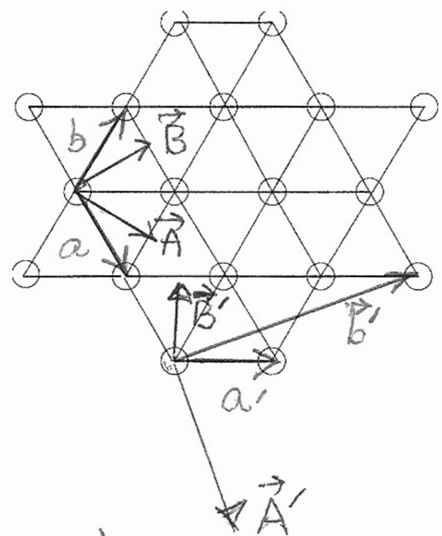
Solutions

Physics 555 **Fall 2007** **HW 1**

due Wednesday Sept 10

1. A primitive 2d lattice consists of a sheet of close-packed atoms forming a triangular lattice. A fragment is shown to the right. The actual sample extends to infinity ("horizontally") and is a single layer thick "vertically." **(a)** What are the primitive translation vectors (pick two permissible sets, one with sensible short vectors and the other not.) **(b)** What are the corresponding reciprocal lattice vectors? Draw the reciprocal lattice in a diagram similar to the one on the right, with spatial x and y coordinates corresponding correctly. Note that either choice of reciprocal lattice basis vectors (the one following from the sensible primitive translations, and the other one) generate the same reciprocal lattice.



(a) sensible

$\vec{a} = \frac{a}{2}(1, -\sqrt{3})$

$\vec{b} = \frac{a}{2}(1, \sqrt{3})$

weird

$\vec{a}' = a(1,0)$

$\vec{b}' = a(\frac{5}{2}, \frac{\sqrt{3}}{2})$

(b) $\vec{A}' = \frac{2\pi}{\sqrt{3}a}(\sqrt{3}, -5)$ $\quad \vec{B}' = \frac{4\pi}{\sqrt{3}a}(0,1)$

A formula you may use in 2d is $\vec{A} = \frac{2\pi(\vec{b}\times\hat{z})}{\vec{a}\cdot(\vec{b}\times\hat{z})}$

(but it is easy to find $\vec{A}\cdot\vec{a} = 2\pi$, $\vec{A}\cdot\vec{b} = 0$ by inspection)

Note that $\vec{a}\times\vec{b} = \vec{a}'\times\vec{b}' = \frac{\sqrt{3}}{2}a^2\hat{z}$ where $\frac{\sqrt{3}}{2}a^2$ = area of unit cell

also $\vec{A}\times\vec{B} = \vec{A}'\times\vec{B}' = \frac{8\pi^2}{\sqrt{3}a^2}\hat{z}$ where $\frac{8\pi^2}{\sqrt{3}a^2}$ = area of Brillouin zone

Reciprocal lattice vectors are

$\vec{G} = m\vec{A} + n\vec{B} = \frac{2\pi}{a}(m+n, \frac{n-m}{\sqrt{3}})$

$\vec{G}' = h\vec{A}' + k\vec{B}' = \frac{2\pi}{a}(h, \frac{2k-5h}{\sqrt{3}})$

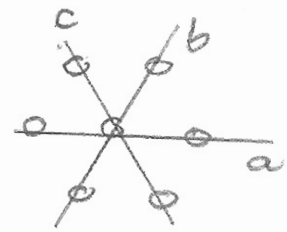
If $h = m+n$ and $k = 2m+3n$

then $\vec{G}' = \vec{G}$ so the 2 lattices are the same.

