Syllabus for Test 08: L 18 (partial) , L 19 (partial) and L20:

L18: Brillouin Zone in 2D/3D

L19: Crystal Defects: Point defects : Vacancy, impurity, Fresnel defects, Schottky defects;

L20: Line defects: Dislocations (Screw and Edge), disclination , Surface defects: Free surface, Grain boundary, Twin Boundary, Stalking Fault, Volume defects: Pores, inclusions, cracks, Problems on crystal structure, Packing fraction of Diamond.

Questions:

1. What is a Brillouin zone?

A unit cell in the space lattice.
A primitive unit cell in the space lattice.
A Wigner-Seitz unit cell in the space lattice.
A unit cell in the scaled reciprocal lattice.
A Wigner-Seitz unit cell in scaled the reciprocal lattice.

Ans: A unit cell in the scaled reciprocal lattice. **Note**: "A Brillouin zone is a unit cell in the (scaled) reciprocal lattice. The Wigner-Seitz unit cell about a lattice point in the (scaled) reciprocal lattice is called the First Brillouin Zone about that point". Hence, in general a Brillouin zone (BZ) may not always be the first Brilouin zone.

2. What is meant by the expression "the first Brillouin zone"?

Wigner-Seitz cell of the reciprocal lattice
A unit cell in the reciprocal lattice
A primmitive unit cell in the reciprocal lattice
A unit cell in the scaled reciprocal lattice.
The cell of closest point to a particular point in the scaled reciprocal lattice.

Ans: The cell of closest point to a particular point in the scaled reciprocal lattice.

3. For a 2D square lattice, the second, third and fourth Brillouin zones are fragmented into:

Two, four, six
Four, six, eight
Four, eight, twleve
Four, six, twelve
Two, six, eight

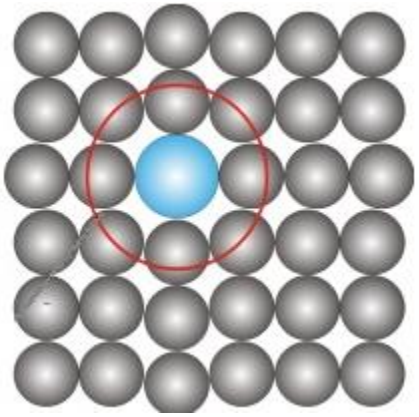
Ans: Four, eight, twelve

4. Vacancy defects in solids is a sub type of _____

Point imperfections
Line imperfections
Volume imperfections
Surface imperfections
May be a volume or point imperfection depending on the size

Ans: Point imperfections. Explanation: The size vacancy defect is taken to be so small (of the size of lattice parameter) that the associated volume is negligible. Hence a point imperfection.

5. Replacement of a foreign atom in the site of parent atom in the crystal is:



Vacancy defect
Substitutional impurity
Volume imperfection
Schottky defect
Frenkel defect

Answer: Substitutional impurity.

Explanation: When an impurity atom of almost the same atomic size of the host atom is being replaced or substituted for the host atoms, it is called a substitutional impurity.

6. A Burgers vector indicates:

Only the Magnitude of a line defect.
Magnitude and direction of a line defect.
Direction of a surface defect.
A general lattice translation vector for a dislocation.
None of the others mentioned.

Ans: Magnitude and direction of a line defect. It also is equal to the shortest lattice translation vector for a full/perfect dislocation.

7. Stacking fault is a:

Point defect
Line defect
Mixed line and point defects
Surface defect
Volume defect

Ans: Surface defect

8. Schottky defect is observed in crystals when:

(a) some cations move from their lattice site to interstitial sites
(b) equal number of cations and anions are missing from the lattice
(c) some lattice sites are occupied by electrons
(d) some impurity is present in the lattice

Only (a) is true
Only (b) is true
Only (c) is true
(a) and (b) both true
All are true.

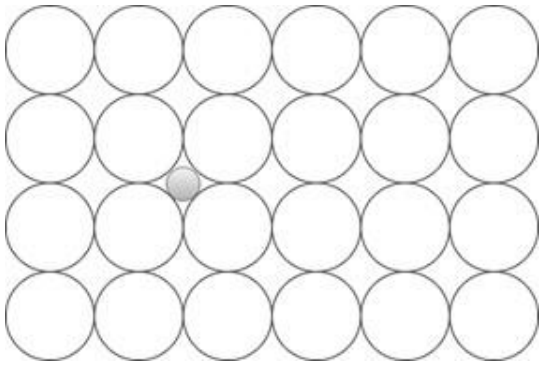
Ans: Only (b) is true.

Explanation: Schottky defect is observed in crystal when equal number of cations and anions are missing from the lattice. Thus, density of solid decreases.

(a) implies: when some cations move from their lattice site to interstitial site is known as Frenkel defect.
(c) implies: when lattice site is occupied by electron, this type of defect is known as **metal excess defect**.
(d) implies: when some impurity is present on crystal is known as impurity defect.

Hence, except (b) all statements are incorrect regarding Schottky defect.

