

**PROBLEM SET 1    Due Wednesday October 9**  
 Physics 240A- FALL 2019

[1.] Construct the matrix which will reflect  $\mathbf{r} = \begin{pmatrix} x \\ y \end{pmatrix}$  about a line through the origin making an angle  $\theta$  with the  $x$ -axis.

[2.] Show that the only allowed rotation angles for a 2D Bravais lattice are  $\theta = \pi, 2\pi/3, \pi/2,$  and  $\pi/3$ . Hint: Write the two lattice vectors

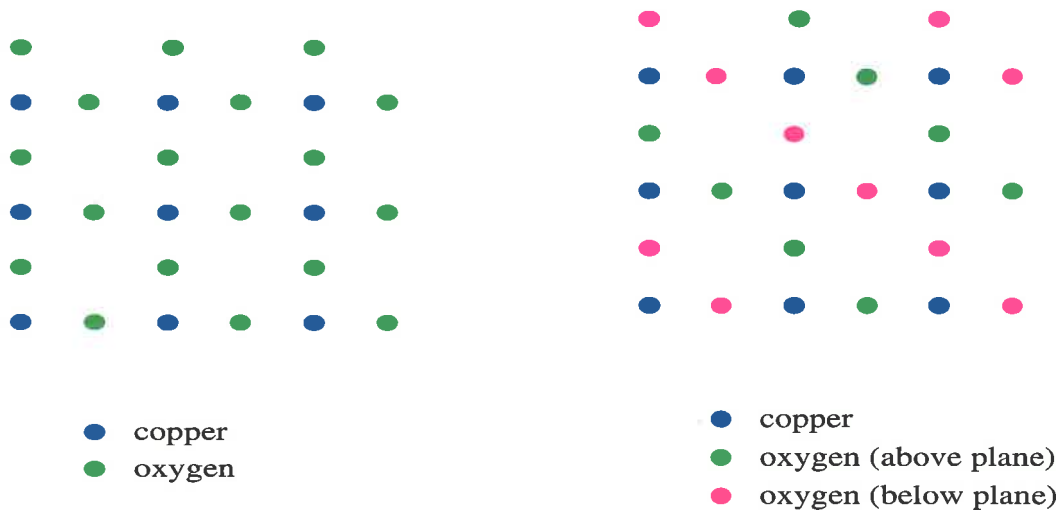
$$\mathbf{a}_1 = \begin{pmatrix} a \\ 0 \end{pmatrix} \quad \mathbf{a}_2 = \begin{pmatrix} b \\ c \end{pmatrix}$$

and demand that when  $\mathbf{a}_1$  is rotated by  $\theta$  and by  $-\theta$  that it lands on another site  $n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$  of the Bravais lattice.

[3.] The “family” of high temperature (cuprate) superconductors contains many compounds.  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  is one example. What is the lattice structure of the “parent” compound,  $\text{La}_2\text{CuO}_4$ ? What is a “perovskite”?  $\text{La}_2\text{CuO}_4$  is an antiferromagnetic insulator. When Sr replaces some of the La, one produces a high temperature superconductor.

[4.] Find the primitive lattice vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  of the real space graphene (hexagonal lattice) and also  $\mathbf{b}_1$  and  $\mathbf{b}_2$  for the reciprocal space lattice. How long are  $\mathbf{b}_1$  and  $\mathbf{b}_2$  if the C-C distance is  $a \sim 0.142 \text{ nm}$ ?

[5.] Sketch the Bravais lattice, find  $\mathbf{a}_1$  and  $\mathbf{a}_2$  and draw the unit cell for the  $\text{CuO}_2$  lattice in Fig. 1(left). Do the same for a lattice in which the oxygen atoms are inequivalent, Fig. 1(right), as is the case in cuprate superconductors when the oxygen tetrahedra tilt. (See problem 3.).



[6.] Find the volumes of the unit cells for *bcc* and *fcc* lattices.

