Chapter 2

Reciprocal lattice

Diffraction of wave by crystal

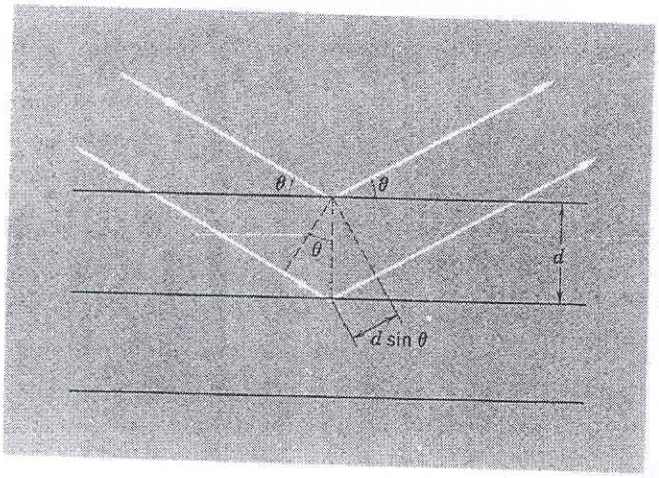


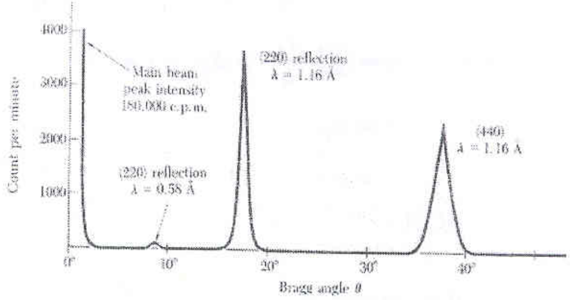
Figure 2 Derivation of the Bragg equation $2d \sin \theta = n\lambda$; here d is the spacing of parallel atomic planes and $2\pi n$ is the difference in phase between reflections from successive planes. The reflecting planes have nothing to do with the surface planes bounding the particular specimen.

constructive interference

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

basis 내부의 원자들은 어떤 기여를 하나?

relative intensity 기여



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

charge concentration

electron number density

magnet moment density

Fourier Analysis

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

1차원

$$n(x) = n_0 + \sum C_p \cos\frac{2\pi x \cdot p}{a} + S_p \sin 2\pi x \cdot \frac{p}{a}$$

$pf.$ $\quad n(x+a) = n_0 + \sum_{p>0} C_p \cos\frac{2\pi(x+a)p}{a} + S_p \sin\frac{2\pi(x+a)p}{a}$

$= n(x)$

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Complex

$$n(x) = \sum_p n_p \exp\left(i\frac{2\pi px}{a}\right)$$

$n(x) is real$

$$\therefore n^*(x) = n(x) \qquad \sum_p n_p^* \exp\left(-i\frac{2\pi px}{a}\right) = \sum_p n_p \exp\left(+i\frac{2\pi px}{a}\right)$$

$$= \sum_p n_{-p} \exp\left(-i\frac{2\pi px}{a}\right)$$

$$\therefore n_p^* = n_{-p}$$

Fourier Series

$$n(\vec{r}) = \sum n_{\vec{G}} \cdot \exp(i\vec{G}\cdot\vec{r})$$

Inversion of Fourier Series

$$\begin{aligned} n_p &= \frac{1}{a}\int_0^a dx n(x) \exp\left(-i\frac{2\pi px}{a}\right) \\ &= \frac{1}{a}\int_0^a dx \sum n_{p'} \exp\left(ip'x\frac{2\pi}{a}\right)\cdot\exp\left(-i\frac{2\pi px}{a}\right) \\ &= \sum\frac{n_{p'}}{a}\int_0^a dx\cdot\exp\left(ix\frac{2\pi}{a}(p'-p)\right) \\ &= \sum\frac{n_{p'}}{a}\cdot\delta_{p'-p}\cdot a \\ &= n_p \end{aligned}$$

$pf.$ 끝

같은 방법으로

$$n_{\vec{G}} = \frac{1}{V_c}\int_{cell} dV \quad n(\vec{r})\exp(-i\vec{G}\cdot\vec{r})$$

Reciprocal lattice vector

$\vec{b_1}, \vec{b_2}, \vec{b_3}$를 $constant$ 라하자.

