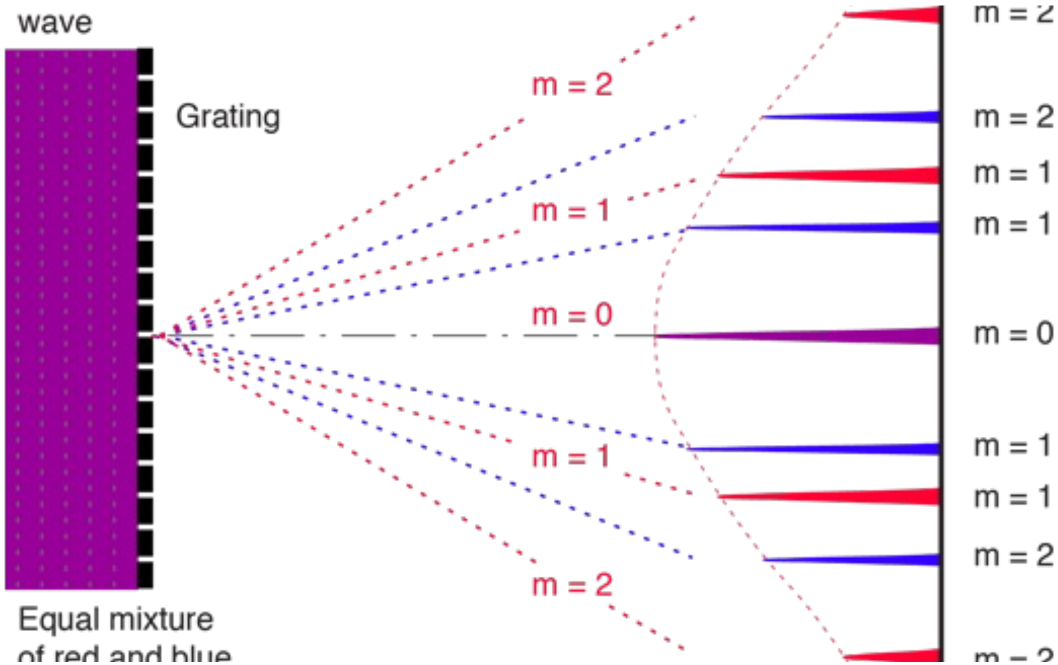
4. Diffraction



Scattering from a sample

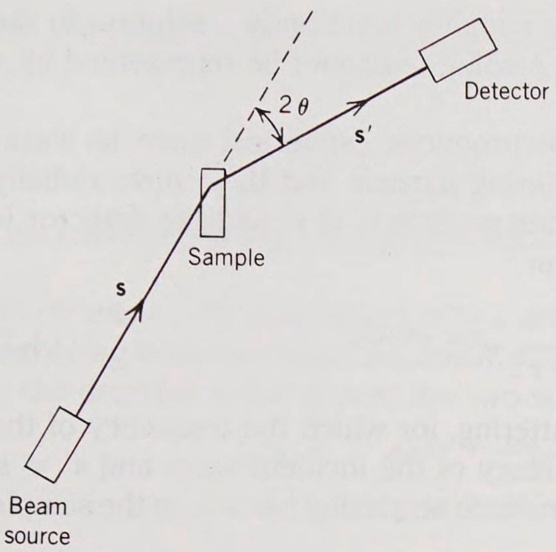
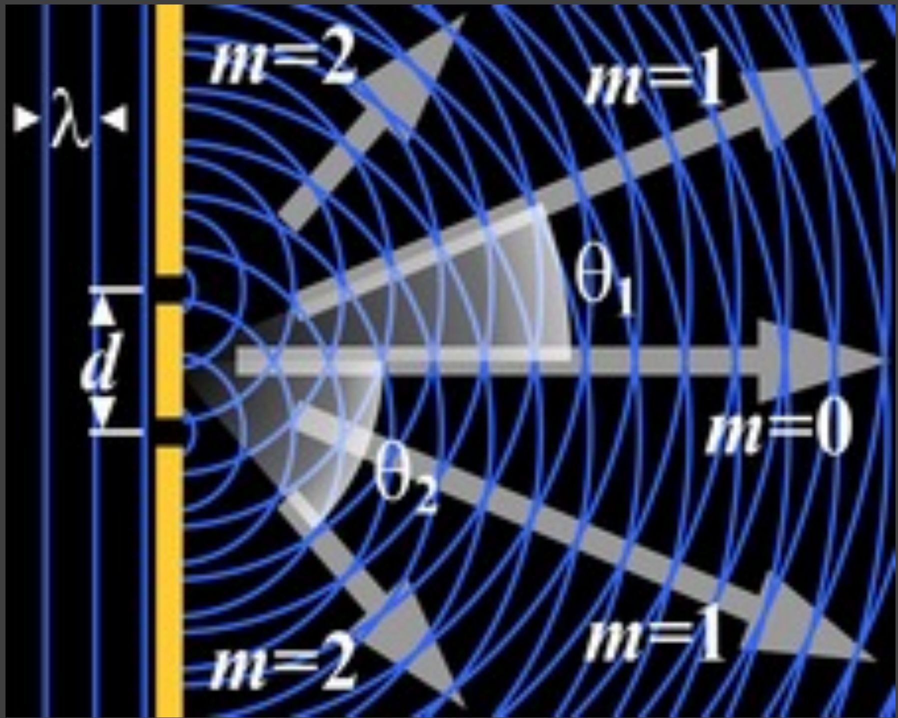
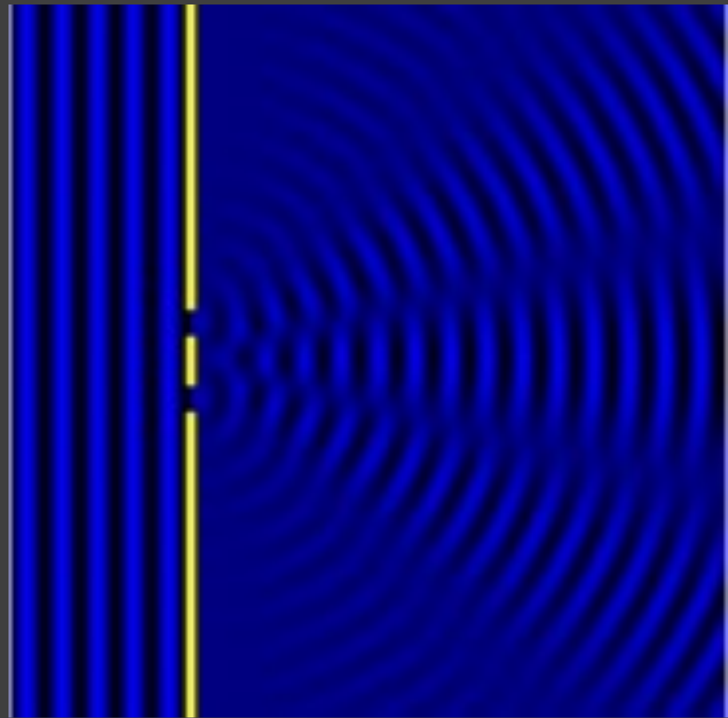


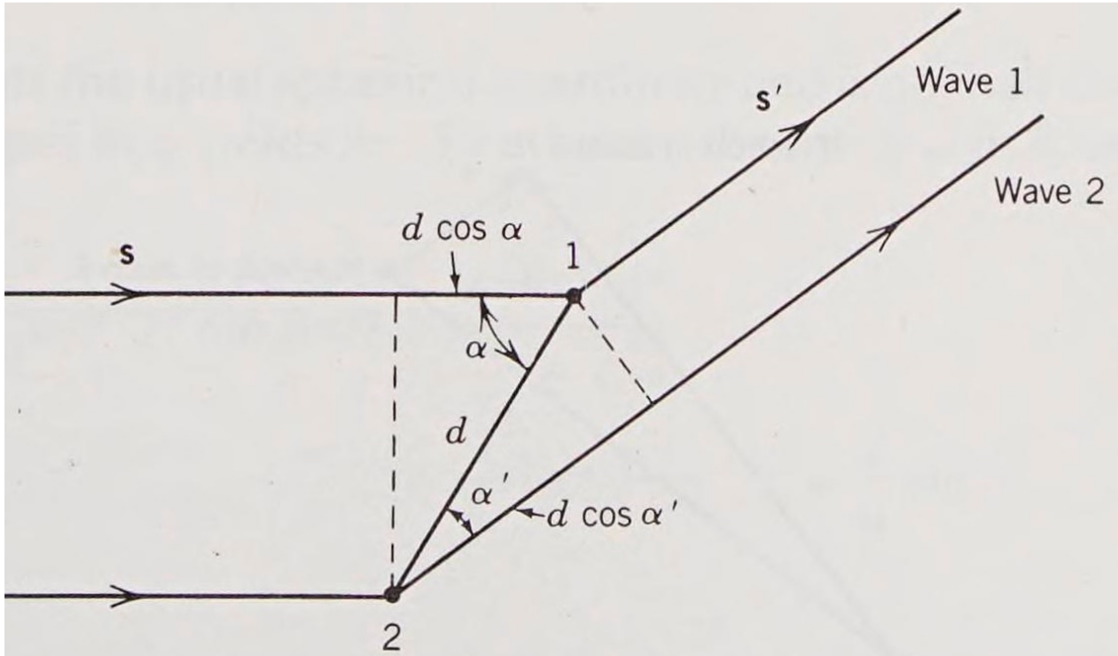
FIGURE 4-1 Scattering from a sample. The beam may consist of x rays, electrons, or neutrons. Propagation vectors for the incident and scattered waves are s and s′, respectively, and the scattering angle is 2θ.