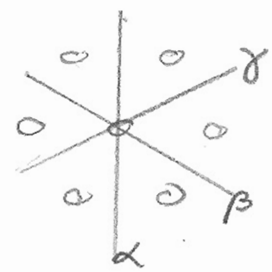
(c) This sheet of atoms lives in a 3d world in which it can translate and rotate, etc. In addition to translational symmetry, this lattice has also some "point symmetry." These are symmetry operations that leave at least one point fixed in space. Counting the identity operation, there are 12 "proper" rotations. What are they? Note that the symmetry operations have a natural multiplication, and form a group. Write out the multiplication table for rotations around a vertical axis. **(d)** Show that not all proper rotations belonging to the "point group" of this object commute with each other. (e) Finally, there are 12 "improper" rotations. One of them, the inversion, can also be expressed as a rotation by π around the vertical axis times a mirror reflection in the plane of the lattice. List the 12 improper rotations, in a simple format of mirrors possibly multiplied by rotations.

(c) Proper rotations

	E	C_6	C_6^2	C_6^3	C_6^4	C_6^5
E	E	C_6	C_6^2	C_6^3	C_6^4	C_6^5
C_6	C_6	C_6^2	C_6^3	C_6^4	C_6^5	E
C_6^2	C_6^2	C_6^3	C_6^4	C_6^5	E	C_6
C_6^3	C_6^3	C_6^4	C_6^5	E	C_6	C_6^2
C_6^4	C_6^4	C_6^5	E	C_6	C_2	C_3
C_6^5	C_6^5	E	C_6	C_6^2	C_3	C_4



C_{2a}
C_{2b}
C_{2c}



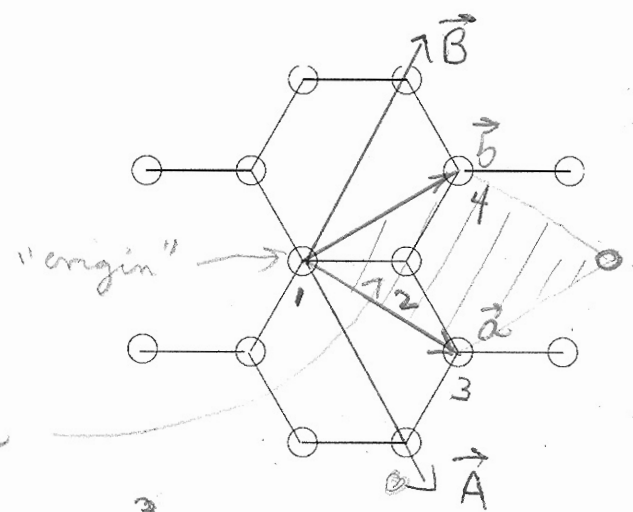
$C_{2\alpha}$
$C_{2\beta}$
$C_{2\gamma}$

(d) $C_{2a}C_6 = C_{2\beta}$
$C_6 C_{2a} = C_{2\gamma}$ } verify by drawing pictures

(e) Improper rotations are

m	mC_{2a}
mC_6	mC_{2b}
mC_6^2	mC_{2c}
mC_6^3 = inversion	$mC_{2\alpha}$
mC_6^4	$mC_{2\beta}$
mC_6^5	$mC_{2\gamma}$

2. Graphite has hexagonal packing of atoms in planes, and a slightly complicated rule for stacking planes on top of each other. The vertical spacing is large and the bonding between planes is weak. In recent years it has been shown that single sheets of graphite (called "graphene") can be separated and mounted on fairly inert substrates where they can be studied. A fragment is shown at the right. **(a)** Choose a simple, symmetrical choice of primitive translations $\vec{a}, \vec{b}$. **(b)** Find the corresponding primitive reciprocal lattice vectors $\vec{A}, \vec{B}$. How many atoms are in a primitive unit cell? Note that not all point symmetries of the previous triangular lattice are available here. For example, no inversion leaving graphene unchanged can leave any atom fixed in space, but inversion through the hexagon center is a symmetry operation. Alternately, you can have an inversion center on an atom, and then "multiply by" a sub-primitive translation. **(c)** Explain this sub-primitive translation. The complete symmetry group contains as many non-pure translations as does the triangular lattice, but there is no simple separation into point operations times translation operations, where both the point operation and the translation operation are also symmetry operations by themselves. Such a space group is called "non-symmorphic."