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

$$\vec{b_i}\cdot\vec{a_j} = 2\pi\delta_{ij}$$

$$\vec{G} = \frac{2\pi P_x}{a}\hat{x} + \frac{2\pi P_y}{a}\hat{y} + \frac{2\pi P_z}{a}\hat{z}$$
$$= P_x\vec{b_1} + P_y\vec{b_2} + P_z\vec{b_3}$$

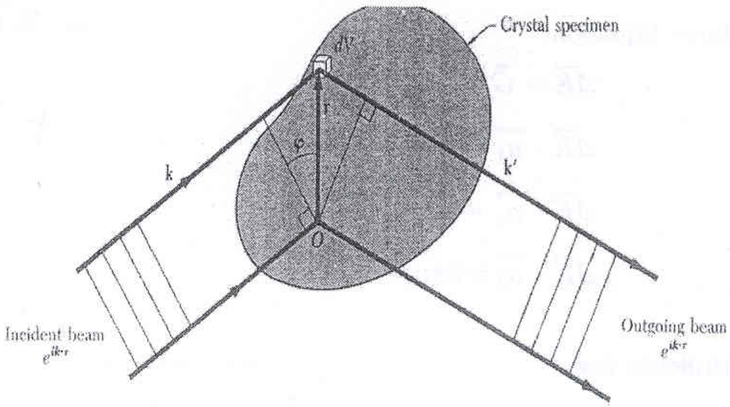
$$\vec{G} = v_1\vec{b_1} + v_2\vec{b_2} + v_3\vec{b_3}$$

v_1, v_2, v_3 : *integer*

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

Diffraction Condition

Scattering amplitude



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$$F = \int dVn(\vec{r})\exp[i(\vec{K} - \vec{K'})\cdot\vec{r}]$$
$$= \int dVn(\vec{r})\exp(-i\Delta\vec{K}\cdot\vec{r})$$

where $\vec{K} + \Delta\vec{K} = \vec{K'}$

Fourier components.

$$F = \int dV \cdot \sum_G n_G \cdot e^{i\vec{G}\cdot\vec{r}} \cdot \exp(-i\Delta\vec{K}\cdot\vec{r})$$
$$= \sum_G \int dV \cdot n_G \cdot \exp[i(\vec{G} - \Delta K)\cdot\vec{r}]$$

$$\therefore \Delta\vec{K} = \vec{G}$$

OR $\vec{K} + \vec{G} = \vec{K'}$

$$K^2 + G^2 + 2\vec{K}\cdot\vec{G} = K^2$$

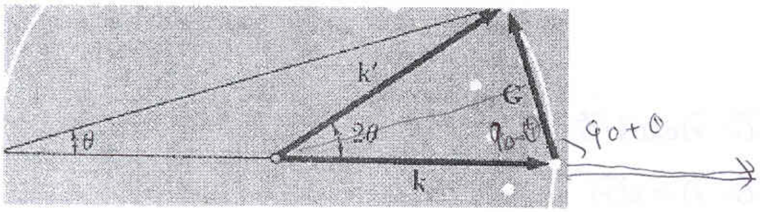
$$\therefore\ 2\vec{K}\cdot\vec{G} = G^2$$

OR $2\vec{K}\cdot\vec{G} + G^2 = 0$

$Th^m.$ $\quad \vec{G} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3}$에 수직인 평면사이의 거리 $= \dfrac{2\pi}{|\vec{G}|}$

$$\therefore 2 \cdot \frac{2\pi}{\lambda} \cdot \sin\theta = \frac{2\pi}{d(hkl)}$$

$$\therefore 2d\sin\theta = \lambda \qquad \text{or} \qquad 2d\sin\theta = n\lambda$$



$\rightarrow 2\vec{k}\cdot\vec{G} = |\vec{k}||\vec{G}|\sin\theta$

$+\ 2|\vec{k}||\vec{G}|\sin\theta = |G|^2$

$2 \cdot \frac{2\pi}{\lambda}\sin\theta = \frac{2\pi}{d}$ $\quad 2d\sin\theta = \lambda$

