Homework ※3.

1. (i) BCC

① primitive translation vector

$a_1 = \frac{1}{2}a(\bar{1}11)$, $a_2 = \frac{1}{2}a(1\bar{1}1)$, $a_3 = \frac{1}{2}a(11\bar{1})$

② reciprocal lattice translation vector.

from equ.

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3} , \quad b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3} , \quad b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3}$$

$b_1 = \frac{2\pi}{a}(011)$, $b_2 = \frac{2\pi}{a}(101)$, $b_3 = \frac{2\pi}{a}(110)$

③ $G = v_1 b_1 + v_2 b_2 + v_3 b_3 = \frac{2\pi}{a}[(v_2+v_3)\hat{x} + (v_1+v_3)\hat{y} + (v_1+v_2)\hat{z}]$

(v_1 , v_2 , v_3 는 정수)

이중 가장 짧은 G vector는

$\frac{2\pi}{a}(\pm\hat{y}\pm\hat{z})$; $\frac{2\pi}{a}(\pm\hat{x}\pm\hat{z})$; $\frac{2\pi}{a}(\pm\hat{x}\pm\hat{y})$

의 12개 이다. [FCC 꼴]

Brillouin zone은 이 12개 vector의 수직 이등분면으로

이루어진다. 따라서 정십이면체이다.

Homework ※.3.

3. (ii) FCC

① primitive translation vector

$a_1 = \frac{1}{2}a(011)$, $a_2 = \frac{1}{2}a(101)$, $a_3 = \frac{1}{2}a(110)$

② reciprocal lattice translation vector

$b_1 = \frac{2\pi}{a}(\bar{1}11)$, $b_2 = \frac{2\pi}{a}(1\bar{1}1)$, $b_3 = \frac{2\pi}{a}(11\bar{1})$

③ $G = v_1 b_1 + v_2 b_2 + v_3 b_3$ (v_1, v_2, v_3 는 정수)

$$= \frac{2\pi}{a}[(-v_1+v_2+v_3)\hat{x} + (v_1-v_2+v_3)\hat{y} + (v_1+v_2-v_3)\hat{z}]$$

이중 가장 짧은 G vector는

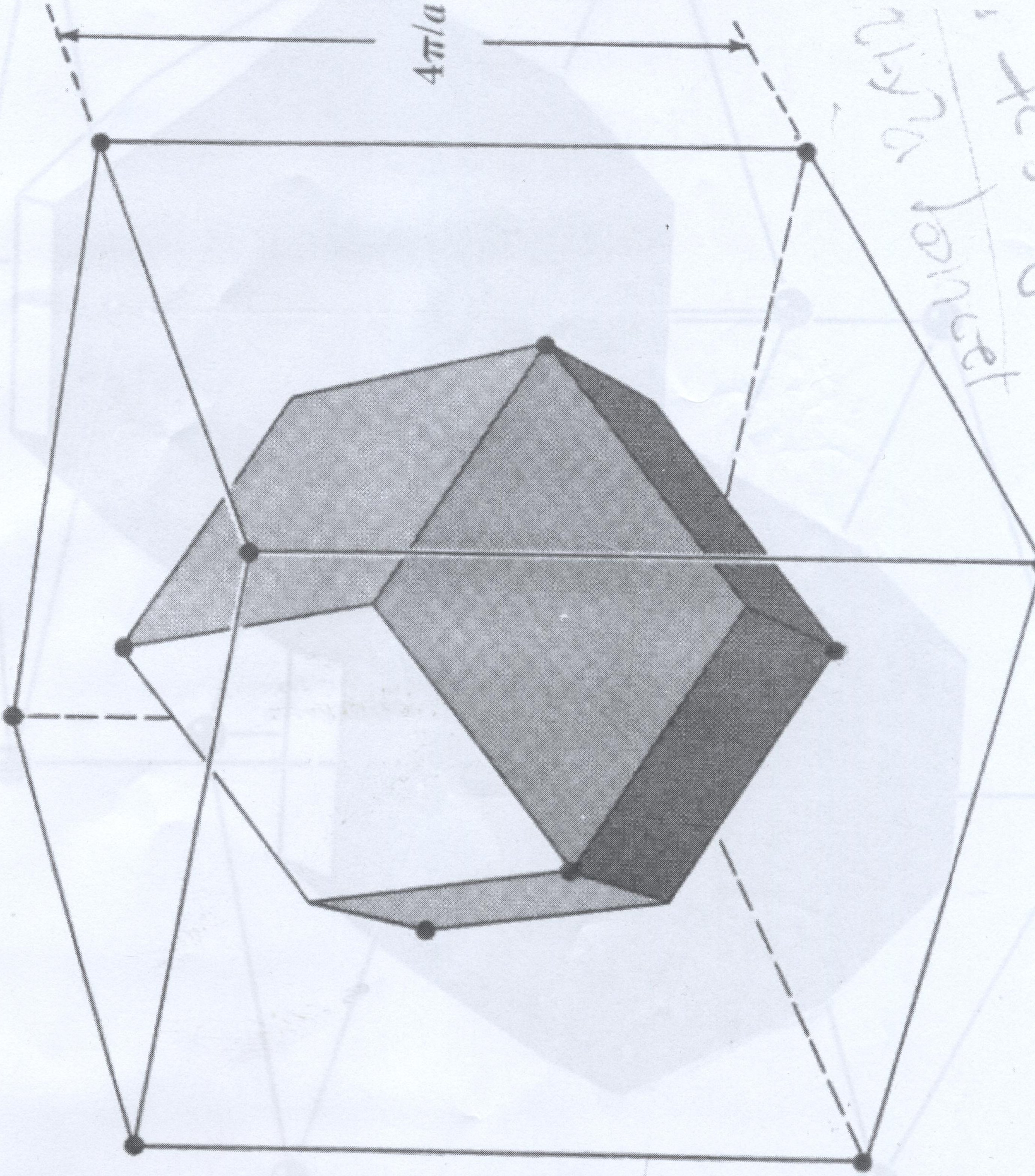
$$\frac{2\pi}{a}(\pm\hat{x} \pm\hat{y} \pm\hat{z})$$

