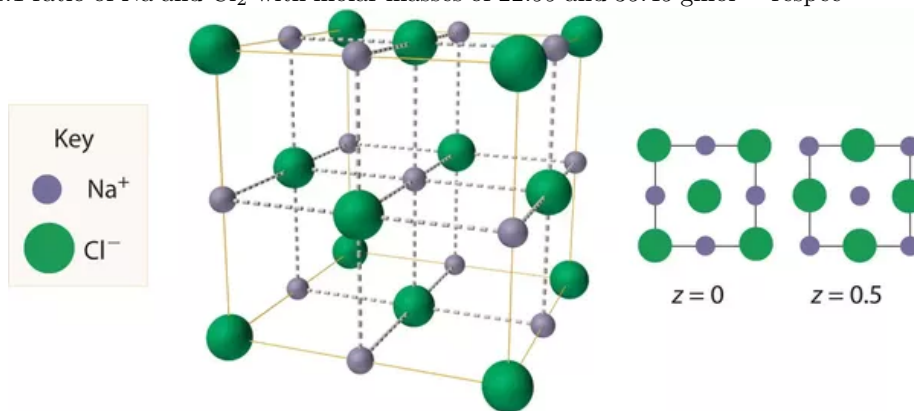
- Face-Centered Cubic (FCC)



- Hexagonal-Closed Packed (HCP)


8. Give full atomic coordinates of NaCl structure.

Sodium chloride is an ionic compound with the chemical formula NaCl, representing a 1:1 ratio of Na and Cl₂ with molar masses of 22.99 and 35.45 gmol⁻¹ respectively.



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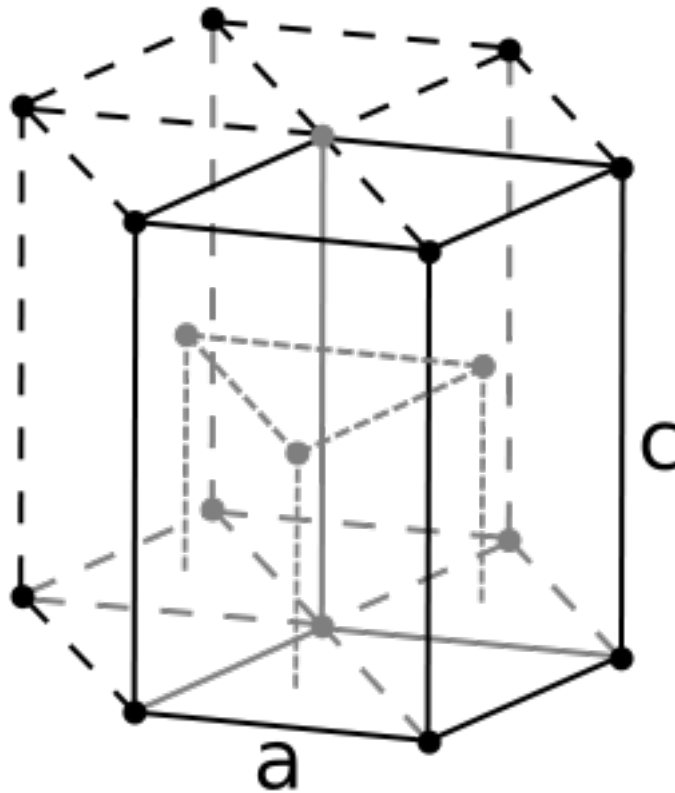
* NaCl has a Cubic-Closed Packed (CCP) arrangement. * The structure of sodium chloride consists of eight ions in a unit cell, four are Na⁺ ions and the other four are Cl⁻

In this structure, each corner of the ion is shared between eight unit cells, each ion at the faces of each cell is shared between two cells, each ion on an edge is shared between four cells, while the ion inside the cell belongs entirely to that unit cell. So the position of the ions is the following (with Na at the center of the axis): * Na^+ $(0\ 0\ 0)$ $(\frac{1}{2}\ \frac{1}{2}\ 0)$ $(\frac{1}{2}\ 0\ \frac{1}{2})$ $(0\ \frac{1}{2}\ \frac{1}{2})$ * Cl^- $(0\ \frac{1}{2}\ 0)$ $(\frac{1}{2}\ 0\ 0)$ $(0\ 0\ \frac{1}{2})$ $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$

10. Calculate the atomic packing fraction of

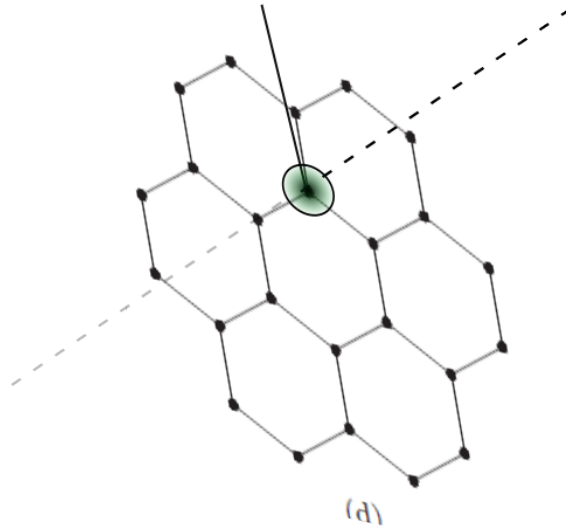
- Hexagonal Crystal lattice
- Hexagonal-Closed Packed structure

Hexagonal-Closed Packed structure Consider the diagram bellow



From the diagram above we notice that each atom at the edge of the hexagon is

Reference atom in 3D



shared between six cells

* 3 cells at the top * 3 cells at the bottom

– each of the 12 edge atoms contributes a total of $\frac{1}{6}$ atoms to the cell

$$\frac{1}{6} \times 12 = 2 \text{ (for the edge atoms)}$$

– we can also see that each of the face atoms is being shared between two adjacent unit cells, thus the two face atoms (at the top and the bottom), contribute a total of $\frac{1}{2}$ atoms.

$$\frac{1}{2} \times 2 = 1 \text{ (for the face atoms)}$$

– we also see that the three inner atoms are not shared with any other unit cell and thus contribute a full atom each to the unit cell

$$1 \times 3 = 3 \text{ (for the inner atoms)}$$

this means the effective number of atom in HCP is

$$2 + 1 + 3 = 6 \text{ atoms}$$

Packing Fraction the packing fraction of a Hexagonal-Closed Packed structure is given by

$$PF = \frac{\text{volume occupied by the atoms}}{\text{volume of the unit cell}}$$

$$\text{volume occupied by the atoms} = z \times \text{volume of an atom}$$