$2d\sin\theta = \lambda$

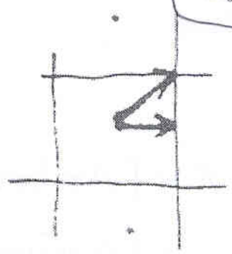
Laue Equation.

$$\Delta\vec{K} = \vec{G}$$

$$\Delta\vec{K} \cdot \vec{a_1} = 2\pi v_1$$

$$\Delta\vec{K} \cdot \vec{a_2} = 2\pi v_2$$

$$\Delta\vec{K} \cdot \vec{a_3} = 2\pi v_3$$

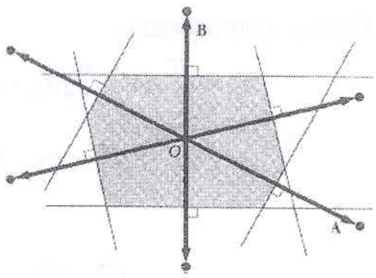


Brillouin zone

$$2\vec{K} \cdot \vec{G} = |\vec{G}|^2 \qquad \therefore \vec{K} \cdot \frac{\vec{G}}{2} = \left(\frac{1}{2}G\right)^2$$

이것이 Wigner-Seitz cell 이다.

Construction of the first Brillouin zone for an oblique lattice



First Brillouin zone.

1-D에서는

$$K = \pm\frac{\pi}{a}$$

Reciprocal lattice to S.C lattice

$$\vec{a_1} = a\hat{x}, \quad \vec{a_2} = a\hat{y}, \quad \vec{a_3} = a\hat{z}$$

$$\vec{b_1} = \frac{2\pi}{a}\hat{x}, \quad \vec{b_2} = \frac{2\pi}{a}\hat{y}, \quad \vec{b_3} = \frac{2\pi}{a}\hat{z}$$

First Brillouin zone of S.C lattice

$$\pm\frac{1}{2}\vec{b_1},\ \pm\frac{1}{2}\vec{b_2},\ \pm\frac{1}{2}\vec{b_3}$$

Reciprocal lattice to B.C.C lattice

$$\vec{a}_1=\frac{1}{2}a(-\hat{x}+\hat{y}+\hat{z}),\quad \vec{a}_2=\frac{1}{2}a(\hat{x}-\hat{y}+\hat{z}),\quad \vec{a}_3=\frac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$$

volume of primitive cell is

$$V=|\vec{a}_1\cdot\vec{a}_2\times\vec{a}_3|=\frac{1}{2}a^2$$

$$\vec{b}_1=\frac{2\pi}{a}(\hat{y}+\hat{z}),\quad \vec{b}_2=\frac{2\pi}{a}(\hat{x}+\hat{z}),\quad \vec{b}_3=\frac{2\pi}{a}(\hat{x}+\hat{y})$$

General reciprocal lattice vector is

$$\vec{G}=v_1\vec{b}_1+v_2\vec{b}_2+v_3\vec{b}_3 = \frac{1}{2}\frac{1}{a}\left[v_1(\hat{y}+\hat{z})+v_2(\hat{x}+\hat{z})+v_3(\hat{x}+\hat{y})\right]$$

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

shortest $\vec{G}$

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

Reciprocal space에서의 volume은?

$$\vec{b}_1\cdot\vec{b}_2\times\vec{b}_3=\left(\frac{2\pi}{a}\right)^3\cdot(\hat{y}+\hat{z})\cdot[(\hat{x}+\hat{z})\times(\hat{x}+\hat{y})]$$

$$=\left(\frac{2\pi}{a}\right)^3\cdot(\hat{y}+\hat{z})\cdot(\hat{y}+\hat{z}-\hat{x})$$

$$=2\cdot\left(\frac{2\pi}{a}\right)^3$$

fcc

에서의 vector (normal to the surface.)

