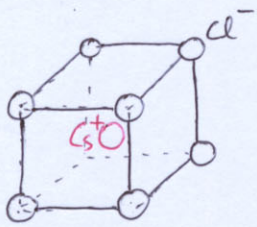
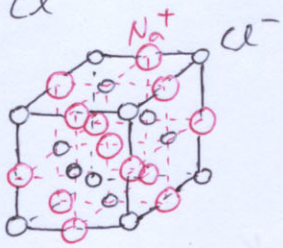
Homework #2

1. $CsCl$



Coordination number = 8

$NaCl$



FCC array of Cl^-

Octahedral sites ~ Na^+

Coordination number = 6

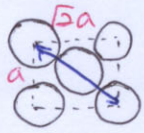
① radius of $Cs^+ = 0.165\ nm$, $Cl^- = 0.181\ nm$ $\Rightarrow r^+/r^- \simeq 0.92$

$0.732 < r^+/r^- < 1$ 이므로 coordination number = 8

② radius of $Na^+ = 0.098\ nm$, $Cl^- = 0.181\ nm$ $\Rightarrow r^+/r^- \simeq 0.54$

$0.414 < r^+/r^- < 0.732$ 이므로 coordination number = 6

2. ① (1 1 0) plane of BCC



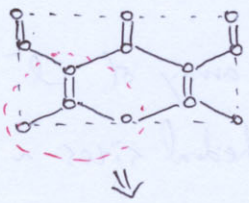
diagonal … $4r = \sqrt{3}\,a$ $\therefore a = \frac{4}{\sqrt{3}}r$

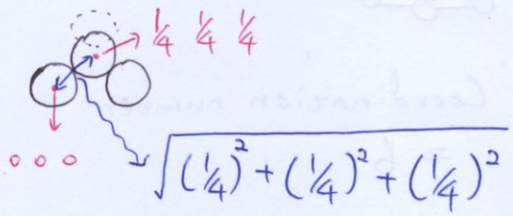
volume of unit cell $= a^3 = \frac{64}{3\sqrt{3}}r^3$

# of atoms in an unit cell = 2 $\Rightarrow$ volume $= 2 \times \frac{4}{3}\pi r^3$

$\therefore APF = \frac{\frac{8}{3}\pi r^3}{\frac{64}{3\sqrt{3}}r^3} = \frac{\sqrt{3}\pi}{8} \simeq 0.68$

② (110) projection of diamond structure





$\therefore a = \frac{8}{\sqrt{3}}r$

volume of unit cell $= a^3 = \frac{8^3}{3\sqrt{3}}r^3$

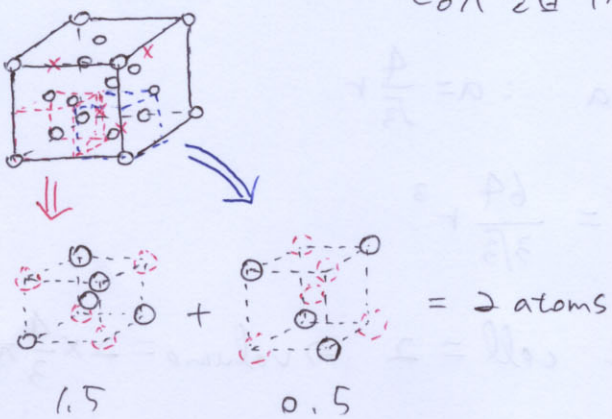
# of atoms in an unit cell $= 8 \rightarrow$ volume $= 8 \times \frac{4}{3}\pi r^3$

$\therefore APF = \frac{8\times\frac{4}{3}\pi r^3}{\frac{8^3}{3\sqrt{3}}r^3} = \frac{4\sqrt{3}\pi}{64} \simeq 0.34$

BCC → coordination number = 8

diamond cubic structure → coordination number = 4 (공유 결합이기 때문)

> bonding과 관련된 설명이 없으면 감점.

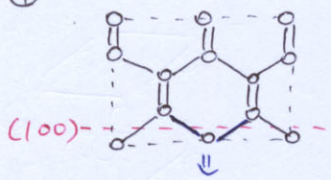


BCC이면 4 atoms/unit cell

∴ bonding nature의 차이 때문에 coordination number가 diamond structure에서 1/2이어서 APF도 1/2이다.

3. (110) projection of diamond structure 이용.

