Physics 140A Winter 2011

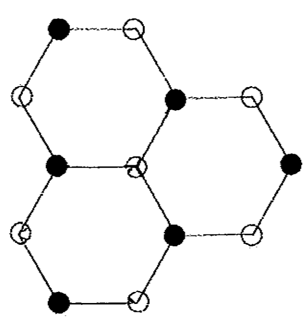
Homework 1 due Wednesday January 12

1. The angles between the tetrahedral bonds of diamond are the same as the angles between the body diagonals of a cube (see Fig. 10 of Chapter 1 of Kittel). Use elementary vector analysis to find the value of this angle.

2. Consider the planes with indices (100) and (001) of the fcc lattice, with reference to the conventional cubic cell. Determine the indices of these planes when referred to the *primitive unit cell axes* as shown in Fig. 11 of Chapter 1 of Kittel.

3. Show that in the ideal hexagonal close packed structure, the ratio $c/a = \sqrt{8/3} = 1.633$. Note that in the ideal structure, the atomic spheres between stacking layers are touching. If the c/a ratio is significantly larger than this ideal ratio, the crystal structure will consist of loosely stacked planes of closely packed atoms.

4. As discussed in class, graphene consists of a single two-dimensional layer of carbon atoms in a honeycomb arrangement as shown below. Determine the lattice structure and basis for this material. Write down the primitive basis vectors for the lattice, and the coordinates of the atoms in the unit cell in that basis.



Homework Solutions #1

Note Title 1/12/2010

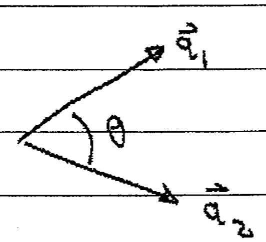
Physics 140A - Winter 2011

① The unit vectors are : $\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$

25 pts

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

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



$$\vec{a}_1 \cdot \vec{a}_2 = |a_1||a_2| \cos\theta$$

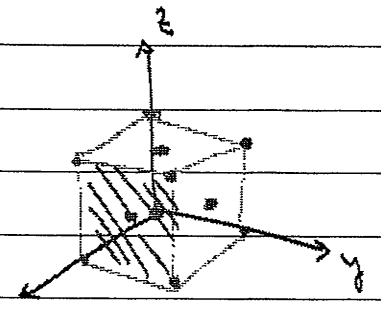
$$\vec{a}_1 \cdot \vec{a}_2 = \frac{a^2}{4}(-1+1-1) = -\frac{a^2}{4}$$

$$\Rightarrow \quad -\frac{a^2}{4} = \left(\frac{a}{2}\sqrt{3}\right)\left(\frac{a}{2}\sqrt{3}\right)\cos\theta$$

$$\Rightarrow \quad \frac{-1}{3} = \cos\theta \quad \text{or} \quad \theta = \cos\left(\frac{-1}{3}\right)$$

$$\boxed{\begin{aligned}\theta &= 109.47^\circ \\ &= 109^\circ\, 28'\, 16.39''\end{aligned}}$$

(2) 25 pts

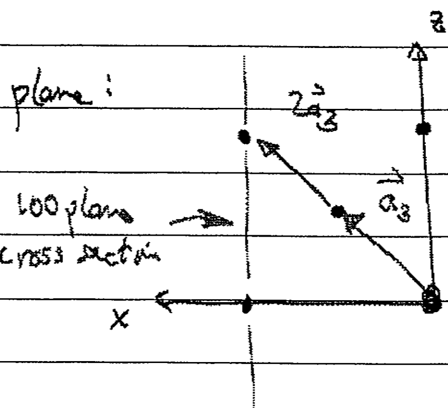


(100) plane of fcc lattice

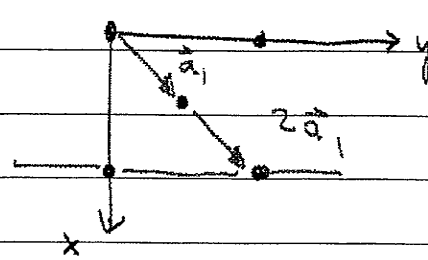
need to find where this plane intercepts axes of primitive lattice vectors:

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

in the x-z plane:



in the x-y plane:



no crossing of the y-z plane

So intercepts at $2\ \infty\ 2$ or $\frac{1}{2}\ 0\ \frac{1}{2}$

but reducing to integers w/ same ratio gives $1:0:1$

So this is the <u>(101) plane of the primitive unit cell</u>

now, the (001) plane of the conventional unit cell:

is the same plane as $z = a$

this intercepts the $\vec{a}_2$ vector at $2a_2$

and $\vec{a}_3$ at $2a_3$

but does not intercept $\vec{a}_1$.