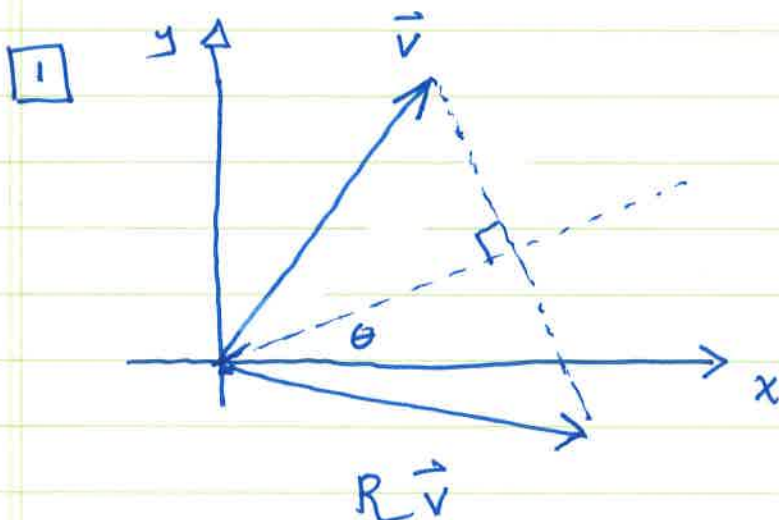
[7.] (a) Find  $c/a$  for an hcp lattice. (b) At temperature  $23^\circ$ , sodium changes from bcc to hcp. If the number density is unchanged, find  $a$  for the high temperature hcp phase if the low temperature bcc phase has  $a' = 4.23 \text{ \AA}$ .

[8.] In a perfect crystal the atoms are located at positions  $\mathbf{R}_n^0 = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$ . Diffraction peaks are  $\delta$ -functions at reciprocal lattice vectors  $\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3$ . Suppose now some "imperfections" are present so that  $\mathbf{R}_n = \mathbf{R}_n^0 + \mathbf{S}_n$  where each component of  $\mathbf{S}_n$  has a Gaussian distribution  $P(S_i) = \exp(-S_i^2/2S_0^2) / \sqrt{2\pi}S_0$ . How are the intensities of the diffraction peaks changed from their perfect delta-function forms?

defect to PS2

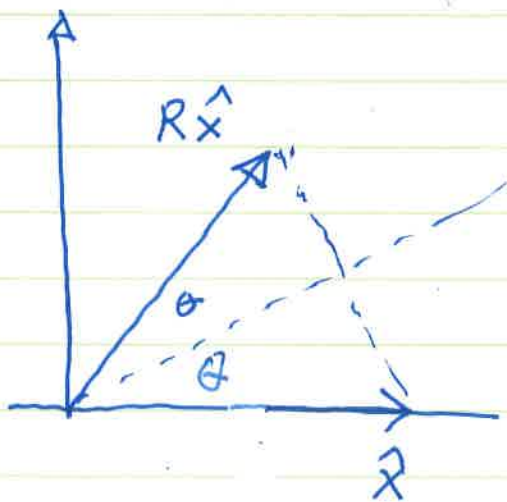
1-1

P240A PS1
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General Rule: Matrix for some operation has columns which are given by vector resulting from action of operator on basis vectors.

What does  $R$  do to  $\hat{x}$ ,  $\hat{y}$ ?



