Lesson 5

- Conditioning the x-ray beam
- How do x-rays interact with matter
- How does the periodic nature of crystals effect this interaction

X-ray Tube Output

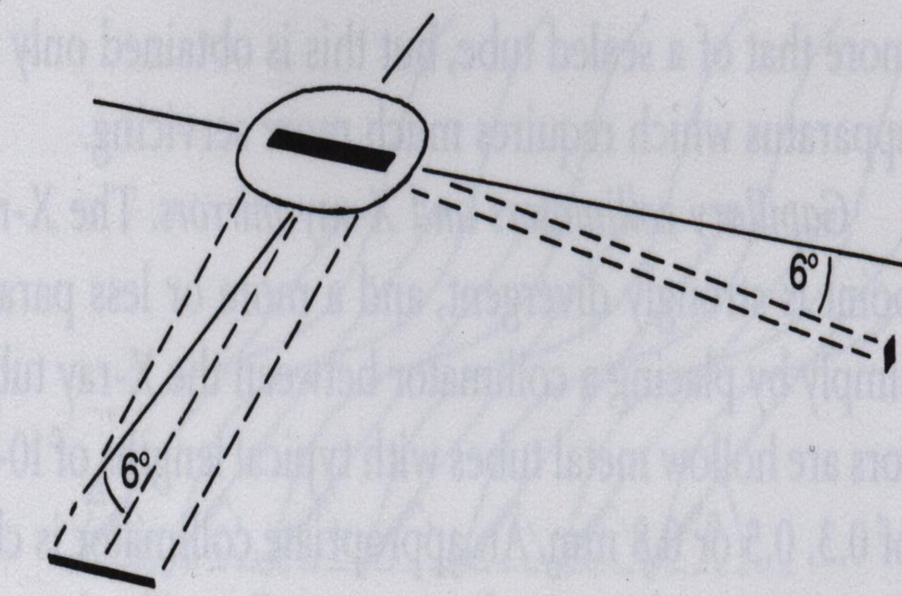


Fig. 3.3. Use of an X-ray tube as a radiation source with a line focus (down) or point focus (right).

Line focus for powder diffraction
Point focus for single crystals
The 6º angle is called the take-off

Desired Properties of the Beam

- Monochromatic
- Parallel
- Coherent
- In phase

Monochromation

- Simplest is β filter
- Crystal monochromator
- Can use a crystal to monochromate by collecting some Bragg spot
- Typically today use graphite (2-dimensional crystal)
- All methods involve considerable loss of intensity

Making the Beam Parallel

- Done using a collimator
- This is a long, narrow tube which eliminates all x-rays that are not travelling down the tube.
- More loss of intensity
- This results in a beam which has a region of uniform intensity the size of the collimator opening. However, there are x-rays that are outside this sweet spot with lesser intensity
- For light this could be done using lens.

Coherence

- This means all the waves are in phase.
- This cannot be achieved for electron beam produced x-rays.
- Therefore, there will be some interference between waves.
- Synchrotron is coherent, parallel and exactly monochromatic!

Polarization

- X-ray source is not polarized
- For light a laser would have all the correct properties.
- No x-ray lasers.
- The energy need to achieve lasing is inversely related to the square of the frequency of radiation to be produced.
- Comparing green light (1/5000) vs x-ray (1/1) it is $2.5x10^7$ times more difficult.

Safety

- Beam is very small
- Hard to get body parts in the beam
- Radiation is lower energy.
- Many interlocks to prevent accidental exposure
- Ba impregnated plexi-glass blocks radiation
- Still—be sure you know what you are doing!!

Simplest Interaction of Radiation with Matter (one photon).

- Transmission—the radiation passes through the material.
- Absorption—the radiation is absorbed by the material. The energy must be dissipated!
- These processes are inverse –that is probability(absorption)=1.-probability(trans)
- Neither play any role in crystallography beyond the fact that absorption is a nuisance that must be corrected.

More complicated Interactions

- In the 1890's J. J. Thompson worked out the scattering of a electromagnetic radiation by a free electron.
- It is this process that is the source of the photons in the x-ray diffraction experiment.
- Note that scattered photons come off in all directions and have a phase 180° to the incident wave.
- Assume elastic scattering—no change in energy

