Introduction to Solid State Physics
(C. Kittel)

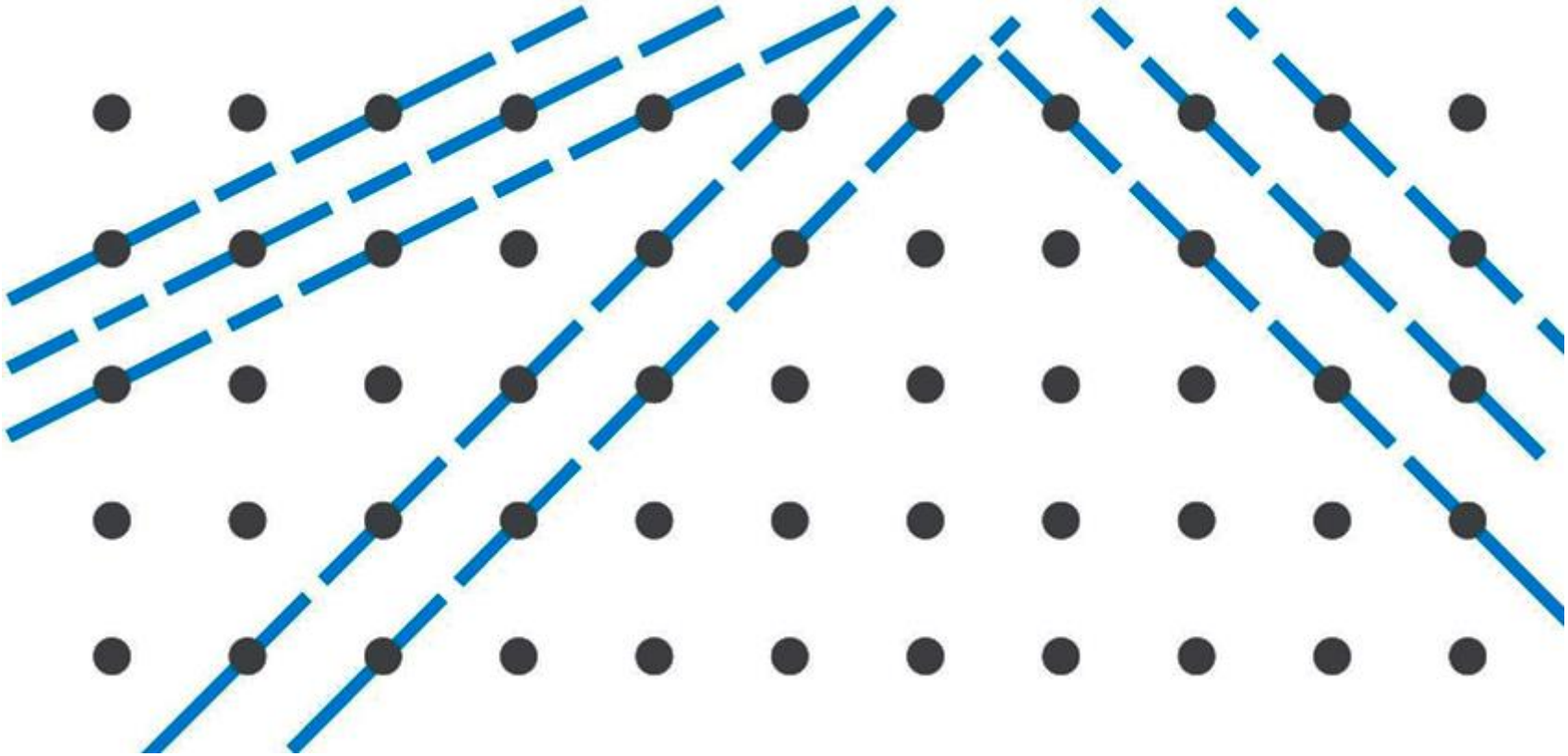
Chapter 2

WAVE DIFFRACTION
AND
THE RECIPROCAL LATTICE

Contents

DIFFRACTION OF WAVES BY CRYSTALS

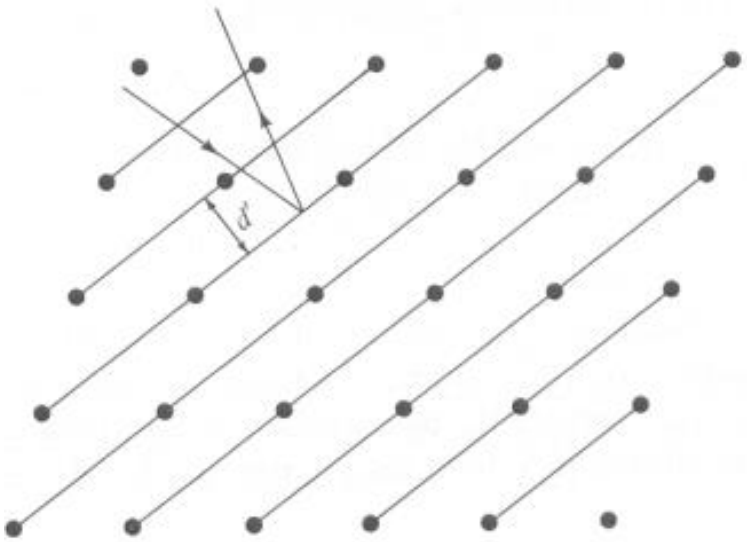
different crystal planes



DIFFRACTION OF WAVES BY CRYSTALS

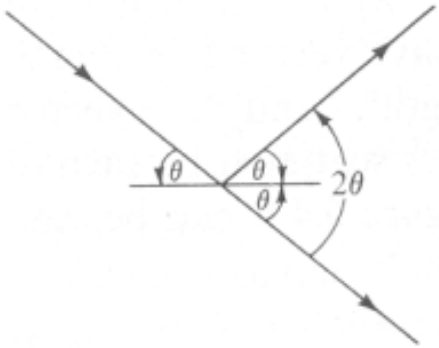
The Bragg law : diffraction condition in terms of **reflection by planes**

reflection by plane



Bragg angle θ

: the half of the total angle 2θ by which the incident beam is deflected



deflected beam
(reflection by plane)

incident beam

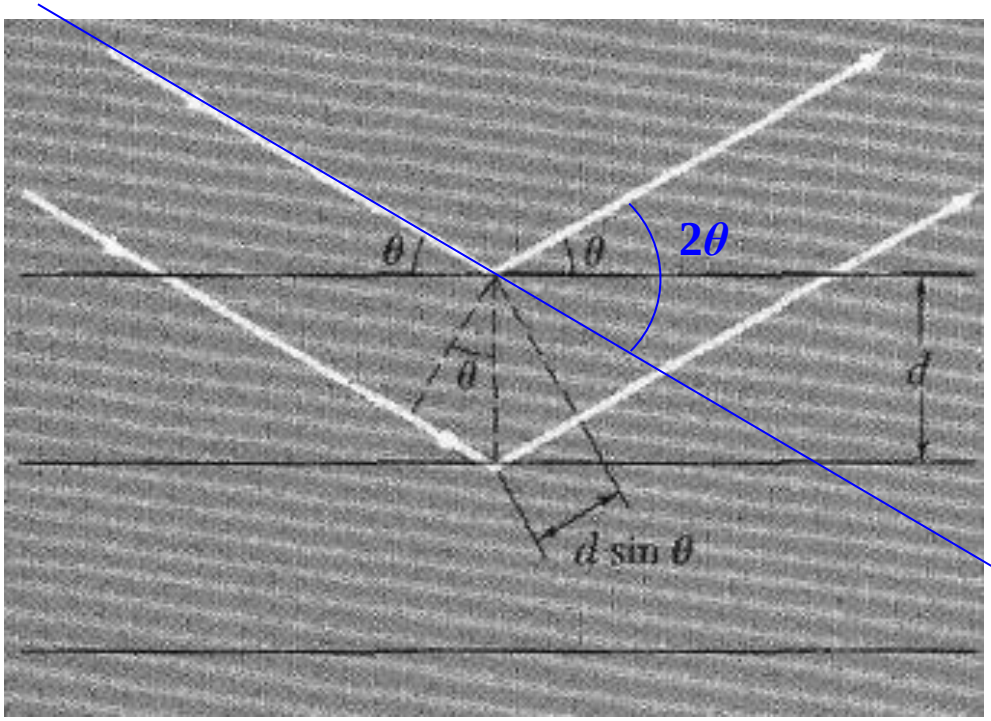
DIFFRACTION OF WAVES BY CRYSTALS

The Bragg law

Bragg condition for diffraction

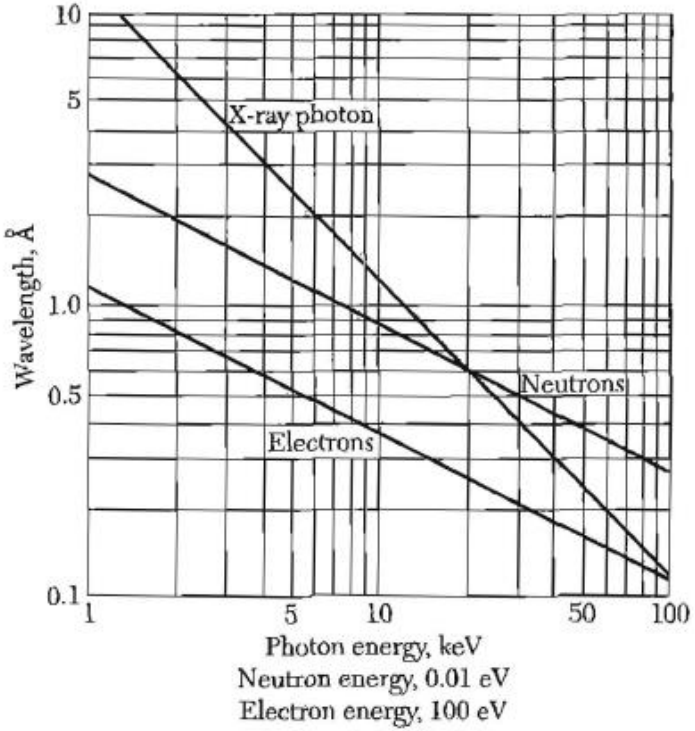
$$2d \sin\theta = n\lambda$$

only for wavelength $\lambda \leq 2d$.



