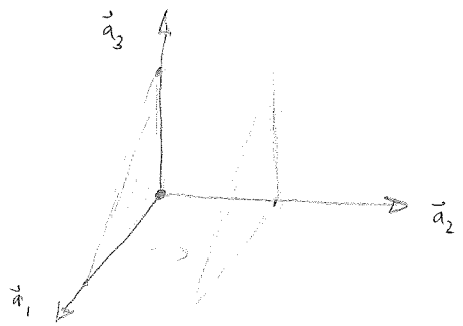
HOMEWORK #1 SOLUTIONS

1a) Plane intersects at $1\vec{a}_1, 0\vec{a}_2, 4\vec{a}_3$ $\quad 1, 0, 4$



you can move it to the right, s.t. it intersects at

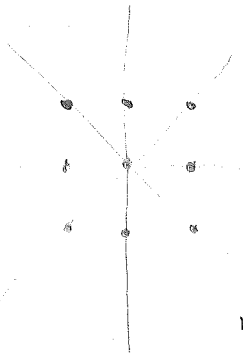
$\vec{a}_1$: ∞
$\vec{a}_2$: 1 $\quad \rightarrow (hkl) = \underline{(0, 1, 0)}$
$\vec{a}_3$: ∞

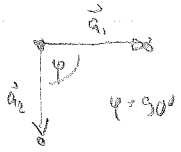
b)

$\vec{a}_1$:	1		$\frac{1}{1}$	12
$\vec{a}_2$:	-3	$\xrightarrow{(\cdot)^{-1}}$	$-\frac{1}{3}$	$\rightarrow$ -4
$\vec{a}_3$:	4		$\frac{1}{4}$	3

$\Rightarrow (hkl) = \underline{(12, \bar{4}, 3)}$

2) a) Square Lattice $\quad |\vec{a}_1| = |\vec{a}_2|$ $\quad \varphi = 90°$



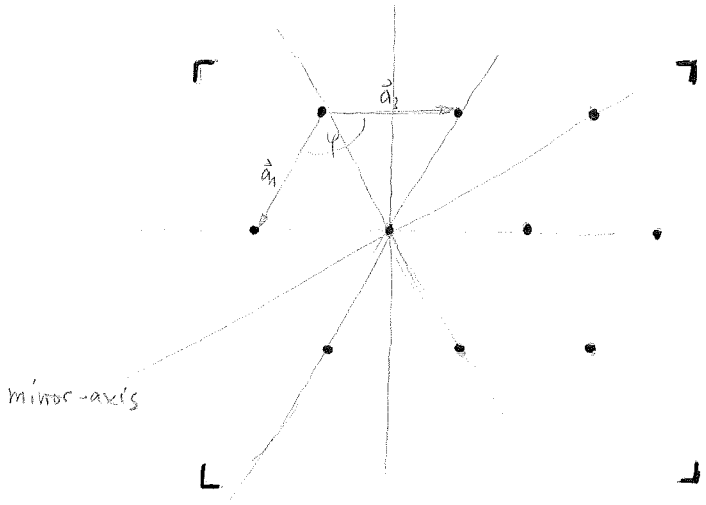


rotation-symmetries : $2\pi, \pi, \frac{\pi}{2}$

mirror symmetrie

n :	1	2	4	$(\frac{2\pi}{n})$

b) Hexagonal lattice $|\vec{a}_1| = |\vec{a}_2|$ $\varphi = 120°$

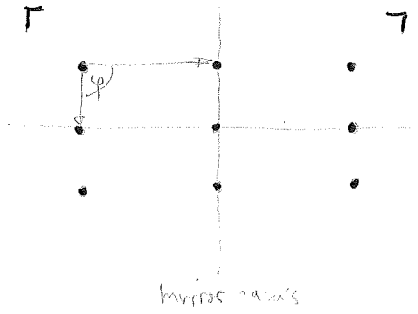


mirror-Symmetrie

rotation Symmetries:

