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

$$\frac{1}{d_{hkl}^2} = \left[\frac{h^2+k^2}{a^2}\right] + \left[\frac{l^2}{c^2}\right]$$

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: tetragonal lattice

2. If 'a' is the length of an edge or side of hexagon in the hexagonal close pack lattice, then the interplanar spacing d of (111) planes is:

a/sqrt(2)	$a/\sqrt{2}$
a/sqrt(8/35)	$a/\sqrt{8/35}$
sqrt(24/41)*a	$a\sqrt{24/41}$
sqrt(35/24)*a	$a\sqrt{35/24}$
sqrt(8/35)*a	$a\sqrt{8/35}$

Answer: $a/\sqrt{8/35}$ Explanation: The formula for the interplanar spacing in hexagonal lattice is:

$$\frac{1}{d_{hkl}} = \sqrt{\frac{4(h^2+k^2+hk)}{3a^2} + \frac{l^2}{c^2}}$$

For hexagonal close pack or HCP structure, we have $c/a = \sqrt{8/3}$; Hence, $l^2/c^2 = (3/8)l^2/a^2$

Hence we have:

$$\frac{1}{d} = \sqrt{4\,(3)/(3a^2) + \;(3/8)\;1/a^2} \;=\; (1/a)\sqrt{4+3/8} \;=\; (1/a)\sqrt{35/8}$$

$$\Rightarrow d = a\sqrt{35/8}$$

i.e.

$$d = a\,/\sqrt{8/35}$$

3. The ratio d100 : d110 : d111 for a FCC structure is:

1: 1/sqrt(3) : 2/sqrt(2)	$1{:}\,1/\sqrt{3} : 2/\sqrt{2}$
1: 1/sqrt(2) : 1/sqrt(3)	$1{:}\,1/\sqrt{2} : 1/\sqrt{3}$
1: sqrt(2) : sqrt(3)	$1{:}\,\sqrt{2} : \sqrt{3}$
1: sqrt(3) : sqrt(2)	$1{:}\,\sqrt{3} : \sqrt{2}$
1: sqrt(6)/2 : sqrt(5)	$1{:}\,\sqrt{6}/2 : \sqrt{5}$

Answer: $1{:}\,1/\sqrt{2} : 1/\sqrt{3}$

Solution: The formula for the interplanar spacing in cubic system is:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Hence,

$d100 \ = \ a = a/\sqrt{1+0+0}$; $d110 = \ a/\sqrt{1+1+0} \ = a/\sqrt{2}$; $d111 \ = \ a/\sqrt{3}$

$$d100{:}\,d110{:}\,d111 = a{:}\frac{a}{\sqrt{2}}{:}\frac{a}{\sqrt{3}} = 1{:}\,1/\sqrt{2} : 1/\sqrt{3}$$

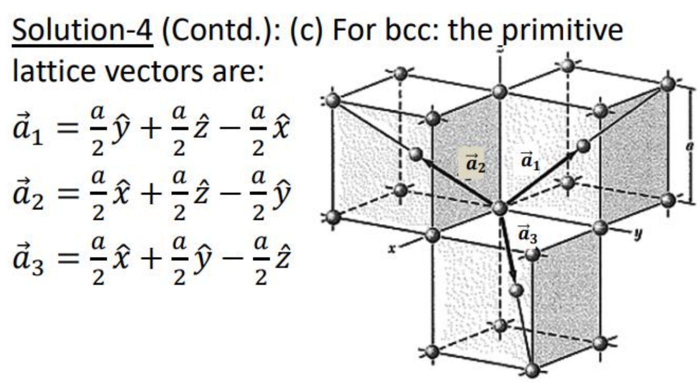
4. A lattice is characterized by the following **primitive lattice** vectors:

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

The reciprocal lattice of the above lattice is a:

FCC lattice with cube edge length 1/2
FCC lattice with cube edge length 2
FCC lattice with cube edge length 1
BCC lattice with cube edge length 1/2
BCC lattice with cube edge length 1/4

Answer: FCC lattice width cube edge length 1/2



Explanation: The primitive lattice vectors for the BCC lattice with edge length l are:

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

Comparing we get $l/2 = 2 \ \Rightarrow l = 4$

Now, we know that the reciprocal lattice vectors for the following set of vectors:

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

are:

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

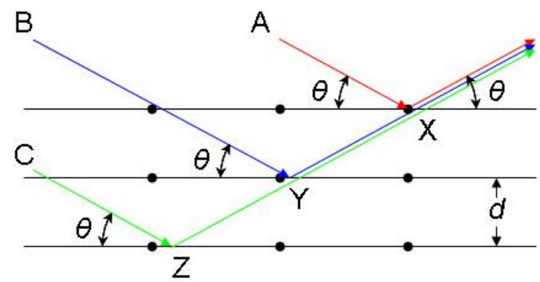
Which are the primitive lattice vectors in the FCC structure with lattice parameter a.