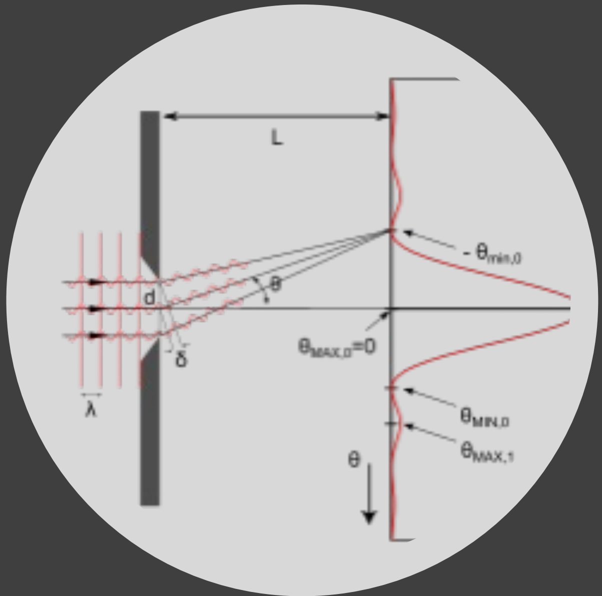




Two slits

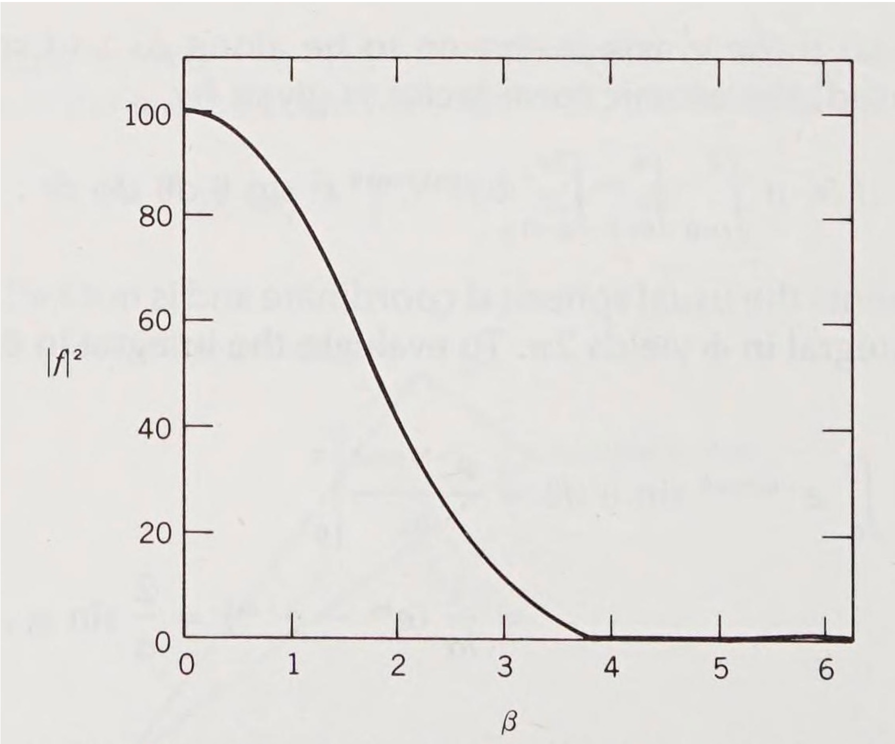
Scattering from two particles

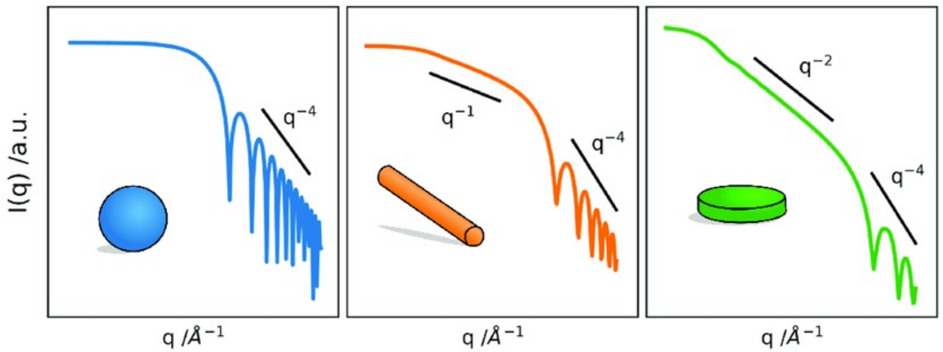


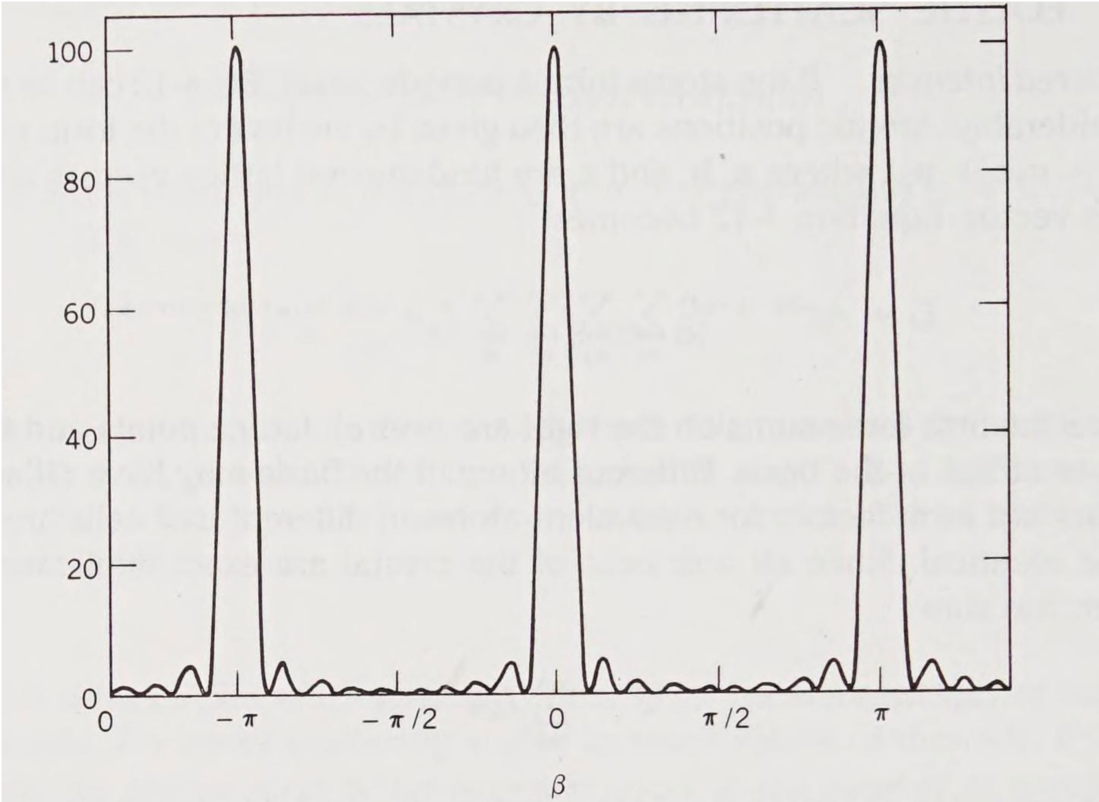


Diffraction from an aperture

Form factor

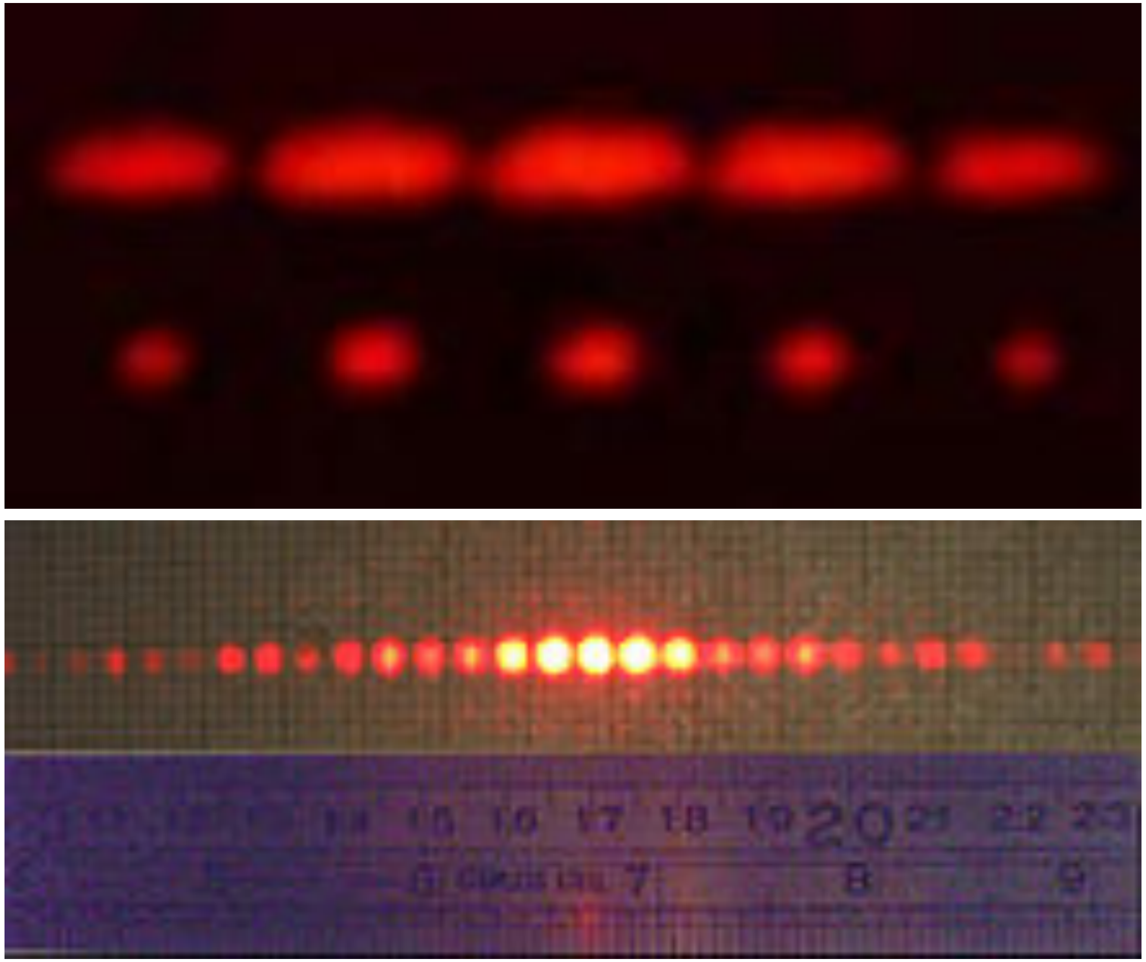