DIFFRACTION OF WAVES BY CRYSTALS

The Bragg law



Bragg condition for diffraction

$\lambda \sim d$ $\quad d \sim 0.1 - 1$ nm

Quiz

With *d* ~ 1 nm, calculate the beam energy (in eV) of each prove beam for diffraction by crystals.

(1) Light (EM wave)

(2) Electron

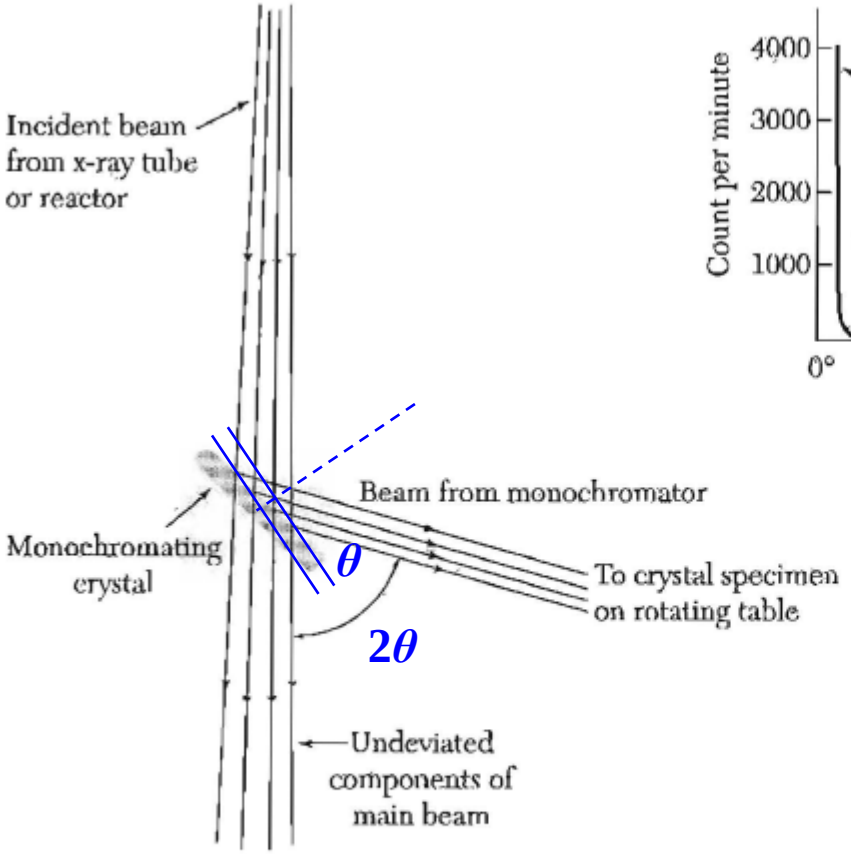
(3) neutron

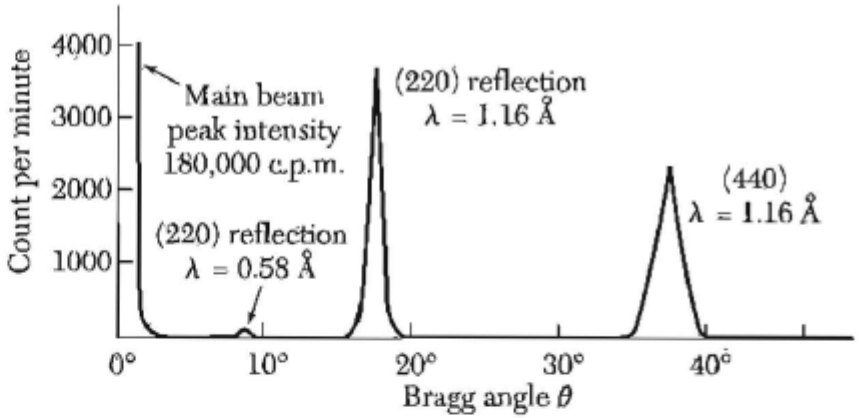
Hint: From *Bragg condition for diffraction*

Observability condition: $\lambda \sim d$

DIFFRACTION OF WAVES BY CRYSTALS

The Bragg law (application: selection of monochromatic beam)





Bragg's condition.

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

Figure 3 Sketch of a monochromator which by Bragg reflection selects a narrow spectrum of x-ray or neutron wavelengths from a broad spectrum incident beam. The upper part of the figure shows the analysis (obtained by reflection from a second crystal) of the purity of a 1.16 Å beam of neutrons from a calcium fluoride crystal monochromator. (After G. Bacon.)

DIFFRACTION OF WAVES BY CRYSTALS

The Bragg law (application: selection of monochromatic beam)

Bragg's condition. $n\lambda = 2d \sin\theta$

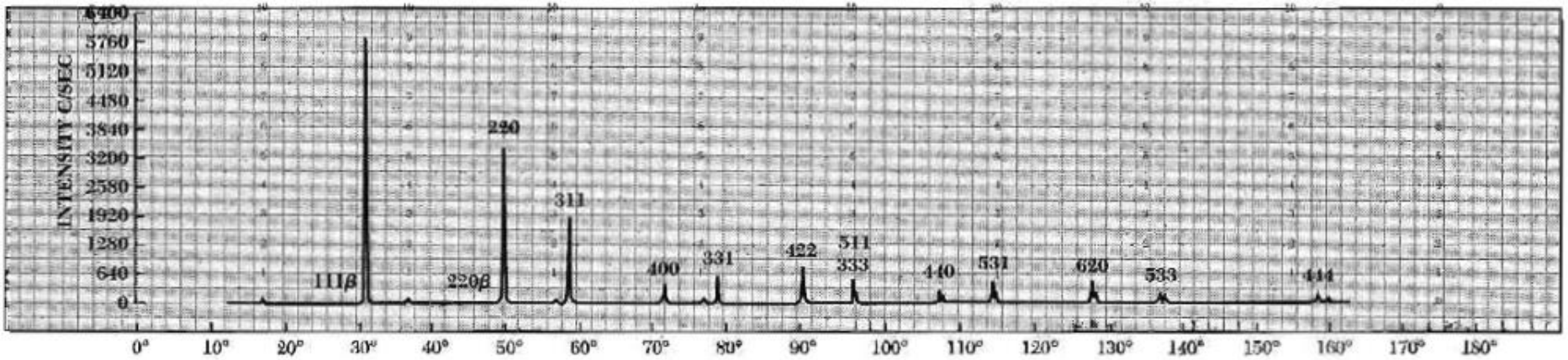


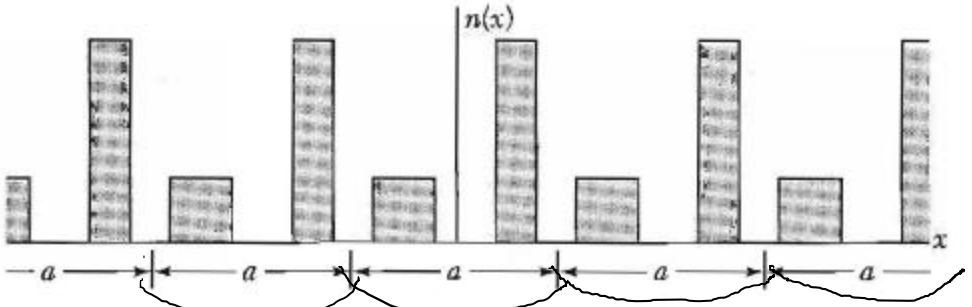
Figure 4 X-ray diffractometer recording of powdered silicon, showing a counter recording of the diffracted beams. (Courtesy of W. Parrish.)

Scattered Wave Amplitude

Fourier analysis

$n(x+a) = n(x)$ $\quad$ T = na

Real space



1-dimensional example

$$n(x) = n_0 + \sum_{p>0} [C_p \cos(2\pi px/a) + S_p \sin(2\pi px/a)]$$

$$n(x+a) = n_0 + \sum [C_p \cos(2\pi px/a + 2\pi p) + S_p \sin(2\pi px/a + 2\pi p)]$$

$$= n_0 + \sum [C_p \cos(2\pi px/a) + S_p \sin(2\pi px/a)] = n(x) \ .$$

$$n(x) = \sum_p n_p \exp(i2\pi px/a)$$: real if $n^*_{-p} = n_p$ is satisfied

Scattered Wave Amplitude

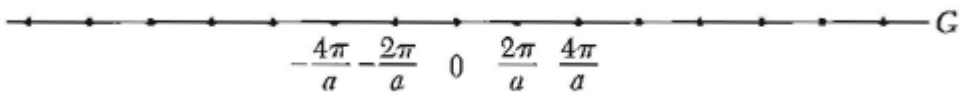
숙제: **Prove** $n(\mathbf{r}+\mathbf{T}) = n(\mathbf{r})$

Fourier analysis

In 1-dimension

$$n(x) = \sum_p n_p \exp(i2\pi px/a)$$: real if $n^*_{-p} = n_p$ is satisfied

$2\pi/a$ is a point in the reciprocal lattice or Fourier space of the crystal.



