

4-2 한 개의 전자의 산란

한 개의 전자는 X선을 두 가지 방법으로 산란한다

- Thomson 공식 - 산란각에 의존, 간섭성 산란
 - 전하 e 와 전자의 질량 m 인 한개의 전자가 전자에서 r 미터 거리(P)에서 산란한 빔의 강도로 표시(I).

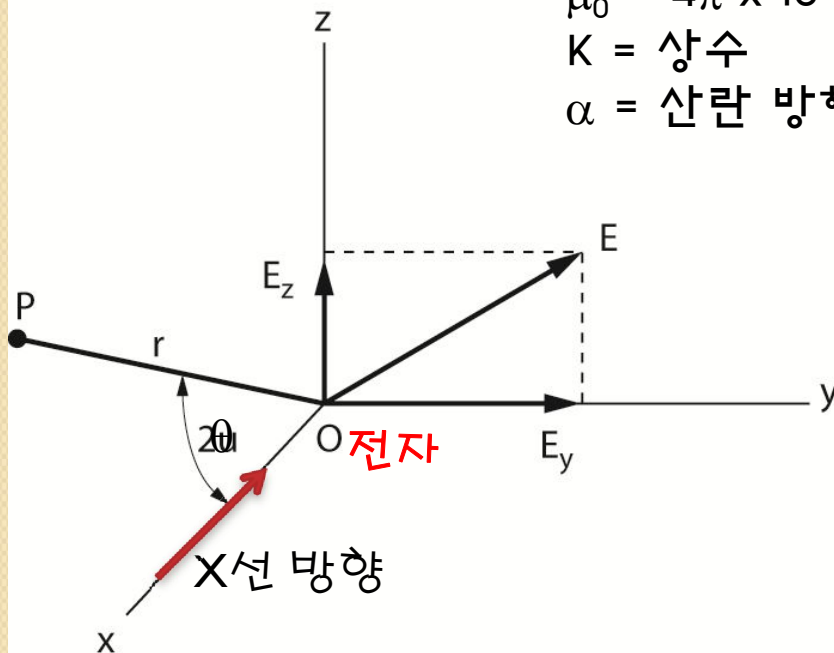
$$I = I_0 \left(\frac{\mu_0}{4\pi} \right)^2 \left(\frac{e^4}{m^2 r^2} \right) \sin^2 \alpha = I_0 \frac{K}{r^2} \sin^2 \alpha$$

I_0 = 입사빔의 강도

$\mu_0 = 4\pi \times 10^{-7} \text{ m kg C}^{-2}$

K = 상수

α = 산란 방향과 전자의 가속 방향 사이의 각 ($\angle yOP$)



