ESE 2021

UPSC ENGINEERING SERVICES EXAMINATION

Preliminary Examination

General Studies and Engineering Aptitude

Basics of Material Science and Engineering

Comprehensive Theory *with* Practice Questions *and* ESE Solved Questions

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ESE 2021 Preliminary Examination : Basics of Material Science and Engineering

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Preface

B. Singh (Ex. IES)

The compilation of this book **Basics of Material Science and Engineering** was motivated by the desire to provide a concise book which can benefit students to understand the concepts of this specific topic of General Studies and Engineering Aptitude section.

This textbook provides all the requirements of the students, i.e. comprehensive coverage of theory, fundamental concepts and objective type questions articulated in a lucid language. The concise presentation will help the readers grasp the theory of this subject with clarity and apply them with ease to solve objective questions quickly. This book not only covers the syllabus of ESE in a holistic manner but is also useful for many other competitive examinations. All the topics are given the emphasis they deserve so that mere reading of the book clarifies all the concepts.

We have put in our sincere efforts to present detailed theory and MCQs without compromising the accuracy of answers. For the interest of the readers, some notes, do you know and interesting facts are given in the comprehensive manner. At the end of each chapter, sets of practice question are given with their keys and detailed explanations, that will allow the readers to evaluate their understanding of the topics and sharpen their question solving skills.

Our team has made their best efforts to remove all possible errors of any kind. Nonetheless, we would highly appreciate and acknowledge if you find and share with us any printing and conceptual errors.

It is impossible to thank all the individuals who helped us, but we would like to sincerely thank all the authors, editors and reviewers for putting in their efforts to publish this book.

With Best Wishes

B. Singh

CMD, MADE EASY Group

Basics of Material Science and Engineering

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Chapter 2

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■■■■

3 Crystallography

3.1 Introduction

- Crystallography is a branch of science in which
  - (i) the internal structure of crystals.
  - (ii) the properties of crystalline metal.
  - (iii) the external and internal symmetries possessed by crystalline solids are studied.
- Before the discovery of X-rays, the crystallography science was limited to the study of external appearance and external symmetries of the crystals. Now with X-rays crystallography, it is possible to ascertain the actual existence of the shape pattern, the exact shape and size of unit cell of a crystalline solid and actual periodic arrangement in space.
- X-ray crystallography could help in revealing that many important materials are crystalline solids.
- The most important crystallography terms are:
  - (i) lattice
  - (ii) space lattice
  - (iii) unit cell
  - (iv) basic symmetry and
  - (v) Miller indices etc.
- Crystallographic methods now depend on the analysis of the diffraction patterns of a sample targeted by a beam of X-rays, neutron or electrons. These three types of radiation interact with the specimen in different ways. Electron beam helps in finding charge distribution.
- Neutron beam is scattered by magnetic field. X-ray beam provides atomic resolution image and an image of strontium titanate as obtained by X-ray beam is as shown in fig. 3.1.

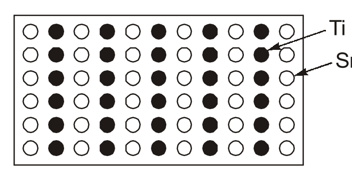
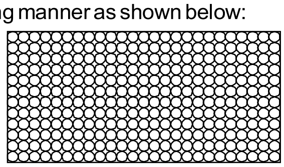
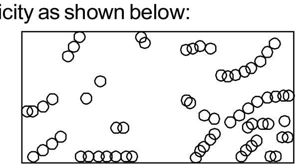


Fig. 3.1 *Atomic resolution image of strontium titanate*

3.2 Comparison of Crystalline and Noncrystalline Solids

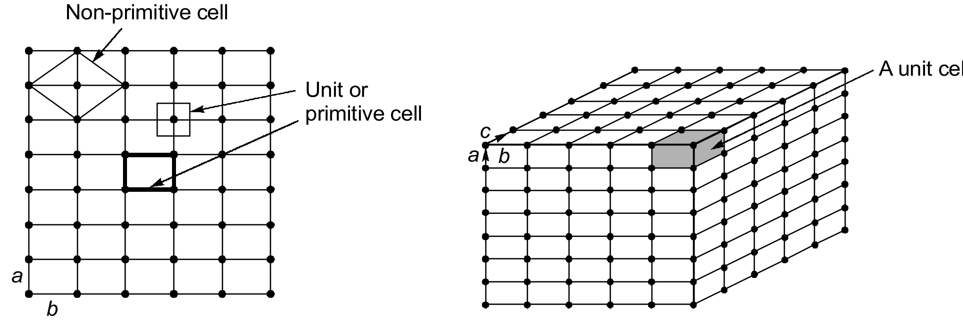
The difference between crystalline and noncrystalline solids are shown in Table 3.1.