Momentum space

In 3-dimension $n(\mathbf{r}+\mathbf{T}) = n(\mathbf{r})$ $\mathbf{T} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$,

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r}) \qquad n_{\mathbf{G}} = V_c^{-1} \int_{\text{cell}} dV\, n(\mathbf{r}) \exp(-i\mathbf{G}\cdot\mathbf{r})$$

G = reciprocal lattice vector in 3D

Reciprocal Lattice Vector

Reciprocal lattice vectors

$\boldsymbol{a}_i$: real-space lattice vector
$\boldsymbol{b}_j$: reciprocal space lattice vector

Construction of reciprocal lattice vectors

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}.$$

➔ If $\mathbf{a}_i$ are primitive, $\mathbf{b}_j$ are primitive.

Reciprocity condition

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

Reciprocal Lattice Vector

Reciprocal lattice vectors

a_i : real-space lattice vector
b_j : reciprocal space lattice vector

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$ **(reciprocity condition)**

u_i, v_j : integers

$$\mathbf{T} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3.$$ Translational vector in **real space**

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

$$\exp(i\mathbf{G}\cdot\mathbf{T}) = 1$$

G: Translational vector in **reciprocal lattice space**

$$\exp(i\mathbf{G}\cdot\mathbf{T}) = \exp[i(v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3)\cdot(u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3)]$$
$$= \exp[i2\pi(v_1u_1 + v_2u_2 + v_3u_3)] = 1$$

$$n(\mathbf{r}+\mathbf{T}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r})\exp(i\mathbf{G}\cdot\mathbf{T})$$

$$n(\mathbf{r}+\mathbf{T}) = n(\mathbf{r}) = \sum n_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r}).$$

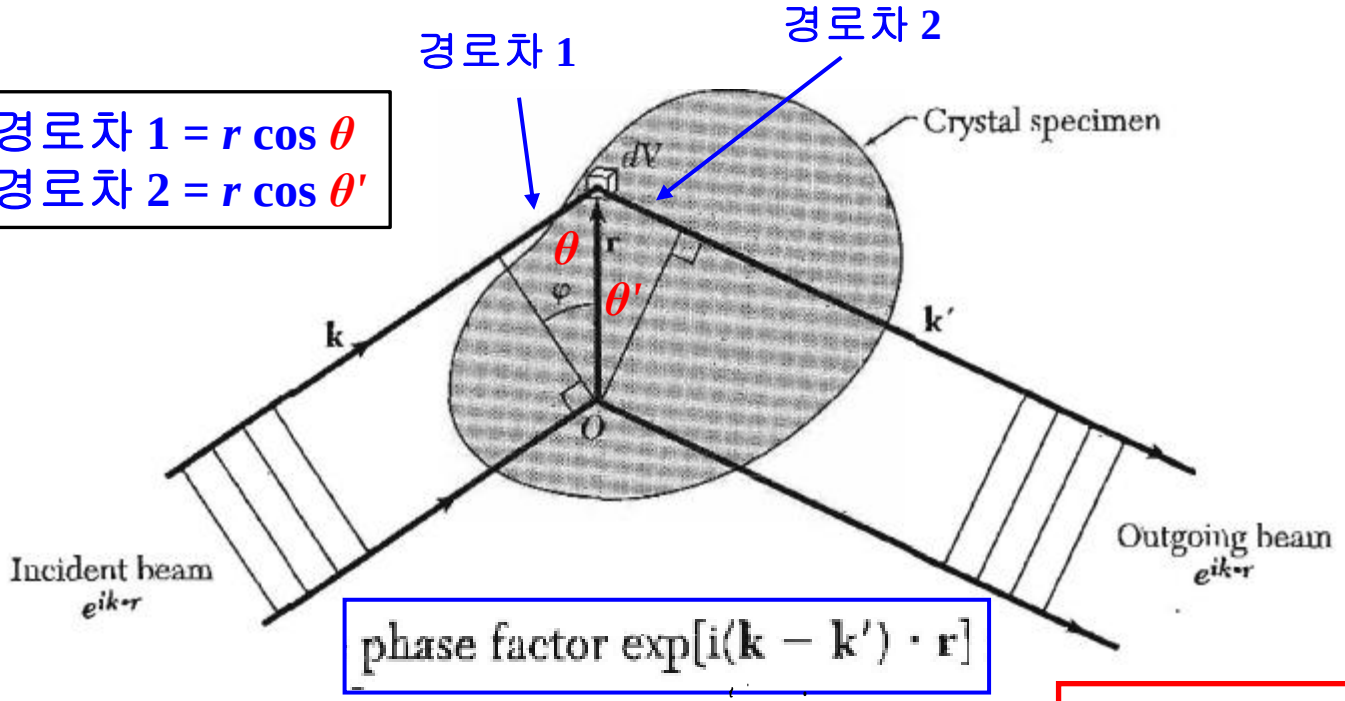
→ ***G*** : non-zero ***k*** in ***Fourier*** **expansion**

Scattered Wave Amplitude

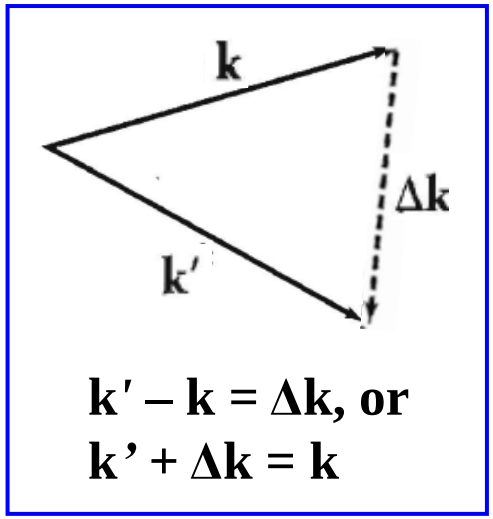
경로차 = 경로차 1 + 경로차 2
위상차 = 위상차 1 + 위상차 2
$= k\,(r\cos\theta + r\cos\theta')$
$= \mathbf{k}\cdot\mathbf{r} - \mathbf{k}'\cdot\mathbf{r}$

- **Diffraction conditions**

경로차 1 = $r\cos\theta$
경로차 2 = $r\cos\theta'$



phase factor $\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]$



$\mathbf{k}' - \mathbf{k} = \Delta\mathbf{k}$, or
$\mathbf{k}' + \Delta\mathbf{k} = \mathbf{k}$

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r})$$

Scattering amplitude

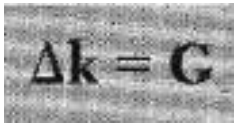
$$F = \int dV\, n(\mathbf{r}) \exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}] = \int dV\, n(\mathbf{r}) \exp(-i\Delta\mathbf{k}\cdot\mathbf{r}) = \sum_{\mathbf{G}} \int dV\, n_{\mathbf{G}} \exp[i(\mathbf{G}-\Delta\mathbf{k})\cdot\mathbf{r}]$$

= 0 unless Δk = G

$F = Vn_G$ **for Δk = G**

Scattered Wave Amplitude

- **Bragg condition**



Diffraction condition

$k' - k = G$, $k' = k + G$, $k'^2 = (k + G)^2$ $2k \cdot G = G^2$ **Another expression of Bragg law**

$d(hkl)$ = **spacing between parallel lattice planes, normal to the direction G (G =** $hb_1 + kb_2 + lb_3$ **)**
= $2\pi/|G|$

$2kG \sin\theta = G^2$ $2(2\pi/\lambda)\sin\theta = 2\pi/d(hkl)$ $2d(hkl)\sin\theta = \lambda$ $2d\sin\theta = \lambda$

Scattered Wave Amplitude

- **Laue Equations**

Simple geometrical interpretation

$\Delta\mathbf{k}$ lies on a certain cone about the direction of $\mathbf{a}_1$

$\Delta\mathbf{k} = \mathbf{G}$ → $\mathbf{a}_1 \cdot \Delta\mathbf{k} = 2\pi v_1$; $\mathbf{a}_2 \cdot \Delta\mathbf{k} = 2\pi v_2$; $\mathbf{a}_3 \cdot \Delta\mathbf{k} = 2\pi v_3$