9. Which defect does the following figure depict?



Vacancy defect
Schottky defect
Frenkel defect
Interstitial defect
Substitutional defect

Ans: Interstitial defect.

Explanation: An interstitial impurity is a point defect that results when an impurity atom occupies hole in the lattice between atoms.
There can be self-interstitial defect and foreign interstitial impurity. In the figure there is a foreign interstitial impurity seen.

10. Which of the following is a line defect?

Disclination
Twins
Screw
Grain boundaries
Schottky defect

Ans: Disclination

11. Frenkel defect is a kind of:

(a) dislocation defect
(b) impurity defect
(c) substitutional defect

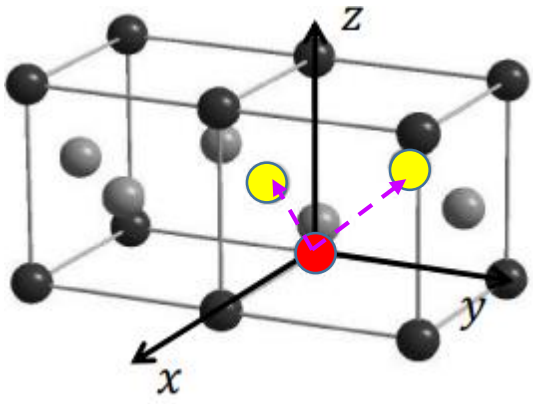
Only (a) is true.
Only (b) is true.
Only (c) is true.
Only (a) and (b) are true
All are true.

Ans: Only (a) is true.

Explanation: A Frenkel defect is a **type of point defect in crystalline solids** named after its discoverer Yakov Frenkel.

The defect forms when an atom or smaller ion (usually cation) leaves its place in the lattice, creating a vacancy, and becomes an interstitial by lodging in a nearby location. It is a kind of dislocation defect.
It is not an impurity defect as the cation is not an impurity in the substance.
It is also NOT a substitutional defect as the cation does not substitute any atom/ion in the crystal.

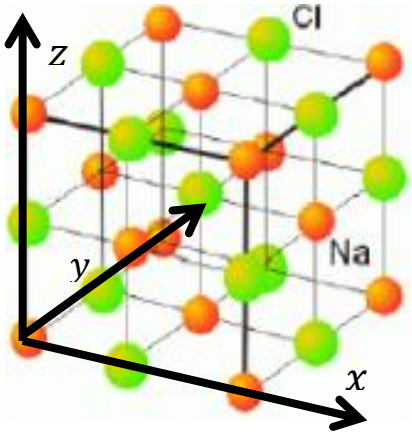
12. What type of Bravais lattice does the lattice in the figure belong and what is the number of atoms in the basis?



FCC, 2 atoms/basis
BCC, 2 atoms/basis
FCC, 3 atoms/basis
SC, 3 atoms/basis
SC, 2 atoms/basis

Ans: SC, 3 atoms/basis
Explanation: It is a side-centered cubic. The Bravais lattice is a simple cubic lattice with 3 atom basis. The position of the atoms are: $a(0,0,0)$, $a(1/2,0,1/2)$ and $a(0,1/2,1/2)$

13. What type of Bravais lattice does the following compound (NaCl) has and what is the number of atoms (including different types/species) in the basis?



FCC, 2 atoms/basis
BCC, 2 atoms/basis
FCC, 4 atoms/basis
SC, 2 atoms/basis
SC, 4 atoms/basis

Ans: FCC, 2 atoms/basis. The atoms are 1 Na atom and 1 Cl atom. The structure can be thought of as two interweaving/interlacing FCC structure each made of either Na or Cl atoms.

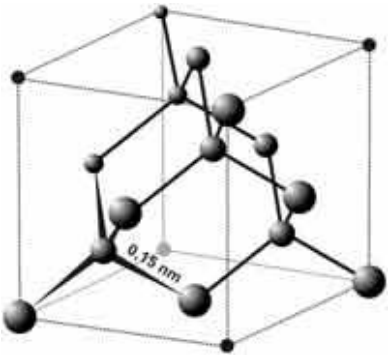
14. When a pair of cation and anion are missing in a crystal, it is called _____

Substitutional impurity
Interstitial defect
Line imperfection
Schottky defect
Frenkel defect

Ans: Schottky defect.

Explanation: Schottky defect, named after its discoverer “Walter H. Schottky”, forms when two atoms of opposite charge (anion and cation) leaves their regular atomic positions thus creating two vacancies. As two atoms of opposite charges are leaving, there is no change in overall charge of the material with Schottky defect. Schottky defect is known for its presence in ionic crystals.

15. What type of Bravais lattice does diamond have and what is the number of atoms in the basis?



FCC, 2 atoms/basis
BCC, 2 atoms/basis
FCC, 4 atoms/basis
SC, 2 atoms/basis
SC, 4 atoms/basis

Ans: FCC, 2 atoms/basis. The atoms are displaced from each other by the vector: $\vec{d} = (a/4)(\hat{\imath} + \hat{\jmath} + \hat{k})$