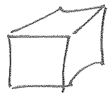
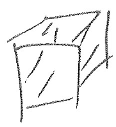
Crystal structure

1/ volume of a cube  $a^3 = (50\cdot 10^{-6})^3 = 1.25\cdot 10^{-13}\ m^3$

volume of one ion  $V = \frac{4}{3}\pi r^3 \approx 4(0.15\cdot 10^{-9})^3 \approx 1.4\cdot 10^{-29}\ m^3$

ions in a grain $N = \dfrac{V_{grain}}{V_{ion}} \approx \dfrac{1.25\cdot 10^{-13}}{1.4\cdot 10^{-29}} \approx 10^{16}$ ions

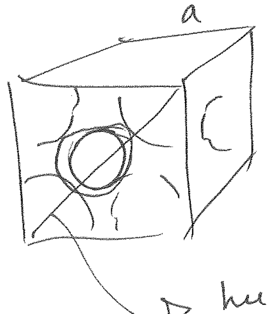
surface area  $6a^2 = 6(50\cdot 10^{-6})^2 = 1.5\cdot 10^{-8}\ m^2$

 cross-sectional area $\pi r^2 = \pi (0.15\cdot 10^{-9})^2 = 7\cdot 10^{-20}$

N at surface $= \dfrac{A_{cube}}{A_{cross}} = \dfrac{1.5\cdot 10^{-8}}{7\cdot 10^{-20}} = 2\cdot 10^{11}$

fraction on surface $= \dfrac{N_{surface}}{N_{volume}} = \dfrac{2\cdot 10^{11}}{10^{16}} \approx 2\cdot 10^{-5}$ i.e. 0.002 %

2/



here, diagonal = 4 radii

$2a^2 = (4r)^2$

$2a^2 = 16r^2$

$a = \sqrt{8}\, r$

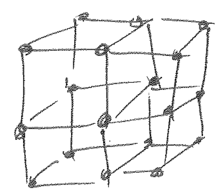
# of atoms $= (6\times\frac{1}{2}) + (8\times\frac{1}{8})$

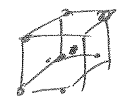
$= 4$ atoms

filling fraction $= \dfrac{V_{atoms}}{V_{cube}} = \dfrac{4\times\frac{4}{3}\pi r^3}{a^3} = \dfrac{16\pi r^3}{3\, 8^{3/2} r^3} = 74\%$

3/ Coordination # is the # of atoms immediately surrounding an atom. It can be thought of as the number of nearest neighbors (all the same distance away)

simple cubic	6
bcc	8
fcc	12
hcp	12





4/ (a) volume of space, defined by lattice vectors, that recreates the entire crystal lattice when repeated end-to-end

(b) a unit cell that contains only one lattice point

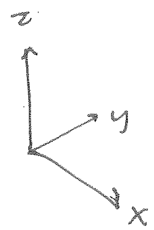
(c) a unit cell that contains more than 1 lattice point

(d) a unit cell that is the one usually chosen to represent a particular lattice, usually since it's visually easy to interpret or it's mathematically the simplest to use

(e) a unit cell that is <u>centered</u> on a lattice point.

See Fig 1.2 in Hofmann

5/



here, $\vec{c} = \frac{d}{2}(\hat{y} + \hat{z})$

$\vec{b} = \frac{d}{2}(\hat{x} + \hat{z})$

$\vec{a} = \frac{d}{2}(\hat{x} + \hat{y})$

points A, B, C can be written in terms of $\hat{x}, \hat{y}, \hat{z}$ or $\vec{a}, \vec{b}, \vec{c}$