An Experiment

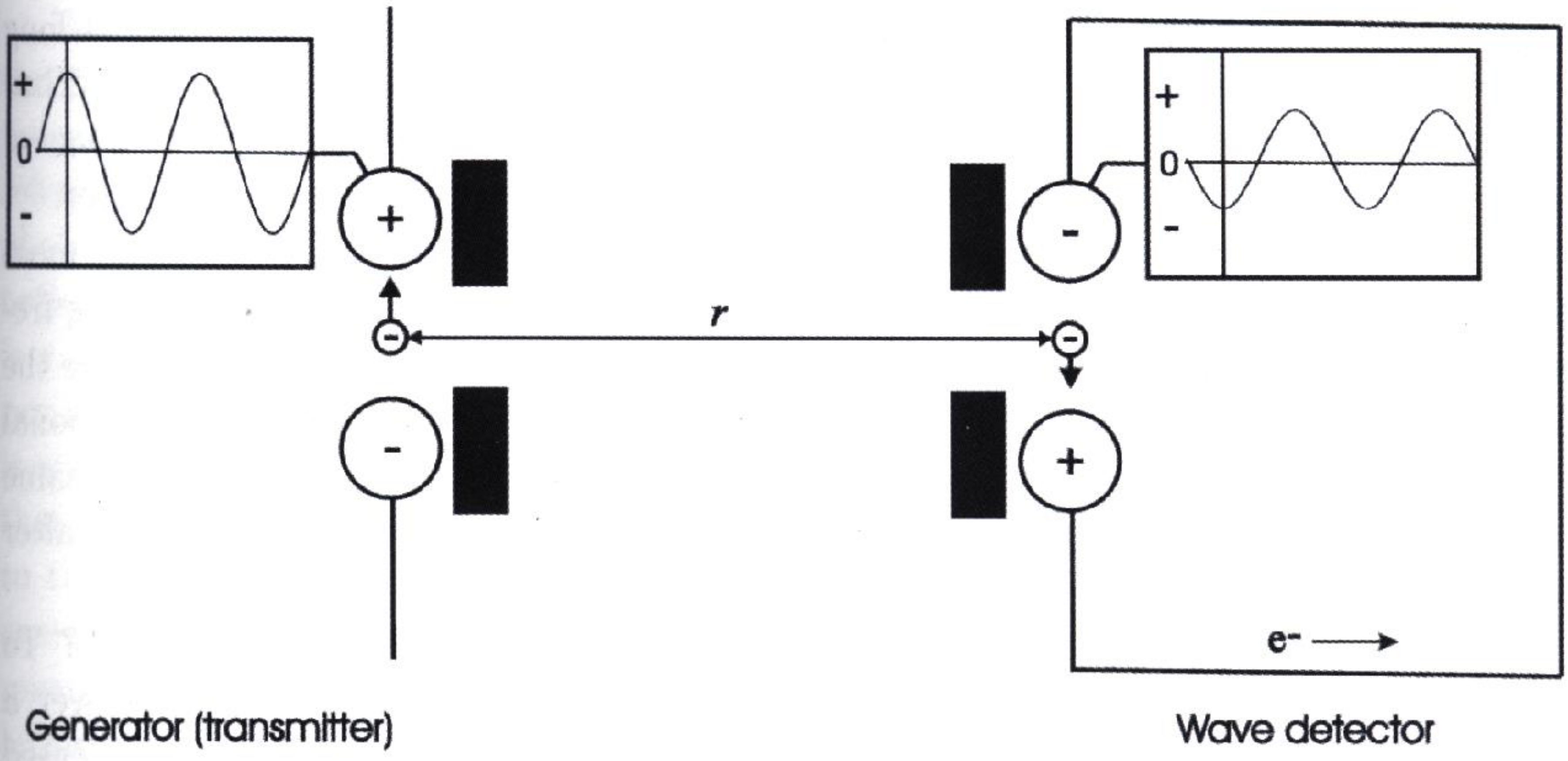


Figure 3.4 Electron oscillator and electron wave-detector.

J.J. Thompson Scattering

The amplitude of the scattered wave is about 2.82×10^{-13} times less than the incoming wave at any point.

This is for elastic scattering where the frequency of the scattered wave is the same as the incoming wave

This is the scattering at a point for 1 electron.

There actually also needs a distance term r (the units are cm) but we will assume we are 1 cm from the scattered electron.

