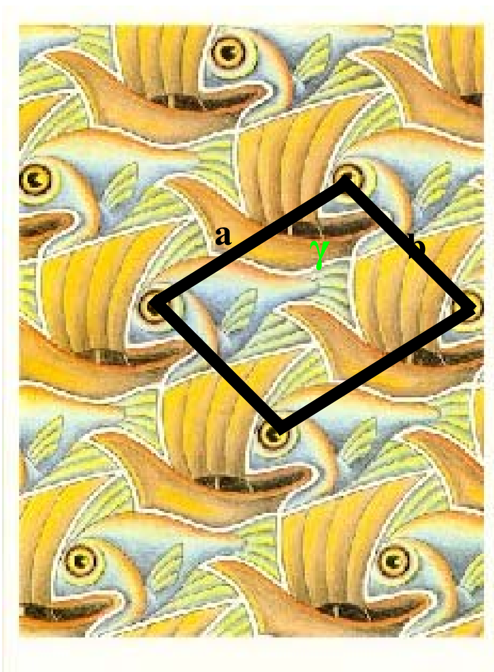
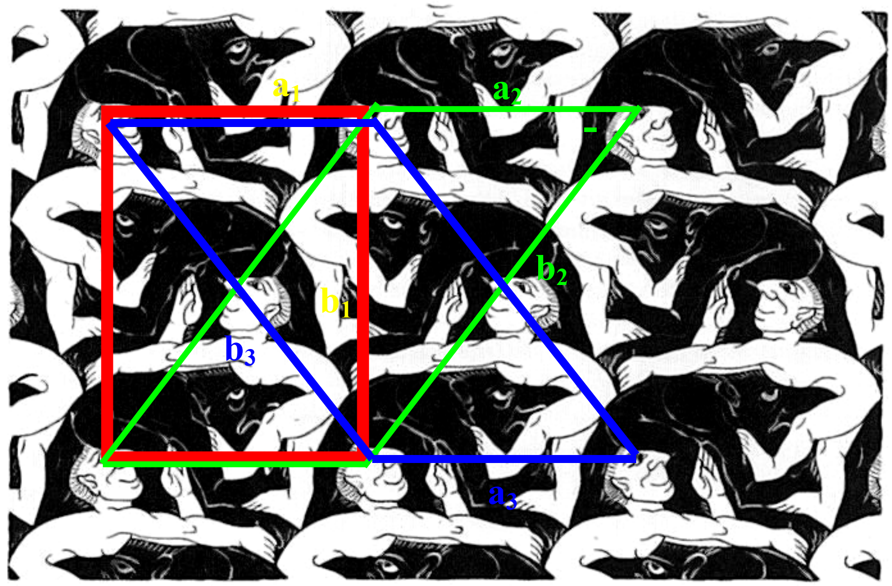
EMSE314--Fall 2003--Homework 1--Name: Changrong Li
Issued: Aug. 29, Due: Sep. 08

Problem 1 (8 points)





48. Regelmäßige Flächenaufteilung für Begegnung. Bleistift und schwarze Tusche. 1944

Unit cell drawing *(2 pts)*

Unit cell parameters *(2 pts)*

a = 2.4 cm
b = 3.1 cm
γ = 103.5°

Unit cell drawing *(2pts)*

Unit cell parameters *(2 pts)*

a_1 = 3.5 cm
b_1 = 4.6cm
γ = 90°

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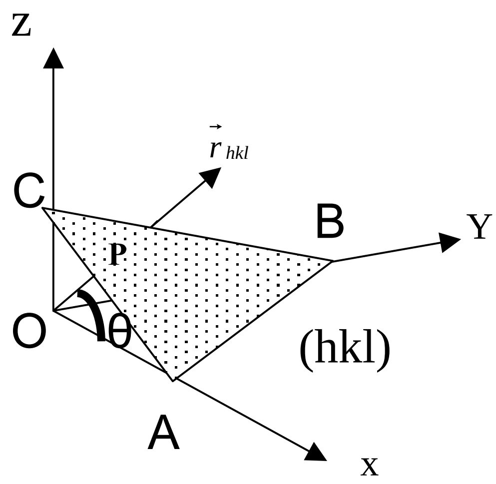
Problem 2 (12 points)



(a) (7pts) As shown in the above sketch, the [*hkl*] direction is defined by vector $\mathbf{r}_{hkl}$ **,** where $\mathbf{r}_{hkl} = h\mathbf{a} + k\mathbf{b} + l\mathbf{c}$**.** Meanwhile, plane (*hkl*) (shown as plane ABC) intersects the *x,y,z* axes at a/h, b/k and c/l by definition. Hence

$\overrightarrow{OA} = \vec{a}/h$, $\overrightarrow{OB} = \vec{b}/k$, $\overrightarrow{OC} = \vec{c}/l$, and

