Syllabus for Test 06:

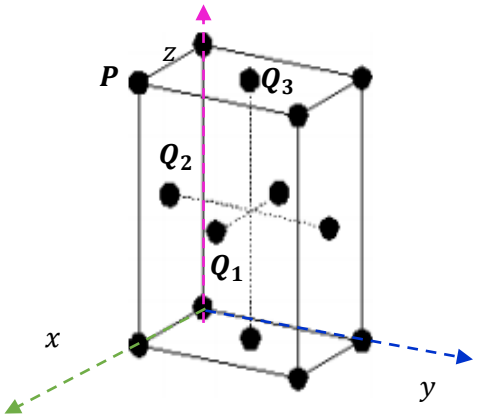
Lecture slides L14 and L 15.
These cover basically the following:

L14: Review of Bravais lattices in 2D and 3D (classification), unit cells, primitive and non-primitive unit cells, close packed structures: HCP, FCC, packing fraction of different crystal structures

L15: Coordination numbers, characteristics of cubic structures, crystal directions, negative directions, family of crystal directions, crystal planes, Miller indices, family of planes.

1. The face-centered orthorhombic lattice in 3D is shown in the figure. What might be the coordination number in this lattice?

2, 4
4, 8
2,6
4
12



Ans: 2, 4. Explanation: Coordination number is a property of a crystal lattice. Hence, if we can find the number if nearest neighbor lattice points ***of any lattice point*** , that will give us the coordination number.

Consider the lattice point $\boldsymbol{P}$, which is a corner lattice point at front-left corner:
The coordinates are: $(a, 0, c)$ where for FC Orthorhombic lattice

$$\alpha = \beta = \gamma = 90°; a \neq b \neq c$$

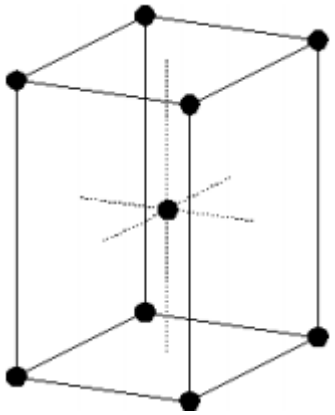
Without loss of generality, we can take $a < b < c$ (according to the figure).
Then the number of nearest neighbor lattice points may be:

A. 2 at distance $a/2$ if $\sqrt{\left(\frac{b}{2}\right)^2 + \left(\frac{c}{2}\right)^2} > a$

B. 4 at a distance $l_1 = \sqrt{\left(\frac{b}{2}\right)^2 + \left(\frac{c}{2}\right)^2}$ if $a > l_1 > a/\sqrt{2}$

Note that: There are three face atoms near to the lattice point P:
A. $\boldsymbol{Q_1}$**:** The distance of the center atom in the front face (parallel to yz-plane) is $= l_1 = \sqrt{b^2 + c^2}/2$
Now, $\frac{a}{2} < \frac{b}{2}; \frac{a}{2} < \frac{c}{2} \Rightarrow l_1 = \sqrt{\left(\frac{b}{2}\right)^2 + \left(\frac{c}{2}\right)^2} > \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} = \sqrt{\frac{a^2}{2}} = a/\sqrt{2}$
Thus, $l_1 > a/\sqrt{2} = 0.707\, a$
Hence, we may have TWO cases:
Case-1: $l_1 > a$ in which case: the coordination number is: 2
Case-2: $a > l_1 > a/\sqrt{2}$; in which case the coordination number is 4 (four face atoms at four different directions , ALL in the same plane)
B. $\boldsymbol{Q_2}$**:** The distance of the center atom in the left-most face i.e. the xz-plane is $= l_2 = \sqrt{a^2 + c^2}/2$
Here, $l_2 = \sqrt{a^2 + c^2}/2 > a$ i.e. $l_2 > a$
C. $\boldsymbol{Q_3}$**:** The distance of the center atom in the top face (parallel to yz-plane) is $= l_3 = \sqrt{b^2 + a^2}$
Here, $l_3 = \sqrt{b^2 + a^2} > a$ i.e. $l_3 > a$

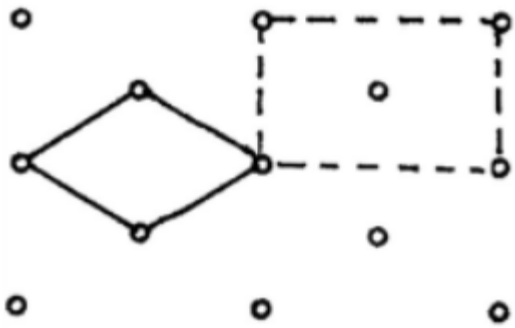
2. What is the coordination number in a body-centered tetragonal lattice in 3D as shown in the figure?