Table 3.1 *Differences between crystalline and noncrystalline solids*

	Crystalline solid		Non-crystalline solid
1.	The arrangement of atoms is in a periodically repeating manner as shown below: 	1.	It possesses entangled chain of atoms without any periodicity as shown below: 
2.	It has high density due to its closed packing of atoms in the structure.	2.	It has lower density as the packing of atoms takes place in a zigzag manner.
3.	It presents a sharp diffraction pattern.	3.	It does not present any sharp diffraction pattern.
4.	It exhibits a pin-pointed melting temperature.	4.	It melts over a range of temperatures.
5.	It has well-defined crystal structure and geometries.	5.	It has varying structure and geometries.

3.3 Lattice Points, Space Lattice and Crystal Structures

- The atoms present in any crystalline material are arranged in a regular three dimensional space in repeating pattern. The three dimensional pattern of atoms present in a crystalline material is called crystal or space lattice.
- Lattice is nothing but a network of lines drawn in space in such a way that:
  (i) the space is divided into equal volume and
  (ii) the points of intersection of these lines are the lattice points on which the atoms (or ions and molecules) of the material are located.
- The essential characteristic of a space lattice is that every point of space lattice has identical surroundings.
- The space lattice of a crystal is described by means of a three dimensional coordinate system in which the coordinate axes coincide with the three edges of the crystal. Hence, space lattice has a finite array of points in three dimensional space in which every point has identical environment.
- A two dimensional square array of points forming a square lattice is as shown in figure 3.2 (a). It is generated by repeated translation of vectors a & b. Similarly, a three dimensional space lattice can be generated by repeated translation of vectors a, b and c as shown in figure 3.2 (b).
- It is found out that there are only 14 distinguishable ways of arranging points in three dimensional space such that each arrangement conforms to the definition of a space lattice. These 14 space lattices are known as Bravais lattices. All crystal structures are based on these 14 Bravais lattices.



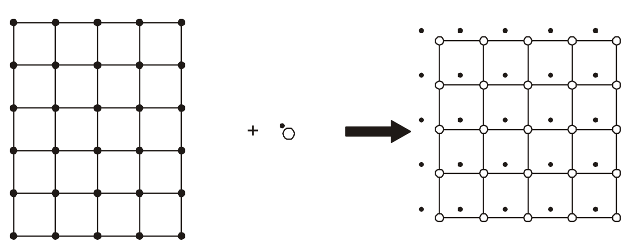
(a) Square array generated by repeated translation of *a* and *b* vectors when both taken as unit

(b) Space lattice dividing space in equal volumes

Fig. 3.2 *Space lattice generated by repeated translation of a, b and c vectors*

- The difference between a lattice and a crystal is that lattice is "a 3-D translationally periodic arrangement of points" while a crystal is "a 3-D translationally periodic arrangement of atoms". Hence, the relation between a crystal and lattice is

Crystal = Lattice + basis or Motif



(a) Lattice (b) Basis (c) Crystal structure

Fig. 3.3 *Generation of crystal structure with lattice and basis (Motif)*

- Motif or basis is an atom or a group of atoms associated with each lattice point, the generation of crystal structure from a lattice and basis is as shown in figure 3.3.

3.4 Unit Cell and Primitive Unit Cell

- A unit cell is the smallest geometrical figure such that the repetition of which in three dimensions will give the actual crystal structure.
- A space lattice can be defined by referring to a unit cell. The unit cell is the smallest unit which, when repeated in space indefinitely, will generate the space lattice. A unit cell in 2 dimensions is the square which can be obtained by joining four neighbouring lattice points as shown in figure 3.2 (a).
- As every corner of the square is common to four unit cell meeting at that corner point, the effective number of lattice point in this unit cell is only one.
- In case, we take the unit cell with one lattice point at the centre of the square as shown in figure 3.2 (a) and with none at the corner, then also the effective number of lattice points in the unit cell remains only one.
- The unit cell that contains one lattice point only is called simple or primitive unit cell. **So primitive unit cells have least number of total atoms and the least volume of atoms per unit cell.**
- The unit cells which contain more than the one lattice points are called non-primitive cells as shown in figure 3.2 (a) where the non primitive cell has two lattice points.