$$I_P = I_{Py} + I_{Pz}$$

$$= I_0 \frac{K}{r^2} \left(\frac{1 + \cos^2 2\theta}{2} \right)$$

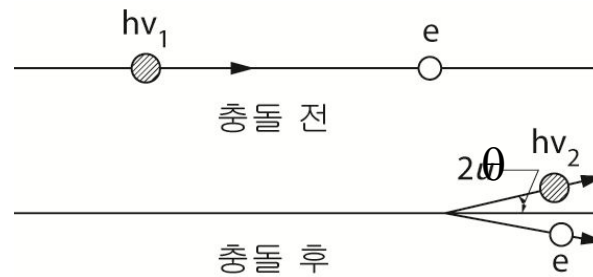
편광인자

4-2 한 개의 전자의 산란

한 개의 전자는 X선을 두 가지 방법으로 산란한다

2. Compton 효과 – 입사빔의 위상과 관계가 일정하지 않다.

- 광자와 전자의 탄성 충돌
- 비간섭성 산란



4-3 한 개 원자의 산란

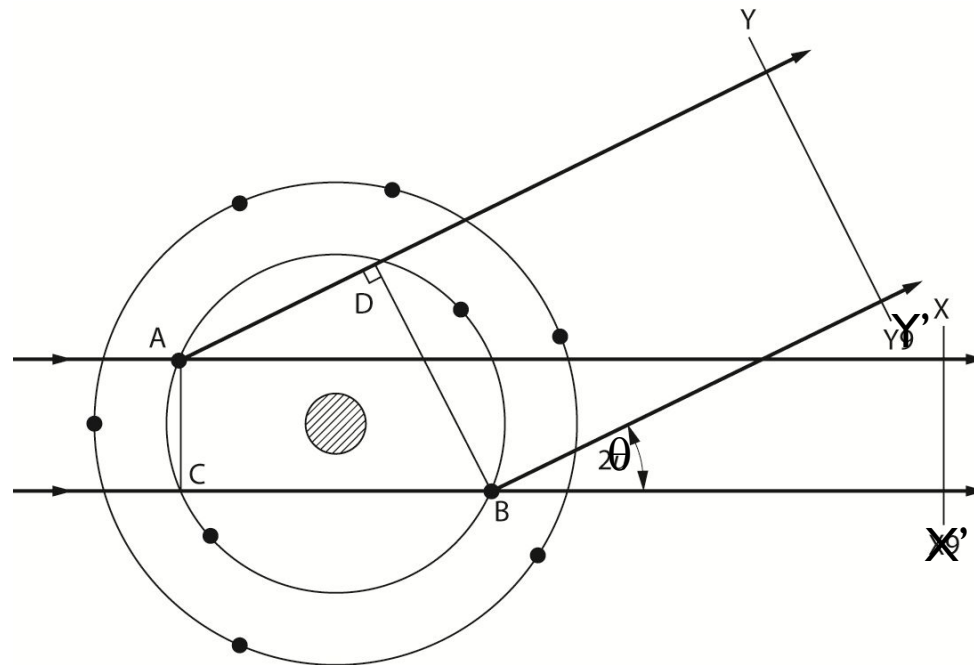
- 원자에 있는 전자들에의 간섭성 산란 발생.
- X선 빔이 한 개 원자에 부딪치면 그 안에 있는 개개의 전자는 Thompson 공식에 따라서 간섭성으로 방사선의 일부를 산란한다.
- $2\theta = 0$ (전방)에서 원자의 모든 전자 산란파 위상 같다

f (원자 산란인자 또는 형식인자)