Diffraction condition

Laue equations

Remember

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

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

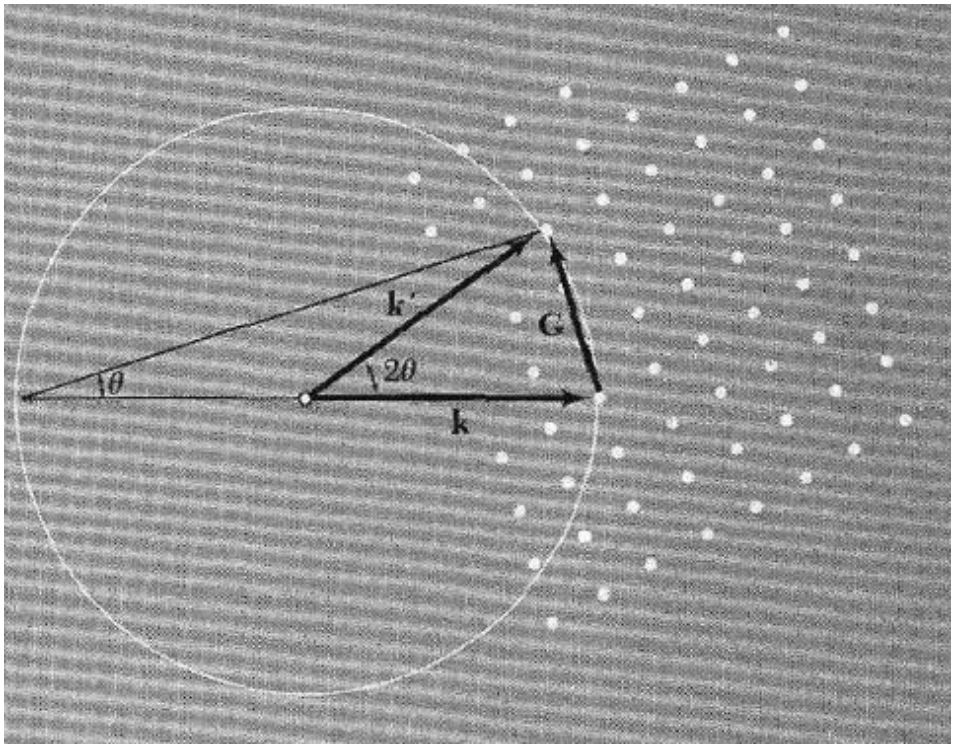
Laue equations

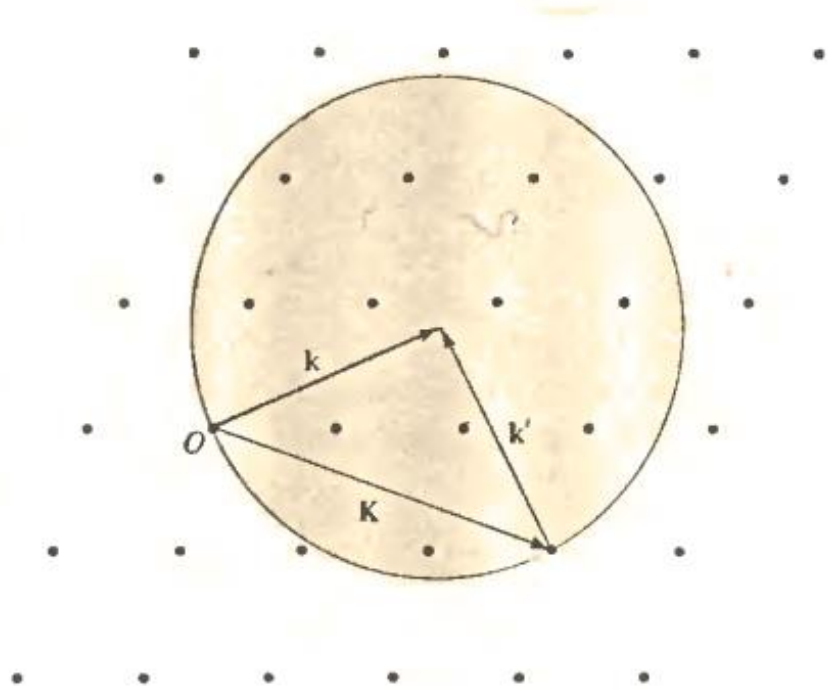
→ **severe condition to satisfy !**

→ **requires systematic sweeping or searching in λ or crystal orientation (or by sheer accident)**

Ewald construction

$$\Delta k = G$$





임의의 ***En***, 임의의 파동 입사 (또는 결정샘플 방향)에 대하여 회절조건을 만족할 수 없다.

Ewald sphere의 반지름 (→ 파동 ***En***), 파동 입사방향 (또는 결정샘플 방향)을 바꿈으로써 회절 관측 가능!

Brillouin Zone

$$\vec{k} - \vec{k}' = \vec{G}$$

Diffraction condition

$$\vec{k}' = \vec{k} - \vec{G}$$

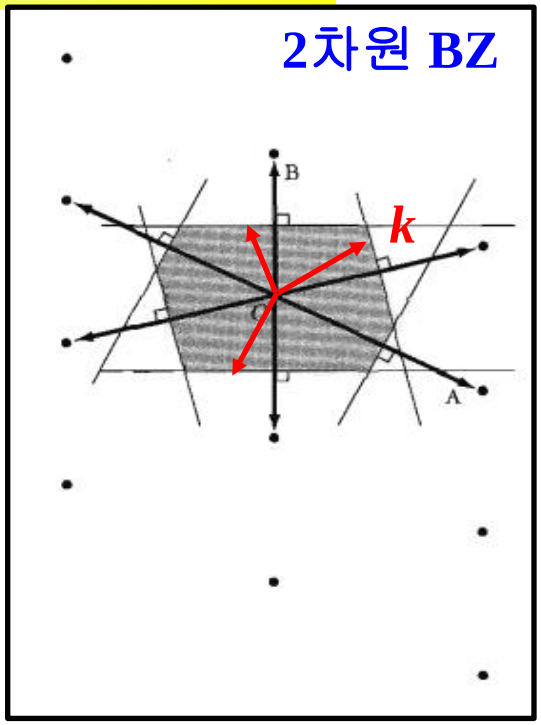
$$\left|\vec{k}\right| = \left|\vec{k}'\right| = \left|\vec{k} - \vec{G}\right| \Longrightarrow k^2 = k^2 + G^2 - 2\vec{k}\cdot\vec{G}$$

Squaring both sides

$$G^2 = 2\vec{k}\cdot\vec{G} \quad \text{or} \quad \frac{G}{2} = \vec{k}\cdot\frac{\vec{G}}{G}$$

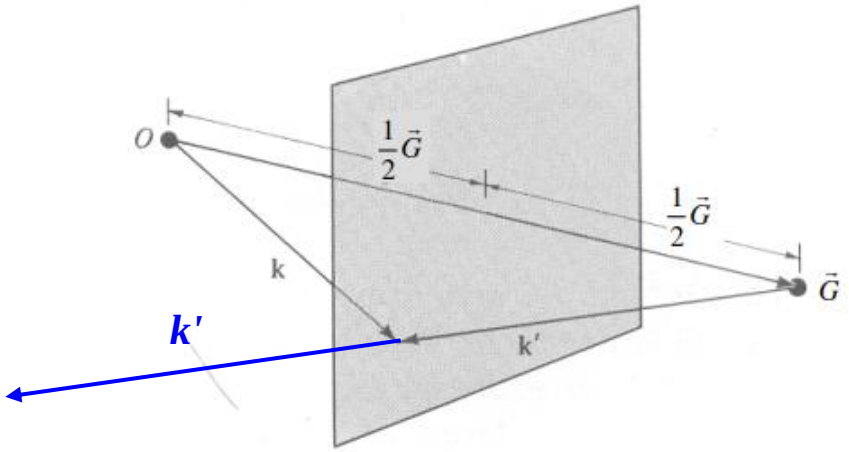
$$2\mathbf{k}\cdot\mathbf{G} + G^2 = 0$$

$$\mathbf{k}\cdot\left(\tfrac{1}{2}\mathbf{G}\right) = \left(\tfrac{1}{2}G\right)^2$$



