Lecture Note

Kittel Introduction to Solid State Physics (6th Edition)

Lectured by

Sung-Ik Lee

 교정본. 이성익 교수

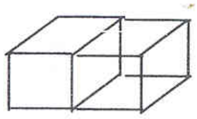
Kittel Introduction to Solid State Physics

Chapter 1

Crystal Structure

고체물리 : 19세기 x-ray diffraction by crystal
Ideal building block이 연속적으로 연결
Laue : Interference effect with Rontger rays
Laue가 x-ray diffraction에 관하여 설명
Friedrich, Knipping : 실험
Amorphous solid, Noncrystalline solid, Glass

Periodic Arrays of atoms
가장 간단한 crystal : unit가 single atom이다.
copper, silver, gold, aluminum



basis라 부른다.

Lattice translation vectors

$$\vec{r'} = \vec{r} + u_1 \vec{a_1} + u_2 \vec{a_2} + u_3 \vec{a_3}$$

u_1, u_2, u_3 arbitrary integers

u_1, u_2, u_3 가 lattice를 결정한다.

lattice + basis = Crystal structure

Translation vector

$$T = u_1 \vec{a_1} + u_2 \vec{a_2} + u_3 \vec{a_3}$$

Point operation : rotations reflection

Basis and the crystal structure

basis

$$\vec{r_j} = x_i \vec{a_1} + y_i \vec{a_2} + z_i \vec{a_3}$$

$$0 \le x_i, y_i, z_i \le 1$$

Primitive lattice cell

6면체 $\vec{a_1}, \vec{a_2}, \vec{a_3}$로 구성 : primitive cell

Volume $V = |\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}|$

primitive cell을 choose 하는 다른 방법 : Wigner Seitz Cell

<u>fundmental type of lattice</u>

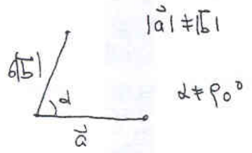
rotation : $2\pi, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$

Two dimensional lattice type

다섯 종류가 있다.

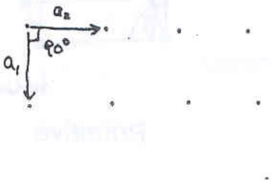
Oblique lattice

$|\vec{a}| \neq |\vec{b}|$, $\alpha = 90^0$



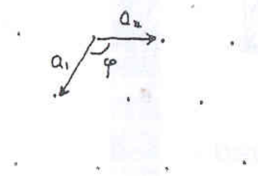
Square lattice

$|\vec{a_1}| = |\vec{a_2}|$, $\phi = 90^0$



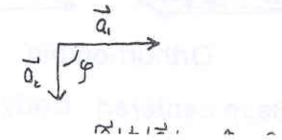
Hexagonal lattice

$|\vec{a_1}| = |\vec{a_2}|$, $\phi = 120^0$



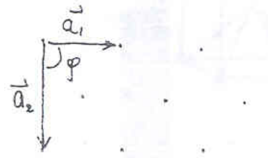
Rectangluar[Quadrangle] lattice

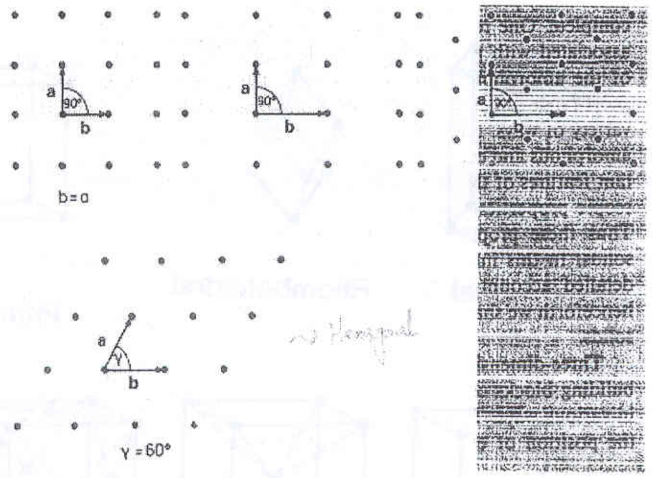
$|\vec{a_1}| \neq |\vec{a_2}|$, $\phi = 90^0$