2π,	$\frac{2\pi}{2}$,	$\frac{2\pi}{3}$,	$\frac{2\pi}{6}$
1	2	3	6

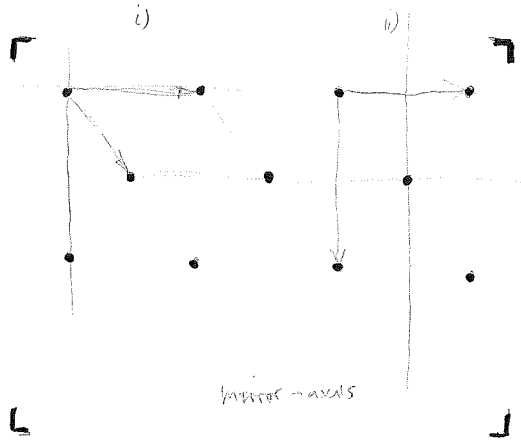
c) $|\vec{a}_1| \neq |\vec{a}_2|$ $\varphi = 90°$



rotation-symmetrie:

2π,	$\frac{2}{2}\pi$
1	2

d) i)



rotation-symmetrie:

2π,	$\frac{2}{2}\pi$
1	2

3

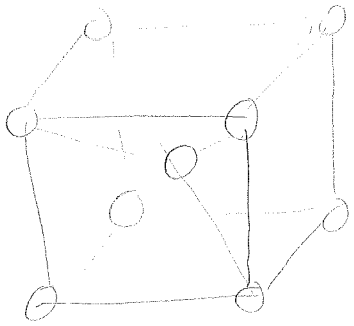
Ionic radia: Cs^+ : 167 pm

Cl^- : 181 pm

Na^+ : 102 pm

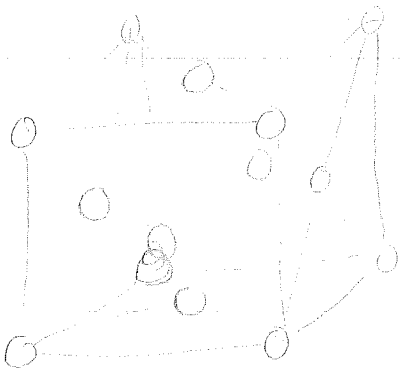
$r_{Cs^+} \approx r_{Cl^-}$ $\quad 2 \cdot r_{Na^+} \approx r_{Cl^-}$

CsCl



the difference in the atomic radii causes the different structures

NaCl



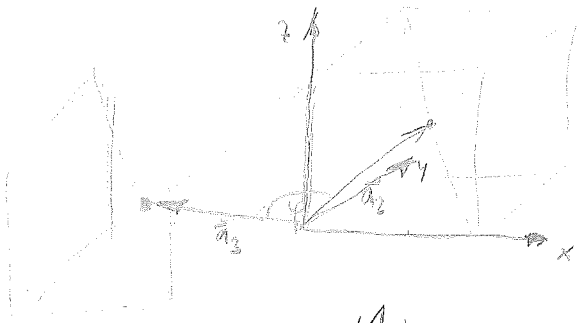
b) in hcp - two Na^+ ions would be nearest neighbours.

1) Tetrahedral angles:

angles between the tetrahedral bonds of diamond

=

angles between body-diagonals of a cube



$$\vec{a}_2 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \qquad |\vec{a}_2| = \frac{1}{2}\cdot\sqrt{1^2+1^2+1^2} = \frac{\sqrt{3}}{2}$$

$$\vec{a}_2 \cdot \vec{a}_3 = \frac{1}{4}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{4}(-1-1+1) = -\frac{1}{4}$$

$$\vec{a}_3 = \begin{pmatrix} -\frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} \qquad |\vec{a}_3| = \frac{1}{2}\sqrt{(-1)^2+(-1)^2+1^2} = \frac{\sqrt{3}}{2}$$