$$\frac{G}{2} = \vec{k}\cdot\frac{\vec{G}}{G}$$

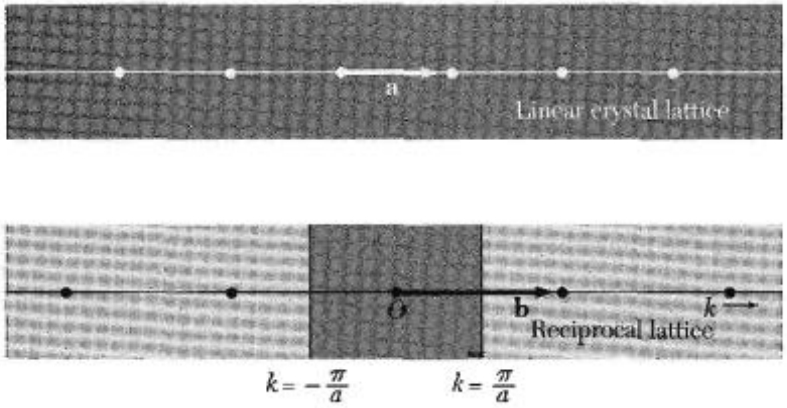
***k* at "Brillouin Zone boundary"**



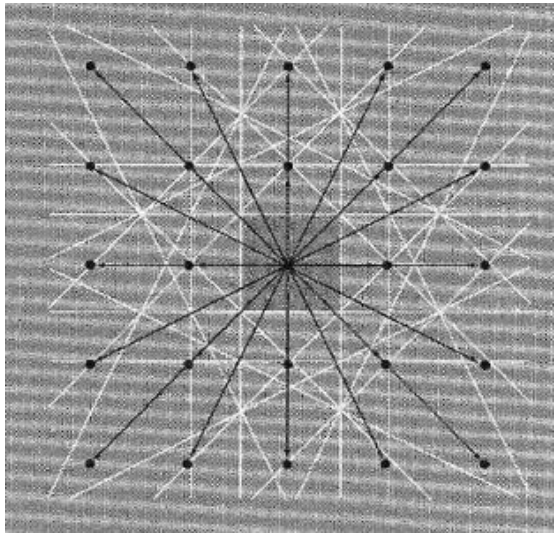
Brillouin Zone

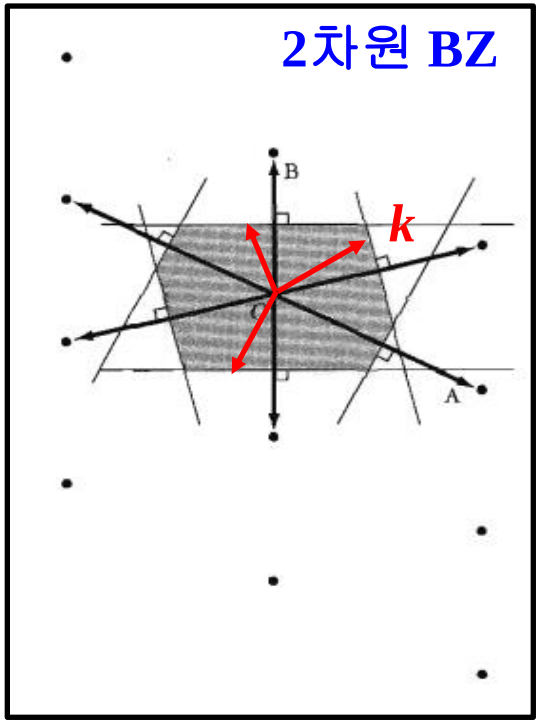
Brillouin zones: Wigner-Seitz cells in k-space

1차원



2차원





Reciprocal Lattice to bcc Lattice

The primitive translation vectors of the bcc lattice (Fig. 12) are

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

$$V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \tfrac{1}{2}a^3$$

$$V_k = \mathbf{b}_1 \cdot \mathbf{b}_2 \times \mathbf{b}_3 = 2(2\pi/a)^3$$

$$V\,V_k = (2\pi)^3$$

***reciprocal* to**

$$\mathbf{b}_1 = (2\pi/a)(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \qquad \mathbf{b}_2 = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{z}}) \; ; \qquad \mathbf{b}_3 = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{y}})$$

➔ **primitive lattice vectors of an fcc lattice**

The shortest **G**'s are the following 12 vectors,

$$(2\pi/a)(\pm\hat{\mathbf{y}} \pm \hat{\mathbf{z}}) \; ; \qquad (2\pi/a)(\pm\hat{\mathbf{x}} \pm \hat{\mathbf{z}}) \; ; \qquad (2\pi/a)(\pm\hat{\mathbf{x}} \pm \hat{\mathbf{y}})$$

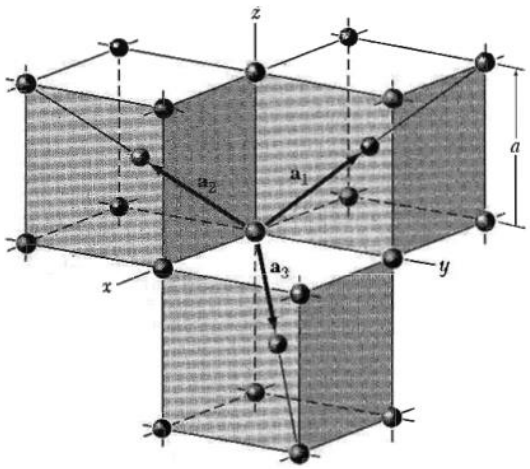


Figure 12 Primitive basis vectors of the body-centered cubic lattice.

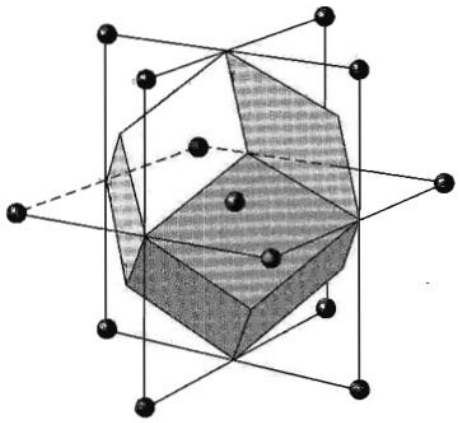


Figure 13 First Brillouin zone of the body-centered cubic lattice. The figure is a regular rhombic dodecahedron.

1st BZ of bcc lattice

Reciprocal Lattice to fcc Lattice

The primitive translation vectors of the fcc lattice of Fig. 14 are

$$\mathbf{a}_1 = \frac{1}{2}a(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a}_2 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a}_3 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \; .$$

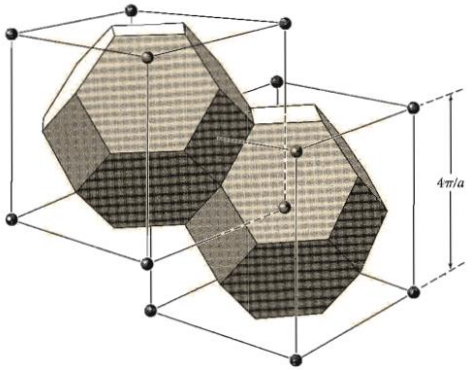
reciprocal to

$$\mathbf{b}_1 = (2\pi/a)(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \qquad \mathbf{b}_2 = (2\pi/a)(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}})$$

$$\mathbf{b}_3 = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \; .$$

➔ **primitive lattice vectors of a bcc lattice**

The shortest **G**'s are the eight vectors: $(2\pi/a)(\pm\hat{\mathbf{x}} \pm \hat{\mathbf{y}} \pm \hat{\mathbf{z}})$



1st BZ of fcc lattice

The volume of the primitive cell is

$$V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \frac{1}{4}a^3$$

Q. What is the volume of the 1st BZ of fcc lattice?

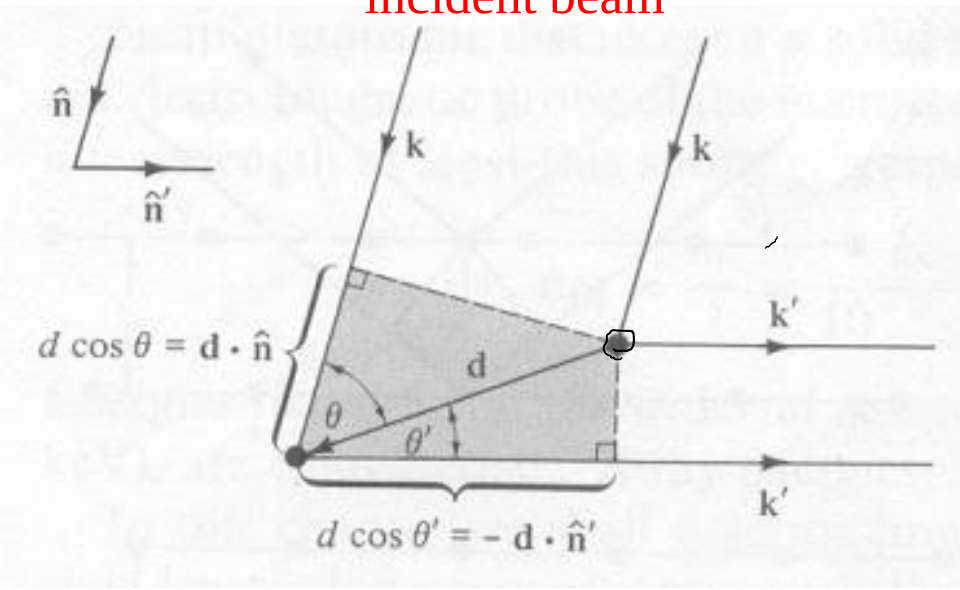
(보충)

Ashcroft & Mermin, Solid State physics, CH. 6

DIFFRACTION OF WAVES BY CRYSTALS

Von Laue formulation

: diffraction condition in terms of **scattering by lattice point (→ charge distribution)**



Incident x-ray: along direction $\hat{n}$

wavelength λ

wave vector $\vec{k} = \frac{2\pi}{\lambda}\hat{n}$

A scattered wave: direction $\hat{n}'$

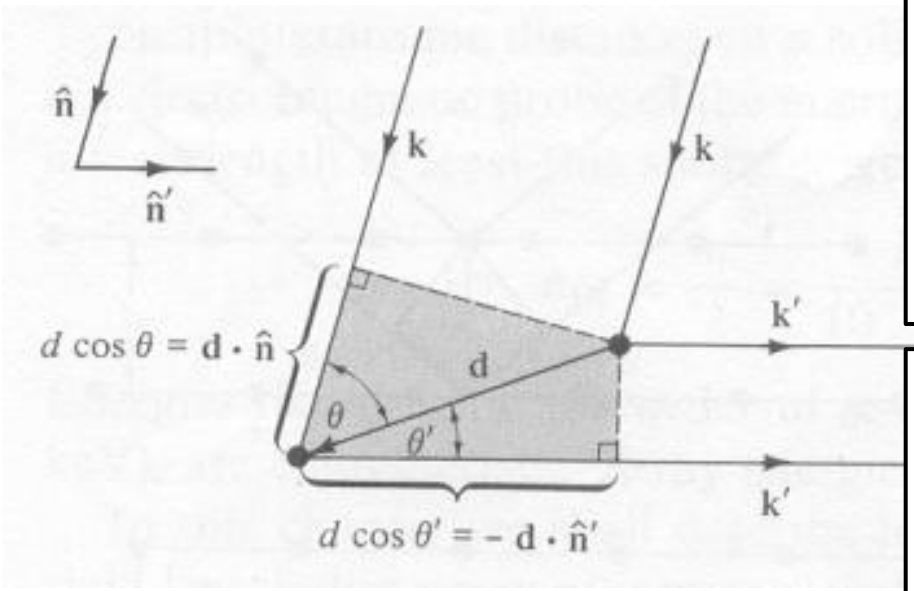
wavelength λ

wave vector $\vec{k}' = \frac{2\pi}{\lambda}\hat{n}'$

(보충)