Centered rectangular lattice

$|\vec{a_1}| \neq |\vec{a_2}|$, $\phi = 90^0$

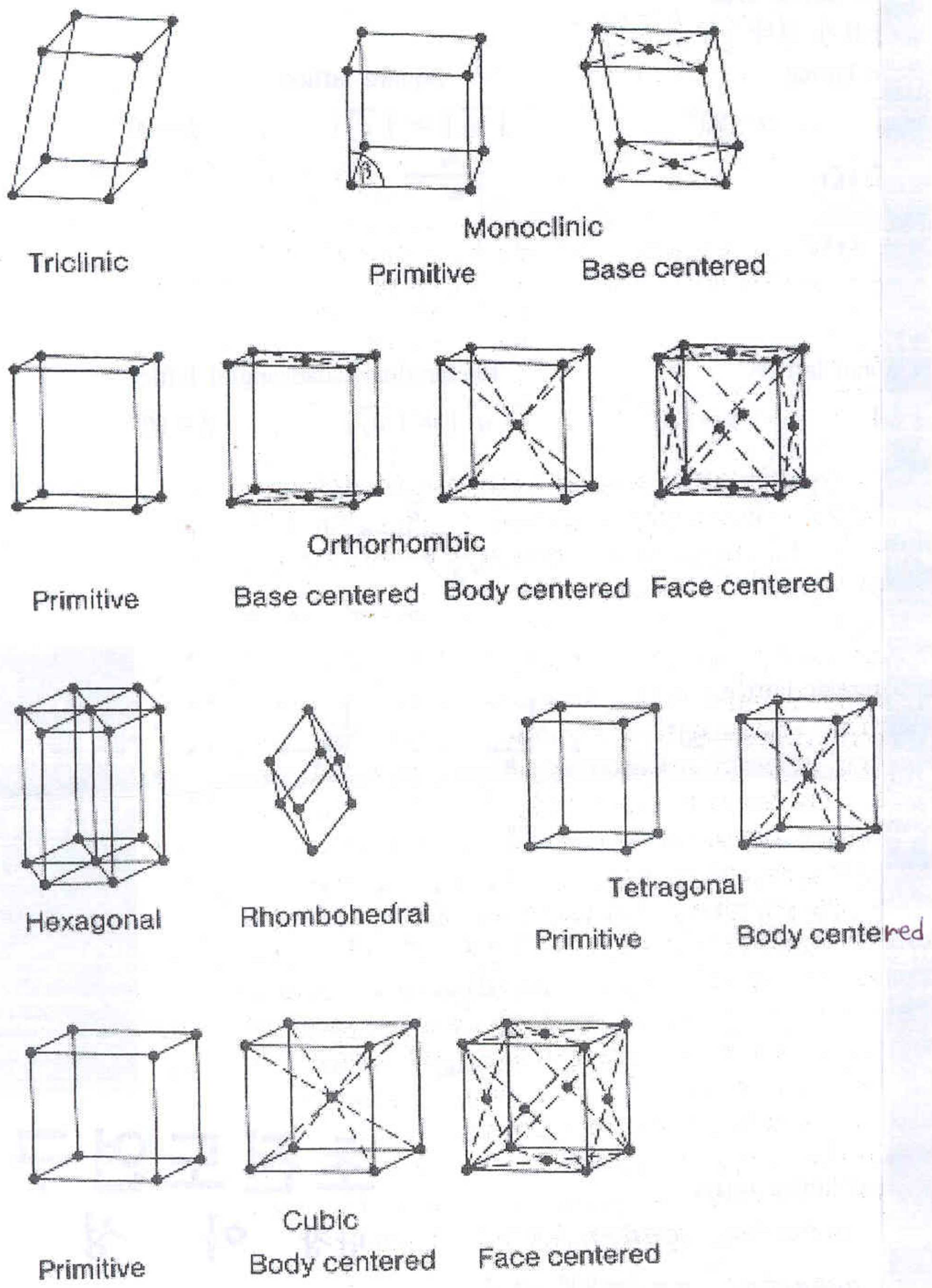




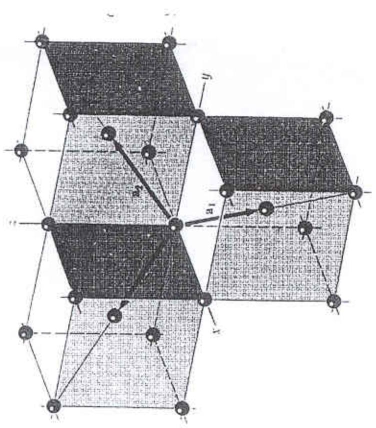
Three dimensional lattice types

Triclinic	$a_1 \neq a_2 \neq a_3,$	$\alpha \neq \beta \neq \gamma$
Monoclinic	$a_1 \neq a_2 \neq a_3,$	$\alpha = \beta = 90^o, \gamma \neq \beta$
Orthorhombic	$a_1 \neq a_2 \neq a_3,$	$\alpha = \beta = \gamma = 90^o$
Tetragonal	$a_1 = a_2 \neq a_3,$	$\alpha = \beta = \gamma = 90^o$
Cubic	$a_1 = a_2 = a_3,$	$\alpha = \beta = \gamma = 90^o$
Trigonal	$a_1 = a_2 = a_3,$	$\alpha = \beta = \gamma < 120^o \neq 90^o$
Hexagonal	$a_1 = a_2 \neq a_3,$	$\alpha = \beta = 90^o, \gamma = 120^o$

참고 : Blackmore의 fig 1-21 (page36)


Triclinic
Monoclinic
Primitive
Base centered
Orthorhombic