$\beta = \frac{1}{2}\,\Delta\mathbf{s} \cdot \mathbf{a}$ and $g(\beta) = \sin^2(N\beta)/\sin^2(\beta)$

Scattering function for N=10



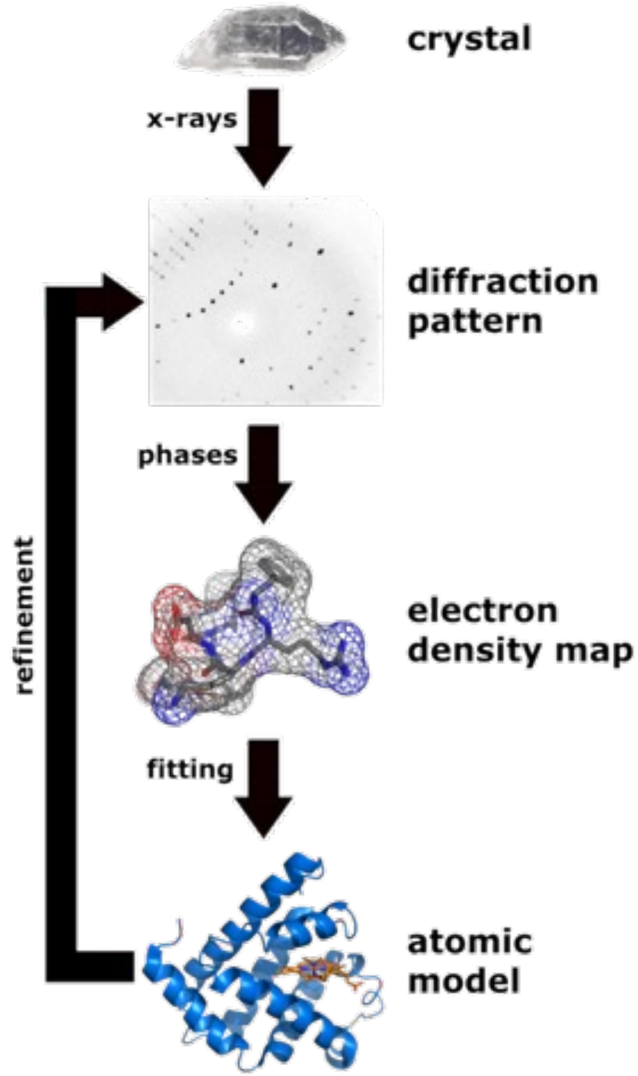
Diffraction patterns for two, five and one hundred and fifty slits

Laue scattering condition

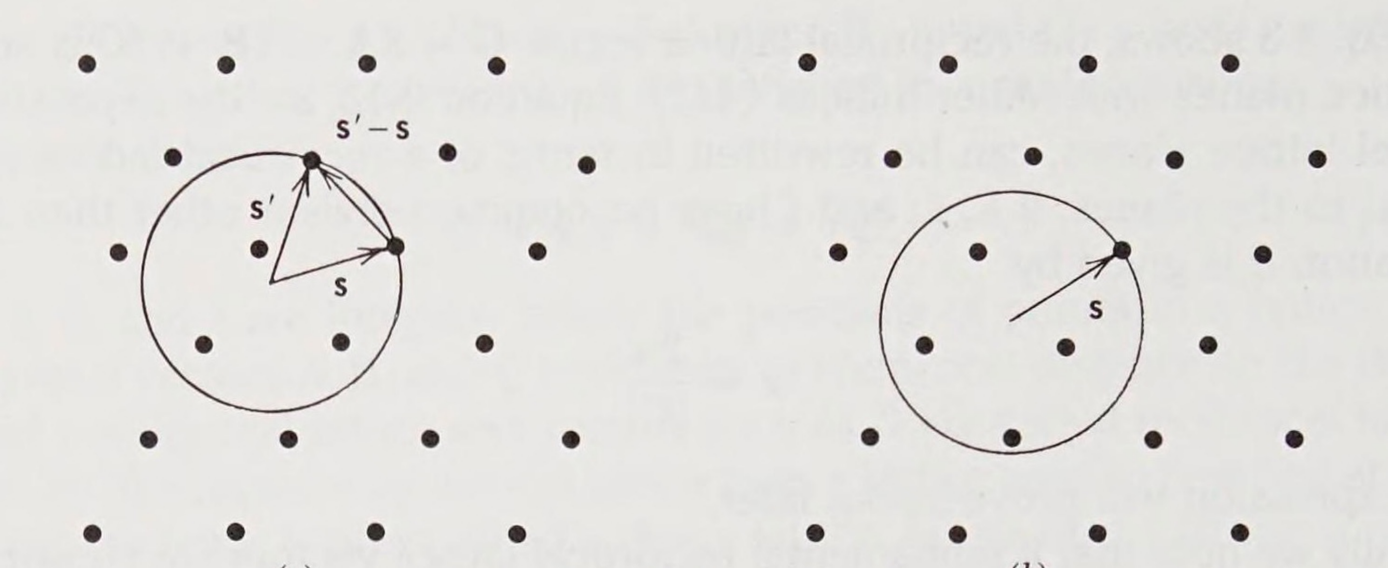
$$\Delta \mathbf{s} = h\mathbf{A} + k\mathbf{B} + \ell\mathbf{C}.$$