의 8개 이다. [BCC 구조]

Brillouin zone은 이 8개 벡터의 수직이등분면으로 결정된다.

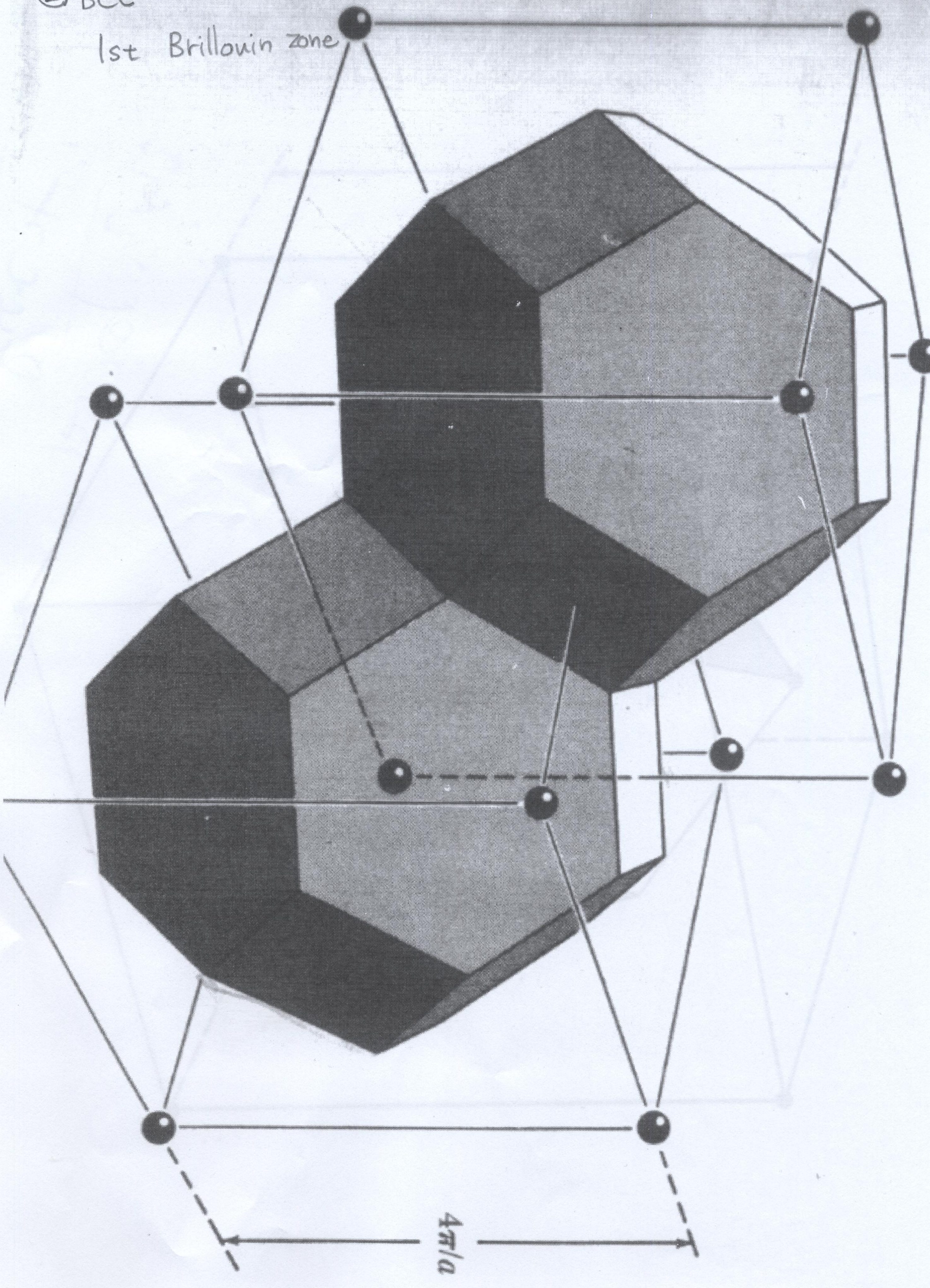
따라서 8면체이다.