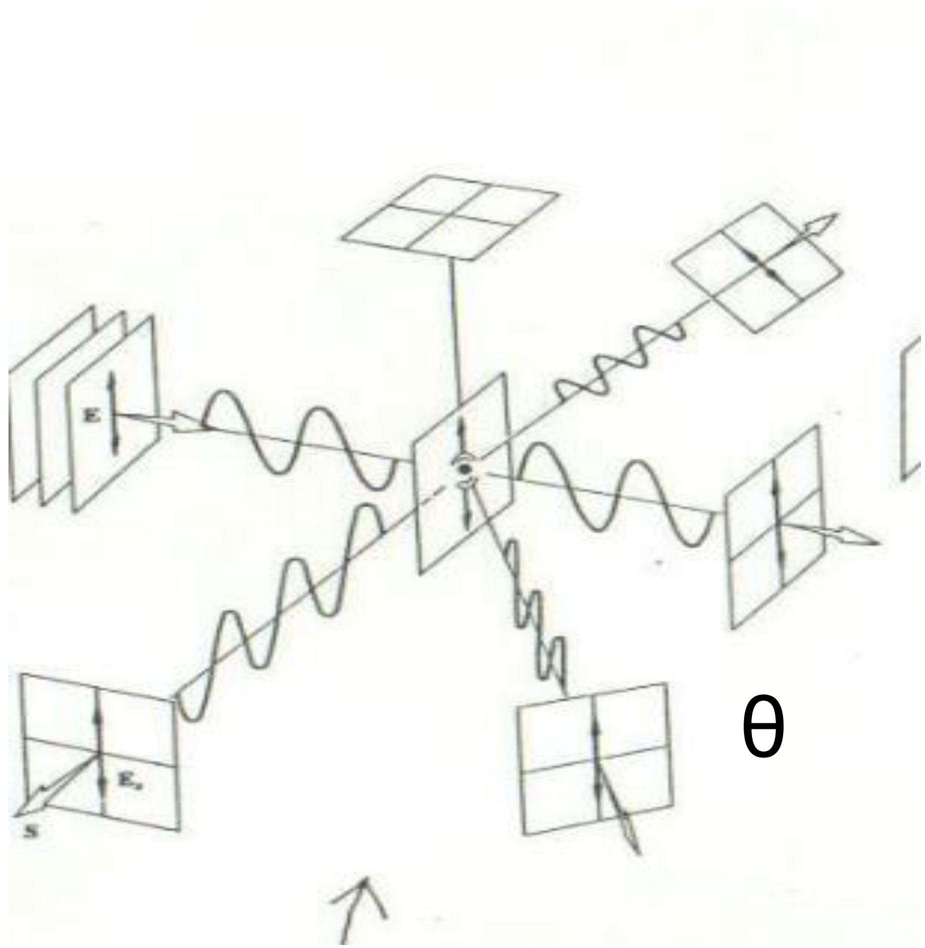
More on Scattering

Scattering where the plane of the scattered wave is the same as the incident radiation has the same probability regardless of the direction

- Scattering out of the plane falls off by $\cos^2(2\theta)$

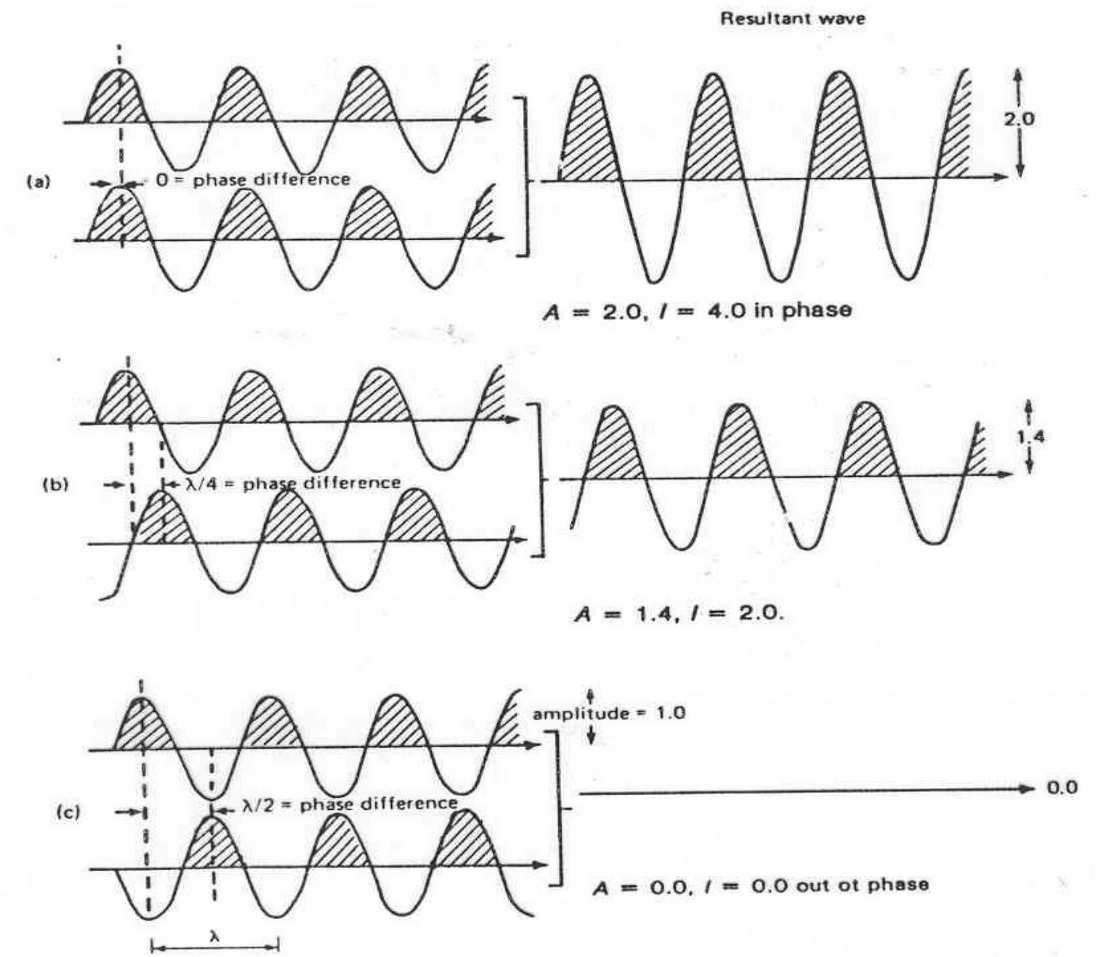
Since any wave can be broken down into two components (in the plane and out of the plane) the fall off for an unpolarized beam is $(1+\cos^2(2\theta))/2$. This is the polarization factor.