by inspection, we can see

$\vec{A} = 2\vec{a}$ which is equivalent to

$= 2(\frac{d}{2})(\hat{x} + \hat{y}) = d(\hat{x} + \hat{y})$

$\vec{B} = \vec{a} + \vec{b}$ which is equivalent to

$= \frac{d}{2}(\hat{x} + \hat{z}) + \frac{d}{2}(\hat{x} + \hat{y})$

$= d\hat{x} + \frac{d}{2}\hat{y} + \frac{d}{2}\hat{z}$

$\vec{C} = d(\hat{x} + \hat{y} + \hat{z})$ which is equivalent to

$= \vec{c} + \vec{b} + \vec{a}$

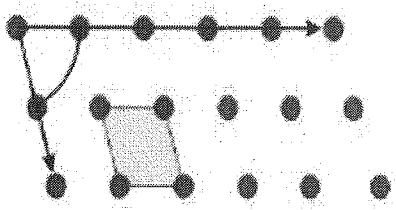
$\vec{D} = 2d\hat{x}$ which is equivalent to

$= \vec{a} + \vec{b} - \vec{c}$

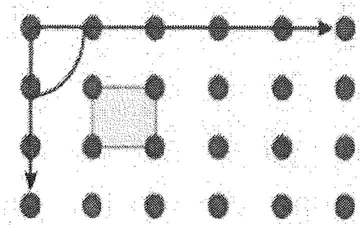
6/

Five Types of Planar 2-D Lattices

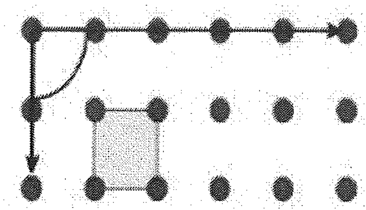
Oblique
a ≠ b
$\gamma \neq 90°$



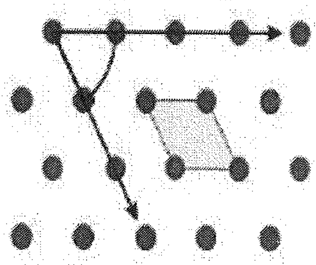
Rectangular P
a ≠ b
$\gamma = 90°$



Square
a = b
$\gamma = 90°$

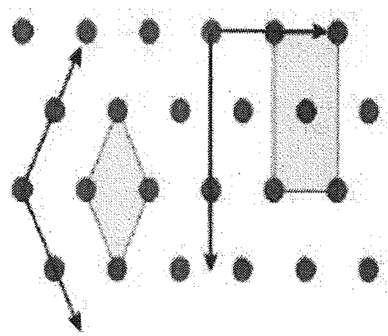


Hexagonal
a = b
$\gamma = 60°$



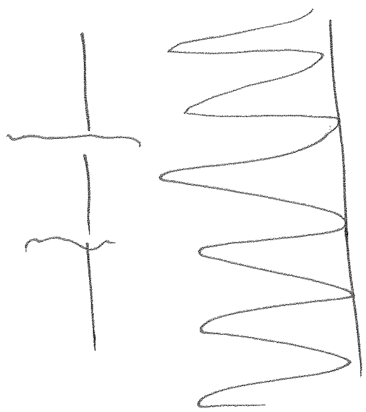
Diamond
a = b
$\gamma \neq 60°, 90°, 120°$

Rectangular C
a ≠ b
$\gamma = 90°$



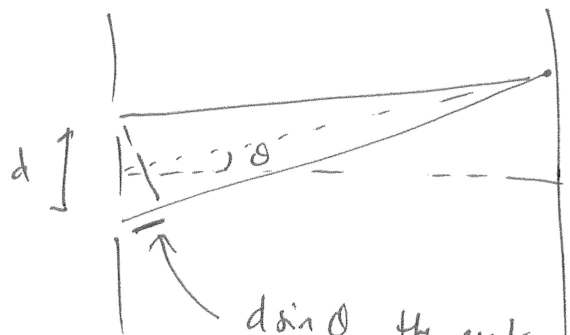
from unf.edu

7/ (a)



The double slit experiment shows that light possess wave characteristics: it can produce an interference pattern. This interference is due to the 2 waves being out of phase, since the 2 waves travel different distances to arrive at the screen.

