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

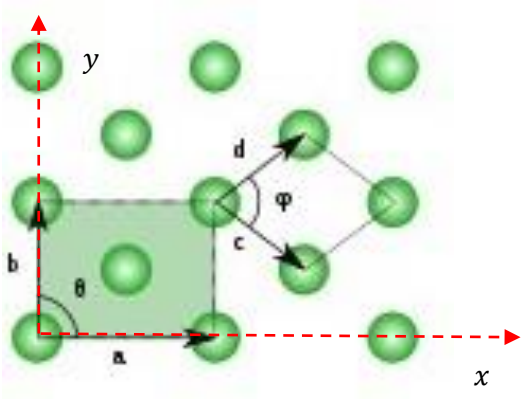
L15: Coordination numbers, characteristics of cubic structures, crystal directions, negative directions, family of crystal directions, crystal planes, Miller indices, family of planes.

1. The lattice vectors of a centered rectangular lattice in a conventional unit cell are $\vec{a} = a\hat{\imath}$, $\vec{b} = b\hat{\jmath}$. The primitive lattice vectors are:

$c = a\hat{\imath};\ d = b(\hat{\imath} + \hat{\jmath})$
$c = \hat{\imath}(a/2) - \hat{\jmath}(b/2);\ d = \hat{\imath}(a/2) + \hat{\jmath}(b/2)$
$c = \hat{\imath}(a/2);\ d = \hat{\imath}(a/2) + \hat{\jmath}(b/2)$
$c = a\hat{\imath};\ d = \hat{\imath}\left(a/\sqrt{2}\right) + \hat{\jmath}\left(b/\sqrt{2}\right)$
$c = \hat{\imath}a + \hat{\jmath}b;\ d = \hat{\imath}(a/2) - \hat{\jmath}(b/2)$

Ans: $= \hat{\imath}(a/2) - \hat{\jmath}(b/2);\ d = \hat{\imath}(a/2) + \hat{\jmath}(b/2)$. Explanation: This is evident from the figure as shown. Also the area covered by the cells with different lattice vectors are: $S = \left|\vec{c} \times \vec{d}\right|$

$\left|\vec{c} \times \vec{d}\right| = \left|(a\hat{\imath}) \times \left(b(\hat{\imath} + \hat{\jmath})\right)\right| = ab$
$\left|\vec{c} \times \vec{d}\right| = \left|\left(\hat{\imath}(a/2) - \hat{\jmath}(b/2)\right) \times \left(\hat{\imath}(a/2) + \hat{\jmath}(b/2)\right)\right| = (ab/4) + (ab/4) = ab/2$
$\left|\vec{c} \times \vec{d}\right| = \left|(\hat{\imath}a/2) \times \left(\hat{\imath}(a/2) + \hat{\jmath}(b/2)\right)\right| = ab/4$
$\left|\vec{c} \times \vec{d}\right| = \left|(\hat{\imath}a) \times \left(\hat{\imath}\left(a/\sqrt{2}\right) + \hat{\jmath}\left(b/\sqrt{2}\right)\right)\right| = ab/\sqrt{2}$
$\left|\vec{c} \times \vec{d}\right| = \left|(\hat{\imath}a + \hat{\jmath}b) \times \left(\hat{\imath}(a/2) - \hat{\jmath}(b/2)\right)\right| = |-ab/2 - ab/2| = ab$



Hence, we see that only for $c = \hat{\imath}(a/2) - \hat{\jmath}(b/2);\ d = \hat{\imath}(a/2) + \hat{\jmath}(b/2)$, we have the area of the unit cell equal to the half of the area of the conventional unit cell, as required.

2. What is the coordination number of a simple cubic structure?

4
6
8
2
12

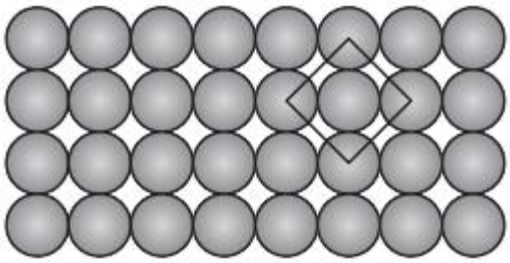
Ans: 6. Explanation: There are six nearest neighbouring atoms for every atom in a simple cubic (SC) unit cell i.e. every atom in a SC unit cell is surrounded by 6 other atoms.

