Syllabus for Test 07: L 16 , L 17 , L 18 (partial) :

L16: Review: Coordination number, crystal directions, family of crystal directions, crystal planes, Miller indices,
New Topics: Interplanar Spacing : Cubic system, Wigner-Seitz unit cells in 2D and 3D, Bragg's law, application of Bragg's law.

L17: Reciprocal Lattice in 3D, Properties of reciprocal lattice, reciprocal lattice vector, interplanar spacing and reciprocal lattice vector, interplanar spacing of Orthorhombic, Tetragonal, Cubic and Hexagonal system. reciprocal lattice of FCC and BCC lattice, reciprocal lattice in 1D and 2D.

L18: Problem on reciprocal lattice (Brillouin Zone not included)

1. The relationship d_{hkl} =a /sqrt(h^2 + k^2 + l^2) gives the interplanar spacing as a function of the Miller indices and the lattice parameter for

cubic lattice
orthorhombic lattice
tetragonal lattice
hexagonal lattice
triagonal lattice

Answer: cubic system

2. If ‘a’ is the length of an edge or side of hexagon in the hexagonal close pack lattice, the interplanar spacing of (101) planes is:

a/sqrt(2)
a/sqrt(4/3)
sqrt(24/41)*a
sqrt(73/24)*a
sqrt(8/35)*a

Answer: sqrt(24/41)*a Explanation: 1/d = sqrt(4 (h^2+k^2+hk)/(3a^2) + l^2/c^2)
For HCP structure we have c/a=sqrt(8/3)
Hence l^2/c^2 = (3/8)l^2/a^2 ; Hence we have: 1/d = sqrt(4 (1)/(3a^2) + (3/8)/a^2) = (1/a) sqrt(4/3 + 3/8) = (1/a) sqrt(32+9)/24) ;
=> d= a* sqrt(24/41)

3. The ratio of lattice parameters in an orthorhombic system is: a:b:c=1:2:3. The ratio of crystal plane separations d100 : d110 : d111 for the system is:

1: 2/sqrt(3) : 4/5
1: sqrt(3)/2 : 6/7
1: sqrt(5)/2 : 4/5
1: sqrt(7)/3 : 3/4
1: sqrt(5)/2 : 6/7

Answer: 1: sqrt(5)/2 : 6/7
Solution: 1/d100 = 1/a ;
1/d110 = sqrt(1/a^2 + 1/b^2) = (1/a)*sqrt(1+1/4)= 2/(sqrt(5)*a)
1/d111 = sqrt(1/a^2 + 1/b^2 + 1/c^2) = (1/a)*sqrt(1+1/4+1/9) = sqrt(49/36)*(1/a) = 7/(6a)
=> d100 : d110 : d111 = 1: sqrt(5)/2 : 6/7

4. A lattice is characterized by the following **primitive lattice** vectors:

$\vec{a}_1 = 2(\hat{\imath} + \hat{\jmath});\ \ \vec{a}_2 = 2(\hat{\jmath} + \hat{k});\ \vec{a}_3 = 2(\hat{k} + \hat{\imath})$

The reciprocal lattice of the above lattice is a:

FCC lattice with cube edge length 1
FCC lattice with cube edge length 2
BCC lattice with cube edge length 1
BCC lattice with cube edge length 1/2
BCC lattice with cube edge length 2

Answer: BCC lattice width cube edge length 1/2

Explanation: The primitive lattice vectors are for the FCC lattice with unit edge length:

$$\vec{a}_1 = \left(\frac{a}{2}\right)(\hat{y} + \hat{z})$$
$$\vec{a}_2 = \left(\frac{a}{2}\right)(\hat{z} + \hat{x})$$
$$\vec{a}_3 = \left(\frac{a}{2}\right)(\hat{x} + \hat{y})$$

Comparing we get $a/2 = 2 \ \Rightarrow a = 4$
The reciprocal lattice vectors are:

$$\vec{a}_1^* = \left(\frac{1}{a}\right)(\hat{z} + \hat{y} - \hat{x})$$
$$\vec{a}_2^* = \left(\frac{1}{a}\right)(\hat{x} + \hat{z} - \hat{y})$$
$$\vec{a}_3^* = \left(\frac{1}{a}\right)(\hat{y} + \hat{x} - \hat{z})$$