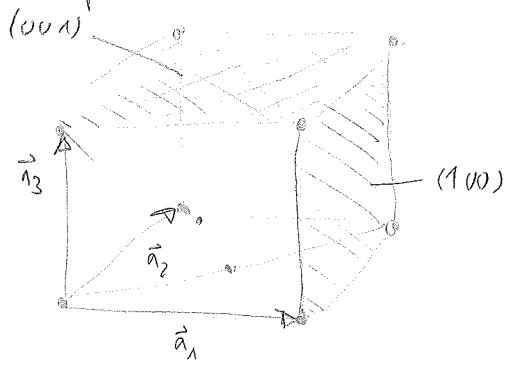
$$|\vec{a}_2 \cdot \vec{a}_3| = |\vec{a}_2|\cdot|\vec{a}_3|\cdot\cos\varphi \quad \Rightarrow \quad \varphi = \arccos\left(\frac{\vec{a}_2\cdot\vec{a}_3}{|\vec{a}_2|\cdot|\vec{a}_3|}\right)$$

$$= \arccos\left(\frac{\vec{a}_2\cdot\vec{a}_3}{\frac{3}{4}}\right)$$

$$= \arccos\left(-\frac{1}{3}\right) = 109{,}5°$$

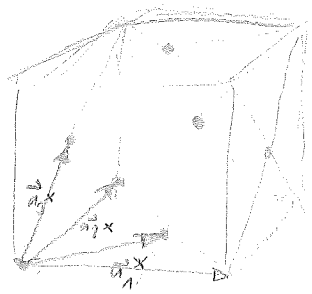
2) Indices of planes: planes (100) and (001) in a fcc lattice

indices refere to conventional cube



plane: (100) → $\frac{1}{n_i}$: 1, ∞, ∞ → 1, 0, 0 $\quad 1\vec{a}_1, 0\vec{a}_2, 0\vec{a}_3$

(001) → . . . → 0, 0, 1 $\quad 0\vec{a}_1, 0\vec{a}_2, 1\vec{a}_3$



primitive axis

$$\vec{a}_1^* : \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} : \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$\vec{a}_2^* : \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \qquad \vec{a}_3^* : \frac{1}{2}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

the (100) plane has intersection $\vec{a}_1^* : 1$

$\vec{a}_2^* : 1$ → (110)

$\vec{a}_3^* : \infty$

the (001) plane:

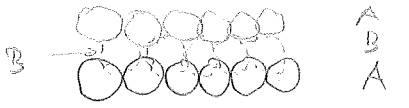
$\vec{a}_1^* : \infty$

$\vec{a}_2^* : 1$ → (011)

$\vec{a}_3^* : 1$

3) Hcp-structure Show $\frac{c}{a} = \left(\frac{8}{3}\right)^{\frac{1}{2}} = \sqrt{\frac{8}{3}} \approx 1.633$

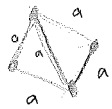
the hcp layers are in the order ABAB... (compare Kittel)



if you look from above:

the B layer is positioned so that it fills up the holes

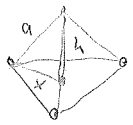
this forms a tetrahedron with an atom at each point



the height of the tetrahedron is $\frac{1}{2}$ of the height of the primitive cell c

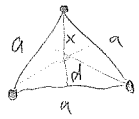
$$c = 2 \cdot h$$

since the atoms touch (dense package) $a = 2 \cdot r$ r: atomic radius



pythagoras: $x^2 + h^2 = a^2$

$$\Rightarrow h = \sqrt{a^2 - x^2}$$



$(x+d)^2 + (\frac{1}{2}a)^2 = a^2$

$$\Rightarrow x + d = \sqrt{\frac{3}{4}}\, a$$

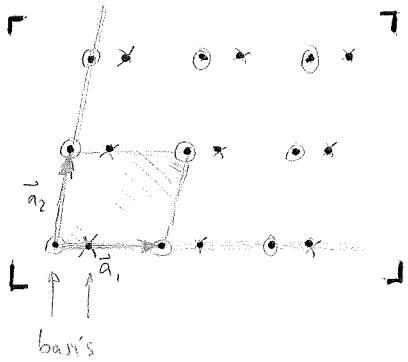
$\boxed{x = 2d}$ (relation for triangle with the same angles)