So we have $\infty, 2, 2$ as the intercepts

$\Rightarrow$ <u>(011) is the index for the prim. cell</u>

3 hcp structure: $\vec{a}_1 = a\hat{x}$

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

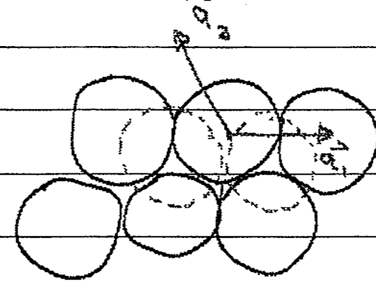
(25 pts) $$\vec{a}_3 = c\hat{z}$$

but have basis: $\vec{r}_1 = 0$

$$\vec{r}_2 = \frac{2}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2 + \frac{1}{2}\vec{a}_3$$

in the ideal case, spheres centered at $\vec{r}_1$ & $\vec{r}_2$ are touching at radius r_0, and spheres at $\vec{r}_1$ and at $\vec{r}_1 + \vec{a}_1$ are touching:

in plane:



so: $2r_0 = |\vec{r}_1 + \vec{a}_1 - \vec{r}_1| = a$

and: $2r_0 = |\vec{r}_2 - \vec{r}_1| = \left|\frac{2}{3}(a\hat{x}) + \frac{1}{3}\left(-\frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}\right) + \frac{1}{2}c\hat{z}\right|$

$$\Rightarrow \quad a = \left|\left(\frac{2}{3} - \frac{1}{6}\right)a\hat{x} + \frac{\sqrt{3}}{6}a\hat{y} + \frac{1}{2}c\hat{z}\right|$$

$$a^2 = \left(\frac{1}{2}\right)^2 a^2 + \frac{3}{36}a^2 + \frac{1}{4}c^2$$

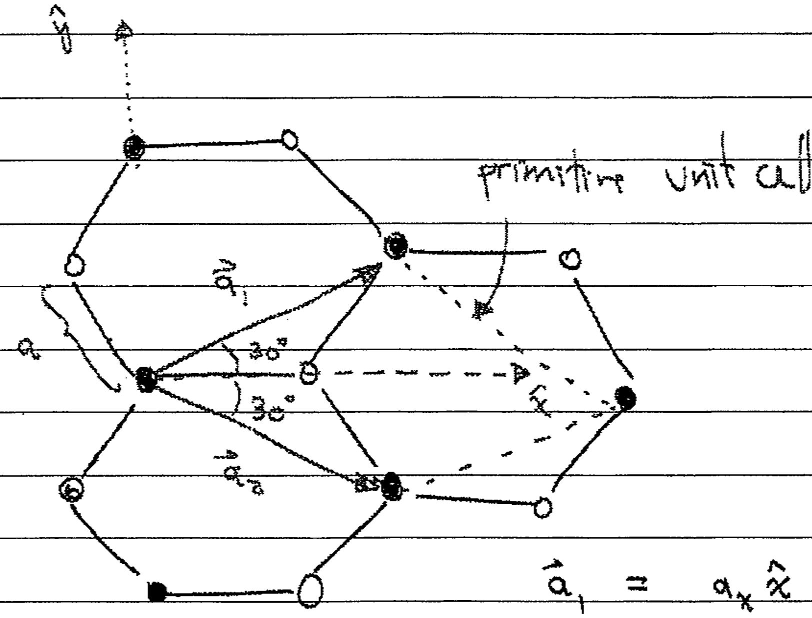
$$(36 - 9 - 3)a^2 = 9c^2$$

$$\frac{\cancel{24}\ 8}{9\ 3} = \left(\frac{c}{a}\right)^2$$

$$\Rightarrow \quad \frac{c}{a} = \sqrt{\frac{8}{3}} = 1.63299$$

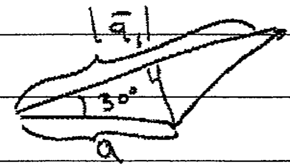
(4)

