

2019. 3. 12.

- 14 Bravais lattice
(5 primitive Bravais lattice)
- Graphen? Non-Bravais lattice.

Structural Determination

- lattice spacing $\sim 1 \text{ \AA}$.
- visible light $10^3 \sim 10^4 \text{ \AA}$
- X-ray 1 \AA
- diffractm of light
- electron
- neutron

Condition for constructive/destructive interference

①

복제 CH의 CIF 해석
a, b, c 크기
vol. of primitive cell 구하기.

a, b, c, lattice parameter 변화.

XRD
peak. 바뀌는 것 식별
< Mercury > 2theta
d 변화.

대부분의 경우.

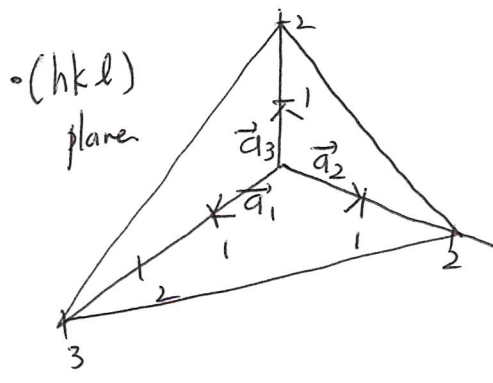
약사 4번 읽는다. 측정치와
측정값에.

바뀌는 방법 [격자변위
시험 + 반복.

질문. 푸어르.

②

Index system for crystal planes



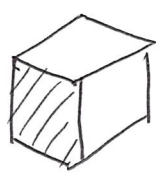
$$3\vec{a}_1, 2\vec{a}_2, 2\vec{a}_3$$

$$\downarrow \frac{1}{3} \quad \frac{1}{2} \quad \frac{1}{2}$$

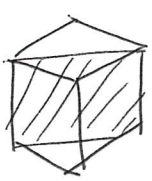
$$\downarrow \times 6 \quad (2 \quad 3 \quad 3)$$

$$(h \quad k \quad l)$$

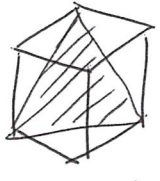
Eg.)



(100)



(110)



(111)



(200)



($\bar{1}$ 00)

Eg.) cube faces of a cubic crystal

- (100) (010) (001)
- ($\bar{1}$ 00) (0 $\bar{1}$ 0) (00 $\bar{1}$)
- ⋮
- {100} {010} {001}

[UVW] a direction in a crystal.

$$[100] = \vec{a}_1$$

$$[0\bar{1}0] = -\vec{a}_2$$

Simple crystal structures

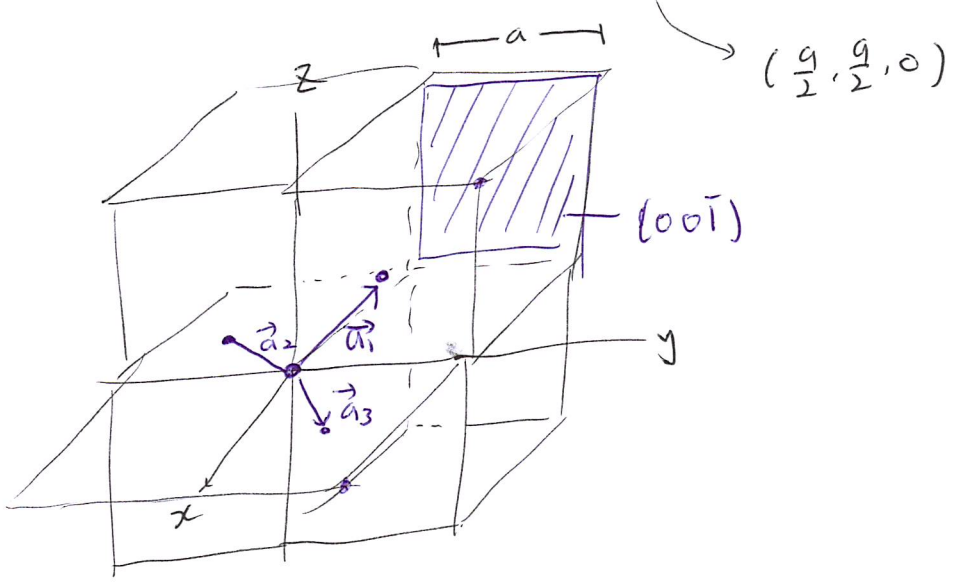
• NaCl.

FCC + $(0, 0, \frac{1}{2})$
basis atom.

$(\frac{1}{2}, 0, 0) \sim (0, \frac{1}{2}, 0)$ 가능.

lattice vector.

$$\begin{aligned}
 \vec{a}_1 &= \frac{a}{2}(\hat{y} + \hat{z}) & \vec{a}_1 &= 0 & (0, 0, 0) \\
 \vec{a}_2 &= \frac{a}{2}(\hat{x} + \hat{z}) & \vec{a}_2 &= 0 & (0, 0, 0) \\
 \vec{a}_3 &= \frac{a}{2}(\hat{x} + \hat{y}) & \vec{a}_3 &= \frac{a}{2}(\hat{z}) & (0, 0, \frac{a}{2})
 \end{aligned}$$



$(hkl) = (0, 0, \bar{1})$

⇒ FCC + 1 basis atom.

| | a |
|------|--------|
| LiH | 4.08 Å |
| MgO | 4.20 Å |
| MnO | 4.43 Å |
| NaCl | 5.63 Å |
| ! | |