Ashcroft & Mermin, Solid State physics, CH. 6

Von Laue formulation of X-ray diffraction by a crystal



Incident x-ray: along direction $\hat{n}$

wavelength λ

wave vector $\vec{k} = \frac{2\pi}{\lambda}\hat{n}$

A scattered wave: direction $\hat{n}'$

wavelength λ

wave vector $\vec{k}' = \frac{2\pi}{\lambda}\hat{n}'$

For all possible *d*,

$$d\cos\theta + d\cos\theta' = \vec{d}\cdot(\hat{n}-\hat{n}') = m\lambda \quad (m : \text{integer}) \qquad \times\left(\frac{2\pi}{\lambda}\right)$$

For all possible ***T***,

$$\vec{T}\cdot(\vec{k}-\vec{k}') = 2\pi m \qquad \Delta k\cdot T = 2\pi m \qquad \Delta k = \vec{k}'-\vec{k}$$

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

$$e^{i(\vec{k}'-\vec{k})\cdot\vec{T}} = 1$$

→ **Diffraction** condition

Reciprocal Lattice Vector

Reciprocal lattice vectors

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

If $\mathbf{a}_i$ are primitive, $\mathbf{b}_j$ are primitive.

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

$$\exp(i\mathbf{G} \cdot \mathbf{T}) = 1$$

Translational vector
in reciprocal lattice space

Laue diffraction condition

$$e^{i(\vec{k}'-\vec{k})\cdot\vec{R}} = 1 \longrightarrow$$

Δk = G

G = reciprocal lattice vector

Reciprocal Lattice Vector

Reciprocal lattice vectors

a_i : real-space lattice vector
b_j : reciprocal space lattice vector

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}.$$

➔ If $\mathbf{a}_i$ are primitive, $\mathbf{b}_j$ are primitive.

Reciprocity condition

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

u_i, v_j : integers

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

Translational vector in **real space**

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

$$\exp(i\mathbf{G} \cdot \mathbf{T}) = 1$$

G: Translational vector in **reciprocal lattice space**

Reciprocal Lattice Vector

숙제: Reciprocal lattice to

(1) sc

(2) fcc

(3) bcc

(4) hcp

SCATTERED WAVE

Fourier analysis of the basis

Scattering amplitude for $\Delta k = G$

Structure factor (integral over a cell)

$$F_{\mathbf{G}} = N \int_{cell} dV\, n(\mathbf{r}) \exp(-i\mathbf{G}\cdot\mathbf{r}) = NS_{\mathbf{G}}$$

$$S_G = n_G = V_c^{-1} \int_{cell} dV\, n(\mathbf{r}) \exp(-i\mathbf{G}\cdot\mathbf{r})$$

$$n(\mathbf{r}) = \sum_{j-1}^{s} n_j(\mathbf{r} - \mathbf{r}_j)$$

$$S_{\mathbf{G}} = \sum_j \int dV\, n_j(\mathbf{r} - \mathbf{r}_j) \exp(-i\mathbf{G}\cdot\mathbf{r})$$

$$= \sum_j \exp(-i\mathbf{G}\cdot\mathbf{r}_j) \int dV\, n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G}\cdot\boldsymbol{\rho})$$

$$S_{\mathbf{G}} = \sum_j f_j \exp(-i\mathbf{G}\cdot\mathbf{r}_j)$$ **Structure factor of the basis**

$$f_j = \int dV\, n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G}\cdot\boldsymbol{\rho})$$ **Atomic form factor**

SCATTERED WAVE (정리)

Fourier analysis of the basis

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

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r})$$

$$n_{\mathbf{G}} = V_c^{-1} \int_{cell} dV\, n(\mathbf{r}) \exp(-i\mathbf{G}\cdot\mathbf{r})$$

Scattering amplitude

(integral over a sample)

$$F = \int dV\, n(\mathbf{r}) \exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}] = \int dV\, n(\mathbf{r}) \exp(-i\Delta\mathbf{k}\cdot\mathbf{r})$$

= 0 unless $\Delta\mathbf{k} = \mathbf{G}$

For $\Delta\mathbf{k} = \mathbf{G}$, $F = N(V_c n_G) = N n_G = N S_G$

Scattering amplitude for $\Delta\mathbf{k} = \mathbf{G}$

Structure factor (integral over a cell)

$$F_{\mathbf{G}} = N \int_{cell} dV\, n(\mathbf{r}) \exp(-i\mathbf{G}\cdot\mathbf{r}) = N S_{\mathbf{G}}$$

$$S_G = n_G = V_c^{-1} \int_{cell} dV\, n(\mathbf{r}) \exp(-i\mathbf{G}\cdot\mathbf{r})$$

$$S_{\mathbf{G}} = \sum_j f_j \exp(-i\mathbf{G}\cdot\mathbf{r}_j)$$

Structure factor of the basis

$$f_j = \int dV\, n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G}\cdot\boldsymbol{\rho})$$

Atomic form factor (for each basis atom)

SCATTERED WAVE

Classical calculation of the scattering factor

$$f_j = \int dV\, n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G}\cdot\boldsymbol{\rho})$$

Atomic form factor (for each basis atom)

For spherically symmetric charge distribution

$$f_j \equiv 2\pi \int dr\, r^2\, d(\cos\alpha)\, n_j(r) \exp(-iGr\cos\alpha)$$

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

$\frac{2\sin Gr}{Gr}$

(i) If $n_j(r) \sim \delta(0)$ $\quad f_j = 4\pi \int dr\, n_j(r) r^2 = Z$

(ii) Forward scattering G = 0, $\quad f_j = Z$

The overall electron distribution in a solid as seen in x-ray diffraction is fairly close to that of the appropriate free atoms. This statement does not mean that the outermost or valence electrons are not redistributed somewhat in forming the solid; it means only that the x-ray reflection intensities are represented well by the free atom values of the form factors and are not very sensitive to small redistributions of the electrons.

SCATTERED WAVE

Fourier analysis of the basis

Homework : Prove

$$S_{\mathbf{G}}(v_1 v_2 v_3) = \sum_j f_j \exp[-i2\pi(v_1 x_j + v_2 y_j + v_3 z_j)]$$

with $\mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3$, $\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3$

Structure Factor of the bcc Lattice

The bcc basis referred to the cubic cell has identical atoms at $x_1 = y_1 = z_1 = 0$ and at $x_2 = y_2 = z_2 = \frac{1}{2}$. Thus (46) becomes

bcc lattice = **2 identical basis atoms in a sc cell**

→ a **sc** reciprocal lattice **(diffraction points)**

(diffraction intensity) $\propto$ **(the structure factor)^2** $\quad \left[S_{\mathbf{G}} = \sum_j f_j \exp(-i\mathbf{G}\cdot\mathbf{r}_j) \right]^2$

$$S_{\mathbf{G}}(v_1v_2v_3) = \sum_j f_j \exp[-i2\pi(v_1x_j + v_2y_j + v_3z_j)]$$

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

$r_1 = (0,0,0)$
$r_2 = (1/2,1/2,1/2)$

$S = 0$ when $v_1 + v_2 + v_3 =$ odd integer ;
$S = 2f$ when $v_1 + v_2 + v_3 =$ even integer .

→ **Non-zero intensities result in *fcc* diffraction points (reciprocal lattice)**