$$\Rightarrow x = \sqrt{\frac{1}{3}}\, a$$

$$\Rightarrow h = \sqrt{a^2 - x^2} = \sqrt{\frac{2}{3}}\, a \qquad c = 2 \cdot h = \sqrt{\frac{8}{3}}\, a$$

$$\Rightarrow \underline{\underline{\frac{c}{a} = \sqrt{\frac{8}{3}}}}$$

5. Sketch in on the figure: a set of lattice points, a choice of primitive axes, a primitive cell and the basis of atoms associated with a lattice point



basis: $(0\,0)$
$(\frac{1}{3}\,0)$

Problem 1: plane indices (hkl) a plane parallel to the (hkl)-plane has the intersection with the $\vec{a}_1, \vec{a}_2, \vec{a}_3$-axis at

$$\left(\frac{1}{h}, \frac{1}{k}, \frac{1}{l}\right)$$

Chapter 2

with the 3 points $\frac{1}{h}\vec{a}_1$, $\frac{1}{k}\vec{a}_2$ and $\frac{1}{l}\vec{a}_3$ you can write the plane in the form

$$\vec{x} = \vec{s} + r\cdot\vec{u} + s\cdot\vec{v}$$

with $\vec{x}$ being a point on the plane and

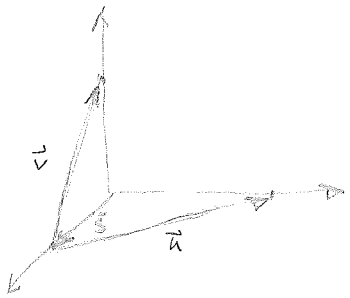
$r, s \in \mathbb{R}$

$\vec{s}$: basis point of the plane

$\vec{u}, \vec{v}$: two different directions on the plane

$(\vec{u}\cdot\vec{v} \neq 0)$

given the 3 points you can calculate $\vec{s}, \vec{u}, \vec{v}$



choose $\vec{s} = \frac{1}{h}\vec{a}_1$

$\vec{u} = \frac{1}{k}\vec{a}_2 - \vec{s} = \frac{1}{k}\vec{a}_2 - \frac{1}{h}\vec{a}_1$

$\vec{v} = \frac{1}{l}\vec{a}_3 - \vec{s} = \frac{1}{l}\vec{a}_3 - \frac{1}{h}\vec{a}_1$

the reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is perpendicular to the plane (hkl) if $\vec{G}\vec{u} = 0$ and $\vec{G}\vec{v} = 0$

relation between lattice vectors $\vec{a}_i$ and reciprocal lattice vectors $\vec{b}_i$

$$\vec{a}_i\vec{b}_j = 2\pi\delta_{ij}$$

① $\vec{G}\vec{u} = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\cdot\left(\frac{1}{k}\vec{a}_2 - \frac{1}{h}\vec{a}_1\right)$

$= \frac{h}{k}\vec{b}_1\vec{a}_2 + \vec{b}_2\vec{a}_2 + \frac{l}{k}\vec{b}_3\vec{a}_2 - \vec{b}_1\vec{a}_1 - \frac{k}{h}\vec{b}_2\vec{a}_1 - \frac{l}{h}\vec{b}_3\vec{a}_1 = 2\pi - 2\pi = 0$

($\frac{h}{k}\vec{b}_1\vec{a}_2 = 0$, $\vec{b}_2\vec{a}_2 = 2\pi$, $\frac{l}{k}\vec{b}_3\vec{a}_2 = 0$, $-\vec{b}_1\vec{a}_1 = -2\pi$, $-\frac{k}{h}\vec{b}_2\vec{a}_1 = 0$, $-\frac{l}{h}\vec{b}_3\vec{a}_1 = 0$)