$$f = \frac{\text{하나의 원자가 산란한 파의 진폭}}{\text{하나의 전자가 산란한 파의 진폭}}$$

$$2\theta = 0 \rightarrow f = Z$$

2θ 증가 \rightarrow 개개의 산란파 위상 같지 않다 $\rightarrow f$ 감소



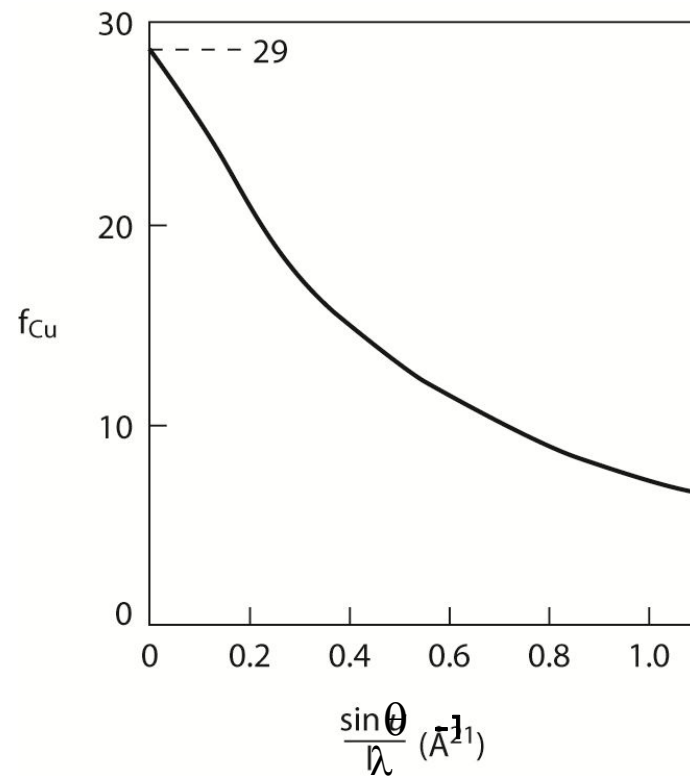
(그림) 구리의 원자 산란인자 계산

: 파장에 의존

: θ 증가 할수록 개개 전자의

산란파는 위상이 같이 않게 된다

→ f 감소



4-4 한 개 단위포의 산란

- 결정을 이루는 모든 원자에서 간섭성 산란 고찰.
- 산란 방사선을 일정한 방향으로 엄격하게 제한 → 회절빔
- 구조인자(structure factor, F) : 단위포의 모든 원자가 산란한 합성파

$$|F| = \frac{\text{단위포의 모든 원자가 산란한 파의 진폭}}{\text{하나의 전자가 산란한 파의 진폭}}$$

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)} \quad u, v, w : \text{분율좌표}(x/a, y/b, z/c)$$

- 단위포의 모든 원자가 Bragg 법칙이 예측하는 방향으로 회절 하게 한 빔의 강도 표현 → 합성빔의 진폭 제곱 $|F|^2$ 에 비례.

Information from peak intensity?

$$I \propto |F|^2$$

$$I_{\text{calc}} = I_{\text{bck}} + S \sum_{hkl} C_{hkl}(\theta) F_{hkl}^2(\theta) P_{hkl}(\theta)$$

background

Scale factor

Miller

Corrections

Structure factor

Profile function

Structure Symmetry

Experimental Geometry set-up

Atomic positions, site occupancy & thermal factors

particle size, stress- strain, texture +

Experimental resolution

4-6 구조인자 계산

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

a) $e^{\pi i} = e^{3\pi i} = e^{5\pi i} = -1$

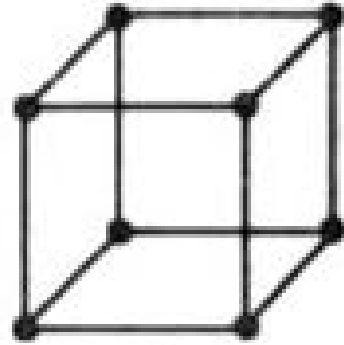
b) $e^{2\pi i} = e^{4\pi i} = e^{6\pi i} = +1$