NOBEL PRIZE IN PHYSICS, 1914

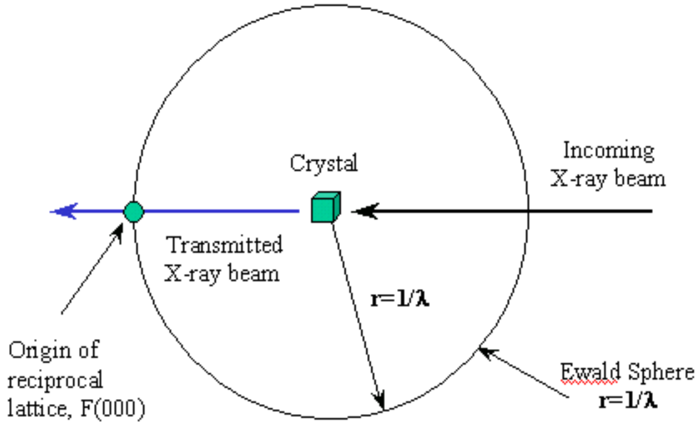
Max von Laue

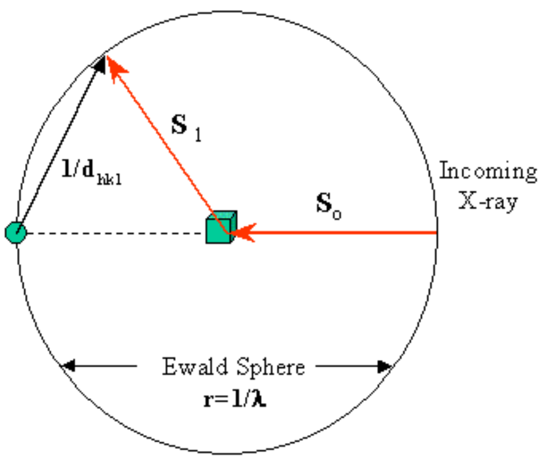


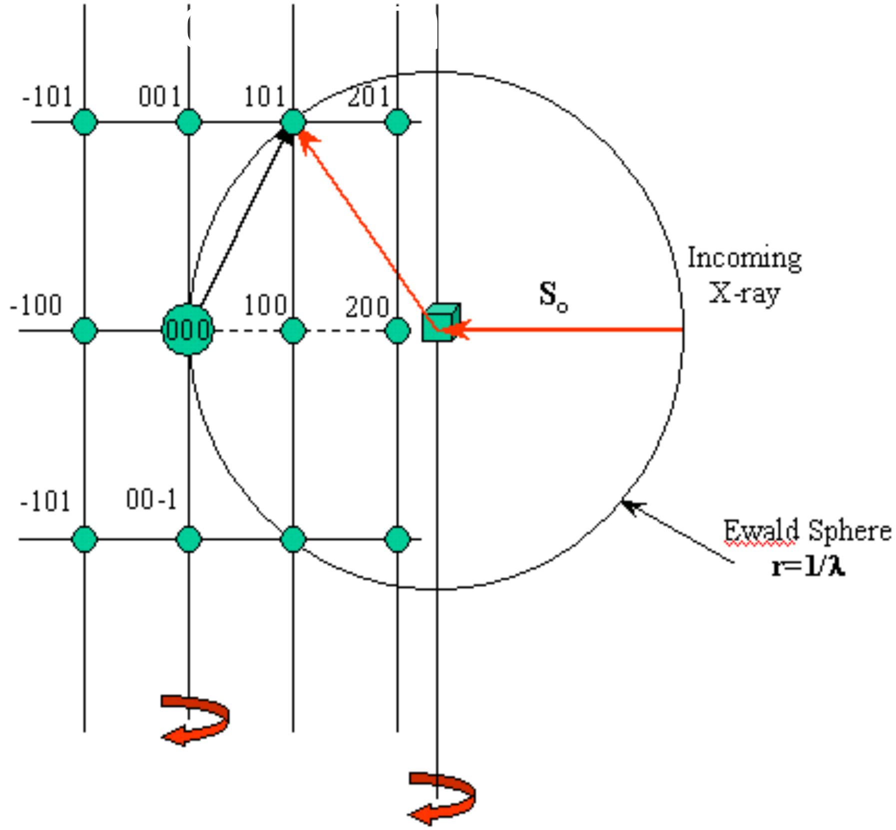
Ewald construction

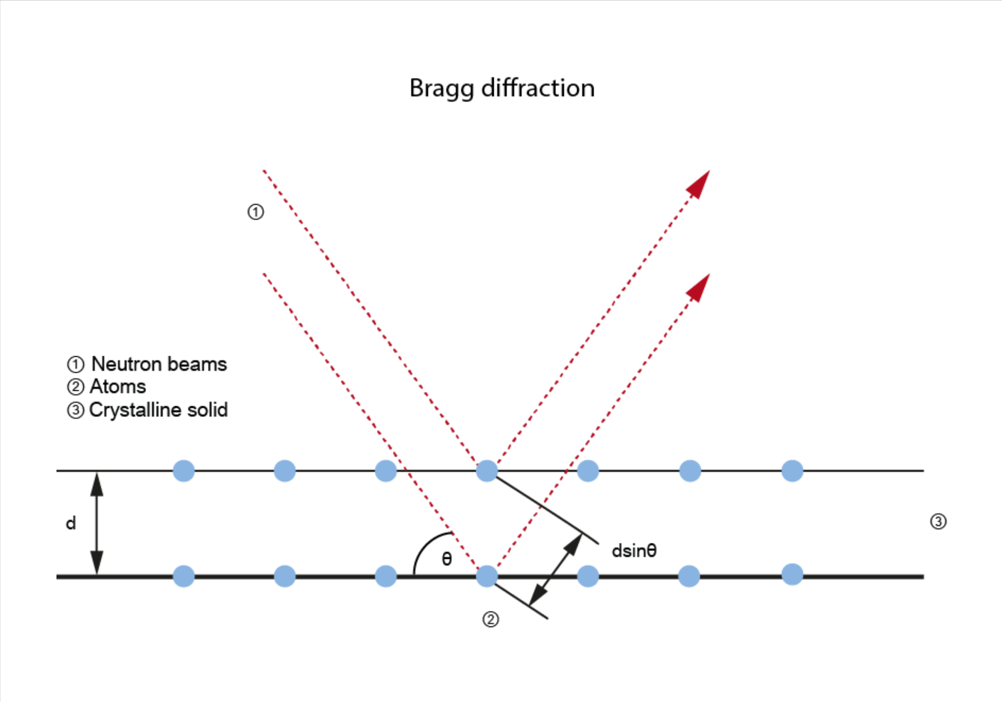


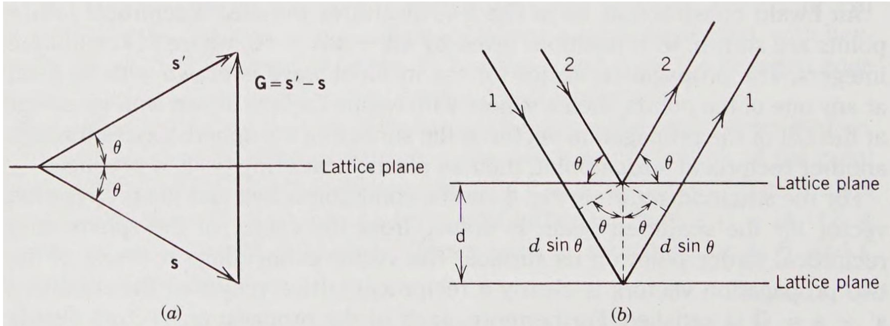
(a) (b)


Crystal
Incoming
X-ray beam
Transmitted
X-ray beam
r=1/λ
Origin of
reciprocal
lattice, F(000)
Ewald Sphere
r=1/λ


