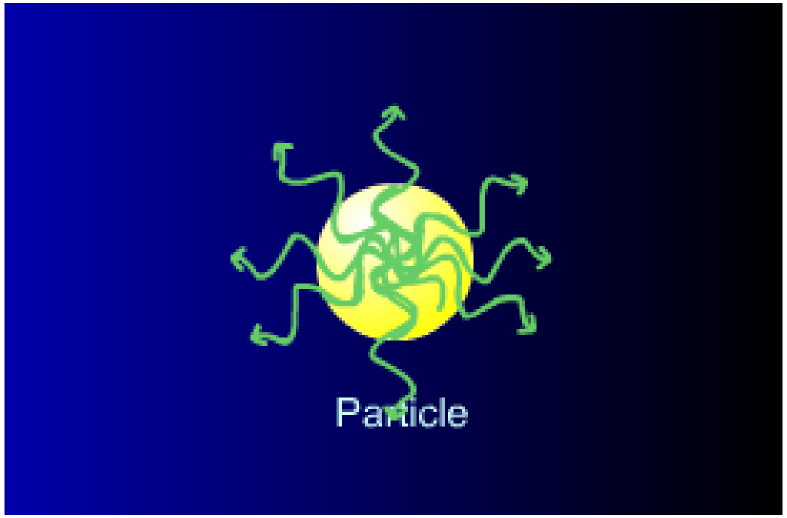
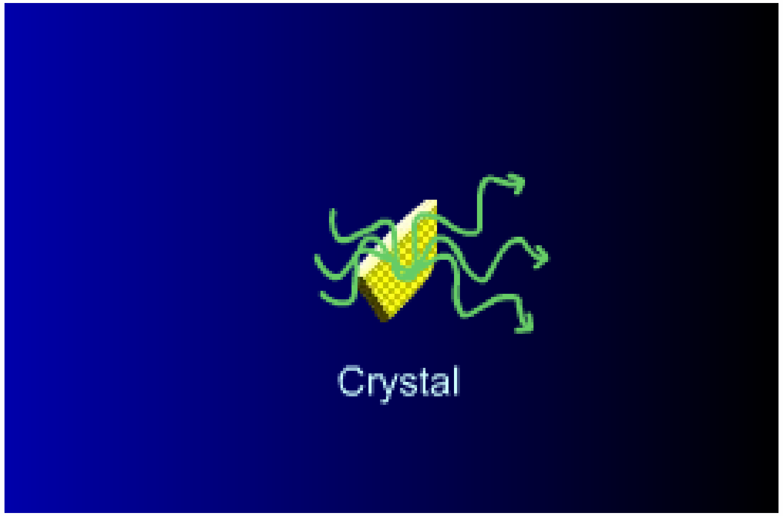
Chapter 10 Diffraction





Reading Assignment:

1. D. Sherwood, Crystals, X-rays, and Proteins-chapter 6

http://www.matter.org.uk/diffraction/Default.htm

Contents

Interaction of waves with obstacles

- interaction of waves with obstacles

  infinite plane wave with wave vector $\vec{k}$ and frequency w

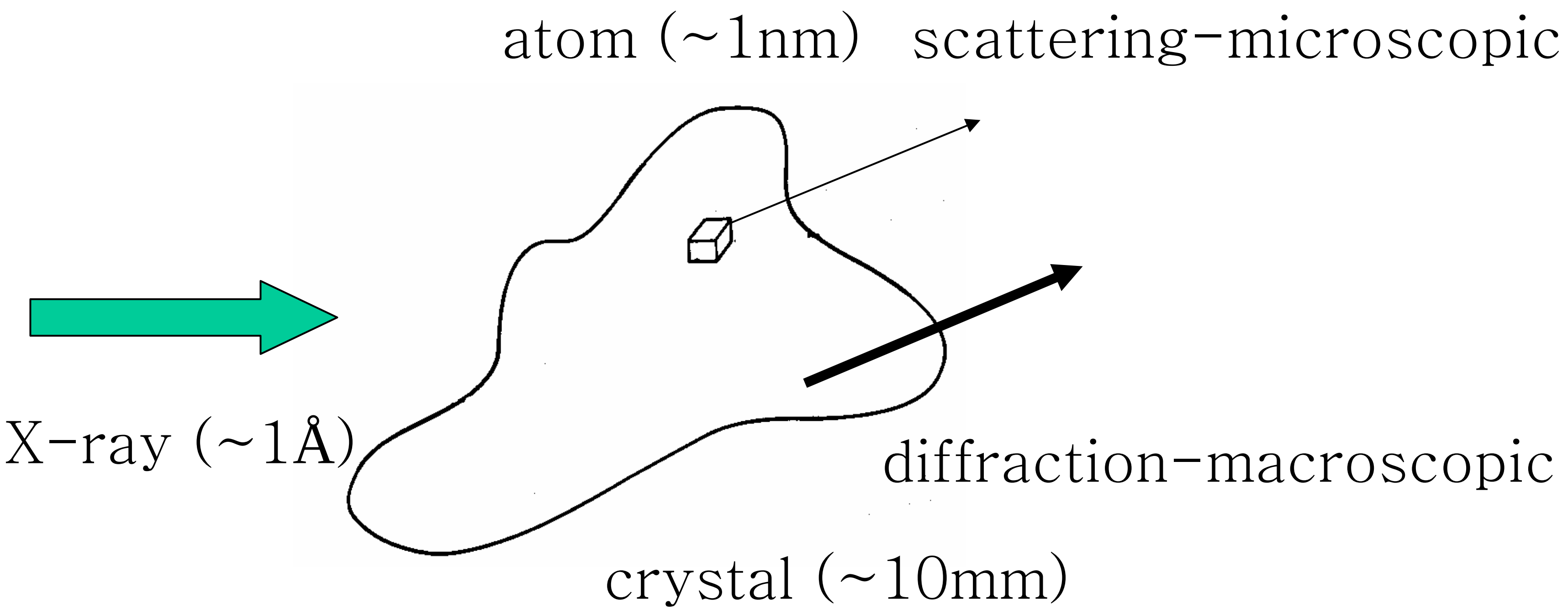
$$\psi = e^{i(\vec{k} \bullet \vec{r} - wt)}$$