Primitive
Base centered
Body centered
Face centered
Hexagonal
Rhombohedral
Tetragonal
Primitive
Body centered
Cubic
Primitive
Body centered
Face centered

	S.C	B.C.C
Volume (conventional cell)	a^3	a^3
Lattice pt. per cell	1	2
Volume (primitive cell)	a^3	$\frac{a^3}{2}$
# of nearest nbd.	6	8
distance(nearest)	a	$\frac{\sqrt{3}}{2}a$
# of 2nd nbd.	12	6
2nd nbd distance	$\sqrt{2}a$	a
packing fraction	$\frac{\frac{4}{3}\pi\cdot(\frac{a}{2})^3}{a^3}=\frac{\pi}{3}$ $=0.52$이다.	$\frac{2\cdot\frac{4}{3}\pi\cdot(\frac{\sqrt{3}}{4}\cdot a)^3}{a^3}=\frac{\pi}{3}$ $=0.68$이다.



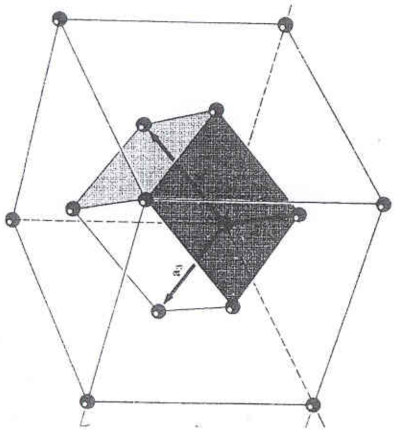
[bcc]

Primitive translation vector

$$\vec{a_1}=\frac{a}{2}(e_x+e_y-e_z)$$

$$\vec{a_2}=\frac{a}{2}(-e_x+e_y+e_z)$$

$$\vec{a_3}=\frac{a}{2}(e_x-e_y+e_z)$$



[fcc]