$R\hat{x}$  has length 1  
and makes angle  $2\theta$   
with  $\hat{x}$  axis

$$\therefore R\hat{x} = \begin{pmatrix} \cos 2\theta \\ \sin 2\theta \end{pmatrix}$$

An "allowed rotation" means that if we rotate a point on the Bravais lattice we should land on another point of the Bravais lattice. That is

$$R_{\theta} \begin{pmatrix} a \\ 0 \end{pmatrix} = \begin{pmatrix} a \cos \theta \\ a \sin \theta \end{pmatrix} = n_1 \begin{pmatrix} a \\ 0 \end{pmatrix} + n_2 \begin{pmatrix} b \\ c \end{pmatrix}$$

$$R_{-\theta} \begin{pmatrix} a \\ 0 \end{pmatrix} = \begin{pmatrix} a \cos \theta \\ -a \sin \theta \end{pmatrix} = n'_1 \begin{pmatrix} a \\ 0 \end{pmatrix} + n'_2 \begin{pmatrix} b \\ c \end{pmatrix}$$

$$a \cos \theta = n_1 a + n_2 b = n'_1 a + n'_2 b$$

$$a \sin \theta = n_2 c = -n'_2 c$$

This tells us  $n'_2 = -n_2$

so

$$a \cos \theta = n_1 a + n_2 b$$

$$a \cos \theta = n'_1 a - n_2 b$$

Adding

$$\cos \theta = \frac{1}{2} (n_1 + n'_1)$$

integer

$$\cos \theta = -1, -\frac{1}{2}, 0, \frac{1}{2}, 1$$

$$\theta = \pi, \frac{2\pi}{3}, \frac{\pi}{2}, \frac{\pi}{3}, 0$$

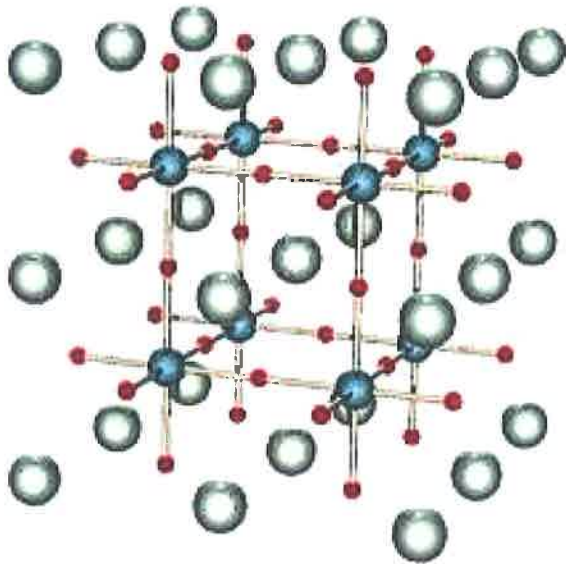
(180, 120, 90, 60, 0 in degrees)

3-1

3. The “family” of high temperature (cuprate) superconductors contains many compounds.  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  is one example. The “parent” compound,  $\text{La}_2\text{CuO}_4$  is an antiferromagnetic insulator. What is the lattice structure of  $\text{La}_2\text{CuO}_4$ ? What is a “perovskite”?

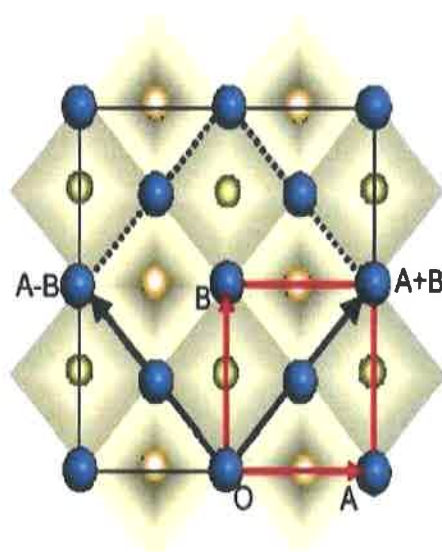
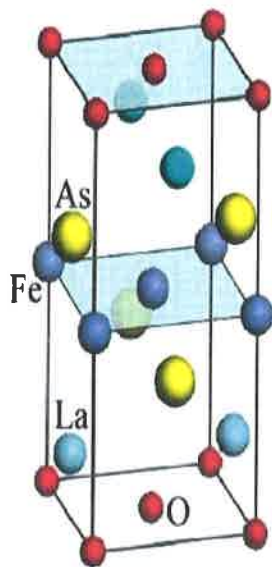
The  $\text{La}_2\text{CuO}_4$  crystal structure is composed of  $\text{CuO}_2$  sheets in which the Cu atoms are at the vertices of a square, with an O atom at the center of each bond. The La atoms, and additional O atoms, lie between these sheets. The  $\text{CuO}_2$  sheets are the common feature of the whole family of cuprates (whilst there are many variants in which La is replaced by other rare earths), suggesting that they must be crucial to the phenomenon of high temperature superconductivity. The additional intersheet O atoms are arranged so that each Cu atom is surrounded by a tetrahedron of O. (See perovskite structure below.)