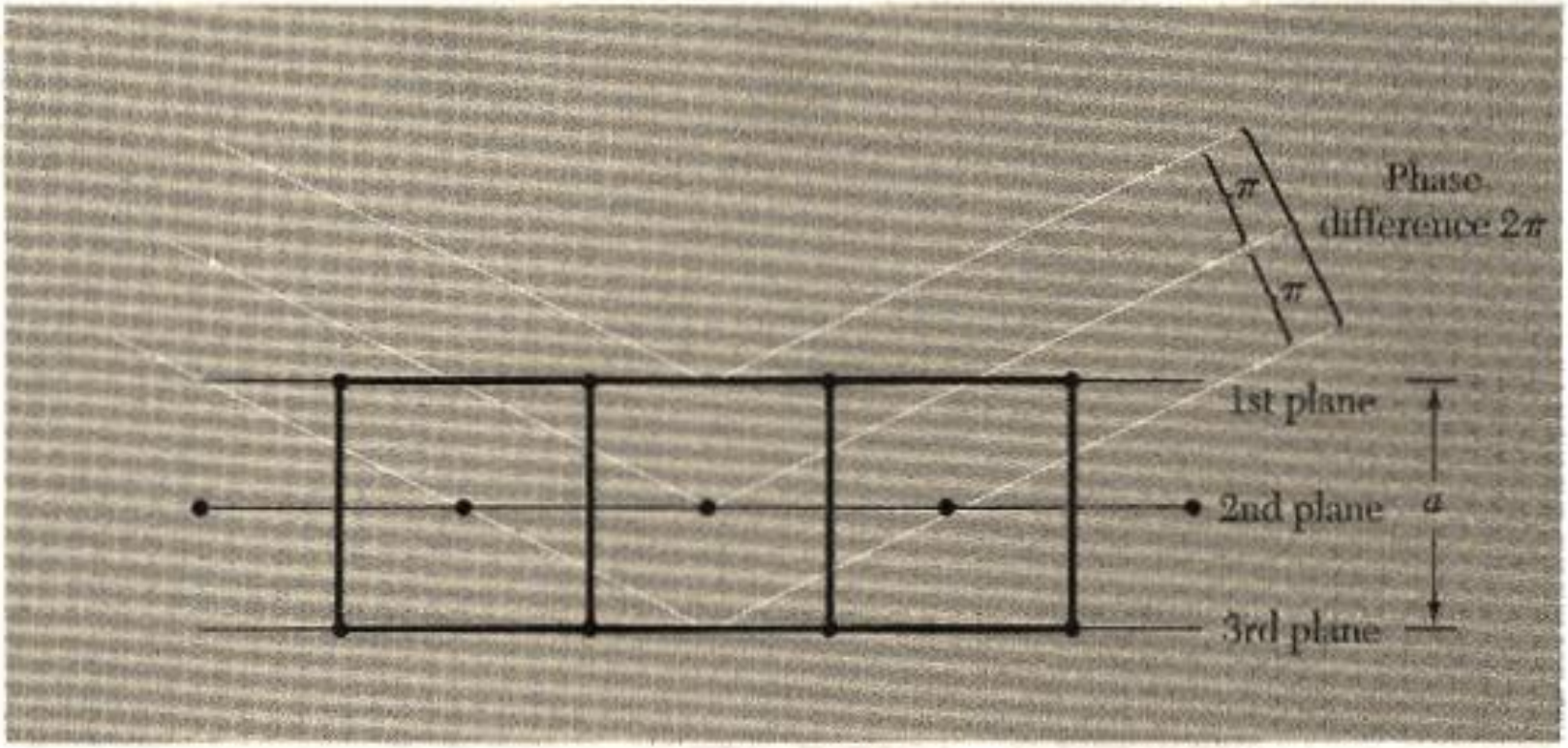


Figure 16 Explanation of the absence of a (100) reflection from a body-centered cubic lattice. The phase difference between successive planes is π, so that the reflected amplitude from two adjacent planes is $1 + e^{-i\pi} = 1 - 1 = 0$.

Structure Factor of the fcc Lattice

The basis of the fcc structure referred to the cubic cell has identical atoms at 000; $0\frac{11}{22}$; $\frac{1}{2}0\frac{1}{2}$; $\frac{11}{22}0$. Thus (46) becomes

$r_1 = (0,0,0)$
$r_2 = (0,1/2,1/2)$
$r_3 = (1/2,0,1/2)$
$r_4 = (1/2,1/2,0)$

fcc lattice = **4 identical basis atoms in a sc cell**

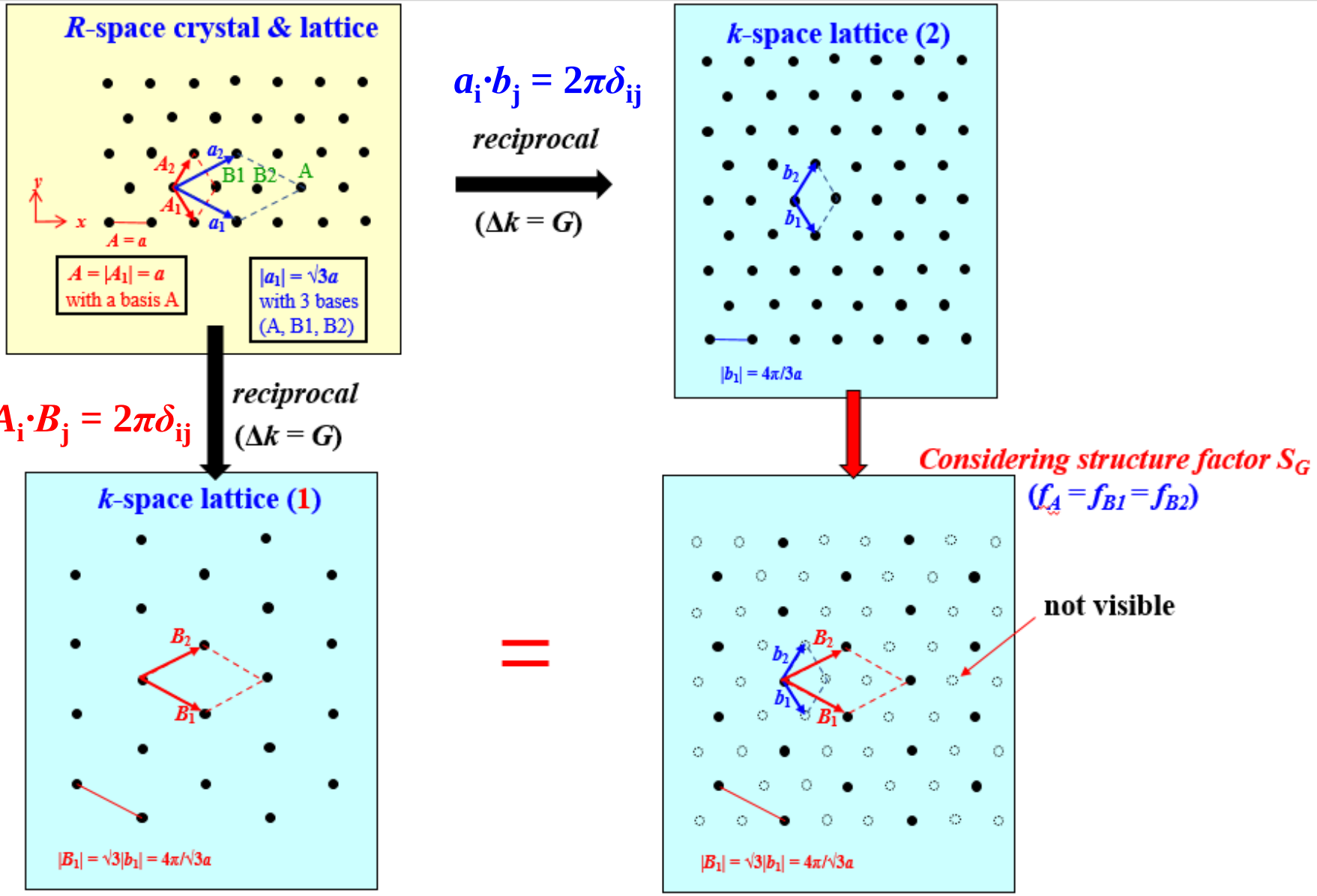
→ a **sc** reciprocal lattice **(diffraction points)**

$$S(v_1v_2v_3) = f[1 + \exp[-i\pi(v_2 + v_3)] + \exp[-i\pi(v_1 + v_3)] + \exp[-i\pi(v_1 + v_2)]] \quad (48)$$

If all indices are even integers, $S = 4f$; similarly if all indices are odd integers. But if only one of the integers is even, two of the exponents will be odd multiples of $-i\pi$ and S will vanish. If only one of the integers is odd, the same argument applies and S will also vanish. Thus in the fcc lattice no reflections can occur for which the indices are partly even and partly odd.

→ **Non-zero intensities result in *bcc* diffraction points (reciprocal lattice)**

2D example


R-space crystal & lattice
A = |A1| = a
with a basis A
|a1| = √3a
with 3 bases
(A, B1, B2)
A = a
B1 B2 A
ai·bj = 2πδij
reciprocal
(Δk = G)
k-space lattice (2)
|b1| = 4π/3a
Ai·Bj = 2πδij
reciprocal
(Δk = G)
k-space lattice (1)
|B1| = √3|b1| = 4π/√3a
Considering structure factor SG
(fA = fB1 = fB2)
not visible
|B1| = √3|b1| = 4π/√3a

- **For a given crystal, there are many way to take "lattice & basis".**
- **For different choices of "lattice & basis", the reciprocal lattices are different.**
- **But, the diffraction pattern and intensity from the crystal should be unique because some reciprocal lattice poits become extinct when the structure factor (diffraction intensity) is taken into account.**