$$\vec{a_1}=\frac{a}{2}(e_x+e_y)$$

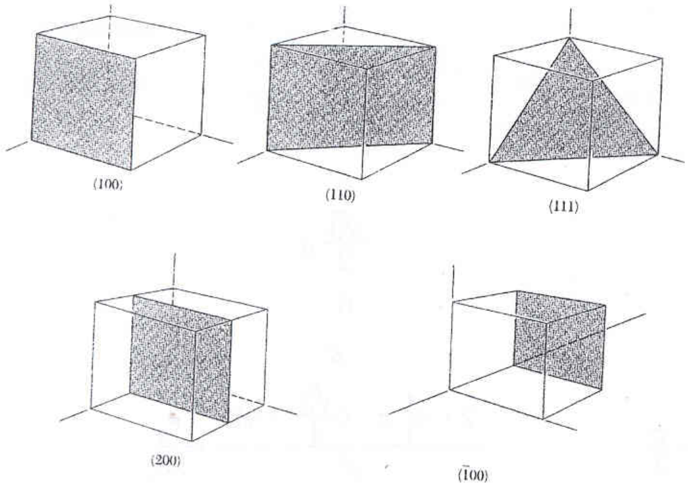
$$\vec{a_2}=\frac{a}{2}(e_y+e_z)$$

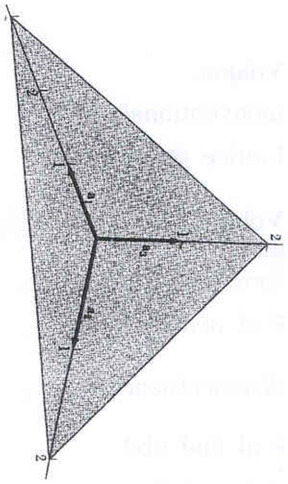
$$\vec{a_3}=\frac{a}{2}(e_z+e_x)$$

Index system for crystal planes

$\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

$2 : 3 : 3$





Simple crystal structure

NaCl structure

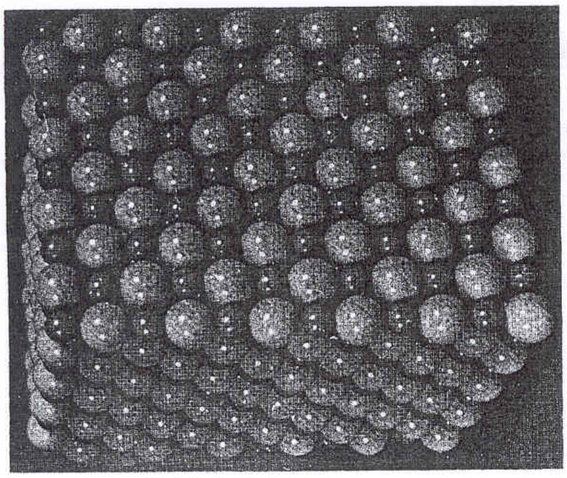


Figure 18 Model of sodium chloride. The sodium ions are smaller than the chlorine ions. (Courtesy of A. N. Holden and P. Singer.)

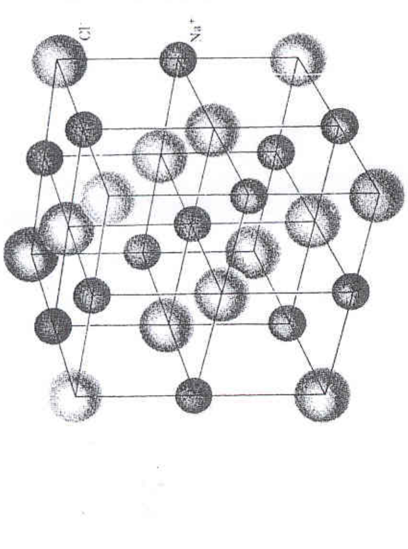
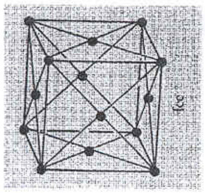


Figure 17 We may construct the sodium chloride crystal structure by arranging Na^+ and Cl^- ions alternately at the lattice points of a simple cubic lattice. In the crystal each ion is surrounded by six nearest neighbors of the opposite charge. The space lattice is fcc, and the basis has one Cl^- ion at 000 and one Na^+ ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. The figure shows one conventional cubic cell. The ionic diameters here are reduced in relation to the cell in order to clarify the spatial arrangement.

face centerd



$8\times\frac{1}{8}+6\times\frac{1}{2}=4$개

two primitive cell속에는 두 개의 Na, Cl이 있다.

Na : $(0\ 0\ 0),(\frac{1}{2}\ \frac{1}{2}\ 0),(\frac{1}{2}\ 0\ \frac{1}{2}),(0\ \frac{1}{2}\ \frac{1}{2})$

Cl : $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}),(0\ 0\ \frac{1}{2}),(0\ \frac{1}{2}\ 0),(\frac{1}{2}\ 0\ 0)$

Cesium Chloride structure

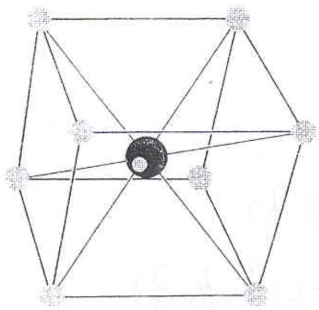


Figure 20 The cesium chloride crystal structure. The space lattice is simple cubic, and the basis has one Cs^+ ion at 000 and one Cl^- ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