I really meant to ask what is the perovskite structure as opposed to what is a perovskite.



The perovskite structure is illustrated at left. The red spheres are typically O, whilst the blue spheres are often a smaller metal atom and the green spheres are larger metal atoms. In the case of the cuprate superconductor, the blue spheres are copper and the green spheres might be, for example, La. Notice the  $\text{CuO}_2$  sheets and the O tetrahedra surrounding each Cu.

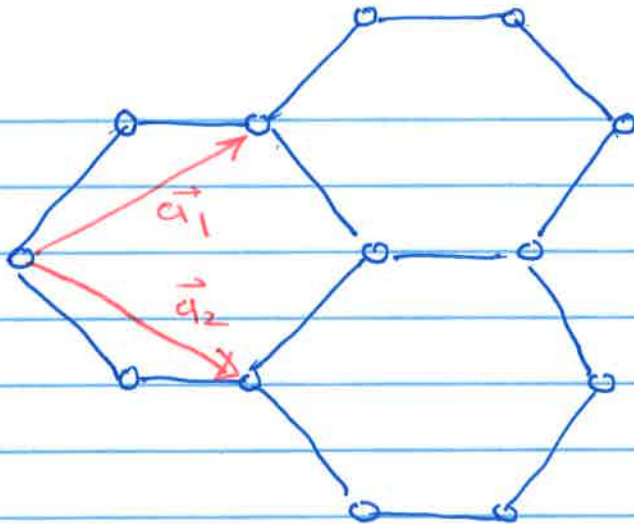
**NOTE:** Another “family” of superconductors are the iron pnictides. What is the structure of the “1111” material  $\text{LaOFeAs}$ ?



The structure of  $\text{LaOFeAs}$  is shown at left. As with the cuprates, the ‘iron superconductors’ are highly layered. The electrons tend to move in the FeAs layers. The Fe atoms form a square lattice in these layers.



4-1



one choice is shown

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

$$\vec{a}_2 = \frac{3}{2} a \hat{x} - \frac{\sqrt{3}}{2} a \hat{y}$$

Reciprocal Lattice vectors obey  $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$

so if  $\vec{b}_1 = b_{1x} \hat{x} + b_{1y} \hat{y}$  we have

$$\vec{a}_1 \cdot \vec{b}_1 = \frac{3}{2} a b_{1x} + \frac{\sqrt{3}}{2} a b_{1y} = 2\pi$$

$$\vec{a}_2 \cdot \vec{b}_1 = \frac{3}{2} a b_{1x} - \frac{\sqrt{3}}{2} a b_{1y} = 0 \quad \leadsto \quad b_{1y} = \sqrt{3} b_{1x}$$

$$\left(\frac{3}{2} a + \frac{\sqrt{3}}{2} a \sqrt{3}\right) b_{1x} = 2\pi \quad \leadsto \quad b_{1x} = \frac{2\pi}{3a}$$

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

Similarly  $\vec{b}_2 = \frac{2\pi}{3a} (\hat{x} - \sqrt{3} \hat{y})$

4-2

The lengths of  $\vec{b}_i$  are the same

$$|\vec{b}_1| = |\vec{b}_2| = \frac{2\pi}{3a} \sqrt{1+3} = \frac{4\pi}{3a}$$

$$a = 0.142 \text{ nm} \quad \frac{4\pi}{3a} = 2.95 \cdot 10^{10} \text{ m}^{-1}$$

