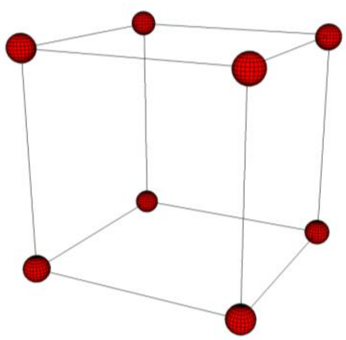
Condensed matter physics 2013
Exercise 2

Release: 24. Sep. 2013
Discussion: 1. Oct. 2013

Problem 6

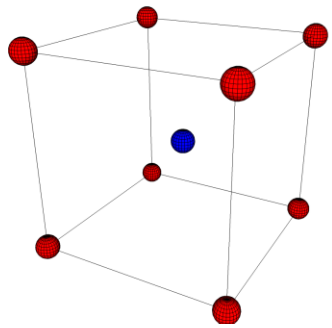
[1p]



Atoms inside the cube:
There is one host atom ("lattice point") at each corner of a cubic unit cell.
1/8 of each atom on the corner is in the cube: therefore total of 1 atom in the cube, Z=1. The unit cell is described by three edge lengths *a*
In this case *a* = 2r is the host atom radius, and ***a* the atom-atom distance**)
Nearest neighbours: 6 two along each of the xyz planes.
Filled Volume ratio:

$$\frac{Z\frac{4}{3}\pi r^3}{a^3} = \frac{\pi}{6}$$

BCC



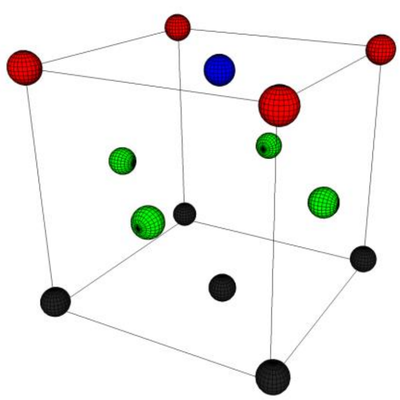
There is one host atom at each corner of the cubic unit cell and one atom in the cell center. **Each atom touches eight other host atoms** along the body diagonal of the cube, show in red relative to the blue atom.

Atom-atom distance: $\frac{\sqrt{3}}{2}a$

There are two atoms inside the unit cell (as for the simple cubic, + one additional atom in the centre, Z = 2).

The filled volume ratio can be calculated from the formula above to be: $\frac{\sqrt{3}\pi}{8}$

FCC



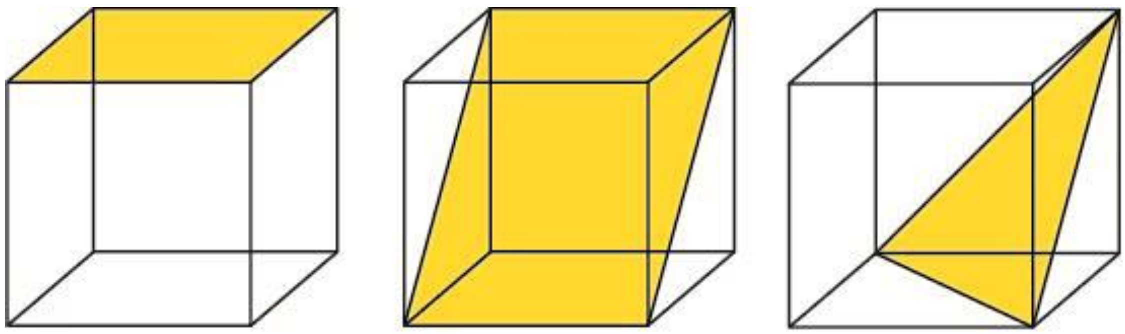
There is one host atom at each corner, one host atom in each face, and the host atoms touch along the face diagonal

Atom-atom distance: $\frac{a}{\sqrt{2}}$

Total number of atoms inside cube is Z= 4.
Each atom touches twelve other host atoms, taking the blue atom as reference:
the nearest neighbours are the red (4 nearest corner atoms) and the green (8 nearest face atoms where only lower atoms are shown here) .
This lattice is "closest packed", because spheres of equal size occupy the maximum amount of space in this arrangement (**$16\pi r^3/[3*(4r/\sqrt{2})^3] = \sqrt{2}\,\pi/6$**); since this closest packing is based on a cubic array, it is called "cubic closest packing": CCP = FCC.