3.5 Bravais Lattices

- There are only fourteen independent ways of arranging points in a three dimensional space on pure symmetry consideration. If all the atoms at the lattice points are identical, the space lattice is said to be a Bravais lattice. These 14 Bravais lattices belong to seven crystal systems. The crystal systems are listed in Table 3.2.

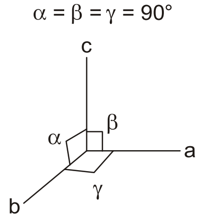
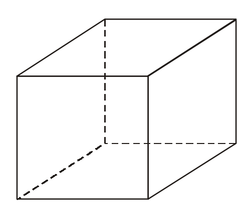
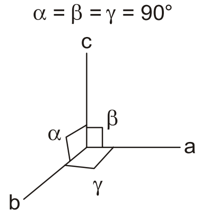
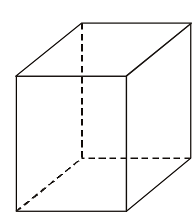
<table>
<tr><th></th><th>Crystal System</th><th>Space Lattice</th><th>Unit Cell</th></tr>
<tr><td>I.</td><td>Cubic
$a = b = c$
$\alpha = \beta = \gamma = 90°$

</td><td>1. Simple (lattice points at the eight corners of the unit cell).
2. Body centred (points a the eight corners and at the body centre).
3. Face centred (points at the eight corners and at the six face centres).</td><td></td></tr>
<tr><td>II.</td><td>Tetragonal
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

</td><td>4. Simple (points at the eight corners of the unit cell).
5. Body centred (points at the eight corners and at the body centres).</td><td></td></tr>
</table>

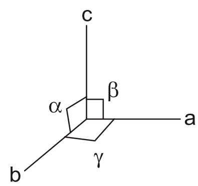
Table 3.2 *Crystal Systems*

<table>
<tr><th></th><th>Crystal System</th><th>Space Lattice</th><th>Unit Cell</th></tr>
<tr><td>III.</td><td>

Orthorhombic

$a \neq b \neq c$

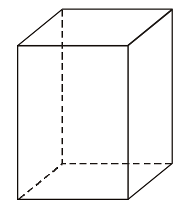
$\alpha = \beta = \gamma = 90°$



</td><td>

6. Simple (points at the eight corners of the unit cell).
7. End centered is also called side centred or base centred (points at the eight corners and at two face centres opposite to each other).
8. Body centred (points at the eight corners and at the body centre).
9. Face centred (points at the eight faces).

</td><td>

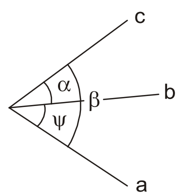


</td></tr>
<tr><td>IV.</td><td>

Rhombohedral

$a = b = c$

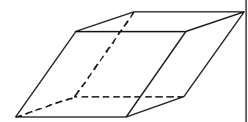
$\alpha = \beta = \gamma \neq 90°$



</td><td>

10. Simple (points at the eight corners of the unit cells).

</td><td>



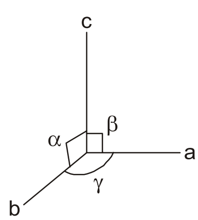
</td></tr>
<tr><td>V.</td><td>

Hexagonal

$a = b \neq c$

$\alpha = \beta = 90°$

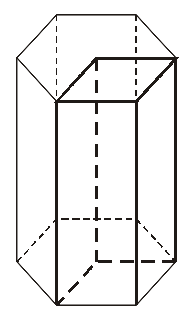
$\gamma = 120°$



</td><td>

11. Simple [(i) points at the eight corners of the unit cell outlined by thick lines. or (ii) points at the twelve corners of the hexagonal prism and at the centres of the two hexagonal faces]

</td><td>

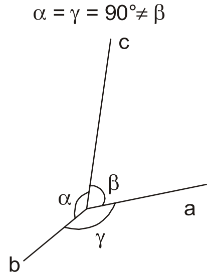


</td></tr>
<tr><td>VI.</td><td>

Monoclinic

$a \neq b \neq c$

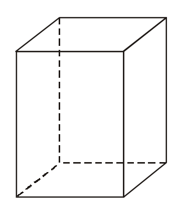
$\alpha = \gamma = 90° \neq \beta$



</td><td>

12. Simple (points at the eight corners of the unit cell).
13. End centred (points at the eight corners and at two face centres opposite to each other).