c) $e^{n\pi i} = (-1)^n,$

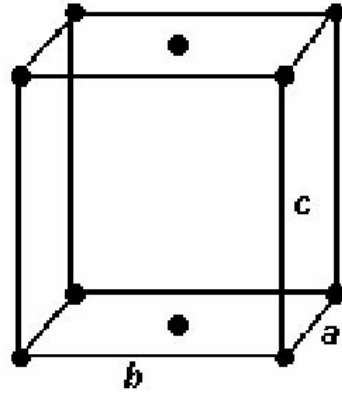
d) $e^{n\pi i} = e^{-n\pi i},$

e) $e^{i\pi} + e^{-i\pi} = 2 \cos x$

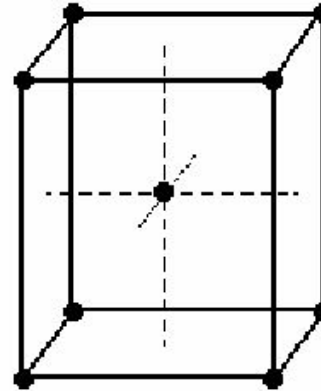
Cubic system



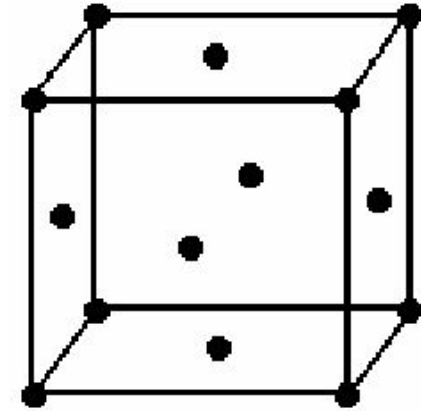
P - 000



C - 000 and $\frac{1}{2}\frac{1}{2}0$

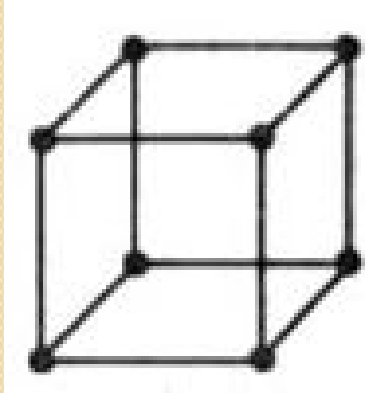


I - 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$



F - 000, $\frac{1}{2}\frac{1}{2}0$,
 $\frac{1}{2}0\frac{1}{2}$ and
 $0\frac{1}{2}\frac{1}{2}$

Cubic system



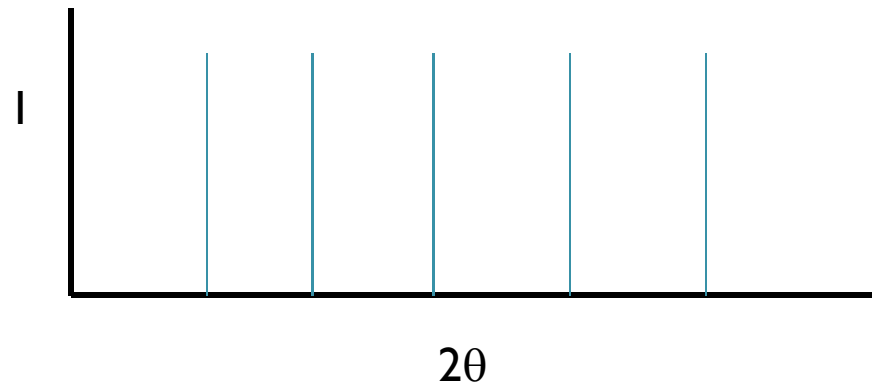
P – 000

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

$$F = fe^{2\pi i(0)} = f$$

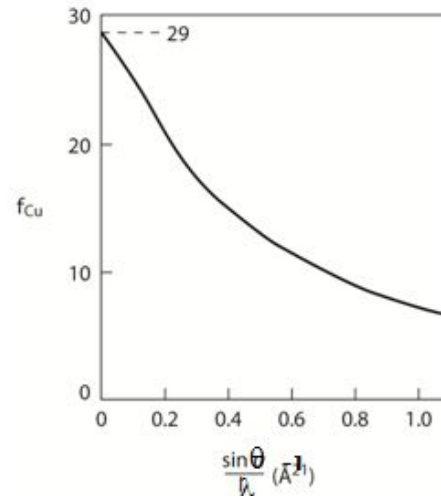
$$F^2 = f^2$$

h,k,l과 무관하며 모든 반사에서 같다.