S 1
1/d hkl
S o
Incoming
X-ray
Ewald Sphere
r=1/λ

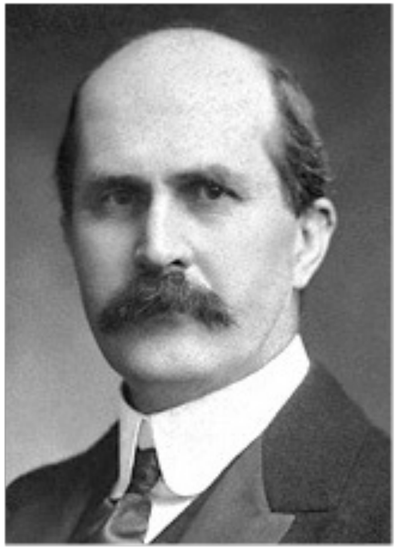

-101
001
101
201
-100
000
100
200
S o
Incoming
X-ray
-101
00-1
Ewald Sphere
r=1/λ



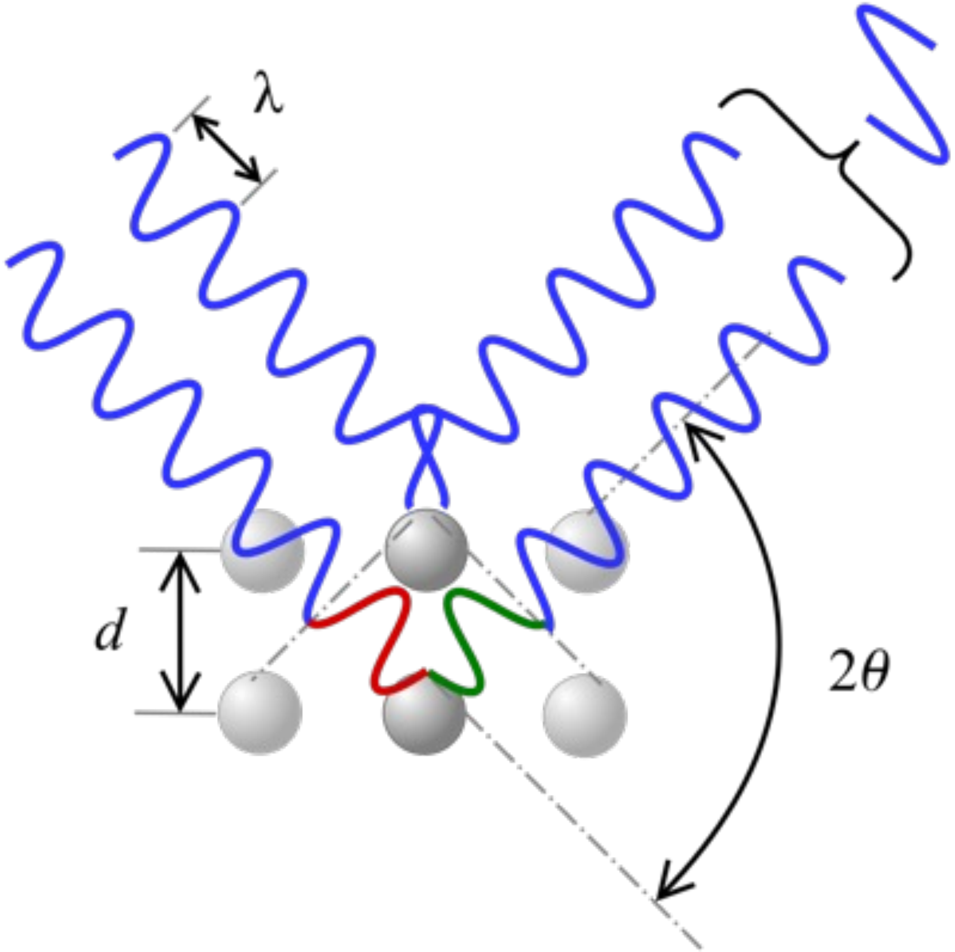


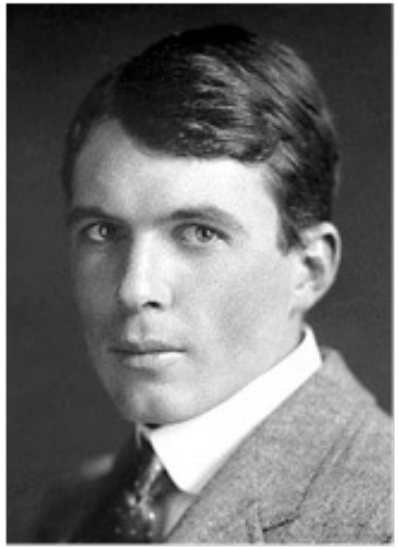
$$2d \sin \theta = n\lambda$$

Bragg scattering



WH BRAGG





WL BRAGG

NOBEL PRIZE IN PHYSICS, 1915

Structure factor

$$F = \sum_{m} f_m e^{-2\pi i (u_m h + v_m k + w_m \ell)} .$$

Structure factor

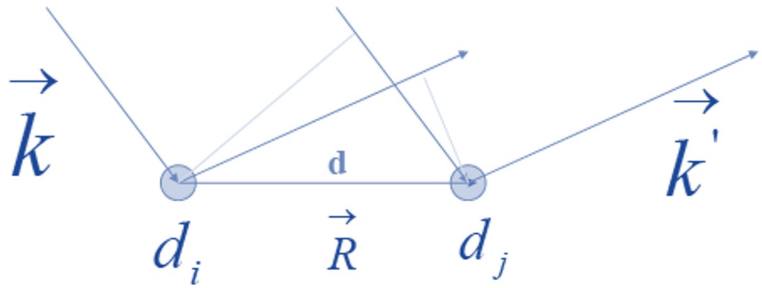
The amplitude of the rays scattered at d_1, d_2, d_3…. are in the ratios :

$$e^{-iK\cdot d_j}$$

The net ray scattered by the entire cell:

$$S_k = \sum_{j=1}^{n} e^{-iK\cdot d_j}$$

$$\boxed{I_{(hkl)} \propto \left|S_k\right|^2}$$



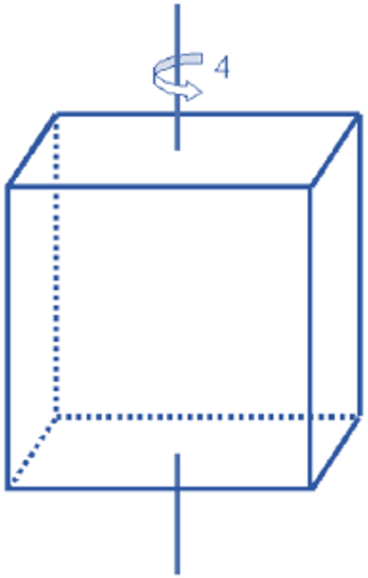
$$\vec{K} = \vec{k}' - \vec{k}$$

Phase difference: $K\cdot(d_i - d_j)$

The amplitude of the two rays differ: $e^{iK\cdot(d_i - d_j)}$

Structure factor SC

For simple cubic: (0,0,0)

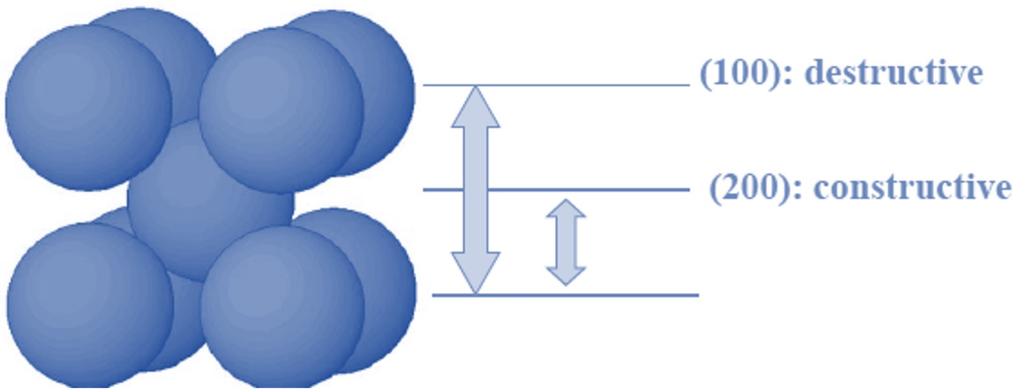


$$S_k = e^{-iK\cdot 0} = 1$$

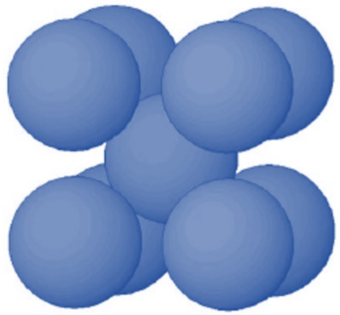
Structure factor BCC

For BCC: (0,0,0), (1/2, ½, ½)…. Two point basis

S=2, when h+k+l even
S=0, when h+k+l odd, systematical absence



For BCC: (0,0,0), (1/2, ½, ½)…. Two point basis



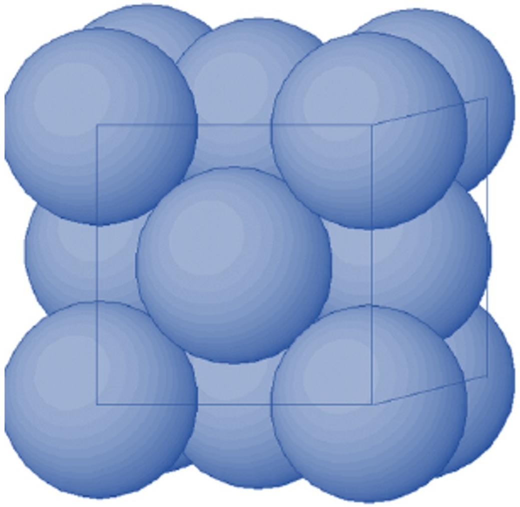
$$S_k = \sum_{j=1}^{2} e^{-iK\cdot d_j} = e^{-iK\cdot 0} + e^{-iK\frac{1}{2}(\vec{x}+\vec{y}+\vec{z})}$$