To put this number in perspective we could ask what type of photon has this  $|\vec{k}|$ .

$$\omega = c|\vec{k}| = (3 \cdot 10^8)(2.95 \cdot 10^{10}) = 8.85 \cdot 10^{18} \text{ sec}^{-1}$$

RED  $\omega = 4.3 \text{ to } 4.8 \text{ THz} \leftarrow 10^{12}$   
 $\lambda = 635 \text{ to } 700 \text{ nm}$   
 $E \sim 1.8 \text{ eV}$

So this is  $\sim 10^6$  the frequency of visible light

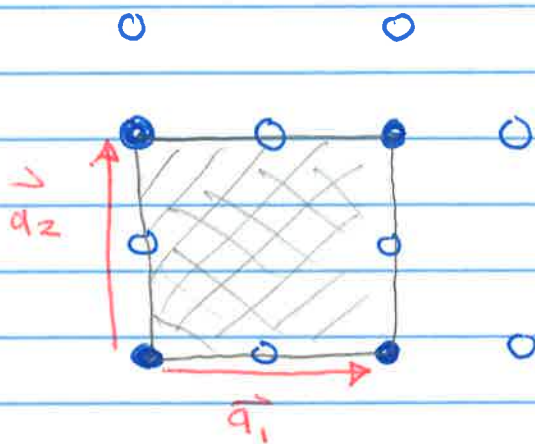
light of the  $\lambda, \omega$  corresponding to these  $g$  would

have very high energy

$$\begin{aligned} E &= \hbar\omega = (1.055 \cdot 10^{-34})(8.85 \cdot 10^{18}) \\ &= 9.34 \cdot 10^{-16} \text{ J} \\ &= 5.84 \cdot 10^3 \text{ eV} \end{aligned}$$

5-1

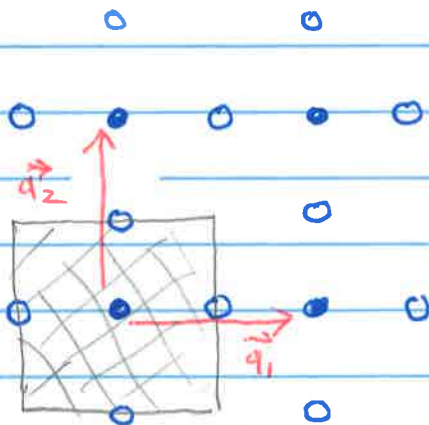
If the two O atoms are equivalent,  
 the repeating unit consists of one Cu atom and two  
 oxygen atoms. One possible unit cell is