Comparing: $l/2 = 1/a$ => $a = \frac{2}{l} = \frac{2}{4} = \frac{1}{2}$

5. Find the wavelength for second order reflection if the angle of incidence is $30°$ and interplanar spacing is d?

d/4
d/3
d
d/2
d/sqrt(2)
Answer: d/2 ; Explanation: Bragg's law states:
"The law states that when the x-ray is incident onto a crystal surface, its angle of incidence, θ, will reflect back with a same angle of scattering, θ. And, when the path difference, d is equal to a whole number, n, of wavelength, a constructive interference will occur" i.e.:

$$2d\sin\theta = n\lambda$$



Here, $2d\sin\theta = 2d\sin(30°) = 2d\ (1/2) = d = n\lambda$
Hence, for second order we get, $\lambda = d/2$

6. What is the minimum interplanar spacing required for Bragg's diffraction if λ is the wavelength of the radiation?

λ/4
2λ
λ
λ/2
sqrt(2) λ

Answer: λ/2
From Bragg's law: $2d\sin\theta = n\lambda \Rightarrow d = n\lambda/(2\sin\theta)$

For interplanar spacing to be the minimum, $\sin(\theta)$ must be a maximum and the order of diffraction n must be the minimum.

Hence we get, $d_{min} = n_{max}\lambda/(2\sin\theta)_{max} = 1.\lambda/(2.1) = \lambda/2$

7. The vector direction normal to the plane (110) in a cubic system is:
[001]
[010]
[100]
[011]
[110]

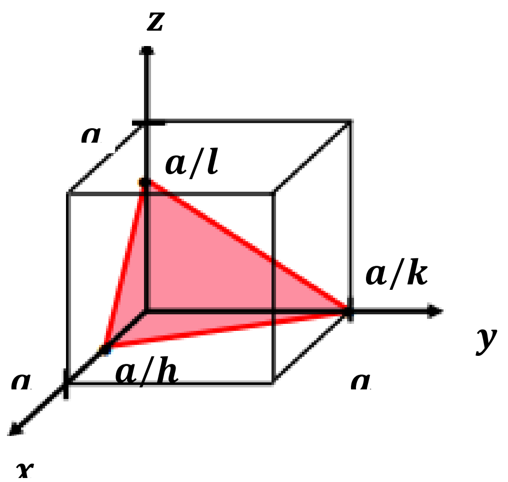
Ans: [110]

Explanation: In the cubic system, a plane (hkl) has intercepts on the x-, y- and z-axis proportional to $1/h$, $1/k$ and $1/l$, respectively.
For cubic lattice system, the crystal axes are along the orthogonal x-, y- and z- axes. A plane (hkl) will have intercepts along the x-, y- and z-axes as:

$$\frac{a}{h}, \quad \frac{a}{k}, \quad \frac{a}{l}$$

A line going through the points $(a/h, 0,0)$ and $(0, a/k, 0)$ will be along the vector:

$$\overrightarrow{AB} = \left(\frac{a}{h}\right)\hat{\imath} - \left(\frac{a}{k}\right)\hat{\jmath}$$



The line representing the direction $[hkl]$ has the vector along it as:

$$\vec{r}_{hkl} = h\,\hat{\imath} + k\,\hat{\jmath} + l\,\hat{k} = h\,\hat{x} + k\,\hat{y} + l\,\hat{z}$$

Hence, the dot product of $\overrightarrow{AB}$ and $\vec{r}_{hkl}$ is:

$$\overrightarrow{AB}\,.\vec{r}_{hkl} = \left(\frac{a}{h}\right)h - \left(\frac{a}{k}\right)k + 0.l = 0$$