Polarization



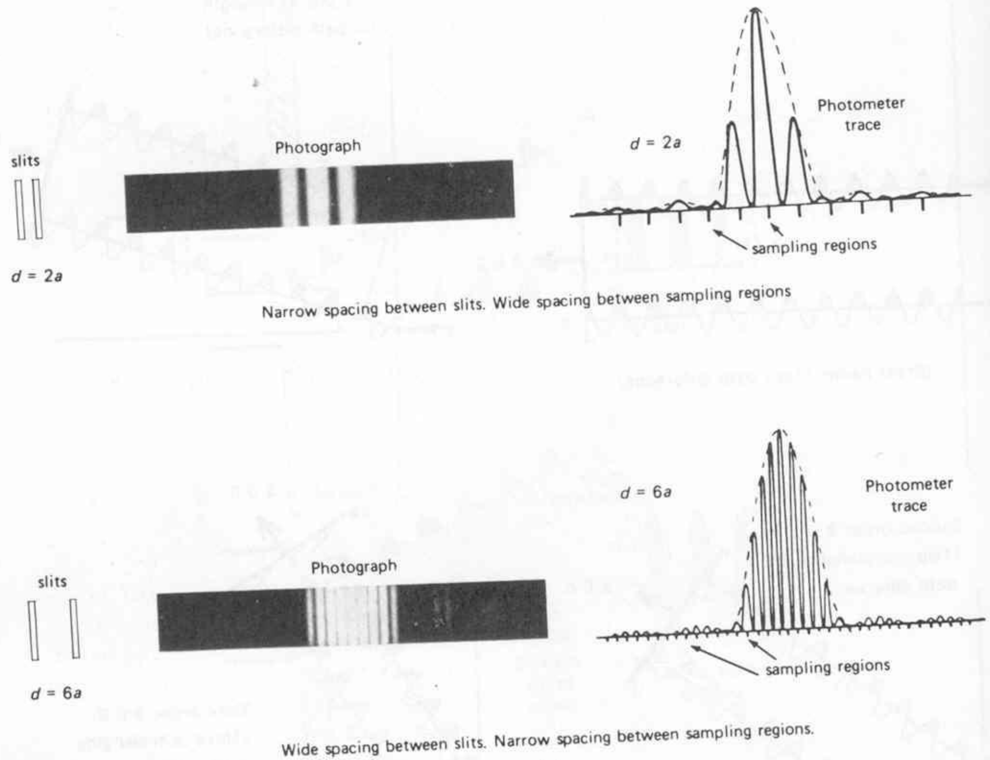
θ

Wave Interference



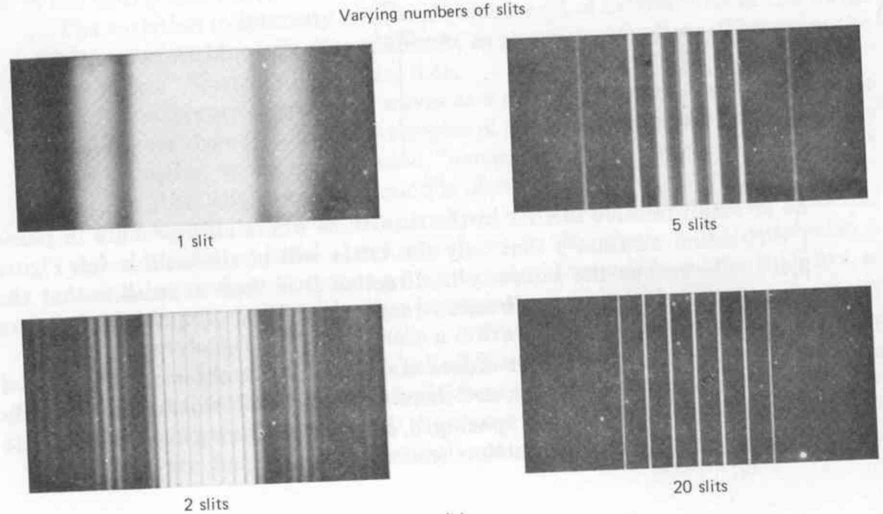
Slits as a Diffraction Substitute

- When electromagnetic, coherent radiation passes through a slit with a width about equal to the wavelength the waves will be diffracted.
- The waves will emerge along a circular wave front.
- Thus the slit will look like an emission source
- NOTE: THIS HAS NOTHING TO DO WITH THE PROCESS OF SCATTERING OF THE X-RAYS BUT IS SIMPLY A MODEL!