$$I \propto |F|^2$$

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$



(그림) 구리의 원자 산란인자 계산

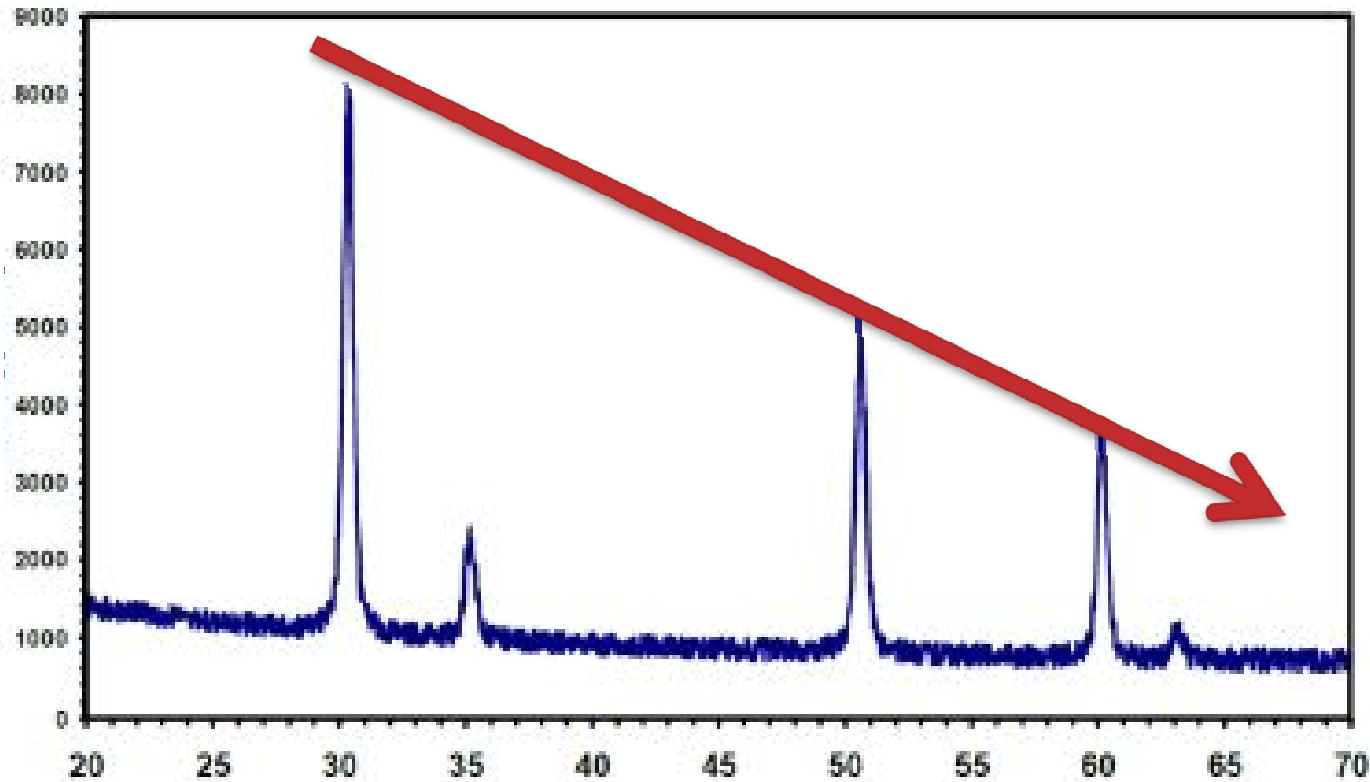
: 파장에 의존

: θ 증가 할수록 개개 전자의

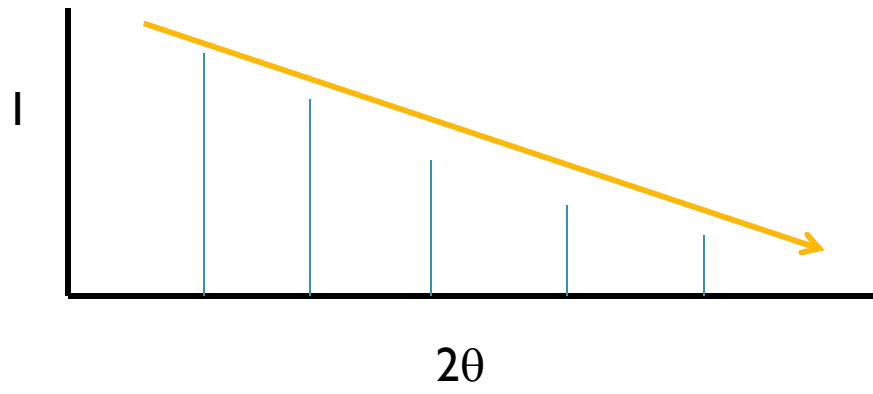
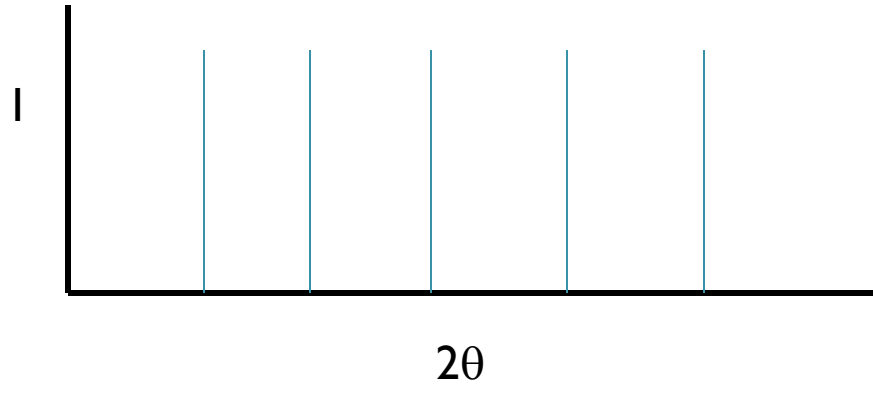
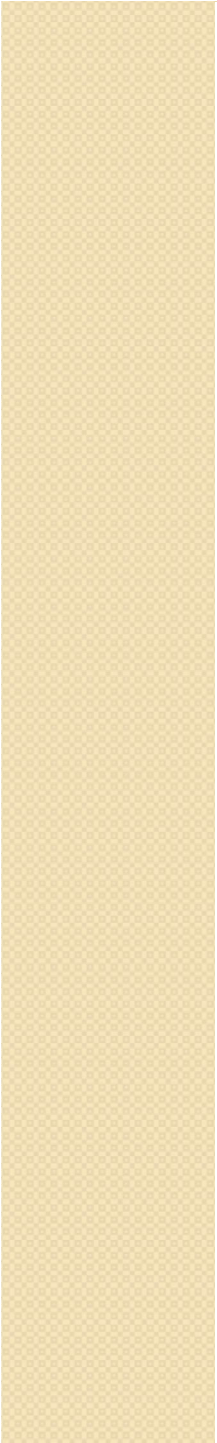
산란파는 위상이 같이 않게 된다

$\rightarrow f$ 감소

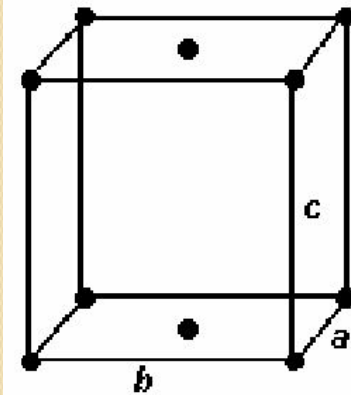
$$I \propto |F|^2$$



2θ



Cubic system



C - 000 and $\frac{1}{2}\frac{1}{2}0$

$$F = fe^{2\pi i(0)} + fe^{2\pi i(h/2 + k/2)}$$
$$= f[1 + e^{\pi i(h+k)}]$$

h,k 둘다 짝수 또는 둘다 홀수 - 비혼합

111, 112, 113, 021, 022, 023

$$F = 2f$$

$$F^2 = 4f^2$$

h,k 하나는 짝수 하나는 홀수 - 혼합

011, 012, 013, 101, 102, 103

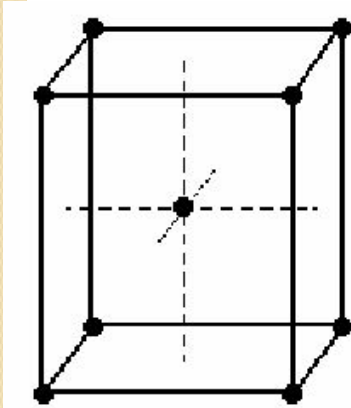
$$F = 0$$

$$F^2 = 0$$

구조인자 영 $\rightarrow I = 0 \rightarrow$ 규칙적 소멸,

systematically absent

Cubic system



1 - 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

$$\begin{aligned} F &= fe^{2\pi i(0)} + fe^{2\pi i(h/2+k/2+l/2)} \\ &= f[1 + e^{\pi i(h+k+l)}] \end{aligned}$$