</td><td>

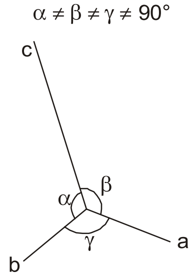


</td></tr>
<tr><td>VII.</td><td>

Triclinic

$a \neq b \neq c$

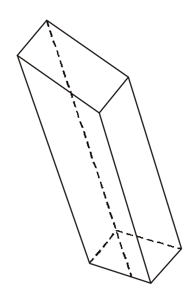
$\alpha \neq \beta \neq \gamma \neq 90°$



</td><td>

14. Simple (points at the eight corners of the unit cell).

</td><td>



</td></tr>
</table>

- **Example:** A polycrystalline material in which the grains or crystals are randomly oriented behaves like isotropic, as its properties are independent of direction.
- A body displaying isotropy has only one refractive index, one dielectric constant and so on. In general, most polycrystalline materials will exhibit isotropic properties.

Previous ESE Prelims Questions

Q.1 What is the volume of an FCC unit cell in terms of its atomic radius R?

(a) $\sqrt{3}R^3$ (b) $16R^3\sqrt{2}$

(c) $16R^3\sqrt{3}$ (d) $\sqrt{2}R^3$

[ESE Prelims : 2018]

Ans. (b)

Volume of unit cell = a^3

In FCC unit cell, $R = \frac{\sqrt{2}a}{4}$

$\Rightarrow$ $a = \frac{4R}{\sqrt{2}}$

$\therefore$ $\text{Volume} = a^3 = \left(\frac{4R}{\sqrt{2}}\right)^3 = 16\sqrt{2}R^3$

Q.2 The number of atoms per unit length whose centres lie on the direction vector for a specific crystallographic direction is called

(a) Linear density (b) Theoretical density

(c) Atomic density (d) Avogadro number

[ESE Prelims : 2019]

Ans. (a)

Linear density: It is defined as number of atoms per unit length whose centres lie on the direction vector for a specific crystallographic direction.

$$\text{Linear density} = \frac{\text{Number of atoms centred on direction vector}}{\text{Length of direction vector}}$$

Q.3 A state for ionic compounds wherein there is the exact ratio of cations to anions as predicted by the chemical formula is

(a) Electroneutrality (b) Stoichiometry

(c) Equiliometry (d) Frankel defect

[ESE Prelims : 2019]

Ans. (b)

Stoichiometry may be defined as a state for any compounds where in there is the exact ratio of cations to anions as predicted by the chemical formula.

Q.4 In a simple cubic structure, atomic packing factor is nearly

(a) 0.9 (b) 0.7

(c) 0.5 (d) 0.3

[ESE Prelims : 2019]

Ans. **(c)**

$$\text{Atomic packing factor} = \frac{\text{Sum of atomic volume in a unit cell}}{\text{Volume of a unit cell}}$$

$$\Rightarrow \quad \text{APF} = \frac{N \times \frac{4}{3}\pi r^3}{a^3}$$

For simple cubic

$$N = \frac{1}{8} \times 8 = 1 \text{ atom/unit cell}$$

$$r = \frac{a}{2}$$

$$\therefore \quad \text{APF} = \frac{1 \times \frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3} = 0.52$$

Q.5 If a pair of one cation and one anion is missing in an ionic crystal such that those pairs of ions are equal to maintain electrical neutrality, then that pair of vacant sites is called

(a) Schottky imperfection
(b) Pair of vacancies
(c) Frenkel defect
(d) Point imperfection

[ESE Prelims : 2020]

Ans. **(a)**

Schottky defect occurs when a pair of cation and anion is missing from crystal such that electrical neutrality is maintained.