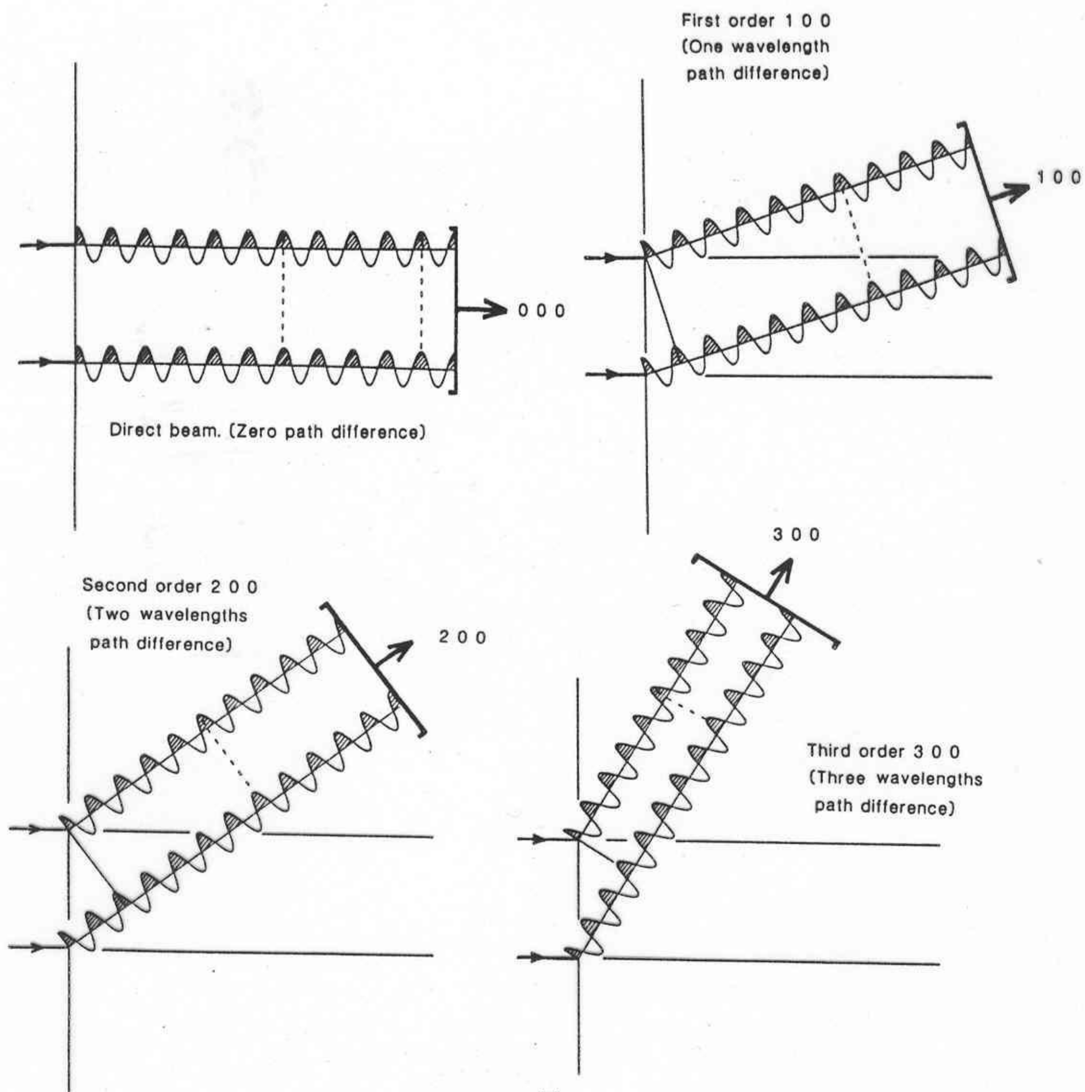


(a)

Varying numbers of slits



(b)