$\overrightarrow{AB} = \overrightarrow{OB} - \overrightarrow{OA} = \vec{b}/k - \vec{a}/h$,

$\overrightarrow{BC} = \overrightarrow{OC} - \overrightarrow{OB} = \vec{c}/l - \vec{b}/k$

Taking the dot products of these plane vectors and $\mathbf{r}_{hkl}$:

$$\overrightarrow{AB} \bullet \overrightarrow{r_{hkl}} = (\vec{b}/k - \vec{a}/h) \bullet (h\vec{a} + k\vec{b} + l\vec{c}) = b^2 - a^2 = 0;$$

$$\overrightarrow{BC} \bullet \overrightarrow{r_{hkl}} = (\vec{c}/l - \vec{b}/k) \bullet (h\vec{a} + k\vec{b} + l\vec{c}) = c^2 - b^2 = 0,$$

where we use the facts that $\vec{a} \bullet \vec{b} = \vec{b} \bullet \vec{c} = \vec{c} \bullet \vec{a} = 0$ and $a = b = c$ in a cubic crystal.

In conclusion, $\overrightarrow{AB} \perp \overrightarrow{r_{hkl}}$ and $\overrightarrow{BC} \perp \overrightarrow{r_{hkl}}$. Therefore the result holds.

(b) (5pts) Suppose $\mathbf{r}_{hkl}$ intersect (hkl) plane at point P.

It is clear that $d = \left|\overrightarrow{OP}\right| = \left|\overrightarrow{OA}\right| \bullet \cos\angle AOP = \overrightarrow{OA} \bullet \overrightarrow{OP} / \left|\overrightarrow{OP}\right| = \overrightarrow{OA} \bullet \overrightarrow{r_{hkl}} / \left|\overrightarrow{r_{hkl}}\right|$

$$= \frac{\vec{a}}{h} \bullet \frac{h\vec{a} + k\vec{b} + l\vec{c}}{\left|h\vec{a} + k\vec{b} + l\vec{c}\right|} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$

Here we use the facts that $\vec{a} \bullet \vec{b} = \vec{b} \bullet \vec{c} = \vec{c} \bullet \vec{a} = 0$ and $a = b = c$ in a cubic crystal again.

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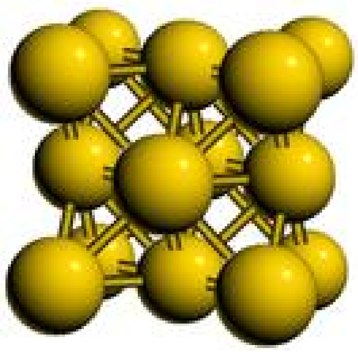
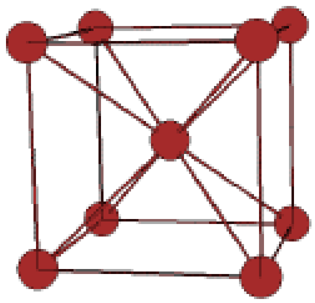
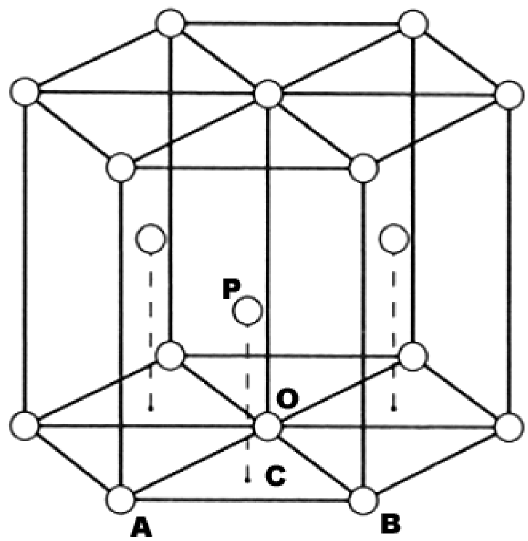
Problem 3 (15 points)







In hard sphere theory, the nearest neighbors touch each other. Suppose the radius of the atoms and lattice parameter of a cubic lattice are r and a, respectively.
(a) For the fcc structure, there are 8*1/8+6*1/2=4 atoms per unit cell.

$$\sqrt{2}a/2 = 2r \Rightarrow r = \sqrt{2}a/4 \Rightarrow APF = \frac{4\times 4\pi r^3/3}{a^3} = 4\times\frac{4}{3}\pi\times\left(\frac{\sqrt{2}}{4}\right)^3 = \frac{\sqrt{2}\pi}{6} \approx 0.740$$

(b) For the bcc structure, there are 8*1/8+1=2 atoms per unit cell.

$$\sqrt{3}a/2 = 2r \Rightarrow r = \sqrt{3}a/4 \Rightarrow APF = \frac{2\times 4\pi r^3/3}{a^3} = 2\times\frac{4}{3}\pi\times\left(\frac{\sqrt{3}}{4}\right)^3 = \frac{\sqrt{3}\pi}{8} \approx 0.680$$

(c) For hcp structure, consider tetrahedron OABP (a, c are lattice parameter.)
OA=a, $OP = \sqrt{PC^2 + OC^2} = \sqrt{(c/2)^2 + (\sqrt{3}a/3)^2} = \sqrt{c^2/4 + a^2/3}$
To reach maximum APF, we must have OA=OP, i.e.
$a^2 = c^2/4 + a^2/3 \Rightarrow c/a = \sqrt{8/3}$ =1.633.