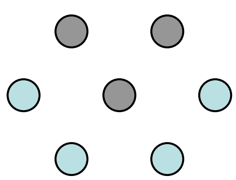
Problem 7

[2p]



(001) (011) (111)

Assume that *a* is the side length of the simple lattice
The rotation symmetry of (100) plane is C_4, the layer spacing is *a*
The rotation symmetry of (110) plane is C_2, the layer spacing is $a/\sqrt{2}$
The rotation symmetry of (111) plane is C_6. This can be understood by considering all the atoms in (111) plane instead of only three of them (in gray). The layer spacing is $a/\sqrt{3}$



See solution to problem 9(c) for spacing equation and proof

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Problem 8

Primitive vectors for hexagonal lattice:

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

a) By direct calculation, the volume of primitive cell is :

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = a\vec{x} \cdot [(\frac{a}{2}\vec{x} + \frac{\sqrt{3}a}{2}\vec{y}) \times c\vec{z}] = a\vec{x} \cdot [\frac{a}{2}c(-\vec{y}) + \frac{\sqrt{3}a}{2}c\vec{x}] = \frac{\sqrt{3}}{2}a^2c$$

[1p]

b) Calculate the reciprocal vector (shown here for b_1 repeat for b_2 and b_3):

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2 \times \vec{a}_3}{\frac{\sqrt{3}}{2}a^2c} = 2\pi\frac{\frac{a}{2}c(-\vec{y}) + \frac{\sqrt{3}a}{2}c\vec{x}}{\frac{\sqrt{3}}{2}a^2c} = \frac{4\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{2}\vec{x} - \frac{1}{2}\vec{y})$$

$$\vec{b}_2 = \frac{4\pi}{\sqrt{3}a}\vec{y}$$

$$\vec{b}_3 = \frac{2\pi}{c}\vec{z}$$

The vectors $\vec{b}_1$ and $\vec{b}_2$ generate a triangular lattice with lattice parameter $\frac{4\pi}{\sqrt{3}a}$ and $\vec{b}_3$ stacks this triangular lattice with layer spacing $2\pi/c$

The lattices are rotated by 30 degrees with respect to eachother:

$$\arccos(\frac{\vec{a_1} \cdot \vec{b_1}}{|\vec{a_1}||\vec{b_1}|})$$

[1p]

c) The first Brillion zone of the hexagonal lattice is also a hexagonal structure. The cross section of the Brillouin zone in xy plane is illustrated by the shaded are in the Figure 8. [1p]