①



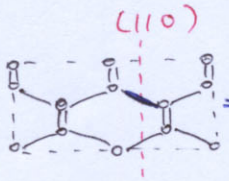
# of broken bonds = 2

areal density = $2/a_0^2$

$\therefore \gamma_{100} = \frac{\varepsilon}{2} \times (\#\text{ of broken bonds}) \times (\text{areal density})$

$= \frac{2\varepsilon}{a_0^2}$

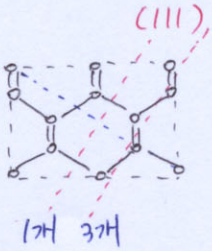
②



⇒ # of broken bonds = 1

areal density = $\frac{4}{\sqrt{2}a_0^2}$ $\quad \therefore \gamma_{110} = \frac{\sqrt{2}\varepsilon}{a_0^2}$

③



~ # of broken bonds = 1 or 3

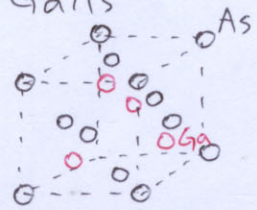
이 중 energy가 낮은 plane으로 cleavage가 일어나므로,

# of broken bonds = 1

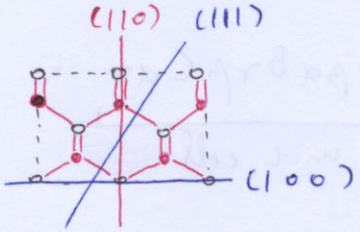
areal density = $\frac{2}{\frac{\sqrt{3}}{2}a_0}$ $\quad \therefore \gamma_{111} = \frac{2\sqrt{3}}{3}\frac{\varepsilon}{a_0^2}$

$\gamma_{111} < \gamma_{110} < \gamma_{100}$ 이므로 (111)면으로 cleavage 된다.

GaAs → ZnS structure

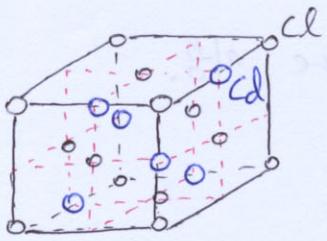


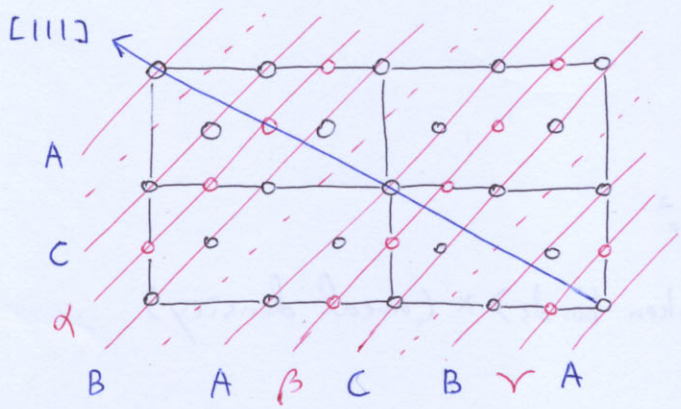
(110) projection ⇒



projection에서와 같이, (111)면으로 잘리면 Ga 또는 As만 surface에 존재하여 불안정 (ionic bonding이 있기 때문). 반면 (110)으로 잘리면 Ga와 As가 1:1로 존재하여 stable. → charge neutrality고려.

4. ① $CdCl_2$



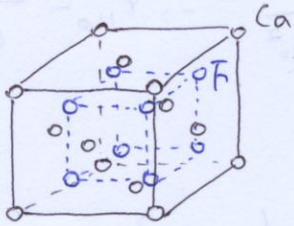


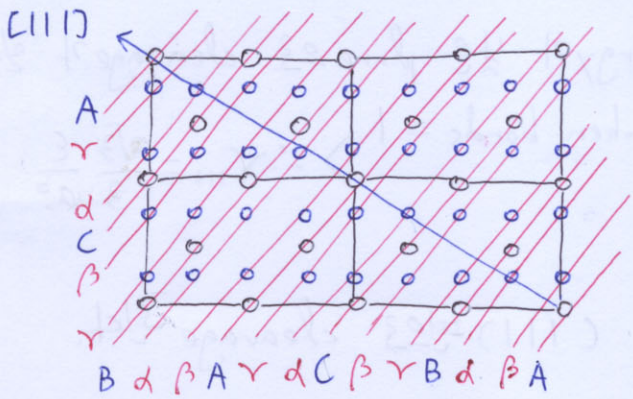
Cd layer ~ 1/2 octahedral site
(교차로 나타남.)

⇒ A γ B C β A B α C ····

unit cell

② CaF_2





⇒ A β α B γ β C α γ ···

unit cell