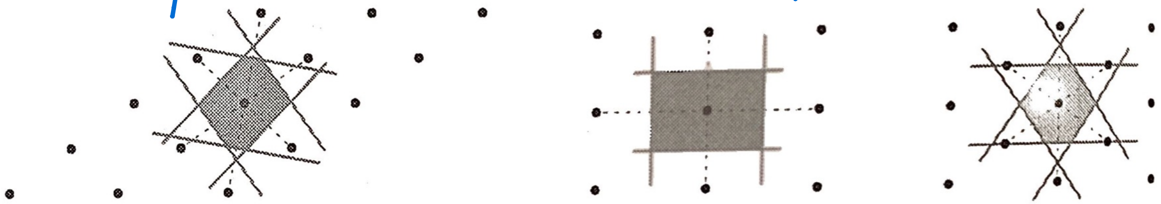
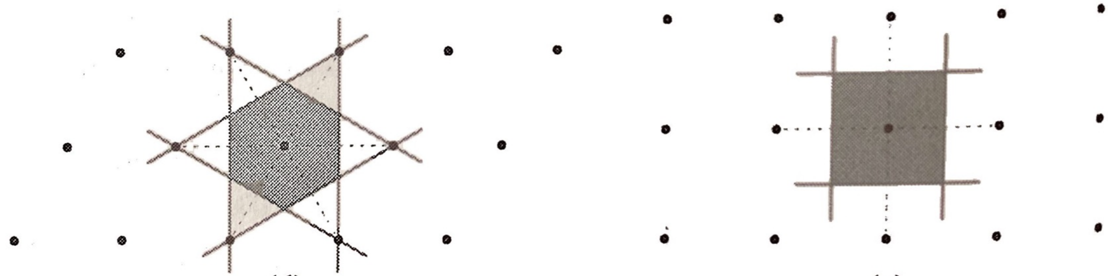
Homework 2 Solutions

P1

Oblique rectangular Centered rectangular



(a) (b) (c)



(d) (e)

Triangular square

For each **Bravais lattice** dotted lines connect the reference lattice point to the nearby lattice points. Solid lines bisect the connecting lines and they also become a part of the boundaries of W-S cells. All W-S. cells are shaded.

p.2 In the diamond structure, there are 8 Sn atoms in a conventional u.c.

Thus the mass density in the diamond structure

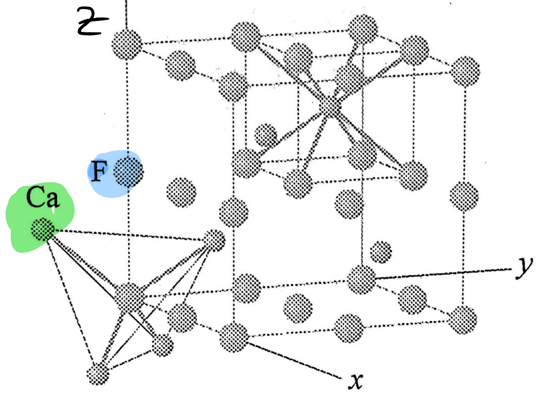
$$\rho_{diamond} = \frac{8\, m_{Sn}}{a^3_{diamond}} \approx 5.768\, \frac{kg}{m^3}$$

In the body-centered tetragonal structure, there are two Sn atoms in a conventional u.c.

Thus the mass density is:

$$\rho_{tetra} = \frac{2\, m_{Sn}}{a^2_{tetra} \cdot c_{tetra}} \cong 3.647\, \frac{kg}{m^3}$$

P.3. The crystal structure of CaF_2 is shown in Figure below:



1) As you see F is 4-coordinated $\Rightarrow Z=4$
and Ca is 8-coordinated $\Rightarrow Z=8$

2) Two Ca lattice planes are along the [111] direction can be seen in the figure:
with one containing Ca $(\frac{1}{4}\ -\frac{1}{4}\ -\frac{1}{4})$
$(-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4})a$, $(-\frac{1}{4}, -\frac{1}{4}, \frac{1}{4})a$
and the other containing Ca ions at:
$(\frac{1}{4}, \frac{3}{4}, \frac{3}{4})a$, $(\frac{3}{4}, \frac{1}{4}, \frac{3}{4})a$
and $(\frac{3}{4}, \frac{3}{4}, \frac{1}{4})a$

But they are <u>not succesive</u> planes b/c the Ca latice plane containing the Ca ion at $(\frac{1}{4}\ \frac{1}{4}, \frac{1}{4})a$ is in between.

Thus the lattice spacing along the [111] direction between the SUCCESIVE PLANES is <u>half</u> the sum of the perpendicular distances from the origin and we get:

$$d_{111}^{Ca} = \frac{1}{2}\frac{(1,1,1)}{\sqrt{3}} \cdot \left[\left(\frac{3}{4},\frac{3}{4},\frac{1}{4}\right)a - \right.$$

$$\left. - \left(\frac{1}{4},-\frac{1}{4},-\frac{1}{4}\right)a\right] = \frac{a}{\sqrt{3}}$$

Another way

On the other hand all the Ca atoms form the FCC B. lattice with the lattice parameter a.

