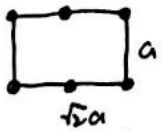
1.1 (a) $\Omega_c = \vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})$

$\vec{a_2} \times \vec{a_3} = \frac{a^2}{4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^2}{4}(\hat{x}+\hat{y}-\hat{z})$

So $\Omega_c = \frac{a^3}{8} \times (1+1) = \frac{a^3}{4}$

(b) (100) Plane : $n = \frac{\frac{1}{4}\times 4 + 1}{a^2} = \frac{2}{a^2}$

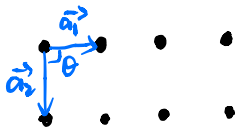
(110) plane : $n = \frac{\frac{1}{4}\times 4 + \frac{1}{2}\times 2}{\sqrt{2}a^2} = \frac{\sqrt{2}}{a^2}$



(111) plane : $n = \frac{\frac{1}{6}\times 3 + \frac{1}{2}\times 3}{\frac{\sqrt{3}}{4}\times(\sqrt{2}a)^2} = \frac{4\sqrt{3}}{3a^2}$

Thus, the (111) plane has the highest atom number densities.

(c)

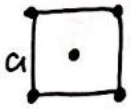


It is a rectangular lattice with a basis of one atom sits at (0,0).

$|\vec{a_1}| = \frac{\sqrt{2}}{2}a$, $|\vec{a_2}| = a$, $\theta = 90°$

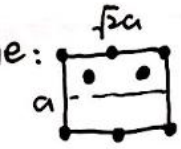
(d)

(100) Plane :



$n = \frac{\frac{1}{4}\times 4 + 1}{a^2} = \frac{2}{a^2}$

(110) plane :



$n = \frac{\frac{1}{4}\times 4 + \frac{1}{2}\times 2 + 2}{\sqrt{2}a^2} = \frac{2\sqrt{2}}{a^2}$

(111) Plane :

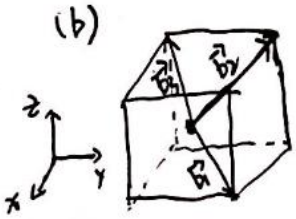
$n = \frac{\frac{1}{6}\times 3 + \frac{1}{2}\times 3}{\frac{\sqrt{3}}{4}(\sqrt{2}a)^2} = \frac{4}{\sqrt{3}a^2}$

1.2 (a) $\vec{b_1} = 2\pi \frac{\vec{a_2} \times \vec{a_3}}{\Omega_c} = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$

$\vec{b_2} = 2\pi \frac{\vec{a_3} \times \vec{a_1}}{\Omega_c} = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$

$\vec{b_3} = 2\pi \frac{\vec{a_1} \times \vec{a_2}}{\Omega_c} = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$

(b)



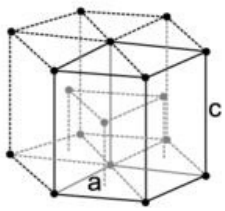
So the reciprocal lattice is a body-centered cubic lattice

(c) The volume of primitive unit cell : $\Omega_R = \vec{b_1} \cdot (\vec{b_2} \times \vec{b_3}) = \frac{8\pi^3}{a^3}(1\,1\,-1)\cdot(2\,2\,0)$

$= \frac{32\pi^3}{a^3}$

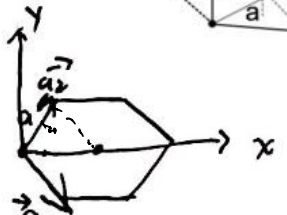
(d) $\Omega_R \cdot \Omega_c = (2\pi)^3$

1.3 (a) The lattice parameters of the conventional unit cell are:



$a=b\neq c$, $\alpha=90°$, $\beta=90°$, $\gamma=120°$

The primitive cell of hcp lattice is:



$\vec{a}_1=\frac{a}{2}\hat{x}-\frac{\sqrt{3}a}{2}\hat{y}$, $\vec{a}_2=\frac{a}{2}\hat{x}+\frac{\sqrt{3}}{2}a\hat{y}$, $\vec{a}_3=c\hat{z}$

with two atoms in the cell located at (000), $(\frac{1}{3},\frac{2}{3},\frac{1}{2})$ which is $\vec{r}=\frac{1}{3}\vec{a}_1+\frac{2}{3}\vec{a}_2+\frac{1}{2}\vec{a}_3$.