② $\vec{G}\cdot\vec{v} = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\left(\frac{1}{l}\vec{a}_3 - \frac{1}{h}\vec{a}_1\right) = \ldots = 2\pi - 2\pi = 0$

$\Rightarrow$ $\vec{G}$ is perpendicular to the (hkl)-plane

b) Since $\vec{G} \perp$ (hkl)-plane you can describe the plane with the following expression

$$\left| \frac{\vec{G}}{|\vec{G}|} \cdot (\vec{x} - \vec{s}) \right| = d$$

with $\vec{s}$ being a point on the hkl-plane

d: distance of the point $\vec{x}$ to the plane

$\forall \vec{x}$ with $d=0 \rightarrow \vec{x}$ is on the plane

to calculate the distance of two adjacent parallel planes you just have to choose two points, one on the first plane ($\vec{s}$) and one on the second plane ($\vec{x}$)

to make the calculation more easy I choose $\vec{s} = \frac{1}{h}\vec{a}_1$

$\vec{x} = 2 \cdot \frac{1}{h}\vec{a}_1$

$$d = \left| \frac{\vec{G}}{|\vec{G}|} \cdot \left(2\frac{1}{h}\vec{a}_1 - \frac{1}{h}\vec{a}_1\right) \right| = \left| \frac{\vec{G} \cdot \frac{1}{h}\vec{a}_1}{|\vec{G}|} \right| = \frac{2\pi}{|\vec{G}|}$$

c) for a simple cubic lattice: $\vec{a}_1 = a\hat{e}_x = a\begin{pmatrix}1\\0\\0\end{pmatrix}$ $\vec{a}_2 = a\hat{e}_y = a\begin{pmatrix}0\\1\\0\end{pmatrix}$ $\vec{a}_3 = a\hat{e}_z = a\begin{pmatrix}0\\0\\1\end{pmatrix}$

the volume of the cell is $V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = a^3$

$\Rightarrow$ reciprocal lattice vectors: $\vec{b}_1 = \frac{2\pi}{a^3}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a}(\hat{e}_2 \times \hat{e}_3) = \frac{2\pi}{a}\hat{e}_1$

$\vec{b}_2 = \frac{2\pi}{a}\hat{e}_2$

$\vec{b}_3 = \frac{2\pi}{a}\hat{e}_3$

$d(hkl) = \frac{2\pi}{|\vec{G}|}$ (a) $\qquad \vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

$|\vec{G}| = \frac{2\pi}{a}\sqrt{h^2 + k^2 + l^2}$

$\Rightarrow d^2 = \frac{4\pi^2}{\frac{4\pi^2}{a^2}(h^2+k^2+l^2)} = \boxed{\frac{a^2}{h^2+k^2+l^2}}$

Problem 2: Hexagonal Space lattice

$$\hat{a}_1 = \frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y$$

$$\hat{a}_2 = -\frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y$$

$$\hat{a}_3 = c \hat{e}_z$$

a) the volume of the cell is $V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$

$$= \left| \left(\frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y\right) \left[\left(-\frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y\right) \times (c \hat{e}_z) \right] \right|$$

$$= a^2 c \left| \left(\frac{\sqrt{3}}{2} \hat{e}_x + \frac{1}{2} \hat{e}_y\right) \left[\underbrace{\left(-\frac{\sqrt{3}}{2} \hat{e}_x \times \hat{e}_z\right)}_{= -\hat{e}_y} + \underbrace{\frac{1}{2} \hat{e}_y \times \hat{e}_z}_{= \hat{e}_x} \right] \right|$$

$$= a^2 c \left| \frac{1}{2} \frac{\sqrt{3}}{2} + \frac{1}{2} \frac{\sqrt{3}}{2} \right| = \frac{\sqrt{3}}{2} a^2 c = \underline{(3^{1/2}/2)\, a^2 c}$$

b) primitive translations:

$$\vec{b}_1 = \frac{2\pi}{V} (\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{V} \left(\left(-\frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y\right) \times (c \hat{e}_z) \right)$$

$$= \frac{2\pi}{V} ac \left(\frac{\sqrt{3}}{2} \hat{e}_y + \frac{1}{2} \hat{e}_x \right) = \frac{2\pi}{\frac{\sqrt{3}}{2} a^2 c} ac \left(\frac{\sqrt{3}}{2} \hat{e}_y + \frac{1}{2} \hat{e}_x \right) = \underline{\frac{2\pi}{\sqrt{3} a} \hat{e}_x + \frac{2\pi}{a} \hat{e}_y}$$

$$\vec{b}_2 = \frac{2\pi}{V} (\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{V} \left(c \hat{e}_z \times \left(\frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y\right) \right) = \frac{2\pi}{V} ac \left(\frac{\sqrt{3}}{2} \hat{e}_y - \frac{1}{2} \hat{e}_x \right)$$

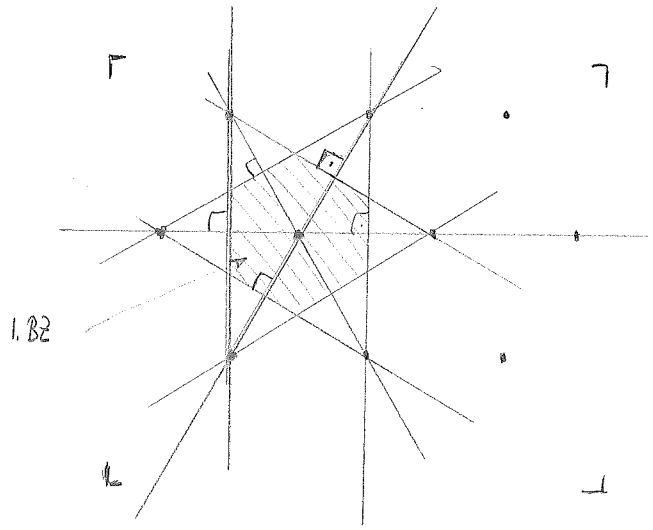
$$= \underline{-\frac{2\pi}{\sqrt{3} a} \hat{e}_x + \frac{2\pi}{a} \hat{e}_y}$$

$$\vec{b}_3 = \frac{2\pi}{V} (\vec{a}_1 \times \vec{a}_2) = \frac{2\pi}{V} \left(\left(\frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y\right) \times \left(-\frac{\sqrt{3}}{2} a \hat{e}_x + \frac{a}{2} \hat{e}_y\right) \right)$$

$$= \frac{2\pi}{V} a^2 \left(-\frac{3}{4} \underbrace{\hat{e}_x \times \hat{e}_x}_{=0} + \frac{\sqrt{3}}{4} \underbrace{\hat{e}_x \times \hat{e}_y}_{=\hat{e}_z} + \frac{\sqrt{3}}{4} \underbrace{\hat{e}_y \times \hat{e}_x}_{=-\hat{e}_z} + \frac{1}{4} \underbrace{\hat{e}_y \times \hat{e}_y}_{=0} \right)$$

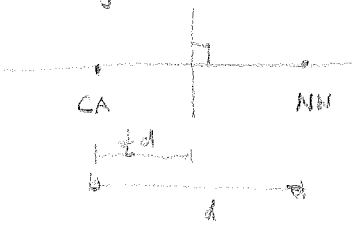
$$= \frac{2\pi}{V} a^2 \frac{\sqrt{3}}{2} \hat{e}_z = \underline{\frac{2\pi}{c} \hat{e}_z}$$

c) the reciprocal lattice of an hexagonal lattice is also hexagonal



hexagonal lattice

Notice! You construct the 1. BZ by connecting the centre atom with its nearest neighbors and then drawing the perpendicular line at the middle of the connecting line



If is just a coincidence that the perpendicular line crosses two nearest neighbors. This is just the case for a hexagonal lattice