Now, the conventional unit cell in BCC lattice with **edge length *l*** has the ***primitive lattice vectors***:

$$\vec{a} = \left(\frac{l}{2}\right)(\hat{z} + \hat{y} - \hat{x})$$
$$\vec{b} = \left(\frac{l}{2}\right)(\hat{x} + \hat{z} - \hat{y})$$
$$\vec{c} = \left(\frac{l}{2}\right)(\hat{y} + \hat{x} - \hat{z})$$

Hence comparing we get:

$$\frac{l}{2} = \frac{1}{a} = \frac{1}{4} \Rightarrow l = \frac{1}{2}$$

5. A lattice is characterized by the following primitive lattice vectors:

$$\vec{a}_1 = \frac{a}{2}(\hat{\imath} + \hat{\jmath});\ \ \vec{a}_2 = \frac{a}{2}(\hat{\jmath} + \hat{k});\ \ \vec{a}_3 = \frac{a}{2}(\hat{k} + \hat{\imath})$$

The volume of the primitive cell of the reciprocal lattice is:

1/a^3
2/a^3
1/(2a^3)
4/a^3
1/(4a^3)
Answer: 4/a^3

Solution: The primitive reciprocal lattice vectors **calculated from** the primitive direct lattice vectors are:

$$\vec{a} = \left(\frac{1}{a}\right)(\hat{z} + \hat{y} - \hat{x})$$
$$\vec{b} = \left(\frac{1}{a}\right)(\hat{x} + \hat{z} - \hat{y})$$
$$\vec{c} = \left(\frac{1}{a}\right)(\hat{y} + \hat{x} - \hat{z})$$

The volume of the **primitive unit cell in the reciprocal lattice** is:

$$V_{RL} = \left|\vec{a}\,.\left(\vec{b} \times \vec{c}\right)\right| = \frac{1}{a^3}\left|(\hat{z} + \hat{y} - \hat{x}).\left((\hat{x} + \hat{z} - \hat{y}) \times (\hat{y} + \hat{x} - \hat{z})\right)\right|$$
$$\Rightarrow V_{RL} = \frac{1}{a^3}\,|(\hat{z} + \hat{y} - \hat{x}).(\hat{z} + \hat{y} - \hat{x} + \hat{y} + \hat{z} + \hat{x})|$$
$$\Rightarrow V_{RL} = \frac{1}{a^3}\,|(\hat{z} + \hat{y} - \hat{x}).(2\,\hat{z} + 2\,\hat{y})\,| = \frac{1}{a^3}|2 + 2| = \frac{4}{a^3}$$

Hence the volume is $V_{RL} = 4/a^3$

6. The interplanar spacing of (220) planes of a Face-centered cubic (FCC) structure is 1.7458 Å. The lattice constant is:

4.938 Å
2.458 Å
0.877 Å
5.262 Å
0.617 Å

Answer: 4.938 Å, Explanation: $d = a/\sqrt{h^2 + k^2 + l^2}$ => $a = d\sqrt{h^2 + k^2 + l^2} = 1.7458 \times (2^2 + 2^2 + 0)^{1/2}$ Å =4.938 Å

7. The primitive lattice vectors of the triangular (or hexagonal) lattice in 2D are:

$$\vec{a} = \alpha\,\hat{x}, \vec{b} = \left(\frac{\alpha}{2}\right)\left(\hat{x} + \sqrt{3}\hat{y}\right)$$

In the reciprocal lattice, the “volume” of the primitive unit cell is:

alpha^2 sqrt(3)/2
sqrt(3)/alpha^2
sqrt(3)/(2 alpha^2)
1/alpha^2
2/(sqrt(3) alpha^2)

Answer: 2/(sqrt(3) alpha^2) . Solution: The reciprocal lattice vectors are:

$$\vec{a}^* = \left(\frac{1}{\alpha}\right)\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right)$$
$$\vec{b}^* = \frac{2}{\alpha\sqrt{3}}\,\hat{y}$$

The “volume” of the primitive unit cell in the reciprocal lattice is:

$$A_{RL} = \left|\vec{a}^* \times \vec{b}^*\right| = \frac{2}{\sqrt{3}}\,\frac{1}{\alpha^2}\left|\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right) \times \hat{y}\right| = \frac{2}{\sqrt{3}\alpha^2}$$

NOTE: The “volume” of the unit cell in the direct lattice is:

$$A_{DL} = \left|\alpha\,\hat{x} \times \left(\frac{\alpha}{2}\right)(\hat{x} + \sqrt{3}\hat{y})\right| = \frac{\alpha^2\sqrt{3}}{2}$$

