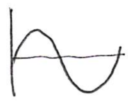
Bravais lattice. (SC = conventional of BCC, FCC)

symmetry of crystals.



과제 #2. : XRD unit conversion q, 2theta, d.
Simulate XRD w/ CH 10%, Ettringite 10%, Clinker 80%

SAXS. , WAXS, Electromagnetic spectrum. $c = \lambda \times f$. $E = h * c / \lambda$.

c: speed of light ($3 \cdot 10^8$ m/s)
λ: wavelength
f: frequency ($\neq T = \frac{1}{f}$ (주기))

분석방법.

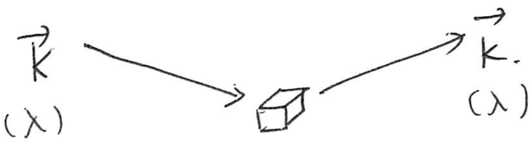
- Diffraction ⊂ Scattering. (total scattering method).
- Spectroscopy
  - Infrared.
  - Raman
  - NMR.
  - Energy-dispersive.
  - XRF

↑ 이전. QXRD, TGA, MIP

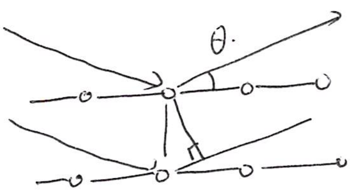
↓ 중간고사 이후

- X-ray
- Ebeam (electron
- Neutron.
- light.

$\boxed{\text{Scattering by an object (crystal)}}$

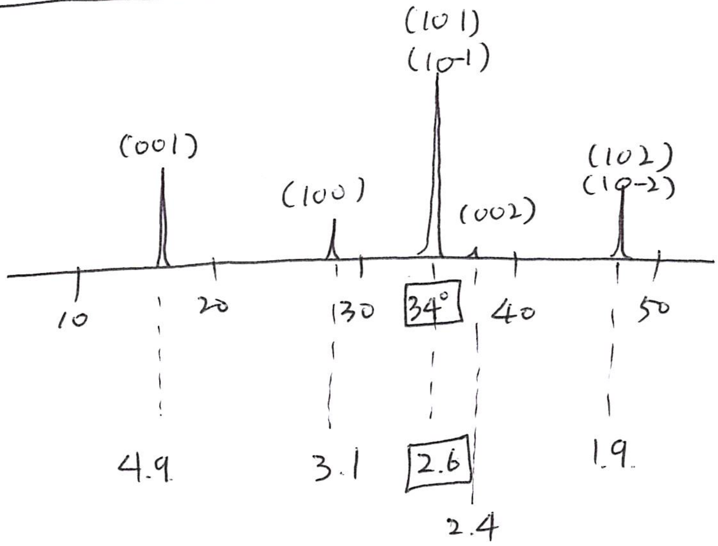


$|\vec{K}| = |\vec{K'}|$



$2d\sin\theta = n\lambda$.

Portlandite $Ca(OH)_2$



2theta (degree) : $\lambda = 1.54056$ Å
Cu-Kα.
Mo-Kα.
0.7107 Å.

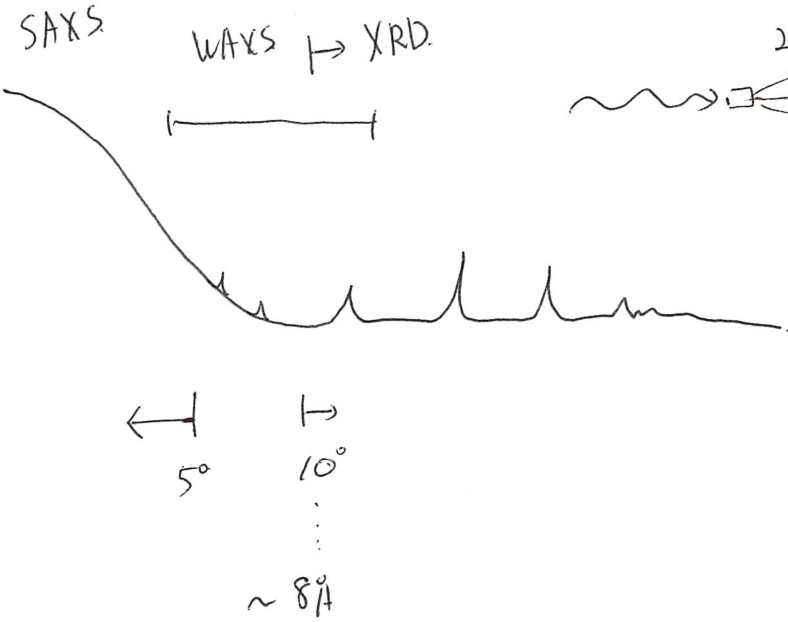
d-spacing (Å)