(b) atom number density: $n=\dfrac{12\times\frac{1}{6}+2\times\frac{1}{2}+3}{\frac{\sqrt{3}}{4}a^2\times 6\times c}=\dfrac{6}{\frac{\sqrt{3}}{4}\times 0.2662^2\times 6\times 0.495}$

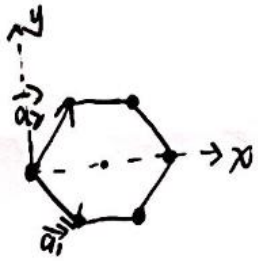
$=65.94$ atoms/nm^3

$=6.594\times10^{28}$ atoms/m^3

(c) mass density $\rho=\dfrac{(12\times\frac{1}{6}+2\times\frac{1}{2}+3)\times 65.38}{\frac{3\sqrt{3}}{2}\times 0.2662^2\times 0.495\times 6.02\times10^{23}}=7.16$ g/cm^3

$=7160$ kg/m^3

1.4



$\vec{a}_1=\frac{a}{2}(\hat{x}-\sqrt{3}\hat{y})$

$\vec{a}_2=\frac{a}{2}(\hat{x}+\sqrt{3}\hat{y})$

$\vec{a}_3=c\hat{z}$

$\vec{b}_1=2\pi\cdot\dfrac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}=\frac{2\pi}{a}(\hat{x}-\frac{\sqrt{3}}{3}\hat{y})$

$\vec{b}_2=2\pi\cdot\dfrac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}=\frac{2\pi}{a}(\hat{x}+\frac{\sqrt{3}}{3}\hat{y})$

$\vec{b}_3=2\pi\cdot\dfrac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}=\frac{2\pi}{c}\hat{z}$

∴ The reciprocal lattice structure is hexagonal lattice.

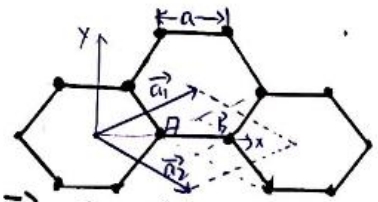
Since $|\vec{b}_1|=|\vec{b}_2|=\frac{4\pi}{a\sqrt{3}}$, $\cos\langle\vec{b}_1,\vec{b}_2\rangle=\frac{1}{2}$, $\langle\vec{b}_1,\vec{b}_2\rangle=60°$

$V_R=\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)=\dfrac{16\pi^3}{\sqrt{3}a^2c}$

$V_\Omega=\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)=\dfrac{\sqrt{3}a^2c}{2}$

So, $V_R\cdot V_\Omega=(2\pi)^3$

1.5 (a)



The 2D structure of graphene is a hexagnol lattice with two atoms associated to with each lattice point. One atom at (0,0), the other atom is at $(\frac{a}{\sqrt{3}}, \frac{a}{\sqrt{3}})$, which means $\vec{r} = \frac{a}{\sqrt{3}}(\vec{a_1} + \vec{a_2})$

(b) $\vec{a_1} = (2a\cos 30^\circ \cos 30^\circ)\hat{x} + (2a\cos 30^\circ \sin 30^\circ)\hat{y} = \frac{\sqrt{3}a}{2}(\sqrt{3}\hat{x} + \hat{y})$