1st
① BCC Brillouin zone



② BCC

1st Brillouin zone



2. $G = 2\pi \left(h_1 \vec{b_1} + h_2 \vec{b_2} + h_3 \vec{b_3} \right)$

For FCC ; $\vec{b_1} = \frac{1}{a}(\bar{1}11)$

$\vec{b_2} = \frac{1}{a}(1\bar{1}1)$

$\vec{b_3} = \frac{1}{a}(11\bar{1})$

Due to periodicity $k' = k + G$

$$E_{k'} = \frac{\hbar^2}{2m}(k+G)^2$$

in the k_x direction ; $k_x = \frac{2\pi}{a}(x i) \quad (0 \leqq x \leqq 1)$

$$E_k = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}(x i) + G\right)^2$$

(a) $h_1/h_2/h_3$: $1\bar{1}\bar{1}$

$$G = 2\pi \left(\vec{b_1} - \vec{b_2} - \vec{b_3} \right)$$

$$= \frac{2\pi}{a}\left(-i \cancel{+j} + k - i + j \cancel{-k} - i \cancel{-j} + k\right)$$

$$= \frac{2\pi}{a}(-3i + j + k)$$

$$\therefore E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}(x i) + \frac{2\pi}{a}(-3i + j + k)\right)^2$$

$$= \underbrace{\frac{\hbar^2}{2m}\cdot\left(\frac{2\pi}{a}\right)^2}_{= C}\left((x-3)^2 + 2\right) \quad \begin{cases} x = 0 \rightarrow 11C \\ x = 1 \rightarrow 6C \end{cases}$$

(b) $h_1/h_2/h_3$: 001

$$G = 2\pi \left(\vec{b_3} \right) = \frac{2\pi}{a}(i + j - k)$$

$$\therefore E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}(x i) + \frac{2\pi}{a}(i + j - k)\right)^2$$