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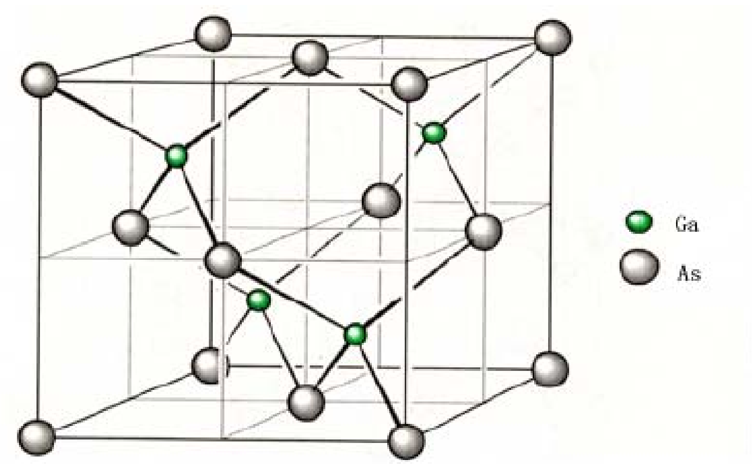
Problem 4 (15 points)

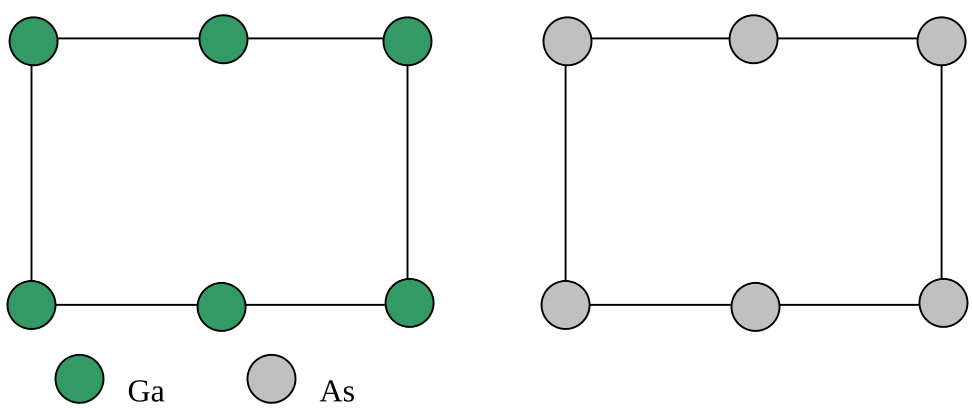
(a) A unit cell of GaAs is shown as the following



Note that the positions of Ga and As atoms are interchangeable.

(b) It is an fcc lattice with 4 lattice point and 8 atoms per unit cell. Suppose the coordinates of As atoms are (000) (1/2 1/2 0) (1/2 0 1/2) and (0 1/2 1/2). Those of Ga atoms are (¼ ¼ ¼), (¾ ¾ ¼), (¾ ¼ ¾) and (¼ ¾ ¾) correspondingly.

(c) There are two possible configurations in a (110) plane of the GaAs structure.



(d) According to the geometry, if two nearest Ga atoms touch each other, we have $\sqrt{2}a/2 = 2*0.126nm \Rightarrow a = 0.356nm$, where a stands for the lattice parameter.

If two nearest As atoms touch, we have $\sqrt{2}a/2 = 2*0.120nm \Rightarrow a = 0.339nm.$

If two nearest Ga and As neighbors touch, $\sqrt{3}a/4 = 0.246nm \Rightarrow a = 0.568nm.$

It is clear that the lattice parameter should be 0.568nm.

Moreover, there are 8 atoms (4 Ga and 4 As atoms) per unit cell, so the density is given by $\rho = \frac{weight\_of\_8\_atoms}{volume\_of\_unit\_cell} = \frac{4\times(69.72+74.92)\times10^{-3}kg/(6.02\times10^{23})}{(0.568\times10^{-9}m)^3}$

$=5.24*10^3$kg/m^3.

(FYI, a= 0.5653 nm, density= $5.318*10^3$ kg.m^{-3}at 300k for GaAs)