3. Co-ordination number of a crystalline solid is:

Number of lattice points in a unit cell
Number of lattice points in a primitive unit cell
Number of nearest neighbours lattice points around any lattice point
Number of voids in a unit cell with lattice point having hard sphere basis
Number of void around a lattice point having hard sphere basis

Answer: Number of nearest neighbours lattice points around any lattice point

4. What is the coordination number in a square lattice?



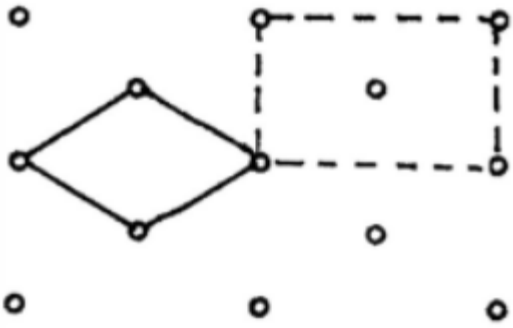
2
3
4
6
8

Ans: 4. Coordination number in a square closed packed structure in two dimensions is equal to 4 as shown in the figure to the right.

5. What is the coordination number of centered rectangular lattice in 2D?

2
4
6
8
12

Ans: 2. Explanation: Since $a \neq b$ for the centered rectangular lattice, we have the coordination number as 2, rather than 4.



6. What is the number of second nearest neighbours in the FCC lattice?

2
4
6
8
12

Ans: 6.

7. Packing efficiency of a crystal structure is the ratio of:

volume occupied by spherical atoms at lattice points within a unit cell to the total volume of the unit cell
volume occupied by spherical atoms at lattice points within a unit cell to that of the voids
total volume of the unit cell to the volume occupied by spherical atoms at lattice points
volume occupied by voids to that of the unit cell
volume occupied by voids to that of the spherical atoms at lattice points within a unit cell

Ans: volume occupied by spherical atoms at lattice points within a unit cell to the total volume of the unit cell.

8. Effective number of atoms in a simple cubic (SC) unit cell is equal to:

2
4
1
8
6

Ans: 1 ; Explanation: Total number of atoms at corners = 8 and each corner atom is shared by total 8-unit cells. Thus, effective number of atoms in an SC unit cell: 8 × 8⁄8 = 1.

9. HCP and BCC are called close-packed structures in 3D. Close packed structures have:
the highest packing efficiency
the highest void fraction
the highest density
the highest number of lattice points per conventional unit cell
all of the others mentioned

Ans: the highest packing efficiency.

10. The atomic packing fraction in a simple cubic unit cell is:

0.740
0.524
0.680
0.907
0.785

Ans: 0.524

11. Atomic radius in a BCC crystal structure (a is the lattice parameter) is:

a/2
a/4
a/√2
a√2/4
a√3/4

Ans: a√3/4

12. A family of directions is represented by:

(hkl)
<hkl>
{hkl}
[hkl]
(h,k,l)

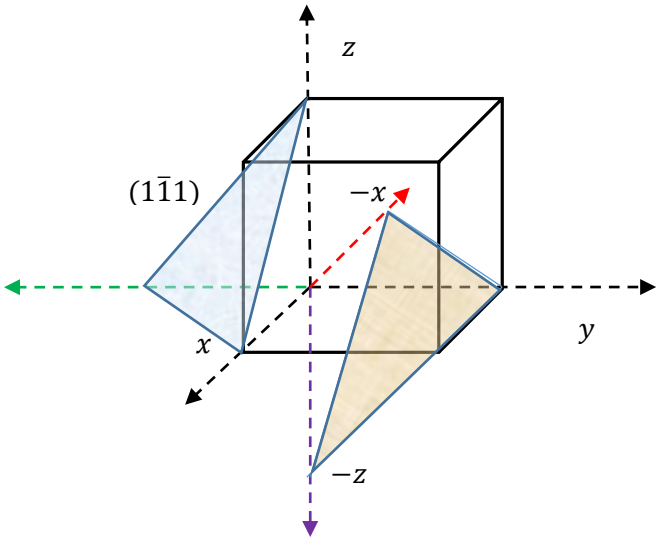
Ans: <hkl> ; Explanation: (hkl) and (h,k,l) represents crystal planes, {hkl} represents family of crystal planes, [hkl] represents crystal directions and finally <hkl> represents family of crystal directions