Objective Brain Teasers

Q.1 The difference between the number of atoms in a unit cell of a BCC crystal and an FCC crystal is

(a) 1
(b) 2
(c) 4
(d) 6

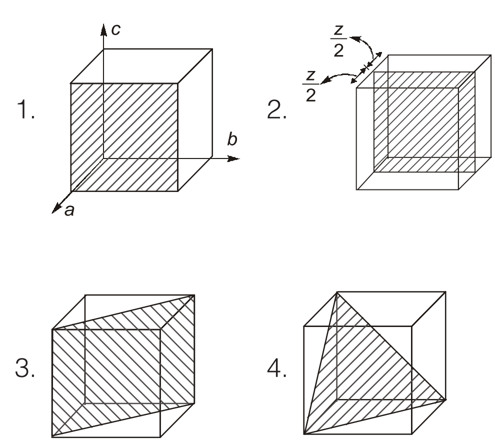
Q.2 When BCC iron is heated, it changes to FCC iron resulting in

(a) contraction in volume
(b) increase in volume
(c) no change in volume
(d) crack in the material

Q.3 Which one of the following helps experimental confirmation of the crystalline state of matter?

(a) shock compression
(b) photo emission
(c) conductivity measurements
(d) x-ray diffraction

Q.4 Consider the following crystallographic planes (shaded) using a cube of size z as shown in the diagram:



(a) Triclinic (b) Ortho-rombic
(c) Cubic (d) Rhombo-hedral

Q.25 Consider the following statements and find the correct ones using the codes given below:
1. When a plane of crystalline structure is parallel to one of the three axes, Miller index of that direction has a value of '0'.
2. When a plane of crystalline structure is parallel to one of the three axes, Miller index of that direction is ∞ (infinity).
3. When a plane of crystalline structure is parallel to one of the three axes, the intercept on that axis is infinity.

(a) 1 and 2 only (b) 2 and 3 only
(c) 1 and 3 only (d) all above

Q.26 Match the following:

Crystalline Structure	Atomic Packing Factor
A. Simple cube	1. $\sqrt{2}\dfrac{\pi}{6}$
B. BCC	2. $\sqrt{3}\dfrac{\pi}{8}$
C. FCC	3. $\dfrac{\pi}{6}$

Codes:

	A	B	C
(a)	1	2	3
(b)	1	3	2
(c)	3	2	1
(d)	3	1	2

Q.27 Consider the following statements and find the correct ones using the codes given below:
1. No change in density of solid in case of Schottky defect while density decreases in case of Frenkel defect.
2. In Frenkel defect, some of the ions of lattice occupy interstitial sites leaving the lattice vacant.
3. Schottky defect occurs when equal number of cations and anions are missing from lattice.

(a) 1 only (b) 1 and 2 both
(c) 1, 2 and 3 (d) 2 and 3 only

Q.28 Statement (I): Germanium and Silicon have diamond cubic crystal structure.

Statement (II): The atomic packing factor of Germanium and Silicon is 0.74.

(a) Both Statement (I) and Statement (II) are individually true and Statement (II) is the correct explanation of Statement (I)
(b) Both Statement (I) and Statement (II) are individually true but Statement (II) is not the correct explanation of Statement (I)
(c) Statement (I) is true but Statement (II) is false
(d) Statement (I) is false but Statement (II) is true

Answers

1. (b)	2. (a)	3. (d)	4. (b)	5. (c)
6. (b)	7. (c)	8. (b)	9. (b)	10. (b)
11. (c)	12. (c)	13. (c)	14. (a)	15. (b)
16. (d)	17. (d)	18. (d)	19. (b)	20. (c)
21. (c)	22. (b)	23. (b)	24. (c)	25. (c)
26. (c)	27. (d)	28. (c)		

Explanations

11. (c)

Copper is an example of FCC structure for which APF is 0.74

12. (c)

Simple cubic $r = \dfrac{a}{2} \Rightarrow a^2 = 4r^2$

BCC $r = \dfrac{a\sqrt{3}}{4} \Rightarrow 16r^2 = 3a^2$

FCC $r = \dfrac{a}{2\sqrt{2}} \Rightarrow 8r^2 = a^2$

13. (c)

Density: $\rho = \dfrac{nA}{V_C N_A}$

where n = number of atoms associated with each unit cell
A = Atomic weight
V_C = Volume of the unit cell
N_A = Avogadro's number (6.023×10^{23} atoms/mol)