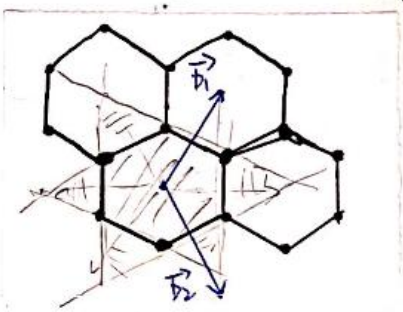
$\vec{a_2} = (2a\cos 30^\circ \cos 30^\circ)\hat{x} - (2a\cos 30^\circ \sin 30^\circ)\hat{y} = \frac{\sqrt{3}a}{2}(\sqrt{3}\hat{x} - \hat{y})$

area $= \frac{\sqrt{3}}{4}(2a\cos 30^\circ)^2 \times 2 = \frac{3\sqrt{3}}{2}a^2$

(c) let $\vec{a_3} = \hat{z}$

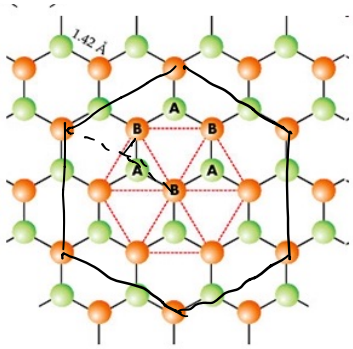
$$\vec{b_1} = \frac{2\pi}{\Omega_c}(\vec{a_2} \times \vec{a_3}) = \frac{2\pi}{\frac{3\sqrt{3}}{2}a^2}\begin{vmatrix} x & y & z \\ \frac{3a}{2} & -\frac{\sqrt{3}a}{2} & 0 \\ 0 & 0 & 1 \end{vmatrix} = \frac{2\pi}{a}\left(-\frac{1}{3}\hat{x} - \frac{\sqrt{3}}{3}\hat{y}\right)$$

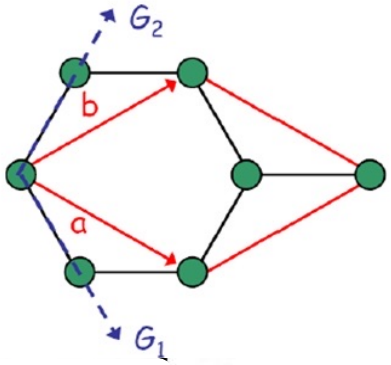
$$\vec{b_2} = \frac{2\pi}{\Omega_c}(\vec{a_3} \times \vec{a_1}) = \frac{2\pi}{\frac{3\sqrt{3}}{2}a^2}\begin{vmatrix} x & y & z \\ 0 & 0 & 1 \\ \frac{3a}{2} & \frac{\sqrt{3}a}{2} & 0 \end{vmatrix} = \frac{2\pi}{a}\left(-\frac{1}{3}\hat{x} + \frac{\sqrt{3}}{3}\hat{y}\right)$$

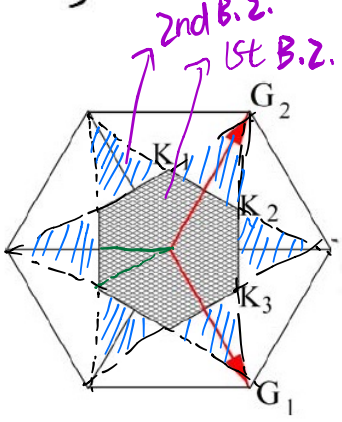


In reciprocal space, the reciprocal lattice is hexagonal lattice

(d)







Source: https://wiki.physics.udel.edu/phys824/Band_structure_of_graphene,_massless_Dirac_fermions_as_low-energy_quasiparticles,_Berry_phase,_and_all_that

(e) $|\vec{b_1}| = \frac{4\pi}{3a}$

Shortest distance: $\frac{1}{2}|\vec{b_1}| = \frac{2\pi}{3a}$

Longest distance: $\frac{2\pi}{3a\sin 60^\circ} = \frac{4\pi}{3\sqrt{3}a}$

Where a is the distance between atom A and B in real space