2
3
4
6
8

Ans: 8. Coordination number is a property of the lattice. Hence it is the same for any lattice point.
The body centered atom is equidistant from 8 corner atoms in BC tetragonal lattice.

3. What is the number of second nearest neighbours in the centered rectangular lattice in 2D?



2
4
6
8
10

Ans: 4 . This is the number of neighbours (of the center atom) situated at the four corners of the rectangle.

4. What is the number of second nearest neighbours in the BCC lattice?

2
4
6
8
12

Ans: 6.

5. The correct order of the packing efficiency in different types of unit cells in 3D is:

fcc < bcc < simple cubic<hexagonal
hexagonal > fcc > bcc > simple cubic
bcc> fcc = hexagonal > simple cubic
fcc = hexagonal > bcc > simple cubic
bcc < simple cubic < fcc = hexagonal

Ans: fcc = hexagonal > bcc > simple cubic

6. The percentage of empty space in a body centred cubic arrangement is (approximately):

48
32
26
22
10

Ans: 32 ; Percentage of empty space = 1- packing efficiency.

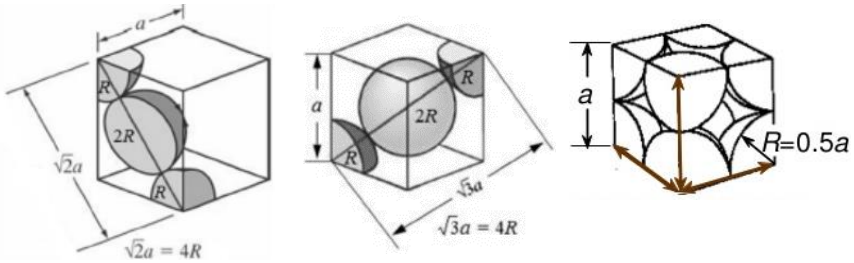
7. Effective number of atoms in a conventional unit cell of honey-comb lattice is:

0.5
1
2
3
6

Ans: 1 ; Explanation: Although the honey comb lattice is not a Bravais lattice, the conventional unit cell can never the less be defined. Each atom at the corner has contribution equal to 1/6 th of an atom. Hence the number of atoms is 1 per conventional cell.

8. The edge lengths of the unit cells in terms of the radius of spheres constituting fcc, bcc and simple cubic unit cells are respectively is:

2r√2 , 4r/√3 , 2r
2r√2 , 2r , 4r/√3
4r/√3 , 2r√2 , 2r
2r , 2r√2 , 4r/√3
2r , 4r/√3 , 2r√2

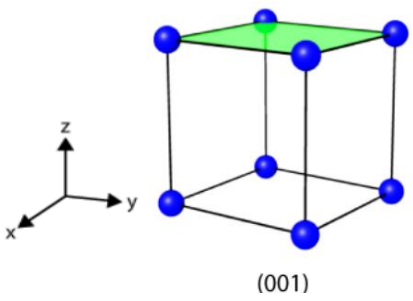


Ans: FCC: a=4r/√2 = 2r√2 ; BCC: a=4r/√3 ; SC: a=2r .

9. (001) is the plane of the cube & is (with z-axis in the vertical direction):

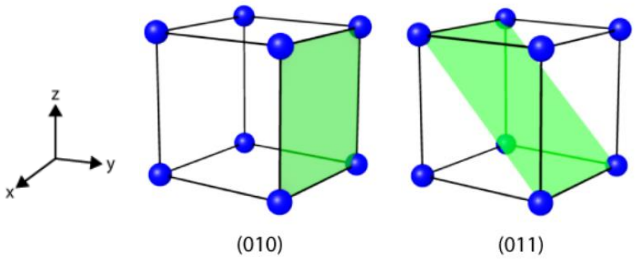
Horizontal and aligned with the xy-plane
Vertical and aligned with the xz-plane
Vertical and inclined to the xz-plane
Neither vertical and nor horizontal
Horizontal and parallel to the xy-plane

Ans: Horizontal and parallel to the xy-plane



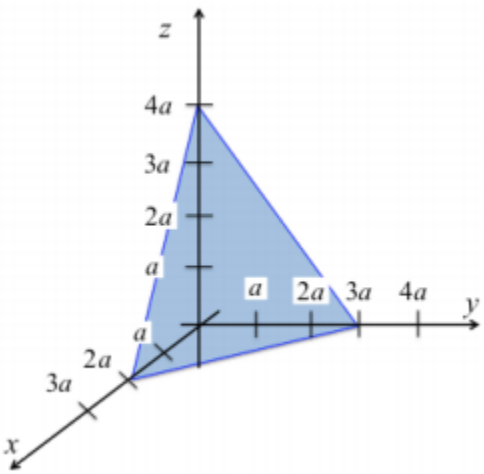
10. The direction on the line that results from the intersection of the planes (011) and (010) within a cubic crystal is:

[100]
[010]
[011]
[101]
[001]