(b), (c)



d = slit separation

θ = refers to the angular position of the interference pattern

$d \sin\theta$, the extra distance traversed by one of the waves

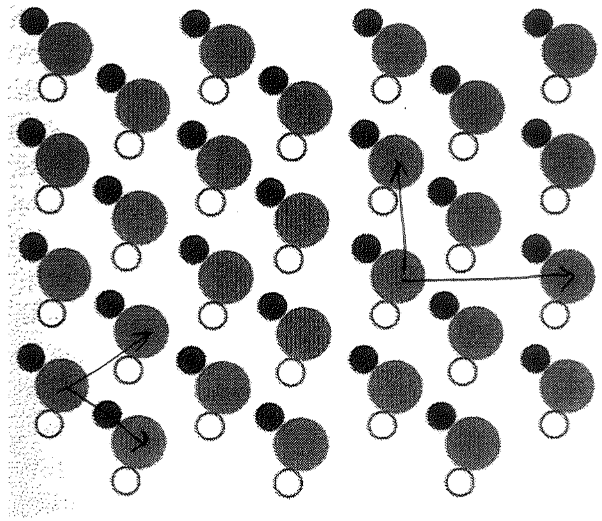
(d) if $d\sin\theta = m\lambda$ integer # of wavelengths, we see constructive interference.

the waves are in phase

if $d\sin\theta = (m+\frac{1}{2})\lambda$ $\frac{1}{2}$ integer wavelengths, it's destructive interference

the waves are completely out of phase

8. In the 2D crystal below, identify



(a) a primitive unit cell and its lattice vectors
(b) a non-primitive rectangular unit cell and its vectors
(c) the bases associated with each of the above
Adapted from Hofmann 1.1

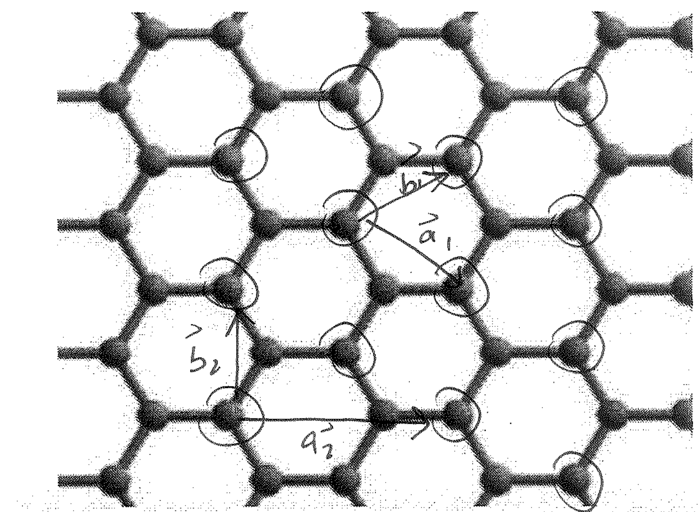
primitive unit cell $\vec{a}$, $\vec{b}$

basis has 3 atoms

non primitive rectangular unit cell $\vec{b}$, $\vec{a}$

basis has 6 atoms (2 sets of 3)

9. The honeycomb lattice is the structure graphene[1].



for $\vec{a}_1, \vec{b}_1$

basis is

(the two opp. atoms on hexagon)