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

Reciprocal lattice to F.C.C lattice

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fcc $\quad \frac{a}{2}(\hat{y}+\hat{z}),\quad \frac{a}{2}(\hat{x}+\hat{z}),\quad \frac{a}{2}(\hat{x}+\hat{y})$

primitive cell 에서의 volume

$$V=|\vec{a}_1\cdot\vec{a}_2\times\vec{a}_3|=a^3/4$$

$$\vec{b}_1=\frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}),\quad \vec{b}_2=\frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}),\quad \vec{b}_3=\frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$$

$$Volume = (\frac{2\pi}{a})^3 \cdot (-\hat{x}+\hat{y}+\hat{z}) \cdot \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix}$$

$$= (\frac{2\pi}{a})^3 \cdot (-\hat{x}+\hat{y}+\hat{z}) \cdot [0 \cdot \hat{x}+2 \cdot \hat{y}+2 \cdot \hat{z}]$$

$$= (\frac{2\pi}{a})^3 \cdot 4$$

가장 짧은 $\vec{G}$는

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

Fourier Analysis of the basis scattering amplitude

$$F_g = N\int dV n(\vec{r})\exp(-i\vec{G}\cdot\vec{r})$$

$$= NS_G$$

S_G : *structure factor*

$$n(\vec{r}) = \sum_{j=0}^{S} n_j(r-r_j)$$

$$S_G = \sum_j \int dv n_j(\vec{r}-\vec{r_j}) \cdot \exp(-i\vec{G}\cdot\vec{r})$$

$$= \sum_j \exp(-i\vec{G}\cdot\vec{r_j}) \int dV n_j(\rho)\exp(i\vec{G}\cdot\vec{\rho})$$

$$= \sum_j f_j \exp(-i\vec{G}\cdot\vec{r_j})$$

$$\text{where} \quad f_j \equiv \int dV n_j(\rho)\exp(-i\vec{G}\cdot\vec{\rho})$$

$$\vec{r_j} = x_j\vec{a_1} + y_j\vec{a_2} + z_j\vec{a_3}$$

$$\vec{G}\cdot\vec{r_j} = (v_1\vec{b_1}+v_2\vec{b_2}+v_3\vec{b_3})\cdot(x_j\vec{a_1}+y_j\vec{a_2}+z_j\vec{a_3})$$

$$= (v_1x_j+v_2y_j+v_3z_j)\cdot 2\pi$$

$$S_G(v_1v_2v_3) = \sum_j f_j\exp[-i2\pi(v_1x_j+v_2y_j+v_3z_j)]$$

$$N_1(cell)\times S_1(basis) = N_2(cell)\times S_2(basis)$$

Structure factor of the bcc lacttice

$$x_1 = y_1 = z_1 = 0 \quad , \quad x_2 = y_2 = z_2 = \frac{1}{2}$$

$$S_G(v_1 v_2 v_3) = f\{1 + \exp[i(v_1 + v_2 + v_3)]\}$$

$S = 0 \quad when\ v_1 + v_2 + v_3 = Odd\ integer$

$S = 2f \quad when\ v_1 + v_2 + v_3 = Even\ integer$

Structual Factor of the fcc lattice

$$000\ ,\ 0\frac{1}{2}\frac{1}{2}\ ,\ \frac{1}{2}0\frac{1}{2}\ ,\ \frac{1}{2}\frac{1}{2}0$$

$$S(v_1 v_2 v_3) = f \cdot \{1 + \exp[-i\pi(v_2 + v_3)] + \exp[-i\pi(v_1 + v_3)] + \exp[-i\pi(v_1 + v_3)]\}$$

all even integer S=4f

all odd integer S=0

KCl, KBr 꼭 simple cubic 같다.

∵ K', Cl ion 은 전자의 수가 다르다.

Atomic form factor

$$f_j = \int dv\, n_j(\vec{r}) \exp(-\vec{G} \cdot \vec{r})$$

$$\vec{G} \cdot \vec{r} = Gr\cos\alpha$$

만약 전자가 spherically symmetric about the origin

$$= 2\pi \int dr r^2 \sin\alpha\ d\alpha n_j(r) \exp(-iGr\cos\alpha)$$

$$= 2\pi \int dr r^2 n_j(r) \frac{\exp(-iGr\cos\alpha)}{iGr}\Bigg|_{\alpha=0}^{\alpha=\pi}$$

$$= 2\pi \int dr r^2 n_j(r) \frac{\exp(iGr) - \exp(-iGr)}{iGr}$$

$$= 4\pi \int dr r^2 n_j(r) \frac{\sin Gr}{Gr}$$

$n(\vec{r})$이 r=0에 응집되어 있다면,

$$f_j = 4\pi \int dr n_j(r) r^2 = 2$$

forward - direction G = 0

f reduce to Z forward direction

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숙제 1 - 7