Ans: The planes will cut at a line parallel to the x-axis. Hence the direction is [100]

11. Deduce the Miller indices for the plane shown in the figure:
(6 4 3)
(3 4 2)
(4 3 6)
(1 2 3)
(1 4 3)



Ans: (6 4 3) ; x-intercept 2a, y-intercept 3a, and z-intercept 4a ;
Intercepts in units of a: 2, 3, 4
Invert the intercepts: 1/2, 1/3, 1/4 ; Multiply by 12: 6, 4,3 => (6 4 3)

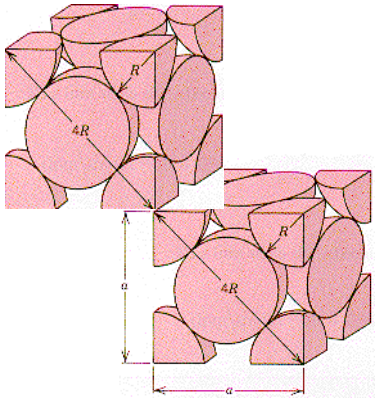
12. Coordination number for closest packed crystal structure in 3D is:

16
12
8
4
10

Ans: 12 . Explanation: In 3D, for both the hexagonal close packed and face centered cubic (FCC) structures, the coordination number is 12.

13. What is the coordination number of the crystal structure shown in the figure?

4
6
8
10
12

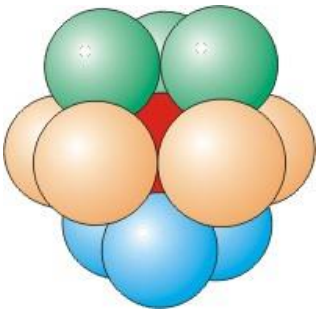


Ans: 12. Explanation: The structure shown is an FCC structure.

A. There are eight atoms, one atom each at the corner of the unit cell and one atom at the centre of each face.
B. For **<u>any corner atom of the unit cell</u>**, the nearest atoms are face-centred atoms.
C. Thus, considering a corner atom (say the top left corner atom in the figure) we get,

The coordination number for an FCC structure =
4 centre atoms below the horizonal plane of a corner atom
+ 4 centre atoms above the horizontal plane
+ 4 centre atoms on the horizonal plane =12 atoms

Hence, the coordination number for an FCC structure is 4 + 4 + 4 = 12

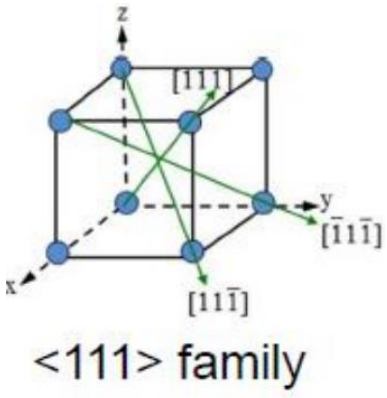


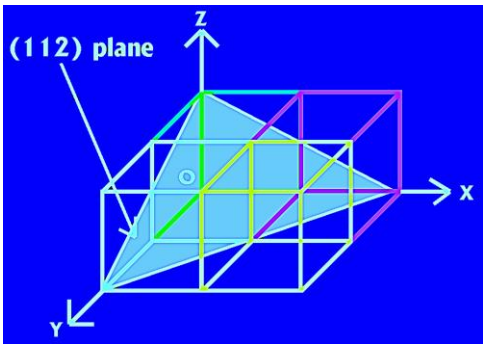
Alternatively, we may consider the structure as shown in the figure:

Each atom in a face-centered cubic unit cell has a coordination number of 12. The 12 particles, which make up the *coordination sphere* of the red particle lie in three planes.

The top and bottom planes each have three particles, while the plane in the middle contains the central particle and six others forming a belt around it.

14. A family of directions is represented by <111>. Which of the direction(s) in the family lie in the (112) plane?





$[111]$
$[1\bar{1}1]$
$[11\bar{1}]$
$[\bar{1}11]$
$[\bar{1}\bar{1}\bar{1}]$

Ans: $[11\bar{1}]$

The direction is given by the vector: $\vec{R} = a\,\hat{\imath} + b\,\hat{\jmath} - c\,\hat{k}$.
The (112) plane is given by the intercepts at 2a, 2b and c and is shown in the figure. Clearly the direction $[11\bar{1}]$ lie in the plane.

15. How many member directions are in the <110> family of directions?

6
8
10
12
24

Ans: 12. The members are:

$$[110],[\bar{1}10],[1\,\bar{1}0],[\bar{1}\,\bar{1}0],[101],[\bar{1}01],[10\,\bar{1}],[\bar{1}0\,\bar{1}],[011],[0\,\bar{1}1],[01\,\bar{1}],[0\,\bar{1}\,\bar{1}]$$

Total number of members: $6 \times 2 = 12$