Hexagonal Closed-packed structure

Hexagonal Closed-packed structure
-> ABABAB

f . c . c
-> ABCABC

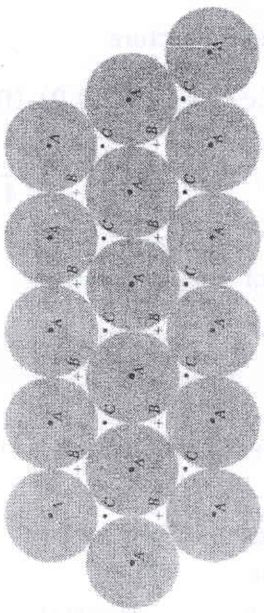


Figure 21 A close-packed layer of spheres is shown, with centers at points marked A. A second and identical layer of spheres can be placed on top of this, above and parallel to the plane of the drawing, with centers over the points marked B. There are two choices for a third layer. It can go in over A or over C. If it goes in over A the sequence is ABABAB. . . and the structure is hexagonal close-packed. If the third layer goes in over C the sequence is ABCABCABC. . . and the structure is face-centered cubic.

Hexagonal Closed-packed structure에서의 primitive cell

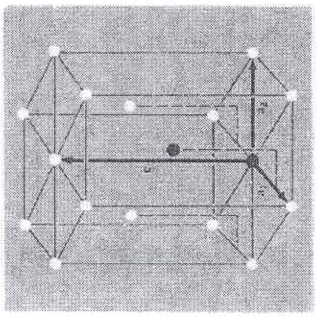
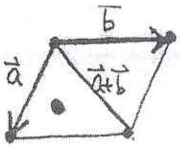


Figure 23 The primitive cell has $a_1 = a_2$, with an included angle of 120°. The c axis (or a_3) is normal to the plane of a_1 and a_2. The ideal hcp structure has $c = 1.633\ a$. The two atoms of one basis are shown as solid circles. One atom of the basis is at the origin; the other atom is at $\frac{2}{3}\frac{1}{3}\frac{1}{2}$, which means at the position $r = \frac{2}{3}a_1 + \frac{1}{3}a_2 + \frac{1}{2}a_3$.



$\vec{a}\ ;\ \vec{a}+\vec{b}$

$$\frac{\vec{a}+(\vec{a}+\vec{b})}{3}=\frac{2}{3}\vec{a}+\frac{1}{3}\vec{b}$$

∴ 중간층에 있는 원자

$$\vec{r}=\frac{2}{3}\vec{a}+\frac{1}{3}\vec{b}+\frac{1}{2}\vec{c}$$

Diamond structure

f.c.c 두 개가 합쳐진 것으로 생각하면 된다.

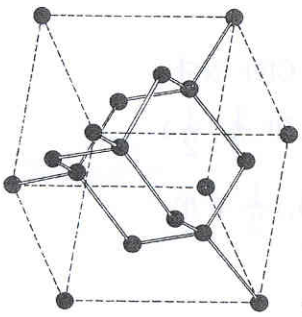


Figure 25 Crystal structure of diamond, showing the tetrahedral bond arrangement.

primitive basis

$(0\ 0\ 0), (\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4})$ 로 출발하는 두 개의 f.c.c.가 있다.

각각은 네 개의 nearest nbd, 12개의 next nearest nbd가 있다.

Cubic Zinc Sulfide structure

Zinc : f.c.c. $(0\ 0\ 0), (0\ \frac{1}{2}\ \frac{1}{2}), (\frac{1}{2}\ \frac{1}{2}\ 0), (\frac{1}{2}\ 0\ \frac{1}{2})$

Sulfide : f.c.c. $(\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}), (\frac{1}{4}\ \frac{3}{4}\ \frac{3}{4}), (\frac{3}{4}\ \frac{3}{4}\ \frac{1}{4}), (\frac{3}{4}\ \frac{1}{4}\ \frac{3}{4})$

Direct imaging of atomic structure

TEM으로 직접 본다.

Nonideal crystal structure

Ideal crystal이 minimum 에너지를 가진 것은 아니다.

Random stacking and Polytypism

ABCABC... two dimensionally crystal

ABABAB... 섞여있다. third axis noncrystal

Polytypism : 45번째 regular sequence가 나타난다.

a = 3.079 Å

c = 989.6 Å

숙제 1, 2, 3