Hence for a cubic system, the plane (hkl) is perpendicular to the direction $[hkl]$

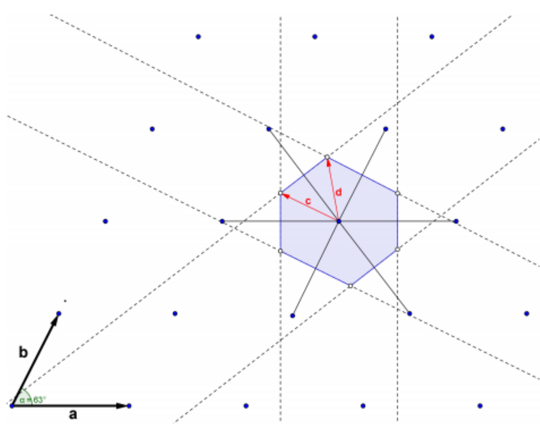
8. In 2D there are five possible classes of Possible Bravais lattice. The Wigner-Seitz unit cells of these are of the shape:

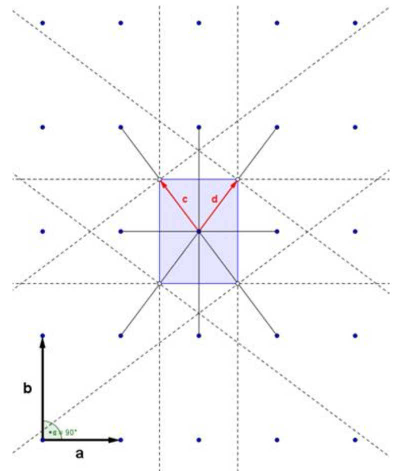
Rectangular, triangular
Hexagonal, triangular
Rectangular, hexagonal
Square, triangular
Pentagonal, hexagonal, triangular

Answer: Rectangular, hexagonal

Explanation: The shape of the Wigner-Seitz unit cells for the five Bravais lattice classes in 2D are shown below:

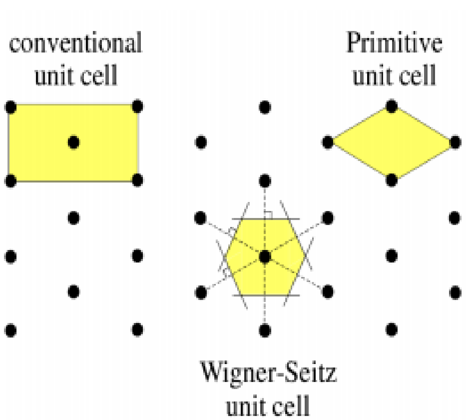
A. **Oblique lattice**: WS cell is a hexagon, although not a regular hexagon:

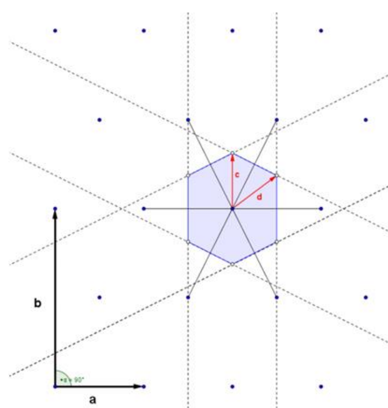


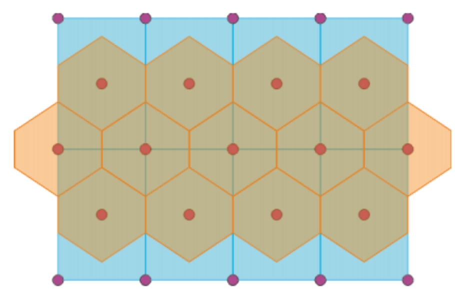


B. **Rectangular lattice**: The WS unit cell is a rectangular cell shown in the above figure.

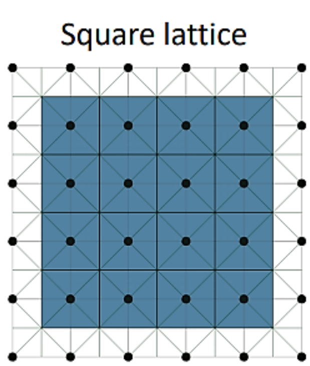
C. **Centered rectangular lattice**: WS unit cell is a hexagonal cell (although not a regular hexagon)