(25 pts)



$$\vec{a}_1 = a_x \hat{x} + a_y \hat{y}$$

$$\vec{a}_2 = a_x \hat{x} - a_y \hat{y}$$



$$|\vec{a}_{1,2}| = a_x^2 + a_y^2 = 2(a\cos 30°)$$

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

length of $|\vec{a}_{1,2}|$

now, $a_x = a_1 \cos 30° = \frac{3}{2}a$

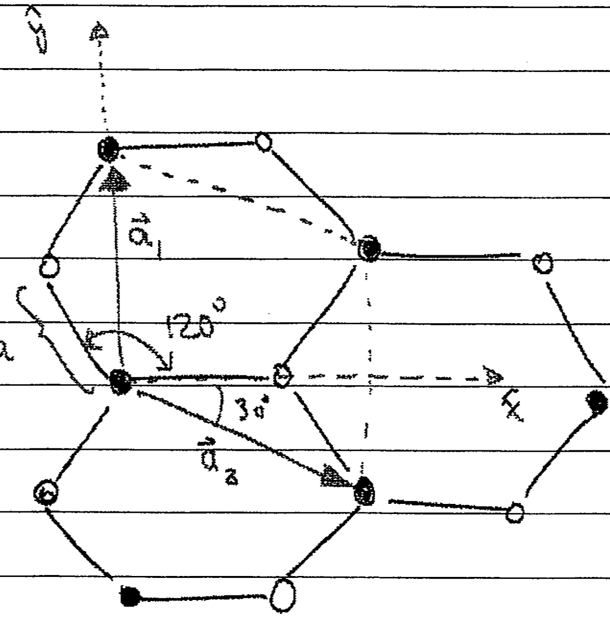
$a_y = a_1 \sin 30° = \frac{\sqrt{3}}{2}a$

So $\boxed{\begin{aligned}\bar{a}_1 &= \tfrac{3}{2} a \hat{x} + \tfrac{\sqrt{3}}{2} a \hat{y} \\ \hat{a}_2 &= \tfrac{3}{2} a \hat{x} - \tfrac{\sqrt{3}}{2} a \hat{y}\end{aligned}}$

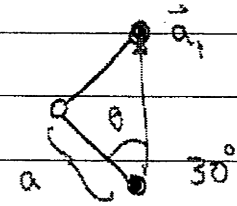
$\boxed{\begin{aligned}&\text{basis:} \\ &\bar{r}_1 = \bar{0} \\ &\bar{r}_2 = a\hat{x}\end{aligned}}$

note that a is the nearest neighbor distance.
In graphene, this is 1.42 Å

{Another way to solve:}



Using geometry:



$$|\vec{a}_1| = 2a\cos 30° = \sqrt{3}a$$

So $\boxed{\vec{a}_1 = \sqrt{3} a \hat{y}}$

to find $\vec{a}_2$, we recognize that $|\vec{a}_2| = |\vec{a}_1| = \sqrt{3}a$

and write $\vec{a}_2 = a_{2x}\,\hat{x} + a_{2y}\,\hat{y}$

where $a_{2x} = \sqrt{3}\,a\cos(-30^\circ) = \frac{(\sqrt{3})^2}{2}a = \frac{3}{2}a$

$a_{2y} = \sqrt{3}\,a\sin(-30^\circ) = -\frac{\sqrt{3}}{2}a$

So $\boxed{\vec{a}_2 = \frac{3}{2}a\,\hat{x} - \frac{\sqrt{3}}{2}a\,\hat{y}}$ The basis is then $\boxed{\begin{array}{l}\vec{r}_1 = \vec{0} \\ \vec{r}_2 = a\,\hat{x}\end{array}}$

Both answers are correct, but the axes of the unit cell are rotated wrt one another. There are other valid answers, too.