Hence, we have as expected:

$$A_{RL} \times A_{DL} = 1$$

8.Consider X-ray diffraction of wavelength lambda=0.7a where a is the lattice parameter in crystal with a face centred cubic lattice. The lattice plane for which there is no diffraction peak is:

(100)
(111)
(201)
(112)
(311)

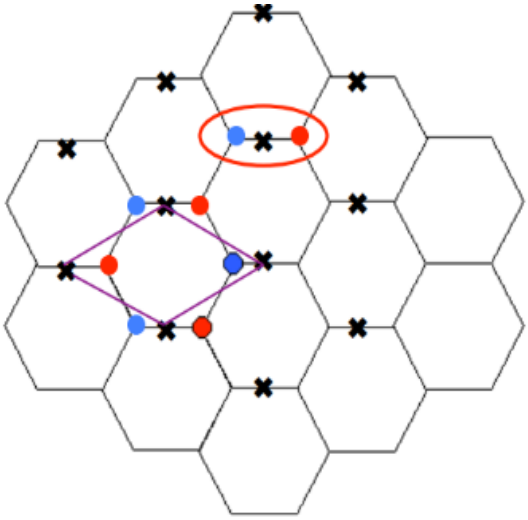
Answer: (311)

For FCC, d=a/sqrt(h^2 +k^2 + l^2)
From Bragg's law: 2d_{hkl} sin(theta) = n \lambda => sin(theta) = n \lambda /(2d_{hkl})

For (311) plane: sin(theta) = n \lambda sqrt(11)/(2*a) = n 0.7*(3.31)/2 >1

Hence there will be no diffraction peak. For all other planes: for n=1
(hkl) = (100) : sqrt(h^2+k^2+l^2)/2 = 0.7/2 <1 ;
(hkl) = (111) : sqrt(h^2+k^2+l^2)/2 =0.7* sqrt(3)/2 <1 ;
(hkl) = (201) : sqrt(h^2+k^2+l^2)/2 = 0.7* sqrt(5)/2 <1 ;
(hkl) = (112) : sqrt(h^2+k^2+l^2)/2 = 0.7* sqrt(6)/2 <1 ;

For higher n values there will be no peak, if for n=1 there is no peak.



9. Graphene has a honeycomb lattice structure which is not a Bravais lattice. To which class of Bravais lattice and with how many atom basis the honeycomb lattice may be considered?

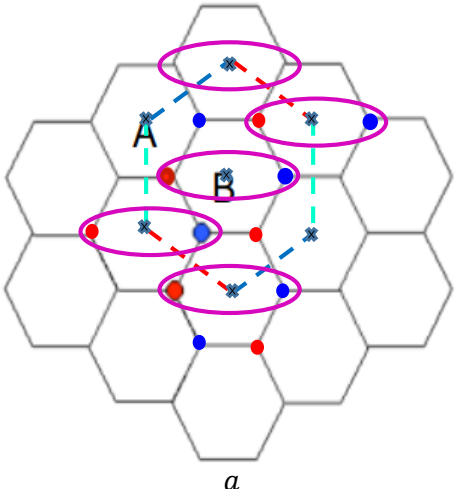
Triangular; 3 atom basis
Oblique; 2 atom basis
Square; 3 atom basis
Orthorhombic; 2 atom basis
Hexagonal; 4 atom basis

Answer: Oblique or monoclinic lattice with 2 atom basis.

It can also be thought of as a triangular or hexagonal lattice with ***2 atom basis***:
The length of the edges of the hexagon would be:

$$\frac{\left(\frac{b}{2}\right)}{\left(\frac{a}{2}\right)} = \tan 60^\circ = \sqrt{3} \Rightarrow b = a\sqrt{3}$$

$$\left(\frac{b}{2}\right)^2 = a^2 - \left(\frac{a}{2}\right)^2 = \frac{a^2 3}{4} \Rightarrow b = a\sqrt{3}$$



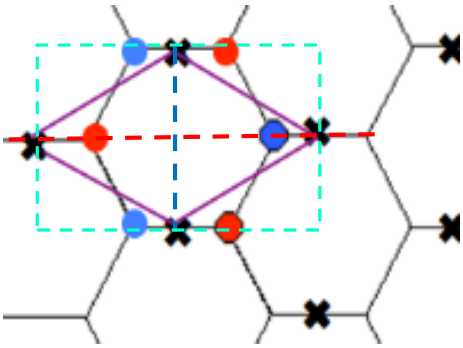
[NOTE: Each unit cell in the hexagonal Bravais lattice would have:
6x(1/3) +1 =3 lattice points per cell
and 6 atoms per cell.