(diffraction intensity) $\propto$ (the structure factor)^2

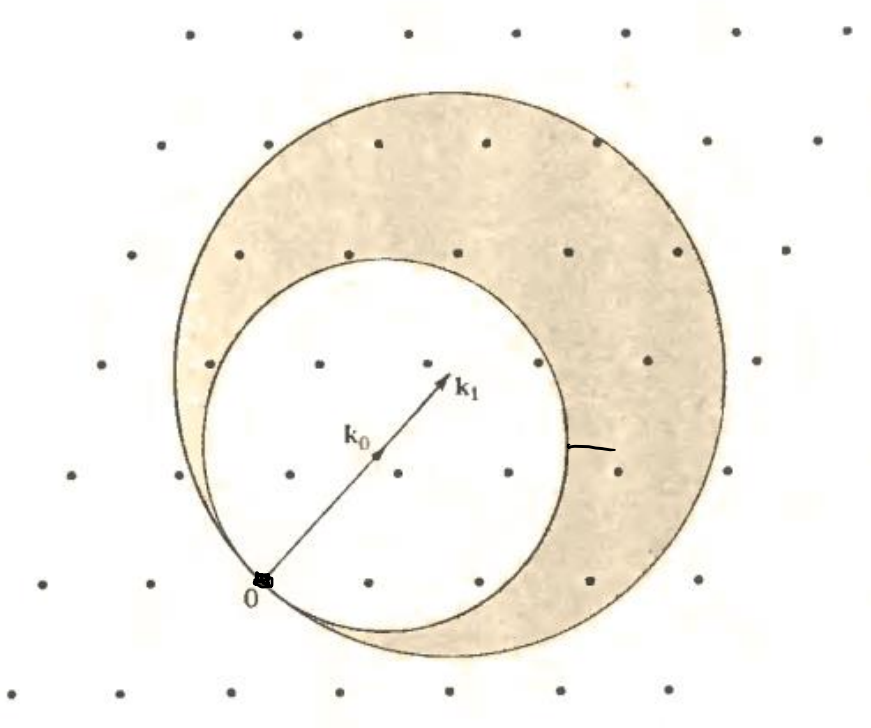
(보충)

Ashcroft & Mermin, Solid State physics, CH. 6

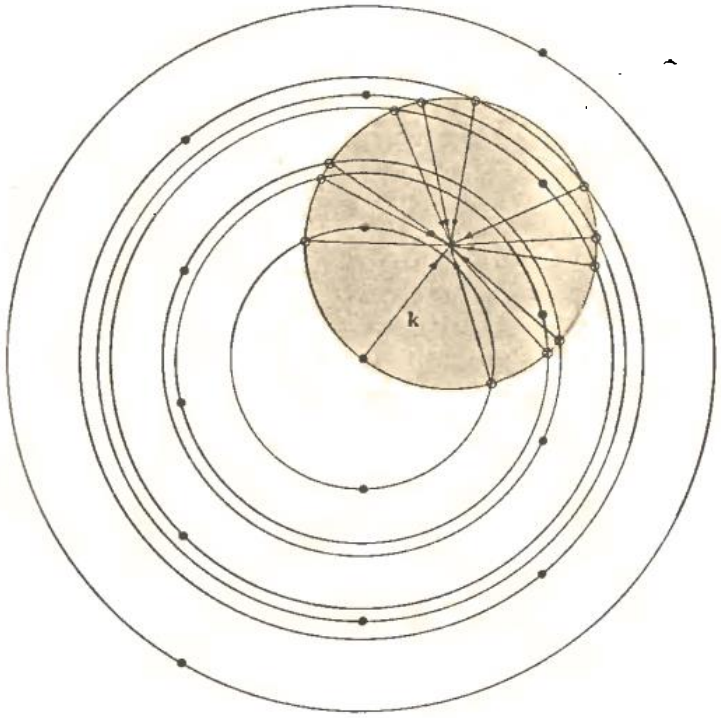
How to do diffraction experiment (XRD)

$$\Delta k = G$$

Laue method



Rotating sample method



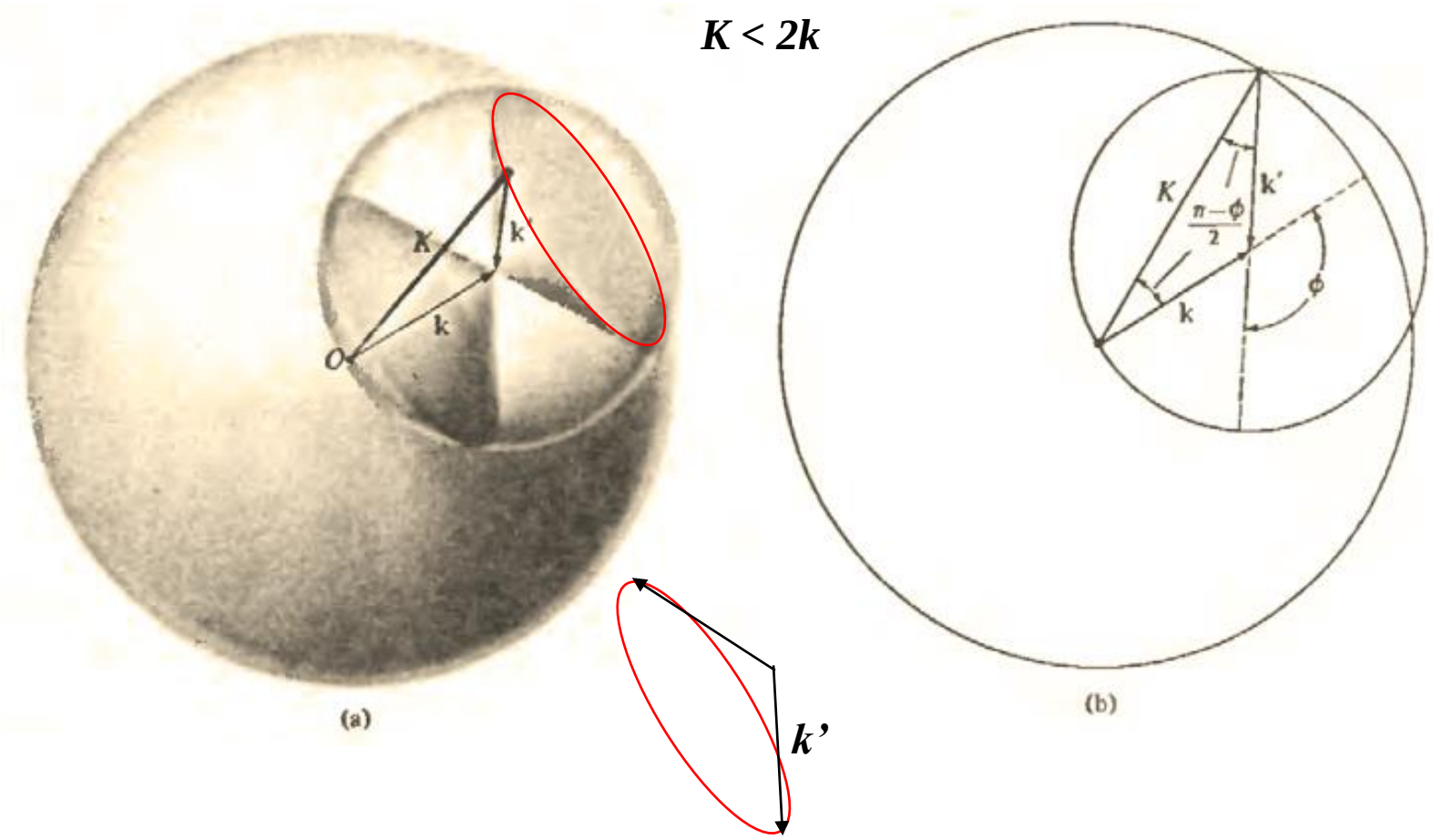
(보충)

Ashcroft & Mermin, Solid State physics, CH. 6

How to do diffraction experiment (XRD)

$$\Delta k = G$$

Powder method



SUMMARY

SUMMARY

- Various statements of the Bragg condition:

$$2d \sin\theta = n\lambda \ ; \qquad \Delta\mathbf{k} = \mathbf{G} \ ; \qquad 2\mathbf{k}\cdot\mathbf{G} = \mathbf{G}^2 \ .$$

- Laue conditions:

$$\mathbf{a}_1\cdot\Delta\mathbf{k} = 2\pi v_1 \ ; \qquad \mathbf{a}_2\cdot\Delta\mathbf{k} = 2\pi v_2 \ ; \qquad \mathbf{a}_3\cdot\Delta\mathbf{k} = 2\pi v_3 \ .$$

- The primitive translation vectors of the reciprocal lattice are

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3} \ ; \qquad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3\times\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3} \ ; \qquad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1\times\mathbf{a}_2}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3} \ .$$

Here $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are the primitive translation vectors of the crystal lattice.

- A reciprocal lattice vector has the form

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

where v_1, v_2, v_3 are integers or zero.

- The scattered amplitude in the direction $\mathbf{k}' = \mathbf{k} + \Delta\mathbf{k} = \mathbf{k} + \mathbf{G}$ is proportional to the geometrical structure factor:

$$S_\mathbf{G} \equiv \sum f_j \exp(-i\mathbf{r}_j\cdot\mathbf{G}) = \sum f_j \exp[-i2\pi(x_j v_1 + y_j v_2 + z_j v_3)] \ ,$$

where j runs over the s atoms of the basis, and f_j is the atomic form factor (49) of the jth atom of the basis. The expression on the right-hand side is written for a reflection $(v_1 v_2 v_3)$, for which $\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3$.

- Any function invariant under a lattice translation $\mathbf{T}$ may be expanded in a Fourier series of the form

$$n(\mathbf{r}) = \sum_\mathbf{G} n_\mathbf{G} \exp(i\mathbf{G}\cdot\mathbf{r}) \ .$$

- The first Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice. Only waves whose wavevector $\mathbf{k}$ drawn from the origin terminates on a surface of the Brillouin zone can be diffracted by the crystal.

Crystal lattice	*First Brillouin zone*
Simple cubic	Cube
Body-centered cubic	Rhombic dodecahedron (Fig. 13)
Face-centered cubic	Truncated octahedron (Fig. 15)

Homework

Problems #1~7