$$= 1 + e^{-i\pi(h+k+l)}$$

$$= 1 + (-1)^{h+k+l}$$

S=2, when h+k+l even
S=0, when h+k+l odd, systematical absence

Structure factor FCC



FCC

S=4 when h+k, k+l, h+l
all even (h,k, l all even/odd)

S=0, otherwise

$$S_k = 1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(l+k)}$$

Rules for diffraction peaks of cubic lattices

Rules for Determining the Diffracting {hkl} Planes in Cubic Crystals

Bravais lattice	Reflections present	Reflections absent
BCC	$(h+k+l)$ = even	$(h+k+l)$ = odd
FCC	(h, k, l) all odd or all even	(h, k, l) not all odd or all even

Miller Indices of the Diffracting Planes for BCC and FCC Lattices

Cubic planes {hkl}	$h^2+k^2+l^2$	Simple cubic Sum $\Sigma(h^2+k^2+l^2)$	Cubic diffracting planes {hkl} FCC	BCC
{100}	$1^2+0^2+0^2$	1		
{110}	$1^2+1^2+0^2$	2	…	110
{111}	$1^2+1^2+1^2$	3	111	
{200}	$2^2+0^2+0^2$	4	200	200
{210}	$2^2+1^2+0^2$	5		
{211}	$2^2+1^2+1^2$	6	…	211
{220}	$2^2+2^2+0^2$	8	220	220
{221}	$2^2+2^2+1^2$	9		
{310}	$3^2+1^2+0^2$	10	…	310

Observable diffraction peaks $h^2+k^2+l^2$

Ratio

SC: 1,2,3,4,5,6,8,9,10,11,12..

BCC: 2,4,6,8,10, 12, 14….
(1,2,3,4,5,6,7…)

FCC: 3,4,8,11,12,16,24….

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

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

Observable diffraction peaks $h^2+k^2+l^2$

Ratio

SC: 1,2,3,4,5,6,8,9,10,11,12..

BCC: 2,4,6,8,10, 12, 14….
(1,2,3,4,5,6,7…)

FCC: 3,4,8,11,12,16,24….

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

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

$$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+l^2)$$

Polyatomic structures

Polyatomic Structures

$$S_k = \sum_{j=1}^{n} f_j(k) e^{-i\vec{K}\cdot\vec{d}_j}$$

$$K = ha^* + kb^* + lc^*$$

$$\vec{d}_j = x\vec{a} + y\vec{b} + z\vec{c}$$

f_j: atomic scattering factor
$\propto$ No. of electrons

$$S_k = \sum_{j=1}^{n} f_j e^{-iK\cdot d_j} = \sum_{j=1}^{n} f_j e^{-2\pi i(hx+ky+lz)}$$

Simple Cubic Lattice

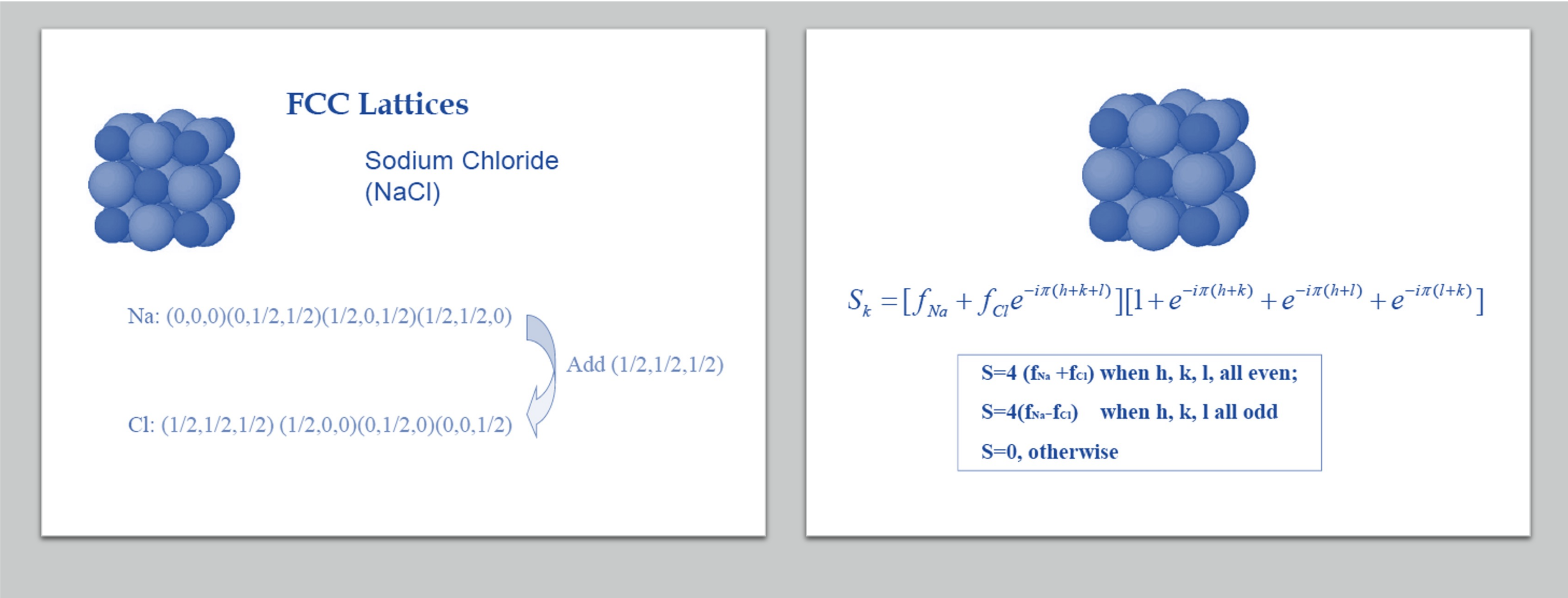
Caesium Chloride (CsCl) is **primitive cubic**

Cs (0,0,0)
Cl (1/2,1/2,1/2)

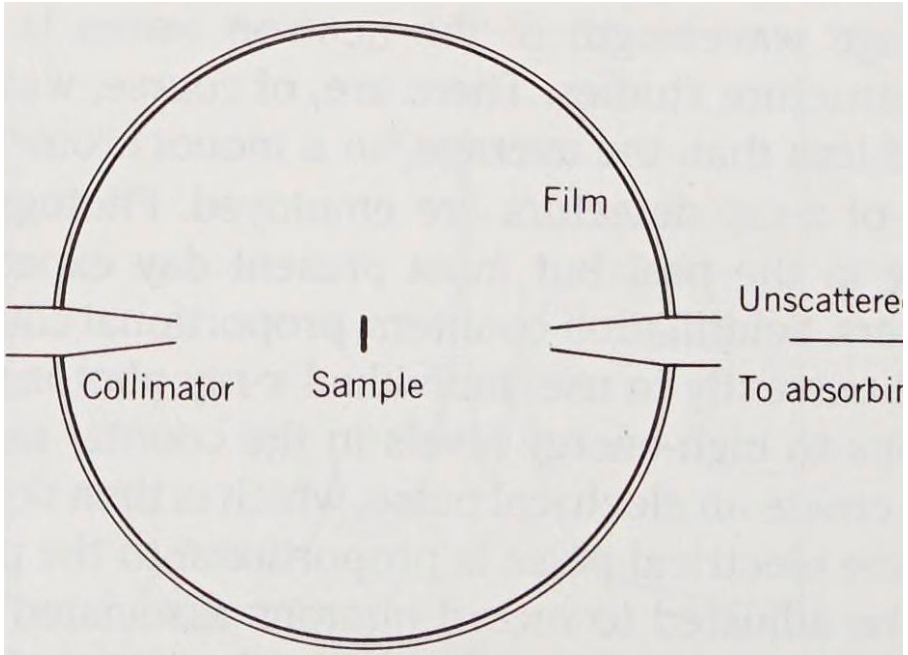
$$S_k = f_{Cs} + f_{Cl} e^{-i\pi(h+k+l)}$$