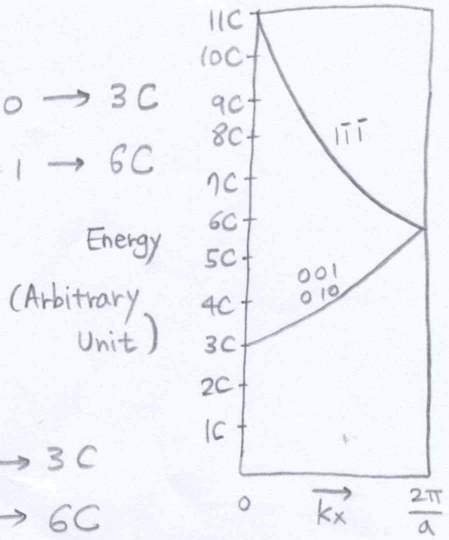
$$= \frac{\hbar^2}{2m}\cdot\left(\frac{2\pi}{a}\right)^2\left((x+1)^2 + 2\right) \quad \begin{cases} x = 0 \rightarrow 3C \\ x = 1 \rightarrow 6C \end{cases}$$

(c) $h_1/h_2/h_3$: 010

$$G = 2\pi \left(\vec{b_2} \right)$$

$$\therefore E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}(x i)^2 + \frac{2\pi}{a}(i - j + k)\right)^2$$

$$= \frac{\hbar^2}{2m}\cdot\left(\frac{2\pi}{a}\right)^2\left((x+1)^2 + 2\right) \quad \begin{cases} x = 0 \rightarrow 3C \\ x = 1 \rightarrow 6C \end{cases}$$



3. 주기성 $k' = k + \underbrace{G}_{\text{translation vector}}$ $G = 2\pi(h_1\vec{b_1} + h_2\vec{b_2} + h_3\vec{b_3})$

· For BCC; $\vec{b_1} = \frac{1}{a}(011)$

$\vec{b_2} = \frac{1}{a}(101)$

$\vec{b_3} = \frac{1}{a}(110)$

$$E_{K'} = \frac{\hbar^2}{2m}(k+G)^2$$

in the k_x direction ; $k_x = \frac{2\pi}{a}(x i)$ $(0 \leqq x \leqq 1)$

$$E_k = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}(x i) + G\right)^2$$

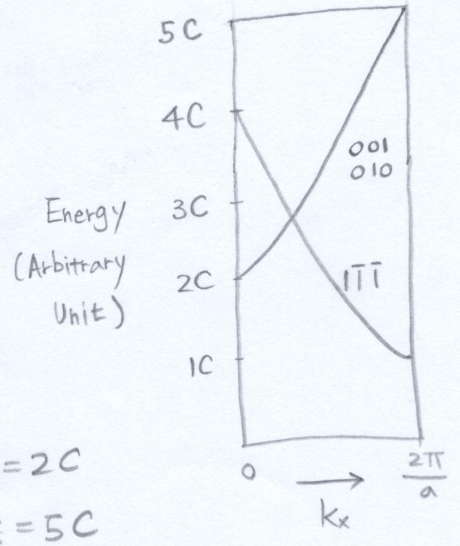
(a) $h_1/h_2/h_3$: $1\bar{1}\bar{1}$

$$G = 2\pi(\vec{b_1} - \vec{b_2} - \vec{b_3})$$

$$= \frac{2\pi}{a}(\cancel{j} + \cancel{k} - i - \cancel{k} - i - \cancel{j})$$

$$\therefore E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}(x i) + \frac{2\pi}{a}(-2i)\right)^2$$

$$= \underbrace{\frac{\hbar^2}{2m}\cdot\left(\frac{2\pi}{a}\right)^2}_{C}(x-2)^2 \quad \begin{cases} x=0 \rightarrow E = 4C \\ x=1 \rightarrow E = C \end{cases}$$



(b) $h_1/h_2/h_3$: 001

$$G = 2\pi(\vec{b_3})$$

$$= \frac{2\pi}{a}(i+j)$$

$$\therefore E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}(x i) + \frac{2\pi}{a}(i+j)\right)^2$$

$$= \frac{\hbar^2}{2m}\cdot\left(\frac{2\pi}{a}\right)^2\cdot((x+1)i + j)^2$$

$$= C\cdot((x+1)^2+1) \quad \begin{cases} x=0 \rightarrow E=2C \\ x=1 \rightarrow E=5C \end{cases}$$