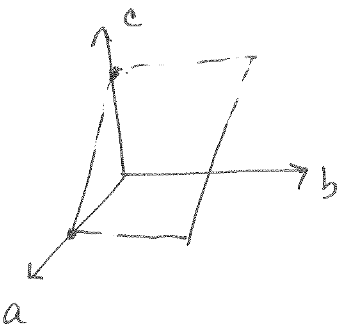
this is a primitive unit cell

for $\vec{a}_2, \vec{b}_2$

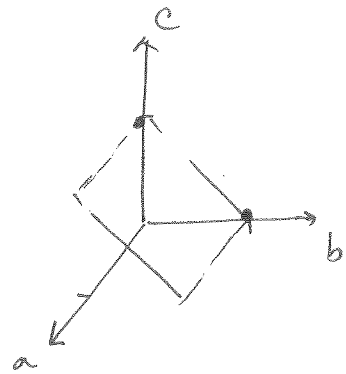
basis is

this is a non-primitive unit cell

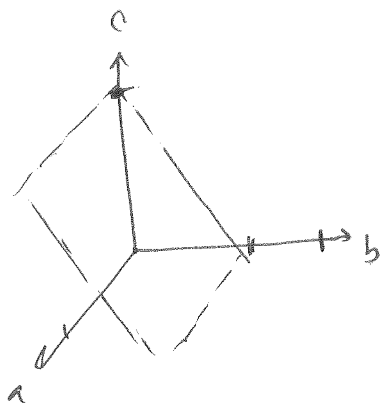
10/



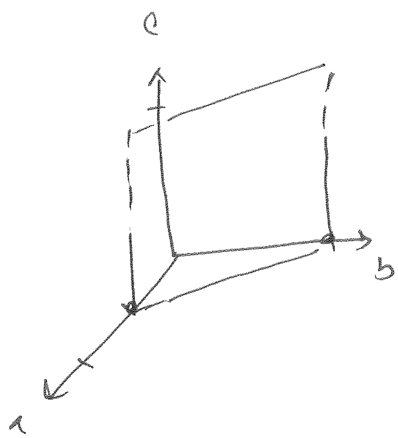
(1 0 1)



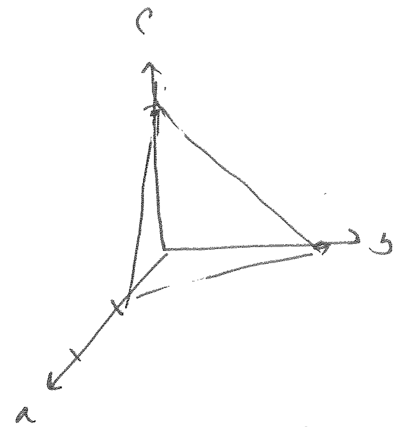
(0 1 1)



(0 2 1)

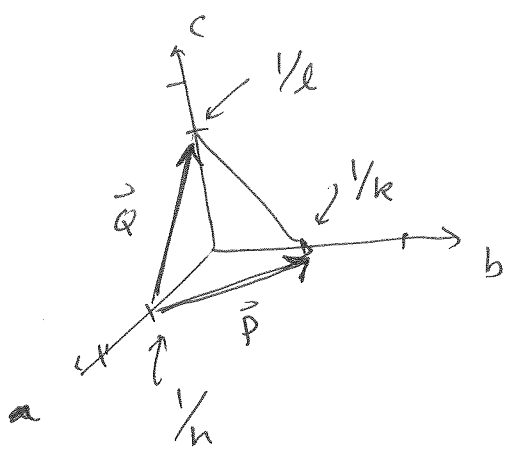


(2 1 0)



(2 1 1)