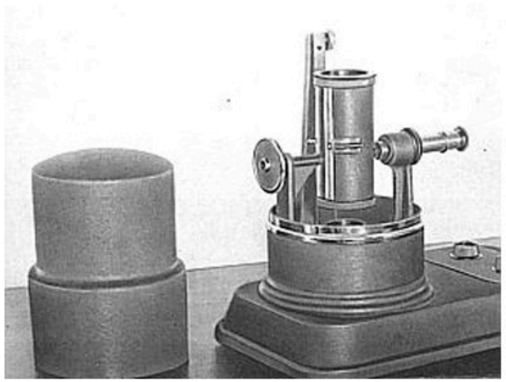
What about CsI?

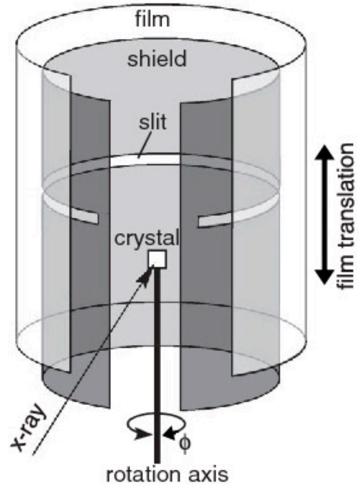
Polyatomic structures



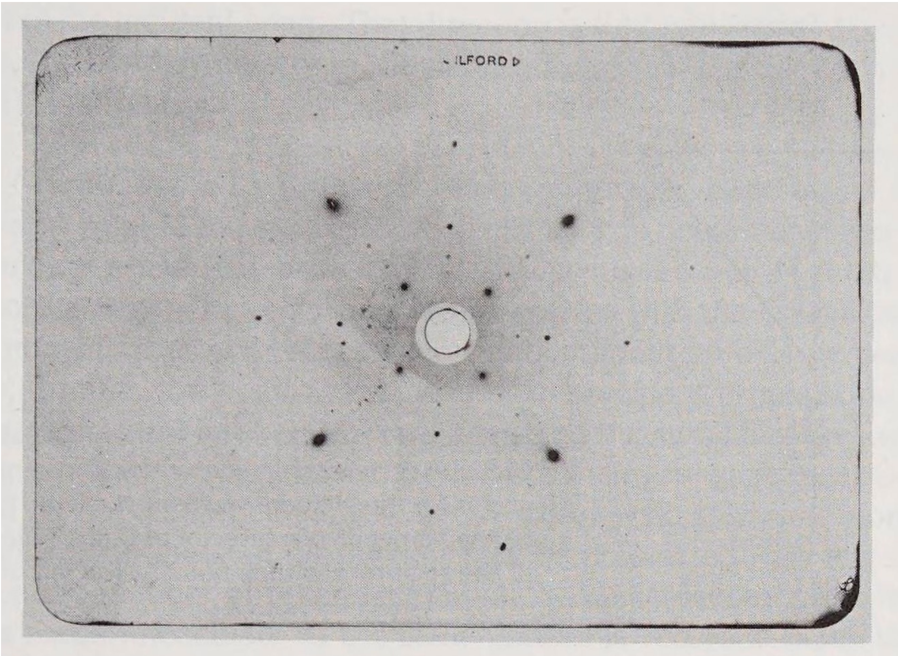
Laue method: cylindrical diffraction camera