The shortest reciprocal lattice vector in the [111] direction in this fcc is $K_0^{Ca} = (1,1,1)\left(\frac{2\pi}{a}\right)$

$^{=\sqrt{3}}$

Thus we can get d_{111}^{Ca}

$$d_{111}^{Ca} = \frac{2\pi}{|K_0^{Ca}|} = \frac{a}{\sqrt{3}}$$

Note, all the F atoms form the simple cubic B. lattice with the lattice constant $a/2$.

The shortest reciprocal lattice vector

$$K_0^F = (111)\left(\frac{4\pi}{a}\right) \Rightarrow d^F_{111} = \frac{2\pi}{|K_0^F|} = \frac{a}{2\sqrt{3}}$$

$|(111)| = \sqrt{3}$

p5. 1) We 1^{st} find the general solution to the homogenious eqn. and then we find the special solution to the inhomogenious eqn.

Thus for the homogeneous case

$$\ddot{r}_j + \gamma \dot{r}_j + \omega_j^2 r_j = 0$$

The characteristic eqn:

$$\lambda^2_j + \gamma \lambda_j + \omega^2_j = 0 \Rightarrow$$

$$\lambda_j^{\pm} = -\gamma/2 \pm i\left(\omega_j^2 - \gamma^2/4\right)^{1/2} =$$

$$\equiv -\gamma/2 \pm i\omega_{z_j}$$

where I call $\omega_{z_j} = \sqrt{\omega_j^2 - \gamma^2/4}$

For weak damping we have

$\omega_j > \gamma/2$ for all j's.

Thus the general solution is

$$r_j^{homog.} = e^{-\gamma t/2}\left(A_j e^{i\omega_{z_j} t} + B_j e^{-i\omega_{z_j} t}\right)$$

For a special case of the inhomo-genious eqn., considering the presence of the exponent $e^{i(\kappa \cdot r_j - \omega t)}$ we set:

$$r_j^s = C_j e^{i(\kappa \cdot r_j - \omega t)}$$

Substituting r_j^s into the homogeneous eqn. yeilds:

$$(-\omega^2 - i\gamma\omega + \omega_j^2)\, C_j = -\left(\frac{e}{m}\right)\epsilon_k E_0$$

$$C_j = -\frac{(e/m)\, E_0 \epsilon_k}{\omega_j^2 - \omega^2 - i\gamma\omega}$$

Thus the general eqn: is

$$r_j = r_j^h + r_j^s =$$

$$= e^{-\gamma t/2}\left(A_j e^{i\omega_{z_j} t} + B_j e^{-i\omega_z t}\right)$$

$$- \frac{\left(\frac{e}{m}\right) E_0 \epsilon_k}{\omega_j^2 - \omega^2 - i\gamma\omega} \cdot e^{i(k\cdot r_j - \omega t)}$$

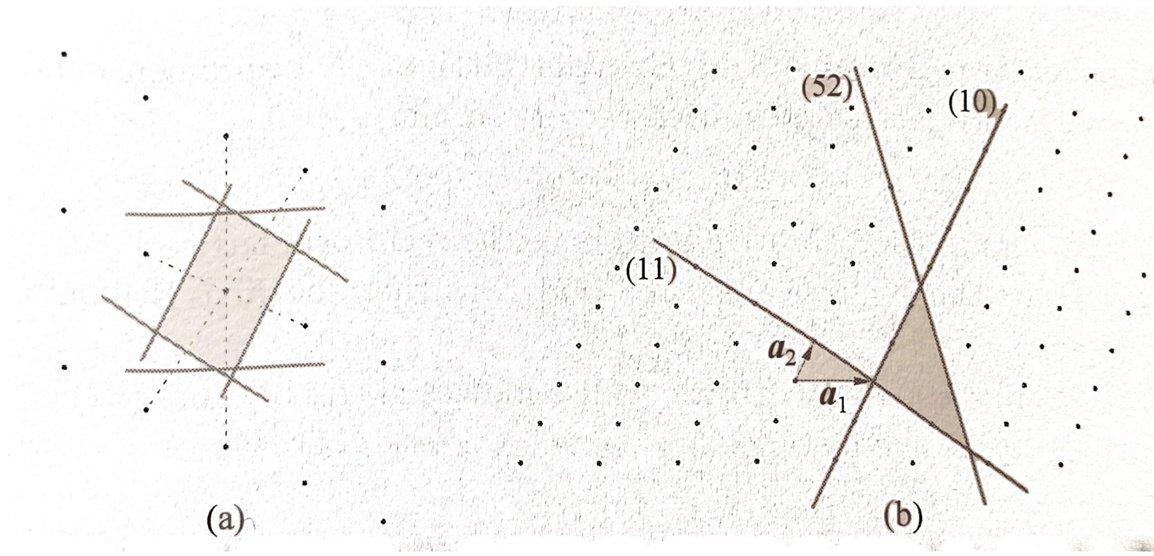
2) The 1^{st} term in the r_j decays rapidly with time. After a short period of t it's undetactable. We then have the steady-state solution:

$$r_j = -\frac{\left(\frac{e}{m}\right) E_0 \epsilon_k}{\omega_j^2 - \omega^2 - i\gamma\omega}\, e^{i(k\cdot r_j - \omega t)}$$

p.6 1) $\bar{b}_1 = \frac{5\pi}{2}(2e_x - e_y) = \frac{5\pi}{2}\begin{pmatrix} 2 \\ -1 \end{pmatrix}$

$$\bar{b}_2 = 10\pi \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 10\pi \, \bar{e}_y$$

2) The reciprocal lattice and the 1^{st} BZ are shown in fig below



The dotted lines are the lines connecting the concerned points with the lattice nearby. The solid lines bisect these connecting lines. The smallest region is the 1^{st} BZ.

3) The direct lattice and (11) and (10) and (52)

planes are given below in the Figure on the previos page

4) The shortest reciprocal vector perpendicular to (11) family of lattice planes is

$$\bar{K}_0 = \bar{b}_1 + \bar{b}_2 = (\bar{e}_x + 3\bar{e}_y/2)\cdot 5\pi$$

Thus $d_{11} = \frac{2\pi}{|K_0|} = \frac{4}{5\sqrt{13}} = 0.22188\,nm$

P7. 1) Evaluating the volume of the primitive cell we get

$$V = a_1 \cdot (a_2 \times a_3)$$

$$= \left(\frac{\sqrt{3}}{2} a e_x + \frac{1}{2} a e_y\right) \cdot \left[\left(-\frac{\sqrt{3}}{2} a e_x +\right.\right.$$

$$+ \frac{1}{2} a e_y \Big) \times (c e_z) \Big]$$

$$= \left(\frac{\sqrt{3}}{2} a e_x + \frac{1}{2} a e_y \right) \cdot \left(\frac{\sqrt{3}}{2} a c e_y + \frac{1}{2} a c e_x \right) = \frac{\sqrt{3}}{2} a^2 c$$

2) For b_1 we have

$$b_1 = 2\pi \frac{a_2 \times a_3}{V} = \frac{2\pi}{\sqrt{3} a^2 c / 2} \cdot$$

$$\cdot \left(-\frac{\sqrt{3}}{2} a e_x + \frac{1}{2} a e_y \right) \times c e_z =$$

$$= \frac{4\pi}{\sqrt{3} a} \left(\frac{1}{2} e_x + \frac{\sqrt{3}}{2} e_y \right)$$

For b_2

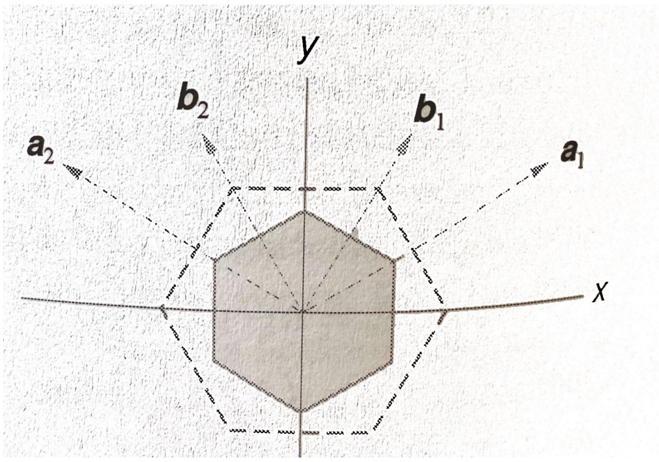
$$b_2 = 2\pi \frac{a_3 \times a_1}{V} = \frac{2\pi}{\sqrt{3} a^2 c / 2} c e_z \times$$

$$\left(\frac{\sqrt{3}}{2} a e_x + \frac{1}{2} a e_y \right) = \frac{4\pi}{\sqrt{3} a} \left(-\frac{1}{2} e_x + \frac{\sqrt{3}}{2} e_y \right)$$

For b_3:

$$b_3 = \frac{2\pi}{c} e_z$$

The 1st two components (x and y) of the above given primitive unit vectors of both the reciprocal and direct lattices are shown in figure below



Solid lines are for reciprocal and dashed lines for direct vectors.

Also I show the W-S. cell of direct and reciprocal spaces.

From the orientation of the W-S cell we see that the reciprocal lattice is 30° rotated about the z axis relative to the direct lattice and if b_1 (b_2) is chosen to be along the positive (negative) axis, then the primitive vectors of the recipr. lattice appear to be rotated by 30° about the z axis relative to the primitive vectors of the direct lattice.

3) The 1^{st} BZ of the simple hexagonal Bravais lattice is shown bellow.