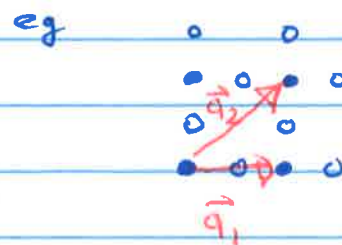
Cu-O distance =  $a$

unit cell volume =  $(2a)^2$   
 $= 4a^2$

Another choice is centered at a copper atom



There are also  
 alternate choices for  $\vec{a}_1, \vec{a}_2$

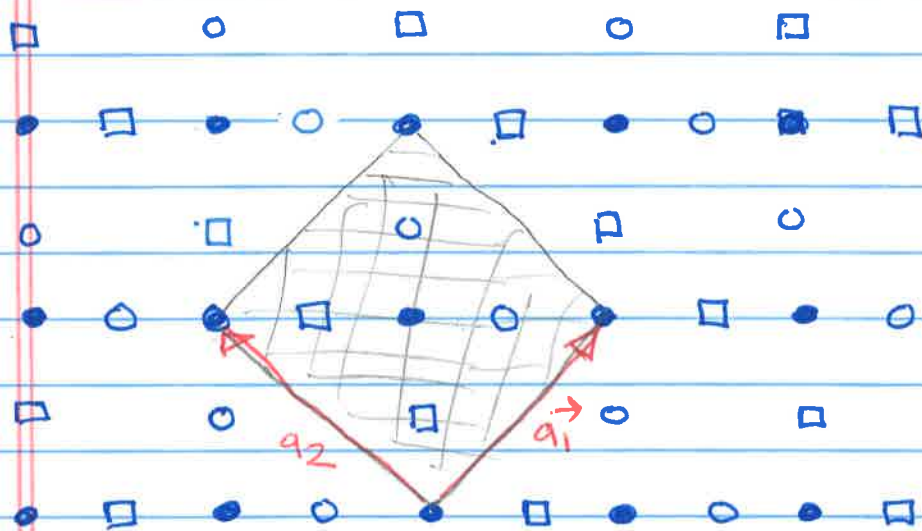


Both types of unit cells have one copper and two oxygens



5.2

Meanwhile, if the two oxygen atoms are inequivalent  
the repeating unit is twice as large, for example



$$\text{Cu-O distance} = a$$

$$|\vec{a}_1| = |\vec{a}_2| = \sqrt{2} 2a$$

$$\begin{aligned} \text{unit cell volume} &= (2\sqrt{2}a)^2 \\ &= 8a^2 \end{aligned}$$

6-1

$$\text{fcc} \quad \vec{a}_1 = \frac{a}{2} (\hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2} (\hat{x} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y})$$

$$V_c = \left| \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \right|$$

$$\vec{a}_2 \times \vec{a}_3 = \frac{a^2}{4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{a^2}{4} (-\hat{x} + \hat{y} + \hat{z})$$

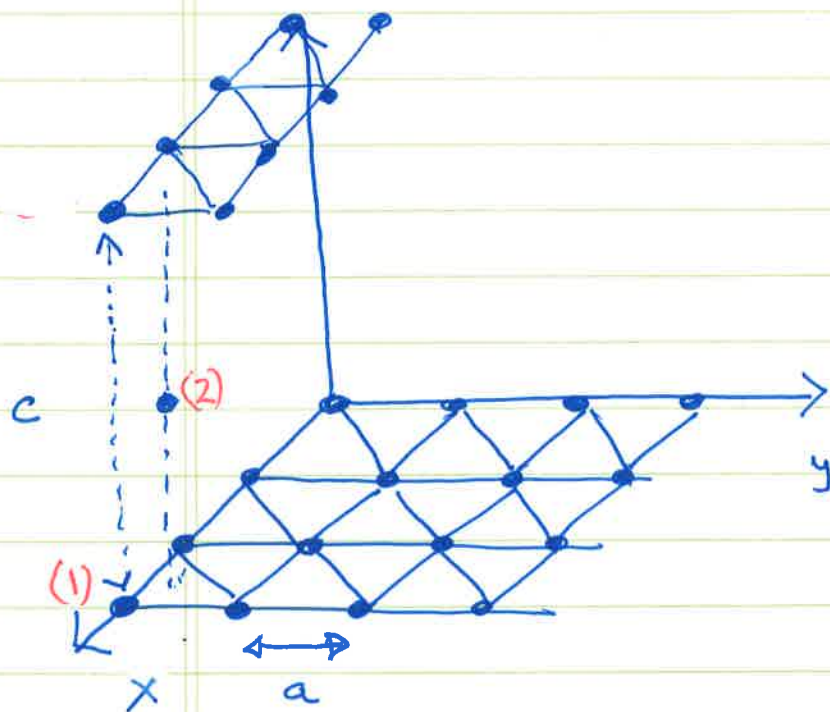
$$\left| \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \right| = \frac{a^3}{8} \{1+1\} = \frac{a^3}{4}$$