h,k,l 짝수

$$F = 2f$$

$$F^2 = 4f^2$$

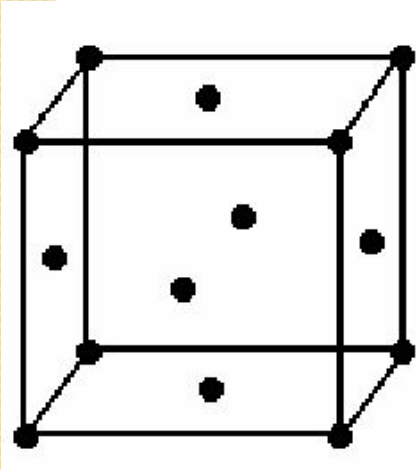
h,k,l 홀수

$$F = 0$$

$$F^2 = 0$$

→ 규칙적 소멸, **systematically absent**

Cubic system



F - 000, $\frac{1}{2}\frac{1}{2}0$,
 $\frac{1}{2}0\frac{1}{2}$ and
 $0\frac{1}{2}\frac{1}{2}$

$$F = fe^{2\pi i(0)} + fe^{2\pi i(h/2+k/2)} + fe^{2\pi i(k/2+l/2)} + fe^{2\pi i(h/2+l/2)}$$
$$= f[1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)}].$$

h,k,l 비혼합

$$F = 4f$$

$$F^2 = 16f^2$$

h,k,l 혼합

$$F = 0$$

$$F^2 = 0$$

→ 규칙적 소멸, **systematically absent**

표 4-1

With certain symmetries reflections from different lattice planes cancel out

→ **Systematic absences.**

Systematic Absences - Centering

If the lattice is not primitive certain classes of hkl peaks will be missing. These are called systematic absences and we can use them to determine the space group (or at least narrow down the possibilities). We will derive this relationship next lecture, but consider that if you have a centered cell it is always possible to draw a smaller primitive cell, and a smaller cell should have fewer peaks.

Centering

Allowed peaks

I-centered → Peaks where $h+k+l$ is an even number

F-centered → Peaks where hkl are either all even #s or all odd #s

C-centered → Peaks where $h+k$ is an even number

B-centered → Peaks where $h+l$ is an even number

A-centered → Peaks where $k+l$ is an even number

R-centered → Peaks where $-h+k+l$ is a multiple of 3

Systematic Absences - Screws & Glides

Screw axes and glide planes also have elements of translation and they will give systematic absences as well. Some examples are given below, others can be deduced from the pattern.

Centering

Allowed peaks

2_1 screw axis \parallel to $a \rightarrow h00$ peaks are only allowed when h is an even #

2_1 screw axis \parallel to $b \rightarrow 0k0$ peaks are only allowed when k is an even #

2_1 screw axis \parallel to $c \rightarrow 00l$ peaks are only allowed when l is an even #

3_1 screw axis \parallel to $c \rightarrow 00l$ peaks are only allowed when $l = 3n$ ($n = \text{integer}$)

4_1 screw axis \parallel to $c \rightarrow 00l$ peaks are only allowed when $l = 4n$ ($n = \text{integer}$)

a glide plane $\perp c \rightarrow hk0$ peaks are only allowed when h is an even #

b glide plane $\perp c \rightarrow hk0$ peaks are only allowed when k is an even #

n glide plane $\perp c \rightarrow hk0$ peaks are only allowed when $h+k$ is an even #

a glide plane $\perp b \rightarrow h0l$ peaks are only allowed when h is an even #

c glide plane $\perp b \rightarrow h0l$ peaks are only allowed when l is an even #

n glide plane $\perp b \rightarrow h0l$ peaks are only allowed when $h+l$ is an even #