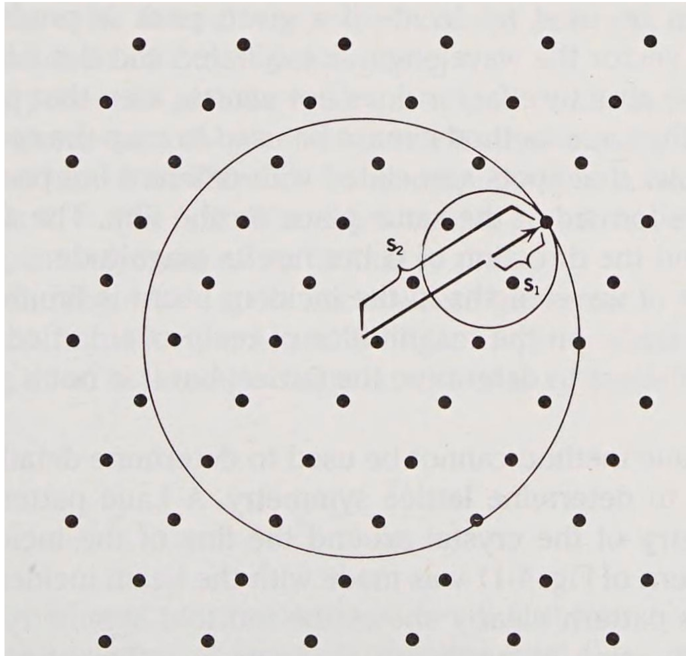






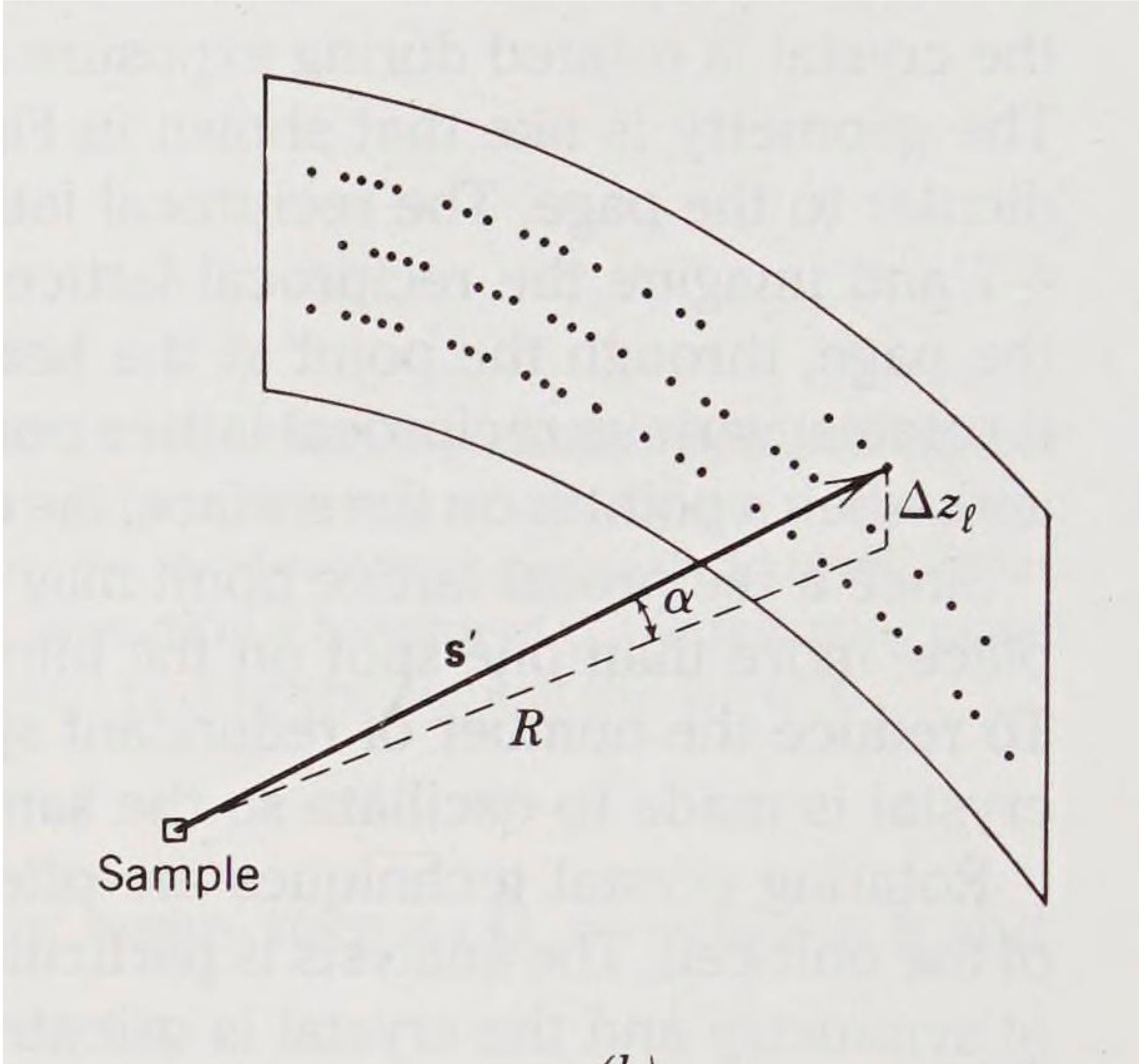
Laue pattern and Ewald construction





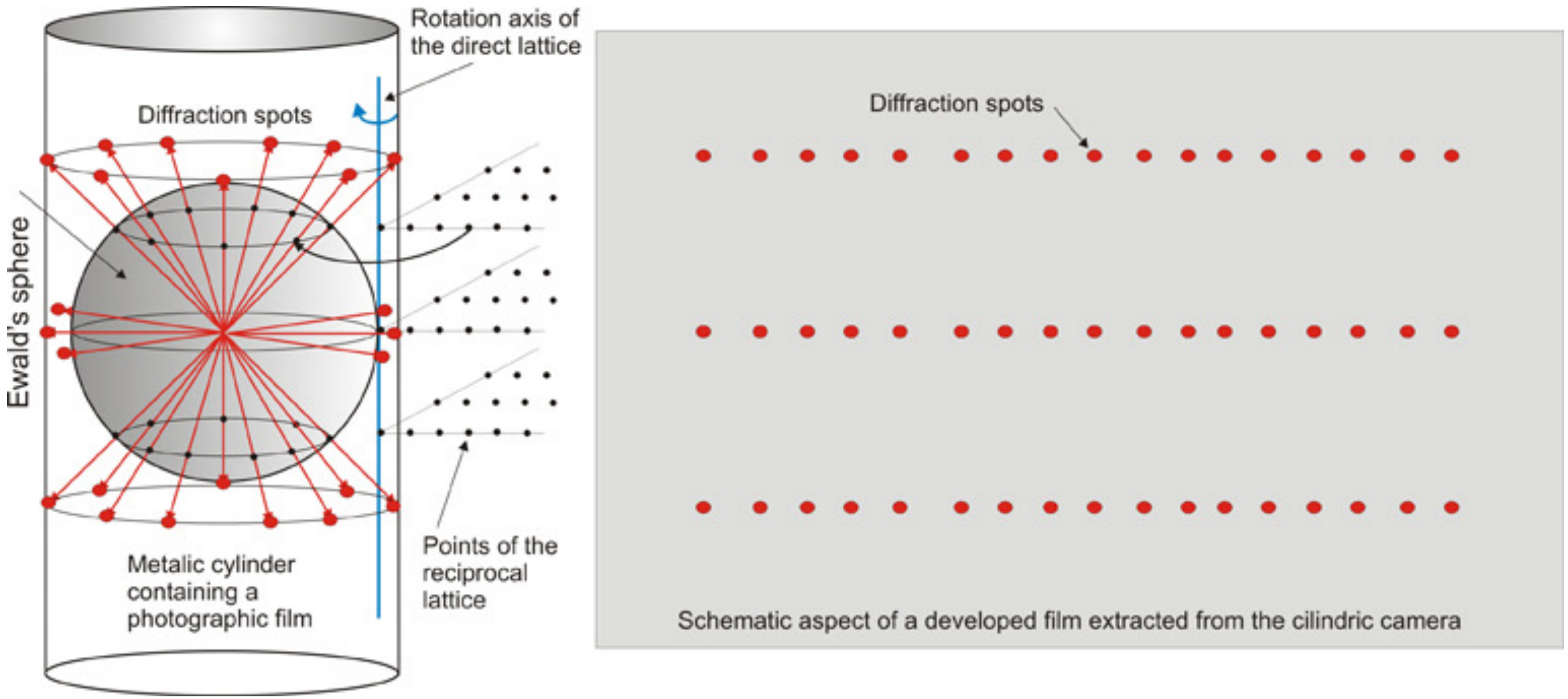
Rotating crystal

Diagram of intensity peaks

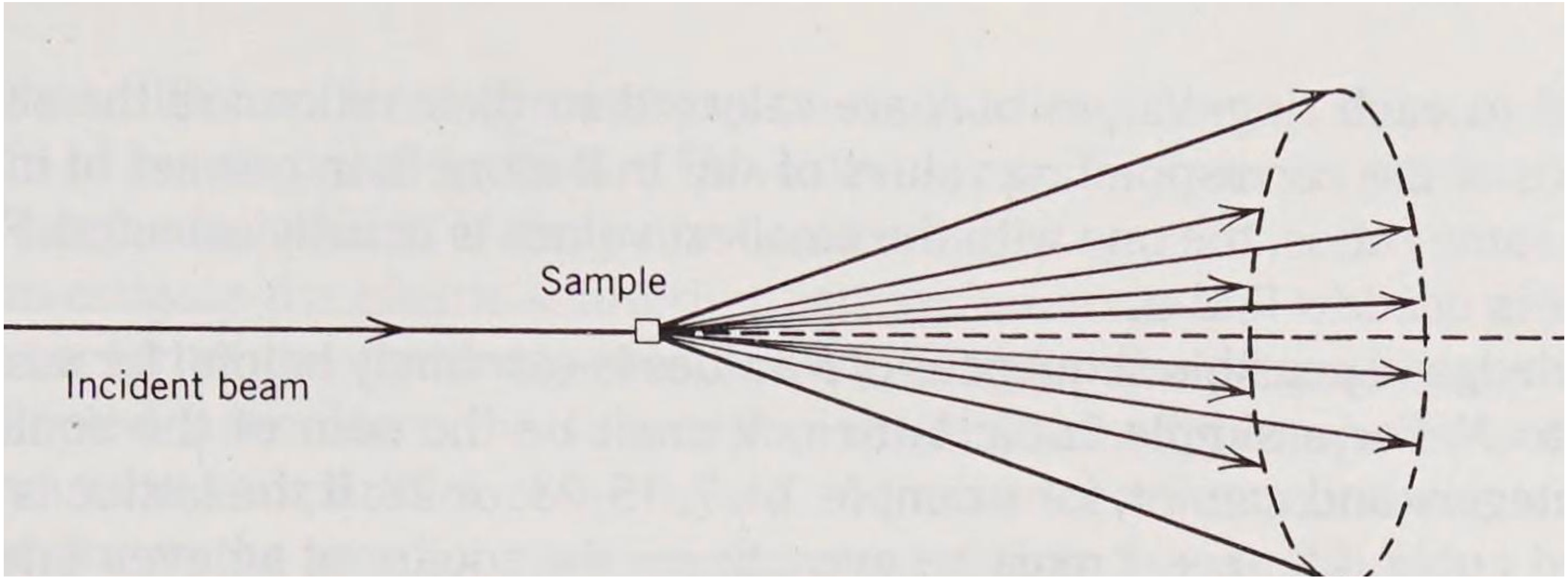


(b)

Rotating crystal



Powder sample



Powder pattern

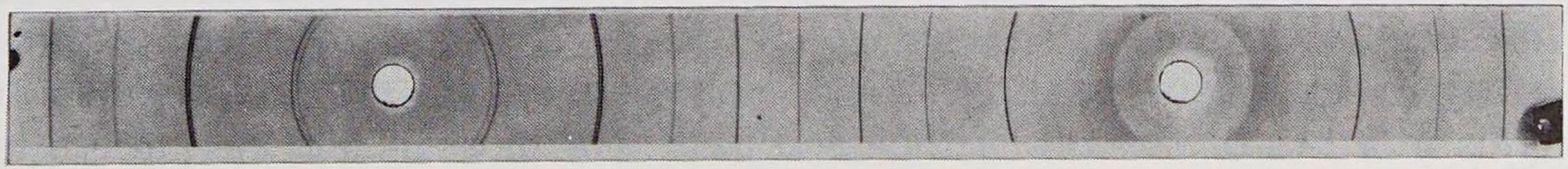


FIGURE 4-16 Powder pattern for tungsten. Each ring corresponds to a different scattering angle. The pattern consists of two sets of rings, for beams scattered in the back (on the left) and forward (on the right) directions, respectively. (From Walter Kiszenick, unpublished. Used with permission.)