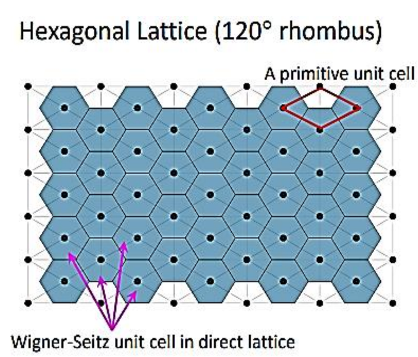






D. **Tetragonal (Square) lattice**: The WS unit cell is a square which is a type of rectangle.





E. **Hexagonal lattice**: The WS unit cell is a regular hexagon.

9. Graphene has a honeycomb lattice structure which is not a Bravais lattice. Let the length of each side of the hexagon be a. The Wigner-Seitz unit cell in the reciprocal lattice has an "area":

3 sqrt(3) a^2 /2	$3\sqrt{3}\,a^2/2$
2/(3 sqrt(3) a^2)	$2/(3\sqrt{3}\,a^2)$
2/(3 a^2)	$2/(3\,a^2)$
2a^2/sqrt(3)	$2a^2/\sqrt{3}$
2/(sqrt(3) a^2)	$2/(\sqrt{3}a^2)$

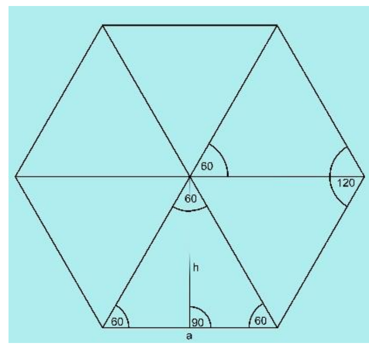
Ans: $2/(3\sqrt{3}\,a^2)$

Solution: The problem is not so difficult if one recalls that:

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

i.e. the product of the "volume" in the direct lattice and that in the reciprocal lattice is unity. Here the "volume" implies area in 2D.

Also recall that, the Wigner-Seitz unit cell in the direct lattice is the hexagonal cell of the honeycomb lattice (**cf. practice questions for test 07**).



The area of the Wigner-Seitz unit cell in the direct lattice is = area of a regular hexagon of side a:

$$A_{DL} = A_{WS-DL} = 3\,\sqrt{3}\,a^2/2$$

$$A_{hex} = 6a\left(\frac{1}{2}\right)h = 3aa \times sin\,(60^\circ) = 3\sqrt{3}\,a^2/2$$

Hence, area of the Wigner-Seitz unit cell of the reciprocal lattice of the honeycomb lattice is:

$$A_{RL} = \frac{1}{A_{DL}} = 2/(3\sqrt{3}\,a^2)$$

<u>Proof of the statement</u>:

In 2D, the reciprocal lattice is defined as:

$$\vec{a}^* = \frac{\vec{b}\times\hat{n}}{|\vec{a}\times\vec{b}|}\,;\vec{b}^* = \frac{\hat{n}\times\vec{a}}{|\vec{a}\times\vec{b}|}$$

where the unit vector perpendicular to $\vec{a}$ and $\vec{b}$ is :

$$\hat{n} = \frac{\vec{a}\times\vec{b}}{|\vec{a}\times\vec{b}|}$$

Area of the unit cell in the reciprocal lattice is:

$$A_{RL} = |\vec{a}^* \times \vec{b}^*| = \frac{1}{|\vec{a}\times\vec{b}|^2}\,|(\vec{b}\times\hat{n})\times(\hat{n}\times\vec{a})| = \frac{1}{A_{DL}^2}\,|(\vec{b}\times\hat{n})\times(\hat{n}\times\vec{a})|$$