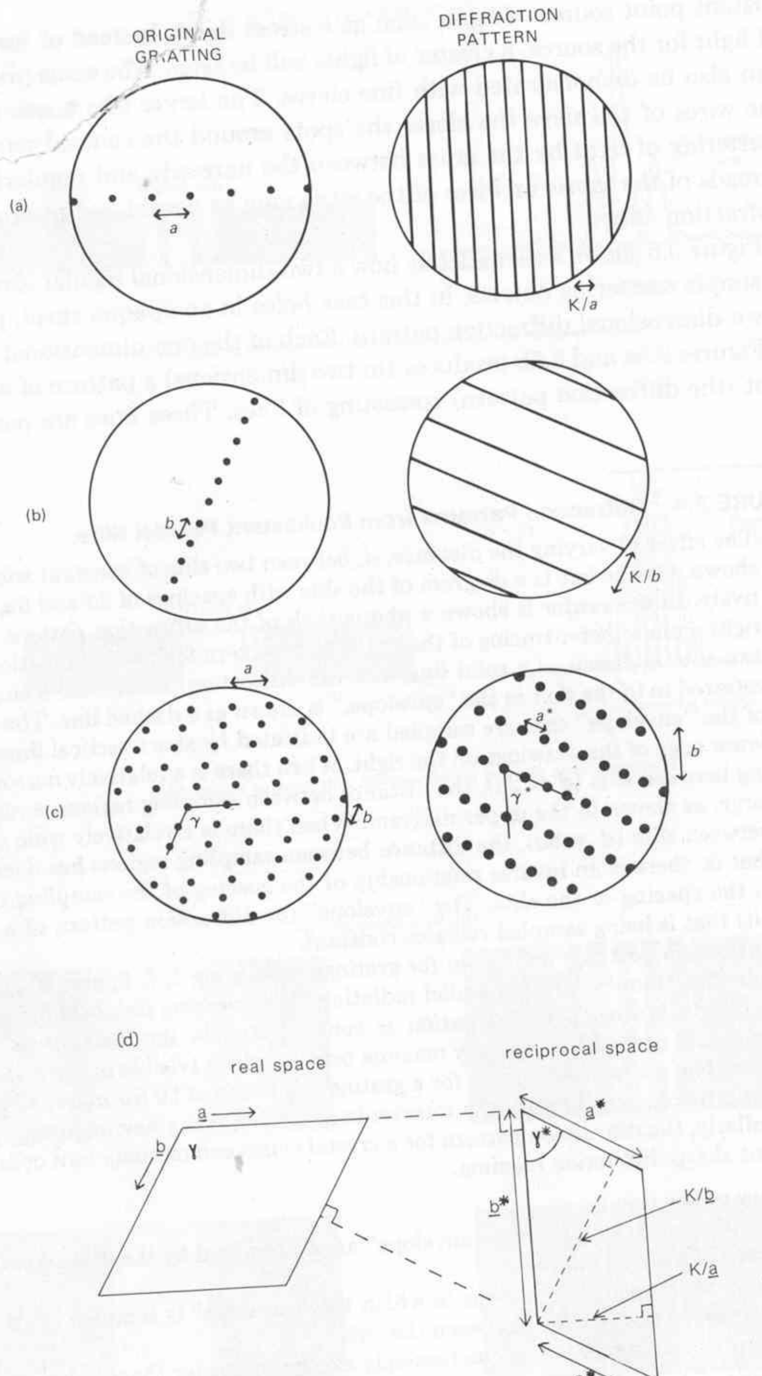

First order 1 0 0
(One wavelength
path difference)
1 0 0
0 0 0
Direct beam. (Zero path difference)
3 0 0
Second order 2 0 0
(Two wavelengths
path difference)
2 0 0
Third order 3 0 0
(Three wavelengths
path difference)

(c)