$$\text{bcc} \quad \left. \begin{array}{l} \vec{a}_1 = \frac{a}{2} (-\hat{x} + \hat{y} + \hat{z}) \\ \vec{a}_2 = \frac{a}{2} (\hat{x} - \hat{y} + \hat{z}) \\ \vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z}) \end{array} \right\} \begin{array}{l} \vec{a}_2 \times \vec{a}_3 \\ = \frac{a^2}{4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} \\ = \frac{a^2}{4} (2\hat{y} + 2\hat{z}) \end{array}$$

$$V_c = \left| \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \right| = \frac{a^3}{8} \{2+2\} = \frac{a^3}{2}$$

7-1

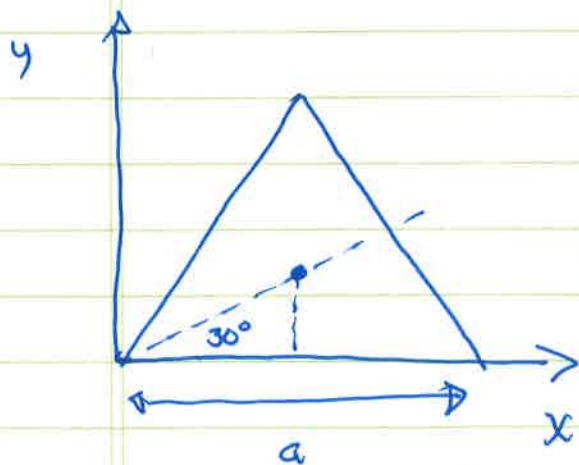
hcp



Atoms in the bottom plane  
touch each other so clearly

$$a = 2R \leftarrow \text{atom radius}$$

Likewise, atoms (1) and (2) touch and so are  $2R$  apart



Position of center of equilateral triangle:  $x = a/2$

$$y/a/2 = \tan 30 = 1/\sqrt{3}$$

$$y = \frac{a}{2\sqrt{3}}$$

(distance)<sup>2</sup> from (1) to (2) is

$$\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = (2R)^2 \quad \begin{matrix} \downarrow \text{atoms (1) and (2) touch} \end{matrix}$$

$$R^2 + \frac{R^2}{3} + \frac{c^2}{4} = 4R^2$$

$$c^2 = 4R^2 \left(3 - \frac{1}{3}\right) = 4R^2 \frac{8}{3} \quad c = \frac{2R}{a} \sqrt{\frac{8}{3}}$$

so  $c/a = \sqrt{8/3}$

7-2

BCC has 2 atoms/unit cell and so density

$$n_{\text{bcc}} = \frac{2}{(a')^3} \quad \text{for cube of side } a'$$

HCP unit cell also has 2 atoms and volume

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

BASIS

$$(0, 0, 0)$$

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

$$\left(\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right)$$

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

$$V_c = \left| \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \right|$$

$$= a \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{vmatrix} = ac \left( \frac{\sqrt{3}}{2} \hat{x} - \frac{1}{2} \hat{y} \right)$$

$$= a^2 c \left\{ \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} \right\} = a^2 c \frac{\sqrt{3}}{2}$$

$$\text{so } n_{\text{hcp}} = \frac{2}{a^2 c \frac{\sqrt{3}}{2}} = \frac{4}{\sqrt{3} a^2 c}$$

$$\text{Equating } \frac{a'^3}{2} = \frac{\sqrt{3} a^2 c}{4} = \frac{\sqrt{3} a^2}{4} \underbrace{\frac{\sqrt{8}}{\sqrt{3}} a}_{\text{ideal } c \text{ from part i}} = \frac{\sqrt{2} a^3}{2}$$

$$a^3 = \frac{(a')^3}{\sqrt{2}} \quad a = \frac{a'}{\sqrt[3]{2}} = \frac{4.23}{1.122} = 3.77 \text{ \AA}$$