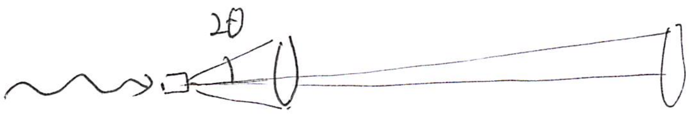
$$q = \frac{2\pi}{d} = \frac{4\pi\sin\theta}{\lambda}$$

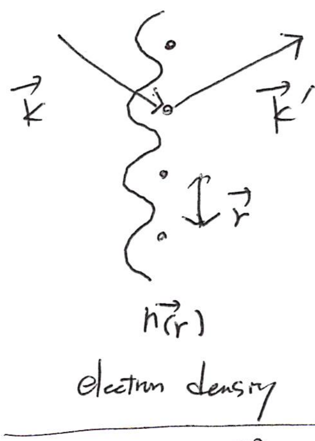
; $$d = \frac{\lambda}{2\sin\theta} = \frac{1.5406}{2\cdot\sin\boxed{17}} \doteqdot 2.63 \text{ Å}$$

34/2.

Scale of Scattering





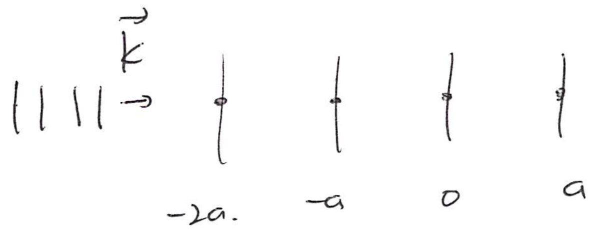


$$\text{Intensity} \propto \left| \int_{\vec{r}} n(\vec{r})\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} \right|^2.$$

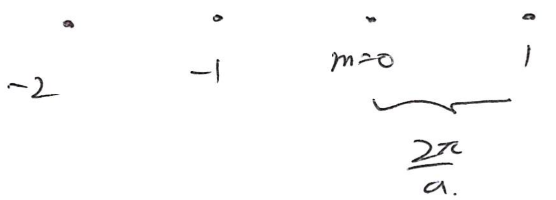
if ; $\vec{G}\cdot r_j = 2\pi n_j$

$$e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} = e^{i\vec{G}\cdot r_j} = e^{i2\pi n_j} = (e^{i2\pi})^{n_j} = 1^{n_j} = 1. \quad \forall j$$

$k-k' = G$; $m_1 G_1 + m_2 G_2 \cdots$ 마찬가지.



real space



Reciprocal space.

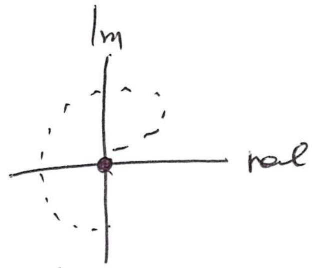
2-2

$$\text{Amplitude} \propto \left| \int n(\vec{r})\, \underbrace{e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}}_{*} \right|^2$$