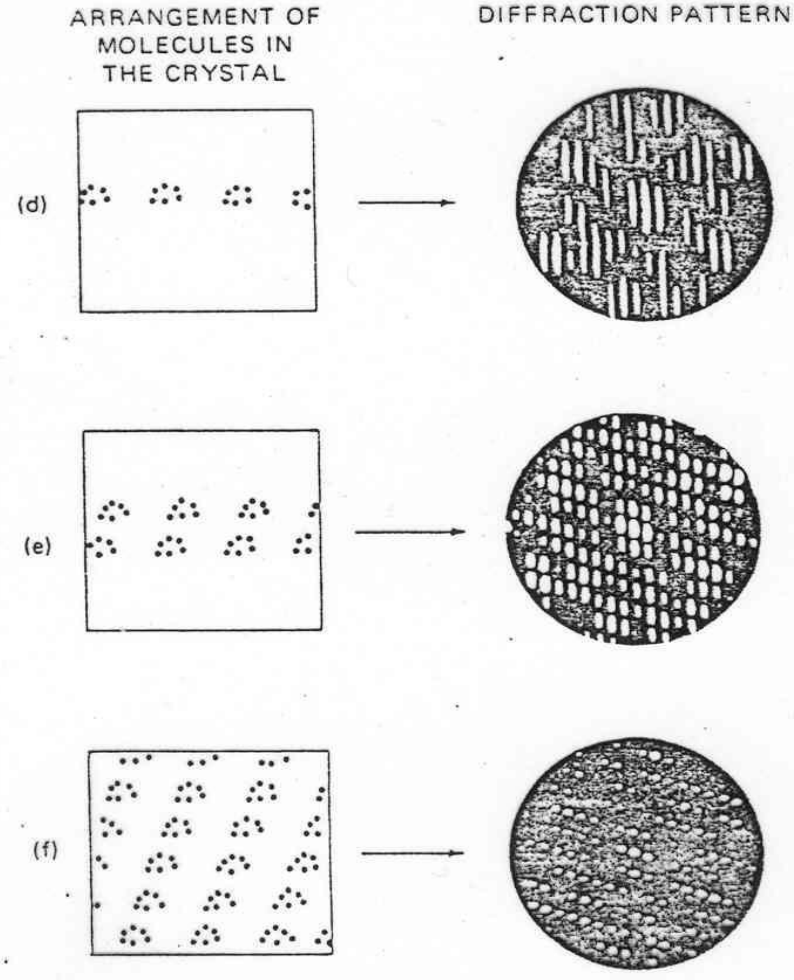
Some Comments

- The pattern from one slit is a function of the slit width and the wavelength of the radiation and is represented by the **intensity**
- The pattern from multiple slits is a series of lines whose separation is a function of the **distance between the slits.**
- The transformational symmetry of the crystal means that there are periodically placed atoms just like the slits. They are separated by the unit cell edges!

- The information about the slit width is still there and is contained in the intensities of the individual lines
- The distance between the diffracted lines and the slits is reciprocal. The greater the distance between the slits the closer the lines of light are.
- Since for a huge number of slits this involves adding up waves this is best thought of as a **Fourier transformation**.



ORIGINAL GRATING
DIFFRACTION PATTERN
(a)
a
K/a
(b)
b
K/b
(c)
a
γ
b
a
b
γ
(d)
real space
reciprocal space
a
b
γ
a*
γ*
b*
K/b
K/a
a*

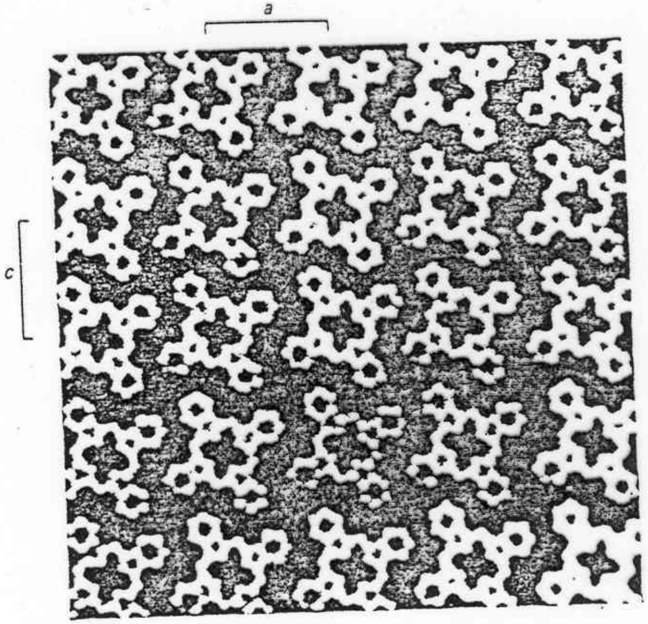


(d) Many molecules horizontally side by side (a one-dimensional crystal).

(e) Two rows of molecules arranged on an oblique lattice. Only parts of the rows are shown.
In comparing (e) with (d), note again the analogy with the relation of the 2-slit and 1-slit patterns of Figure 6b.

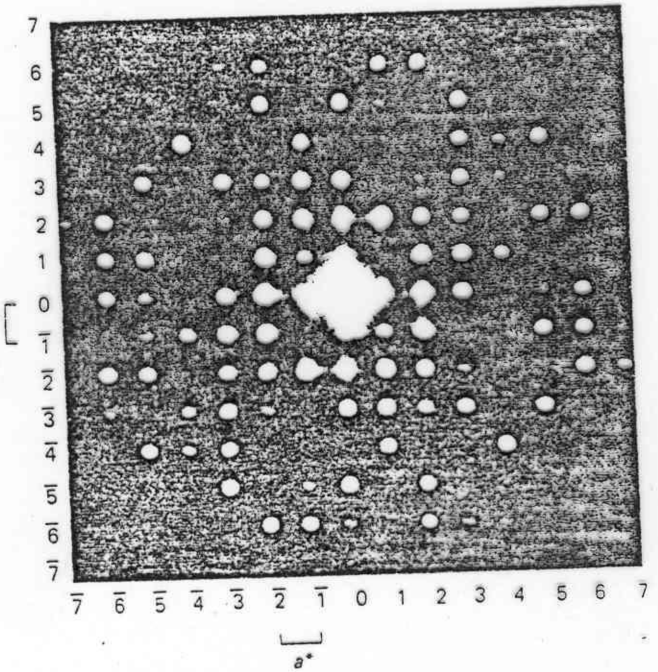
(f) Two-dimensional crystal of molecules. Only part of the crystal is shown.