  obstacle- perturb the wave motion in some way

-scattering- wave-obstacle interaction such that the dimensions of obstacles and wavelength are comparable

diffraction- wave-obstacle interaction such that the dimensions of obstacles are much larger than the wavelength of the wave motion

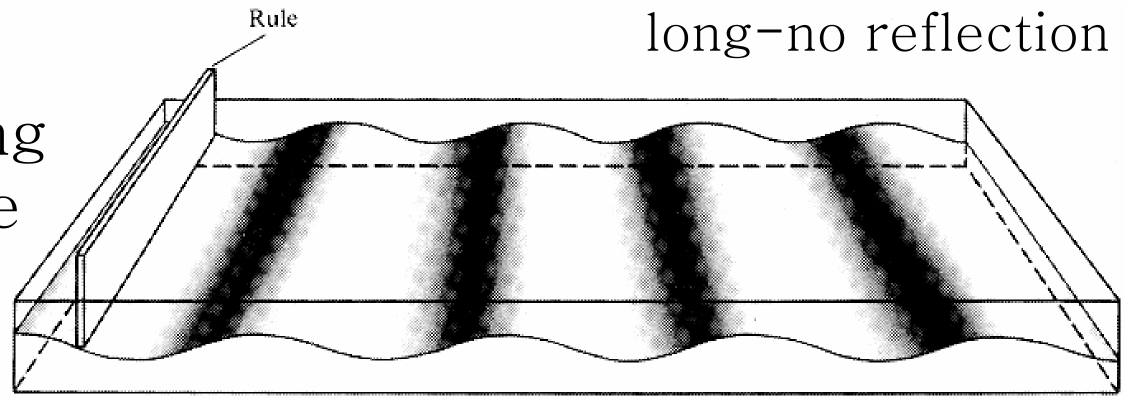