(c) $h_1/h_2/h_3$: 010

$$G = 2\pi(\vec{b_2}) = \frac{2\pi}{a}(i+k)$$

$$\therefore E = \frac{\hbar^2}{2m}\cdot\left(\frac{2\pi}{a}(x i) + \frac{2\pi}{a}(i+k)\right)^2$$

$$= \frac{\hbar^2}{2m}\cdot\left(\frac{2\pi}{a}\right)^2((x+1)^2+1) \quad \begin{cases} x=0 \rightarrow E=2C \\ x=1 \rightarrow E=5C \end{cases}$$

4. $n=1$; $E = \frac{\hbar^2}{2m}\left(k_x + \frac{2\pi}{a}\right)^2$

$k_x = 0$ $\quad E = \frac{4\pi^2\hbar^2}{2ma^2} = 4\left(\frac{\pi^2\hbar^2}{2ma^2}\right)$

$k_x = \frac{\pi}{a}$ $\quad E = \frac{9\pi^2\hbar^2}{2ma^2} = 9\left(\frac{\pi^2\hbar^2}{2ma^2}\right)$

$n = -2$; $E = \frac{\hbar^2}{2m}\left(k_x - \frac{4\pi}{a}\right)^2$

$k_x = 0$ $\quad E = \frac{16\pi^2\hbar^2}{2ma^2} = 16\left(\frac{\pi^2\hbar^2}{2ma^2}\right)$

$k_x = \frac{\pi}{a}$ $\quad E = \frac{9\pi^2\hbar^2}{2ma^2} = 9\left(\frac{\pi^2\hbar^2}{2ma^2}\right)$

5. (a) metal 내부의 전체 전자 개수를 구하려면 $N = 2\cdot Z(E)F(E)$ 를 $[0, E_F]$ 구간에서 적분해주어야 한다. 즉 제대로 계산하는 식은 $N^* = \int_0^{E_F} 2\cdot Z(E)F(E)\,dE$ 이다. 따라서 Fermi Energy level 에서 density of state 인 $Z(E_F)$ 의 2배인 2×10^{21} electrons $/cm^3$ 는 옳지 않은 답이다. cf.) electron의 maximum $E_K = E_F \rightarrow T=0K$

(b) $N^* = \int_0^{E_F} 2\cdot Z(E)F(E)$

$\hbar = 1.054\times10^{-34}$ J.s

$m_e = 9.11\times10^{-31}$ kg

$= \int_0^{E_F} 2\cdot \frac{V}{4\pi^2}\times\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}\,dE$

$= \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\cdot E_F^{3/2}$

$\therefore \frac{N^*}{V} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_F^{3/2}$

$= 8.41\times10^{22}\ /cm^3$

이 값을 문제에서 주어진 $Z(E_F) \simeq 10^{21}\ /cm^3$ 과 비교해 보면 Fermi Energy 근처에 굉장히 많은 density of state 가 존재하고 따라서 $\underline{\text{전자밀도 } 2Z(E_F)}$ 값과 N^* 값이 비슷함을 알 수 있다. $\quad \simeq 2\times10^{21}\ /cm^3$

6. (a) $N^* = \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot E_F^{3/2}$

$$= \frac{10^{-6}\,m^3}{3\pi^2}\left(\frac{2\times 9.11\times 10^{-31}\,kg \times 7eV}{(6.582\times 10^{-16}eV\cdot s)^2 \times 1.602\times 10^{-19}\,(kg\cdot m^2/s^2/eV)}\right)^{3/2}$$

$$= 8.413\times 10^{22}/cm^3$$

(b) $N_a = \frac{N_0 \cdot \rho}{M} = \frac{6.022\times 10^{23}\,/mol \times 8.94\,g/cm^3}{63.546\,g/mol}$

$$= 8.47\times 10^{22}/cm^3$$

(c) 자유공간에서의 질량 m_0와 crystal 내부에서의 effective mass의 차이가 (a), (b) 두 결과값의 차이를 가져왔다. crystal 내에서 원자와의 충돌로 인해 느려진 mass를 반영한 좀더 큰 effective mass를 m_0 대신 사용해주면 discrepancy를 수정할수있다.

(d) 문헌에 따르면 $\left(\frac{m^*}{m_0}\right) = 1.42$ 이다.
(a), (b) 계산 결과와 잘 맞지는 않지만, $m^* > m_0$ 인 effective mass를 사용하면 오차를 줄일 수 있다.