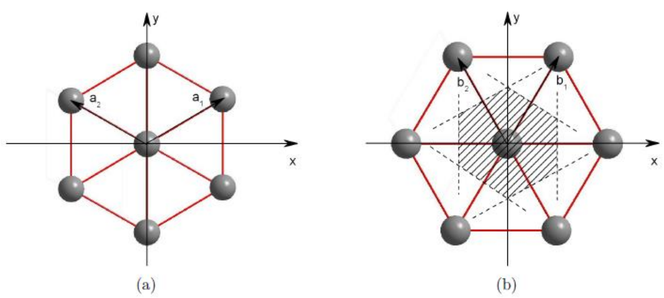
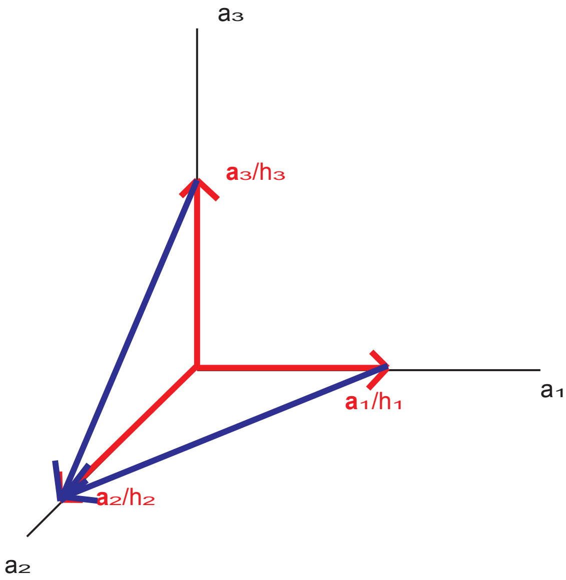


Figure 8: (a) xy plane of hexagonal lattice. (b) xy plane of the reciprocal lattice for hexagonal lattice. Shaded area indicates the Brillouin zone.

Problem 9



The reciprocal lattice vector $\vec{q}$ is normal to a plane.
Take two vectors in the plane (shown here in blue). The cross product of these two vectors gives another vector normal to the plane.

a)

$$\vec{q} = \sum_i h_i \vec{b}_i$$

for

$$(\frac{\vec{a}_1}{h_1} - \frac{\vec{a}_2}{h_2}) \times (\frac{\vec{a}_3}{h_3} - \frac{\vec{a}_2}{h_2}) = -\frac{1}{h_1 h_2}(\vec{a}_1 \times \vec{a}_2) - \frac{1}{h_2 h_3}(\vec{a}_2 \times \vec{a}_3) - \frac{1}{h_3 h_1}(\vec{a}_3 \times \vec{a}_1)$$

if we multiply by:

$$\frac{-2\pi h_1 h_2 h_3}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)}$$

we get

$$2\pi(\frac{h_1 \vec{a}_2 \times \vec{a}_3}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)} + \frac{h_2 \vec{a}_3 \times \vec{a}_1}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)} + \frac{h_3 \vec{a}_1 \times \vec{a}_2}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)}) = \vec{q}$$

b) Remember: $\vec{a} \cdot \vec{b} = |\vec{a}||\vec{b}|Cos\theta$
Take a vector to the plane: $\vec{a_i}/h_i$
The angle between this vector and the reciprocal lattice vector is:

$$\frac{\vec{a_1} \cdot \vec{q}}{|\vec{a_i}||\vec{q}|} = Cos\theta$$

The distance to a point on the plane is the length of the vector multiplied by the cosine of the angle:

$$\frac{|\vec{a_i}|}{h_i} Cos\theta$$

Therefore:

$$d = \frac{|\vec{a_i}|}{h_i} \cdot \frac{\vec{a_i} \cdot \vec{q}}{|\vec{a_i}||\vec{q}|} = \frac{\vec{a_i} \cdot \vec{q}}{h_i |\vec{q}|} = 2\pi / |\vec{q}|$$

c)

$$d = 2\pi / |\vec{q}\,|$$

for a simple cubic lattic:

$$|\vec{b}_i|^2 = (\frac{2\pi}{a})^2$$

this gives:

$$d^2 = (2\pi/|\vec{q}\,|)^2 = \frac{4\pi^2}{(h_1^2 b_1^2 + h_2^2 b_2^2 + h_3^2 b_3^2)} = a^2/(h_1^2 + h_2^2 + h_3^2)$$

Problem 10

The edge directions of the {111} plane-bounded inverted pyramids are {110}, this can be easily understood if we check our Problem 7. The top angle of the pyramid is:

$$\alpha = 180^\circ - arccos \left[\frac{\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}}{\left| \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right| \left| \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} \right|} \right] = 70.5^\circ$$