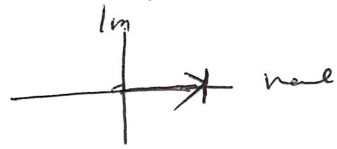
$$e^{ix} = \cos x + i\sin x$$

$$e^{-ix} = \cos x - i\sin x.$$

$$* = 1 + e^{i\phi} + e^{i2\phi} + e^{iN\phi} \Rightarrow$$



$$+1 + e^{i2\pi\phi} + e^{i2\pi 2\phi} \cdots e^{i2\pi N\phi} \Rightarrow$$



$$1 + 1 + 1 + \cdots$$

Reciprocal lattice

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \; ; \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \; ; \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij} \qquad \left(\delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i \neq j \end{cases} \right)$$

$$\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$$

Set of reciprocal lattice vectors

Example

$$\vec{T} = u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3$$

Translation

$$n(\vec{r}) = \sum_G n_G \exp(i \vec{G} \cdot \vec{r})$$

n_G : X-ray scattering amplitude.

$$n(\vec{r} + \vec{T}) = \sum_G n_G \exp(i \vec{G} \cdot \vec{r}) \exp(i \vec{G} \cdot \vec{T})$$

electron density

$$= n(\vec{r})$$

$$\exp(i \vec{G} \cdot \vec{T}) = \exp[i(v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3) \cdot (u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3)]$$

$$= \exp[i 2\pi (v_1 u_1 + v_2 u_2 + v_3 u_3)]$$

$$= 1.$$

$$\begin{cases} e^{ix} = \cos x + i \sin x \\ e^{-ix} = \cos x - i \sin x \end{cases}$$

Example

BCC.

$$\begin{cases} \vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x}) \\ \vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y}) \\ \vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) \end{cases}$$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\cancel{\vec{b}_2 = 2\pi}$$

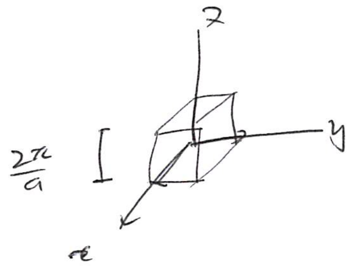
$$\begin{cases} = \frac{2\pi}{a}(\hat{y} + \hat{z}) \\ \vec{b}_2 = \frac{2\pi}{a}(\hat{x} + \hat{z}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y}) \end{cases}$$

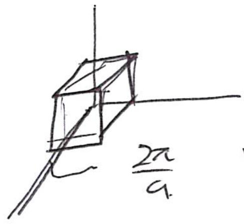
Bravais lattice vector of FCC.

SC.

$$\begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{cases}$$

$$\begin{cases} \vec{b}_1 = \frac{2\pi}{a}\hat{x} \\ \vec{b}_2 = \frac{2\pi}{a}\hat{y} \\ \vec{b}_3 = \frac{2\pi}{a}\hat{z} \end{cases}$$



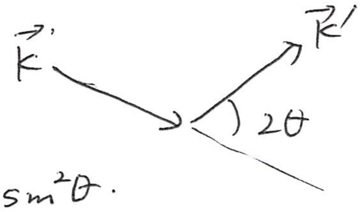


Vol. of 1st Brillouin zone $= \left(\frac{2\pi}{a}\right)^3$

$\boxed{\text{Laue condition}}$

$$|\vec{k}| = |\vec{k}'| = k = \frac{2\pi}{\lambda}.$$

Laue condition $\vec{k}' - \vec{k} = \vec{G} = \frac{2\pi}{d} n \hat{z}$



$$|\vec{k}' - \vec{k}| = \sqrt{\vec{k}^2 + \vec{k}'^2 - 2\vec{k}\cdot\vec{k}'}$$

$$= \sqrt{2k^2 - 2k^2\cos 2\theta}.$$

$$= 2k\sin\theta.$$

$\swarrow$ $1-\cos 2\theta = 2\sin^2\theta.$

$$= 2\,\frac{2\pi}{\lambda}\sin\theta.$$

$$= \frac{2\pi}{d} n.$$

$\swarrow$ $2d\sin\theta = n\lambda.$

$\boxed{\text{Bragg's condition}}$