Area of the hexagonal Bravais lattice:

$$A_{HEX} = b^2 \frac{3\sqrt{3}}{2} = 3a^2 \frac{3\sqrt{3}}{2} = \frac{9\sqrt{3}}{2} a^2 = 3A_{HCM}$$

where $A_{HCM} = a^2 3\sqrt{3}/2$ is the area of the unit cell of the honeycomb lattice.

Area covered by each atom =$A_{HCM}/2$ which can also be found from $A_{HEX}/6$

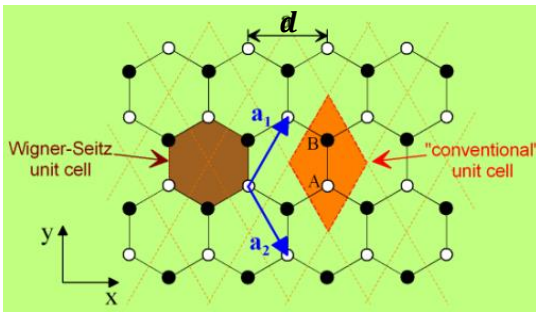


Also note that: For the oblique lattice unit cell, area of the monoclinic or oblique lattice is:

$$A_{Obli} = \frac{1}{2}(2a + a) \times d = \frac{3}{2}a \times a\tan(60°) = \frac{3\sqrt{3}}{2}a^2$$
$$\Rightarrow A_{obli} = A_{HCM}$$

There are of course 2 atoms per cell in the oblique/monoclinic unit cell.]

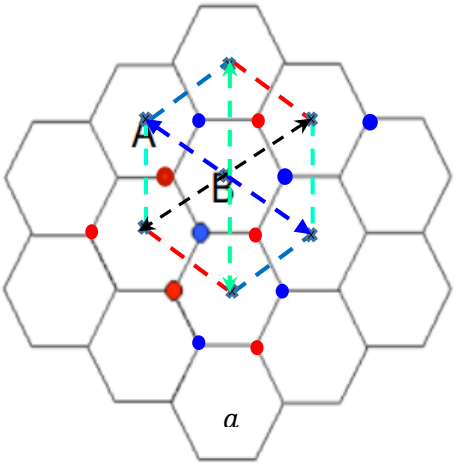
10. Graphene has a non-Bravais lattice structure known as the honeycomb lattice. It may be thought of as a hexagonal Bravais lattice in 2D with three lattice points per hexagonal cell. The area of the Wigner-Seitz unit cell of Graphene has the area (when a is the length of a side of the honeycomb hexagon):



3 sqrt(3) a^2
3 sqrt(3) a^2 /2
a^2 /sqrt(3)
a^2/(3 sqrt(3))
a^2/3

Answer: 3 sqrt(3) a^2 /2
Explanation: The Wigner-Seitz unit cell may be found from the hexagonal Bravais lattice using the given prescription:

A. Connect one lattice point to all lattice points nearest to it.
B. Draw perpendicular bisector lines.
C. The cell created by the perpendicular bisectors is the Wigner-Seitz unit cell.

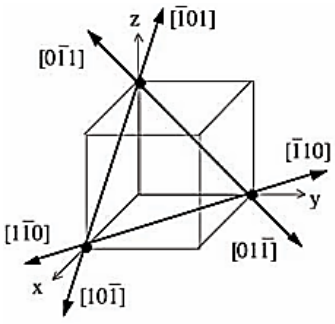


The Wigner-Seitz unit cell is seen to be the same as the hexagon in the honeycomb lattice.

Hence the area of the Wigner-Seitz unit cell is =$A_{HCM} = 3\sqrt{3}a^2/2$

Note that, the Wigner-Seitz unit cell has exactly one lattice point (at the center) per cell. Since the honeycomb lattice is a non-Bravais lattice, the WS unit cell has 2 atoms/cell.

11. Review question: Consider a (111) plane in an FCC structure. How many different [110]-type
directions lie in this (111) plane?



1
3
4
6
12
Answer: 6
There are six [110]-type directions in the (111) plane. Their indices are:
[10-1] , [-101] , [-110] , [1-10] , [0-11] , [01-1]