11/



Plane is defined by 2 vectors

$$\vec{P} = -\frac{1}{h}\hat{a} + \frac{1}{k}\hat{b}$$

$$\vec{Q} = -\frac{1}{h}\hat{a} + \frac{1}{l}\hat{c}$$

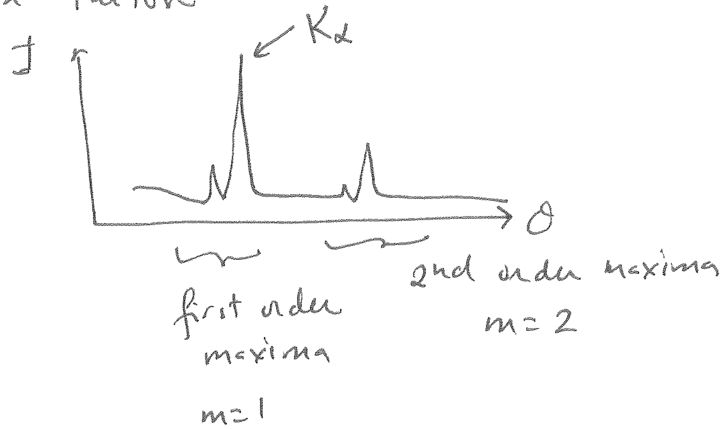
A vector $\perp$ to both $\vec{P}$ & $\vec{Q}$ is created by the cross product

$$\vec{N} = \vec{P} \times \vec{Q} = \begin{vmatrix} \hat{a} & \hat{b} & \hat{c} \\ -\frac{1}{h} & \frac{1}{k} & 0 \\ -\frac{1}{h} & 0 & \frac{1}{l} \end{vmatrix}$$

$$= \left(\frac{1}{kl}\hat{a}\right) + \left(\frac{1}{hl}\right)\hat{b} + \left(\frac{1}{kh}\right)\hat{c}$$

$$\hat{N} = h\hat{a} + k\hat{b} + l\hat{c}$$

12/ 2.9 in Turton



- since x-ray diffraction is described by $d\sin\theta = m\lambda$, a larger λ corresponds to higher θ. So K_α is the 2^{nd} peak.

- $2d\sin\theta = m\lambda$

$$d = \frac{m\lambda}{2\sin\theta} = \frac{(1)(0.15393\cdot 10^{-9})}{\sin 15.8^\circ} = 0.28 \text{ nm}$$

- to find Δd:

$$\left.\begin{aligned} d_+ &= \frac{m\lambda}{2\sin(15.8+0.05)} \\ d_- &= \frac{m\lambda}{2\sin(15.8-0.05)} \end{aligned}\right\} \quad \begin{aligned} &0.2818 - 0.2835 \\ &\Delta d = 0.0009\text{nm} \end{aligned}$$

13/ 2.10 in Turton

Consider just first part of problem on spacing between planes

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

$$d = \frac{m\lambda}{\sin\theta} = \frac{(1)(0.09\cdot 10^{-9})}{\sin(8.9^\circ)} = 0.291 \text{ nm}$$

14/ (a) $2d\sin\theta = m\lambda$

$$\lambda_{max} = \frac{2d\sin\theta}{m} = \frac{2(0.36\cdot10^{-9})(\sin 90°)}{(1)}$$

λ_{max} is when $\theta = 90°$

$= 0.72\text{ nm}$

(b) photons have energy $E = hf$
using wavelength, $c = \lambda f$

$$E = \frac{hc}{\lambda} = \frac{(6.63\cdot10^{-34})(3\cdot10^{8})}{0.72\cdot10^{-9}}$$

$= 2.8\cdot10^{-16}\text{ J}$

in eV: $2.8\cdot10^{-16}\text{ J}\ \frac{1\text{ eV}}{1.6\cdot10^{-19}} = 1750\text{ eV}$

(c) to use neutrons, $p = \frac{h}{\lambda}$ and $E = \frac{p^2}{2m}$

substituting p into E $\quad E = \frac{h^2}{2m\lambda^2} = \frac{(6.63\cdot10^{-34})^2}{2(1.67\cdot10^{-27})(0.72\text{nm})^2}$

$= 2.5\cdot10^{-22}\text{ J}$ or 1.6 meV

much smaller energy req'd

15/ $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$

and $p = \frac{h}{\lambda}$

$$E = \left(\frac{h}{\lambda}\right)^2\frac{1}{2m}$$

solve for λ

$$\lambda^2 = \frac{h^2}{2mE}$$

$$\lambda = \frac{h}{\sqrt{2mE}}$$