(a)



a
c

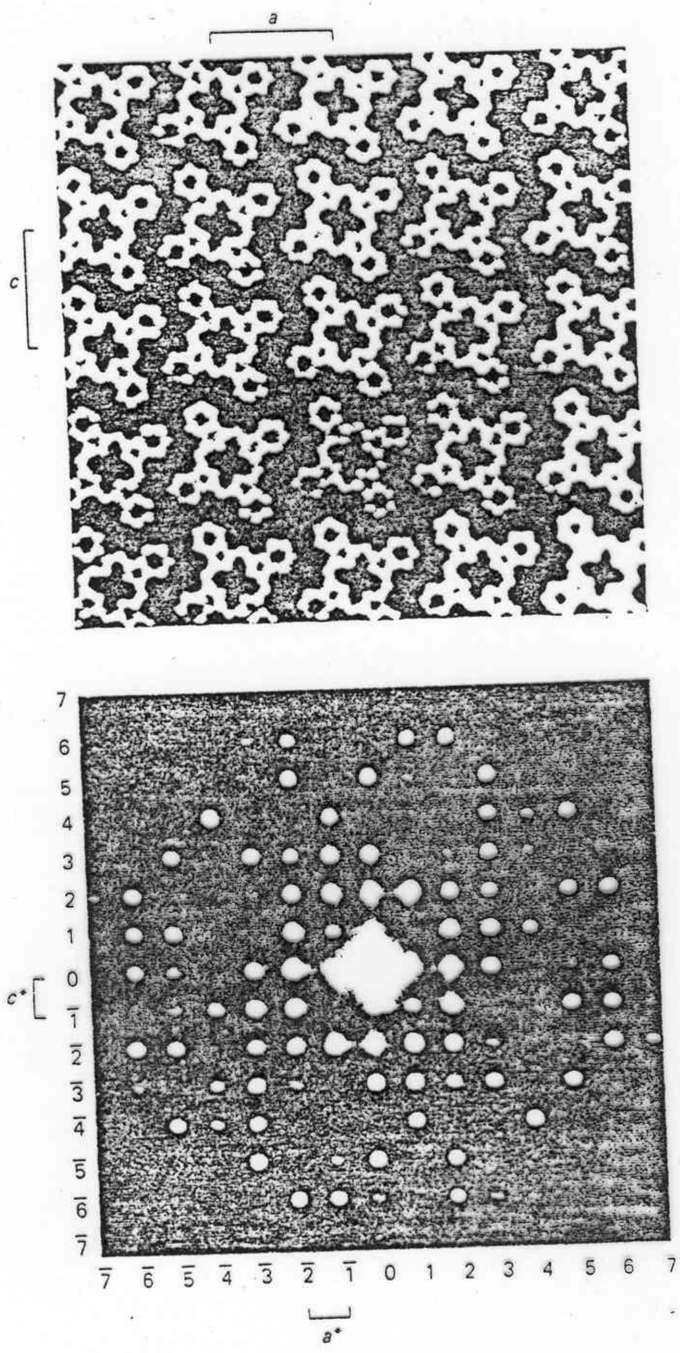
(b)



7
6
5
4
3
2
1
0
$\bar{1}$
$\bar{2}$
$\bar{3}$
$\bar{4}$
$\bar{5}$
$\bar{6}$
$\bar{7}$
c^*
$\bar{7}$ $\bar{6}$ $\bar{5}$ $\bar{4}$ $\bar{3}$ $\bar{2}$ $\bar{1}$ 0 1 2 3 4 5 6 7
a^*

(a)

(b)



a
c
c*
a*
7 6 5 4 3 2 1 0 $\bar{1}$ $\bar{2}$ $\bar{3}$ $\bar{4}$ $\bar{5}$ $\bar{6}$ $\bar{7}$
$\bar{7}$ $\bar{6}$ $\bar{5}$ $\bar{4}$ $\bar{3}$ $\bar{2}$ $\bar{1}$ 0 1 2 3 4 5 6 7

The Take Home Message

- The electrons scatter the x-ray radiation. Each atom scatters proportional to its atomic number
- The scattered waves interfere with each other because of the periodic nature of the crystal.
- The distance between the spots is inversely related to the repeat distance.
- The pattern of the individual scatterers is contained in the intensity of each spot.
- By applying a Fourier series the intensity can be converted to the scattering arrangement.