7. (a) (i)

n	$E-E_F = nk_BT$
1	$k_BT = 2.59 \times 10^{-2} eV$
2	$2k_BT = 5.18 \times 10^{-2} eV$
3	$3k_BT = 7.76 \times 10^{-2} eV$
4	$4k_BT = 10.35 \times 10^{-2} eV$
5	$5k_BT = 12.94 \times 10^{-2} eV$
6	$6k_BT = 15.53 \times 10^{-2} eV$

$k_B = 1.38 \times 10^{-23} J$

$T = 300K$

$1eV = 1.6 \times 10^{-}$

(ii) Calculate the error in F(E) for neglecting "1" in the denominator.

n	$\underbrace{\left[\frac{1}{\exp\left(\frac{E-E_F}{kT}\right)}\right]}_{A} - \underbrace{\left[\frac{1}{1+\exp\left(\frac{E-E_F}{kT}\right)}\right]}_{B}$	Error (%) $= \frac{A-B}{B} \times$
1	$\frac{1}{e} - \frac{1}{1+e}$	37
2	$\frac{1}{e^2} - \frac{1}{1+e^2}$	14
3	$\frac{1}{e^3} - \frac{1}{1+e^3}$	5
4	$\frac{1}{e^4} - \frac{1}{1+e^4}$	2
5	$\frac{1}{e^5} - \frac{1}{1+e^5}$	0.7
6	$\frac{1}{e^6} - \frac{1}{1+e^6}$	0.2

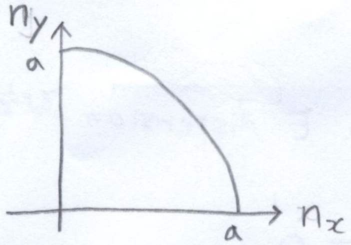
(b) $\frac{E-E_F}{k_BT} = 4 = n$

(a) 에서 n= 4 에서 오차가 2% 정도이므로 Boltzmann Statistics 로 나타낼 수 있는 E 값이다.

$E = E_F + 4k_BT = 5 + 10.35 \times 10^{-2}$

$\simeq \underline{5.103 \ eV}$

8. (a), (b)



$$E_n = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2)$$

$\eta = \frac{1}{4}\pi n^2$ (E_n 보다 작거나 같은 E 갖는 states의 수)

$$\therefore Z(E) = \frac{d\eta}{dE} = \frac{d}{dE}\left(\frac{\pi}{4}\cdot\frac{2ma^2}{\pi^2\hbar^2}E\right)$$

$$= \underline{\frac{ma^2}{2\pi\hbar^2}}$$

density of state
= number of energy states per unit energy

(c) $N(E) = 2\cdot Z(E)\cdot F(E)$

$$= 2\cdot\frac{ma^2}{2\pi\hbar^2}\cdot\frac{1}{\exp\left(\frac{E-E_F}{k_BT}\right)+1} = \frac{ma^2}{\pi\hbar^2}\cdot\frac{1}{\exp\left(\frac{E-E_F}{k_BT}\right)+1}$$

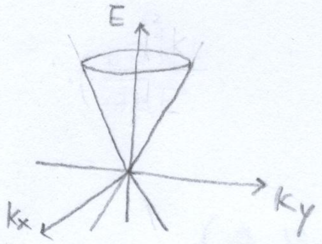
(d) $N^* = \int_0^{E_F} N(E)\,dE = \int_0^{E_F}\frac{ma^2}{\pi\hbar^2}\,dE = \frac{ma^2}{\pi\hbar^2}E_F$

($\because T\to 0$ $E<E_F$ 상황)
$\exp\left(\frac{E-E_F}{k_BT}\right)\to 0$

$$\therefore \left(\frac{N^*}{a^2}\right) = \frac{m}{\pi\hbar^2}(E_F)$$ //

9. effective mass $m^* = \hbar^2 \left(\frac{d^2E}{dk^2}\right)^{-1}$

graphene 은 $E=\hbar v_F|\vec{k}_\perp|$ 인 linear low E dispersion 갖는다.



$\therefore \frac{d^2E}{dk^2} = \infty$ $\quad\therefore m^* = 0$