Now, using the vector triple product rule: $\vec{a}\times(\vec{b}\times\vec{c}) = \vec{b}\,(\vec{a}\,.\,\vec{c}) - \vec{c}\,(\vec{a}\,.\vec{b})$, we get,

$$\vec{b}\times\hat{n} = \vec{b}\times\frac{(\vec{a}\times\vec{b})}{|\vec{a}\times\vec{b}|} = \frac{[\vec{a}\,(\vec{b}.\vec{b}) - \vec{b}\,(\vec{a}.\vec{b})]}{|\vec{a}\times\vec{b}|} = \frac{1}{A_{DL}}[\vec{a}\,(\vec{b}.\vec{b}) - \vec{b}\,(\vec{a}.\vec{b})]$$

$$\hat{n}\times\vec{a} = \frac{(\vec{a}\times\vec{b})}{|\vec{a}\times\vec{b}|}\times\vec{a} = -\vec{a}\,\times\frac{(\vec{a}\times\vec{b})}{|\vec{a}\times\vec{b}|} = -\frac{[\vec{a}\,(\vec{a}.\vec{b}) - \vec{b}\,(\vec{a}.\vec{a})]}{|\vec{a}\times\vec{b}|} = -\frac{1}{A_{DL}}\,[\vec{a}\,(\vec{a}.\vec{b}) - \vec{b}\,(\vec{a}.\vec{a})]$$

$$(\vec{b}\times\hat{n})\times(\hat{n}\times\vec{a}) = -\frac{1}{A_{DL}^2}[\vec{a}\,(\vec{b}.\vec{b}) - \vec{b}\,(\vec{a}.\vec{b})]\times[\vec{a}\,(\vec{a}.\vec{b}) - \vec{b}\,(\vec{a}.\vec{a})]$$

$$\Rightarrow (\vec{b}\times\hat{n})\times(\hat{n}\times\vec{a}) = -\frac{1}{A_{DL}^2}\left\{-(\vec{a}\times\vec{b})(b^2a^2) - (\vec{b}\times\vec{a})(\vec{a}.\vec{b})^2\right\} = \frac{1}{A_{DL}^2}(\hat{n}\,|\vec{a}\times\vec{b}|)\left(a^2b^2 - (\vec{a}.\vec{b})^2\right)$$

$$\Rightarrow (\vec{b}\times\hat{n})\times(\hat{n}\times\vec{a}) = \frac{1}{A_{DL}^2}\,\hat{n}\,A_{DL}a^2b^2(1-\cos^2(\theta)) = \frac{\hat{n}}{A_{DL}}\,a^2b^2\sin^2\theta = \frac{\hat{n}}{A_{DL}}A_{DL}^2 = \hat{n}A_{DL}$$

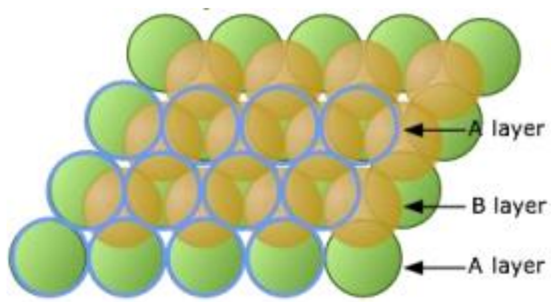
where $A_{DL} = |\vec{a}\times\vec{b}| = ab\sin\theta$ and the angle between $\vec{a}$ and $\vec{b}$ is θ.
Hence we get,

$$A_{RL} = \frac{1}{A_{DL}^2}\,|(\vec{b}\times\hat{n})\times(\hat{n}\times\vec{a})| = \frac{1}{A_{DL}^2}\,|\hat{n}A_{DL}| = \frac{1}{A_{DL}}$$ (Proved)

10. Stacking sequence in hexagonal close packed (HCP) structure is?

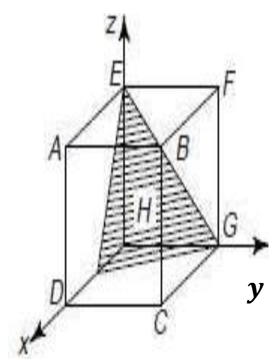
AABAABAA
ABABABAB
ABCABCABC
AABBAABBAA
ABBBABBBA

Answer: ABABABAB



ABA hexagonal close packed

11. What are the Miller indices of a plane that makes intercepts with a, b and c axes equal to 1Å, 2Å and 3Å in a tetragonal crystal with c/a ratio of 1.5?