(a) $\vec{a} = a\left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right)$

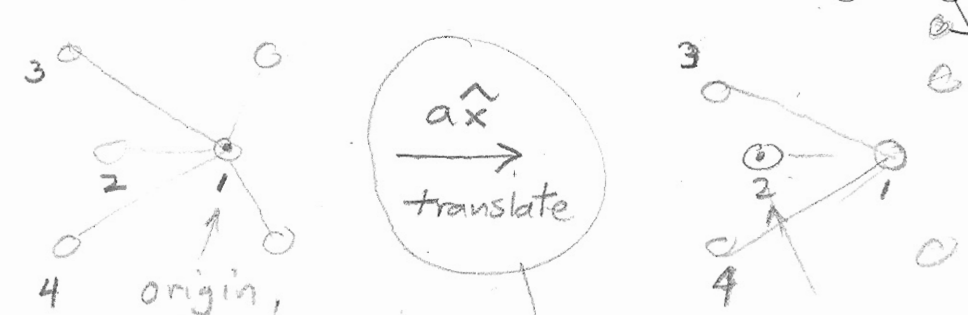
$\vec{b} = a\left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right)$

(b) $\vec{A} = \frac{2\pi}{a}\left(\frac{1}{3}, -\frac{1}{\sqrt{3}}\right)$

$\vec{B} = \frac{2\pi}{a}\left(\frac{1}{3}, \frac{1}{\sqrt{3}}\right)$

unit cell has 2 atoms

(c)



origin, after inversion through the origin

"sub-primitive" translation.

origin after translation of lattice keeping origin fixed.

The net effect of inversion through the atom at the origin and translation by $a\hat{x}$ is an inversion through $\frac{a}{2}\hat{x}$.

wrong definition. Sorry
should be $\frac{\text{volume inside spheres}}{\text{total volume}}$

3. For the hexagonal closed packed (hcp) structure, **(a)** what is the lattice and the basis? **(b)** If atoms are regarded as hard spheres, what should be the choice of axial ratio *c/a* to make the hard spheres touch? **(c)** what is the "packing fraction" (ratio of volume inside spheres to volume not inside spheres). **(d)** what is the packing fraction of the fcc and the bcc crystal structures?

(a) hcp $\vec{a} = \frac{a}{2}(1, -\sqrt{3}, 0)$

$\vec{b} = \frac{a}{2}(1, \sqrt{3}, 0)$

$c = c(0\ 0\ 1)$

basis: one atom at the origin, one at

$\tau = a\left(\frac{1}{2}, \frac{1}{2\sqrt{3}}, \frac{c}{2a}\right)$

(b) The atom spacing in plane is $|\vec{a}| = a$

The atom spacing to the next layer is $|\vec{\tau}|$

$|\vec{\tau}| = a\left[\frac{1}{3} + \frac{c^2}{4a^2}\right]$

These are equal if $\frac{c^2}{4a^2} = \frac{2}{3}$ $\quad c = \sqrt{\frac{8}{3}}\, a$

(c) volume of cell is $\frac{\sqrt{3}}{2} a^2 c = \sqrt{2} a^3$

This contains 2 atoms of volume $2 \cdot \frac{4\pi}{3}\left(\frac{a}{2}\right)^3 = \frac{\pi a^3}{3}$

ratio is $\frac{\pi}{3\sqrt{2}}$ = packing fraction $= 0.74$

(d) fcc has 8 atoms in a cube whose face diagonal is 2a

Length $= \sqrt{2} a$, volume $= 2\sqrt{2} a^3$

atom volume $= 4 \cdot \frac{4\pi}{3}\left(\frac{a}{2}\right)^3 = \frac{2\pi}{3} a^3$

packing fraction $= \frac{\pi}{3\sqrt{2}}$ same as hcp

bcc has 2 atoms in a cube whose body diagonal is 2a

Length $= \frac{2a}{\sqrt{3}}$ volume $= (2a/\sqrt{3})^3 = 8a^3/3\sqrt{3}$

atom volume $= 2\, \frac{4\pi}{3}\left(\frac{a}{2}\right)^3 = \pi a^3/3$

packing fraction is $\sqrt{3}\pi/8 = 0.68$