13. The plane $(\bar{1}1\bar{1})$ is parallel to:

$(1\bar{1}1)$
$(\bar{1}\bar{1}1)$
(111)
$(1\bar{1}1)$
$(1\bar{1}\bar{1})$

Ans: $(1\bar{1}1)$, Explanation: The plane $(\bar{1}1\bar{1})$ cuts the x- and z-axes at the negative sides. The intercepts with the axes may be (ignoring the scaling), -1, 1, -1 units:

Obviously, ***any multiple of the Miller indices will represent a parallel plane***.
Hence if we multiply by -1, we get the Miller indices of a parallel plane as: $(1\bar{1}1)$



14. The x-, y-, and z intercepts of a plane are 2,1, and 3. Its Miller Indices are:
(3 6 2)
(3 6 1)
(2 1 3)
(2 6 3)
(6 3 9)
Ans: (3 6 2)

15. Which plane is perpendicular to a $[1\bar{1}0]$ direction in cubic lattices?

(001)
$(\bar{1}01)$
$(01\bar{1})$
$(0\bar{1}1)$
$(1\bar{1}0)$

Ans: The plane given by $(1\bar{1}0)$. Explanation: In cubic lattice, the primitive lattice vectors are parallel to the axes. The key point here is that the direction $[hkl]$ Is perpendicular to the plane represented by the Miller indices (hkl).

This is because a direction ***within a plane given by*** $(\boldsymbol{hkl})$ ***may be taken as:*** $\overrightarrow{AB} = -\left(\frac{1}{h}\right)\hat{\imath} + \left(\frac{1}{k}\right)\hat{\jmath}$

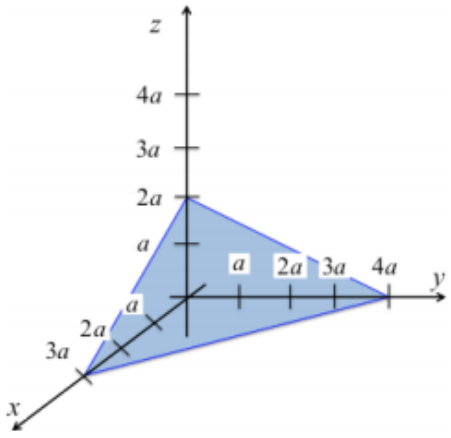
where we may take the coordinates in 3D of the points as:
$A \equiv \left(\frac{1}{h}, 0,0\right)$ $B \equiv \left(0, \frac{1}{k}, 0\right)$ and we have the result $\Delta\vec{r} = \overrightarrow{AB} = \vec{r}_B - \vec{r}_A$

Since the intercepts of the plane (hkl) are proportional to $\left(\frac{1}{h}\right)$, $\left(\frac{1}{k}\right)$ and $\left(\frac{1}{l}\right)$.
Hence the cosine of the angle between the directions given by $[hkl]$ and $[pqr] = [\frac{1}{h}\frac{1}{k}\ 0]$ is:

$$\cos\alpha = \frac{(ph + qk + rl)}{\sqrt{p^2 + q^2 + r^2}\sqrt{h^2 + k^2 + l^2}} = \frac{\left(-\frac{h}{h} + \frac{k}{k} + 0.l\right)}{\sqrt{p^2 + q^2 + r^2}\sqrt{h^2 + k^2 + l^2}} = 0$$

This result is specifically true for CUBIC LATTICES where the lattice vectors are parallel to the axes. For other lattices, this may not be true.

16. The Miller indices for the plane shown in the figure are:
(3 4 2)
(4 3 6)
(1 2 3)
(1 4 3)
(3 4 1)



Ans: (4 3 6)
Explanation: Intercepts:3a,4a,2a
Intercepts in units of a: 3, 4, 2
Invert the intercepts: 1/3, 1/4, 1/2
Multiply by 12: 4, 3,6
Put in parentheses since this is a specific plane: (4 3 6)