(436)
(123)
(321)
(211)
(231)

Ans: (211)
Solution: In the tetragonal crystal, the lattice vectors are of length a, b and c where $a = b$ and $c/a = 1.5$.
Thus in terms of the lattice vectors, the intercepts are: $1Å/a$, $2Å/a$ and $3Å/c$
But we have $c/a = 3/2$ which gives $c = 3a/2$ and in terms of the lattice parameter a , the intercepts are:

$$1Å/a,\ 2Å/a \text{ and } 3Å/c = (3Å)2/3a = 2Å/a$$

Hence the Miller indices are found by multiplication of 2 with

$$\left(\frac{1}{1},\frac{1}{2},\frac{1}{2}\right)\to(211)$$

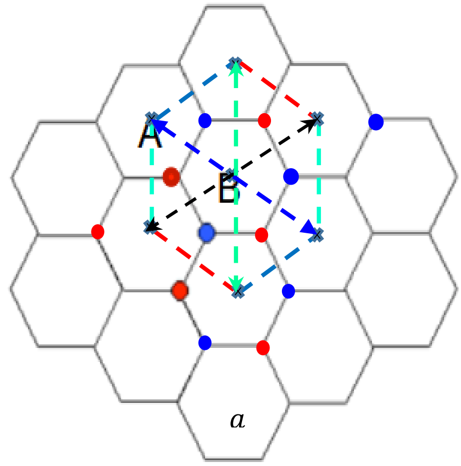
12. The interplanar spacing of (210) planes of a Face-centered cubic (BCC) structure is 1.458 Å. The lattice constant is:

3.260 Å
2.458 Å
0.877 Å
5.262 Å
0.617 Å

Answer: 3.260 Å, Explanation: $d = a/\sqrt{h^2+k^2+l^2}$ => $a = d\sqrt{h^2+k^2+l^2} = 1.458\times(2^2+1^2+0)^{1/2}$ Å =3.260 Å

13. 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 spanned by the reciprocal lattice vectors to form a unit cell is (when a is the length of a side of the honeycomb hexagon):

2/(sqrt(243)a^2)	$2/(\sqrt{243}a^2)$
3 sqrt(3) a^2	$3\sqrt{3}a^2$
3 sqrt(3)/(2 a^2)	$3\sqrt{3}/(2a^2)$
sqrt(3)/a^2	$\sqrt{3}/a^2$
a^2/(3 sqrt(3))	$a^2/(3\sqrt{3})$



Answer: $2/(\sqrt{243}a^2)$=2/(sqrt(243)a^2)
Solution: First of all, the "area" of the unit cell in the reciprocal lattice will have a dimension of $[1/L^2]$.

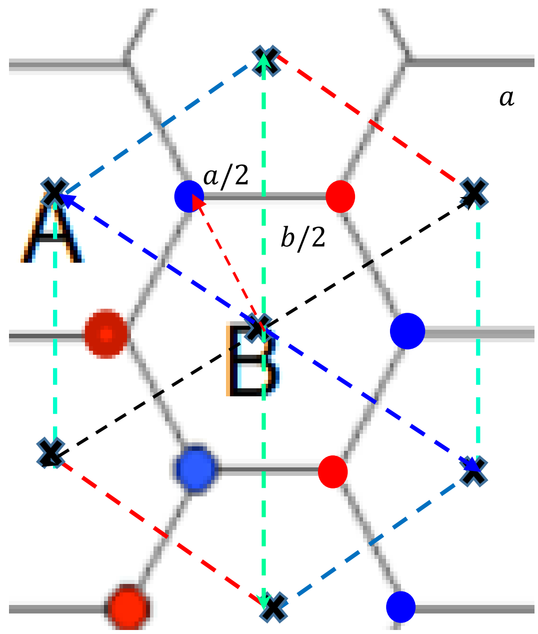
Hence a few of the choices will be ruled out. The remaining choices are:

$$2/(\sqrt{243}a^2),\ 3\sqrt{3}/(2a^2) \quad \text{, and } \sqrt{3}/a^2$$

The conventional unit cell is a bigger hexagonal cell with side length of each side equal to $AB = b$, where

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

There are six atoms and three lattice points per unit cell.



The area of the conventional unit cell is thus that of a regular hexagon of side length b i.e.

$$A_{HEX} = 3\sqrt{3}\,b^2/2$$

The area of the unit cell spanned by the reciprocal lattice is then found from the relation:

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

Thus

$$A_{RL} = \frac{1}{A_{DL}} = 2/(3\sqrt{3}b^2) = 2/(3\sqrt{3}a^2 3) = 2/(\sqrt{3 \times 81}a^2)$$