Diffraction of X-rays



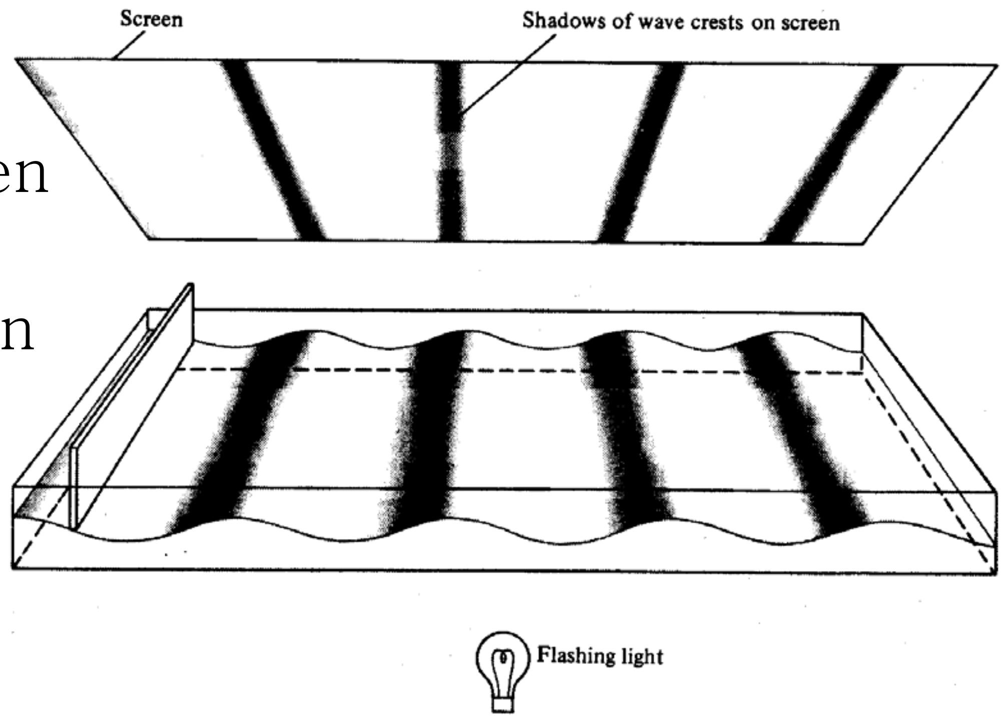
Diffraction of Water Waves

- ripple tank
  rule-periodic dipping
  → plane water wave

long-no reflection

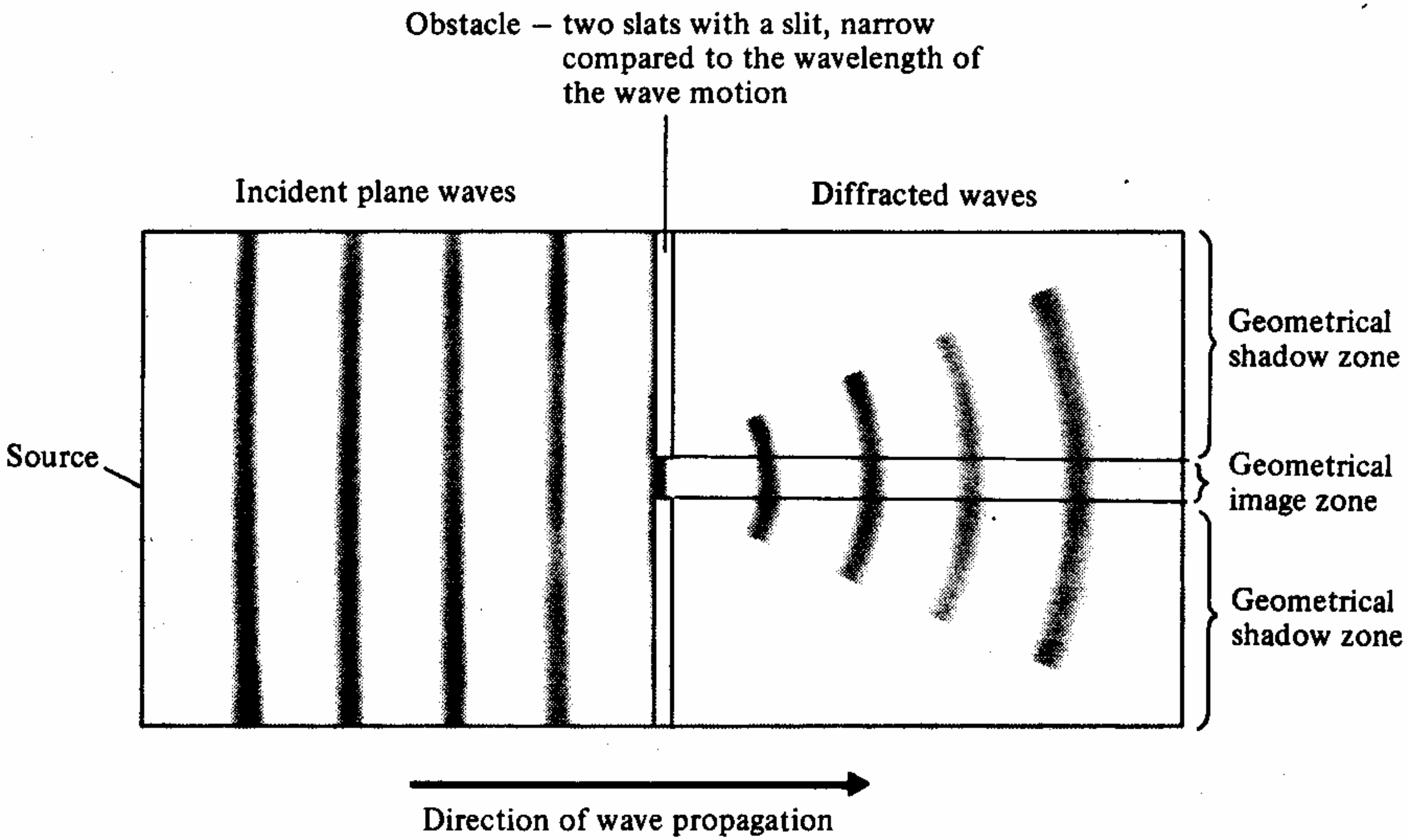


- transparent base-light
  → shadow on the screen
- synchronize light with
  wave motion- frozen in
  → stroboscopic ripple
  tank

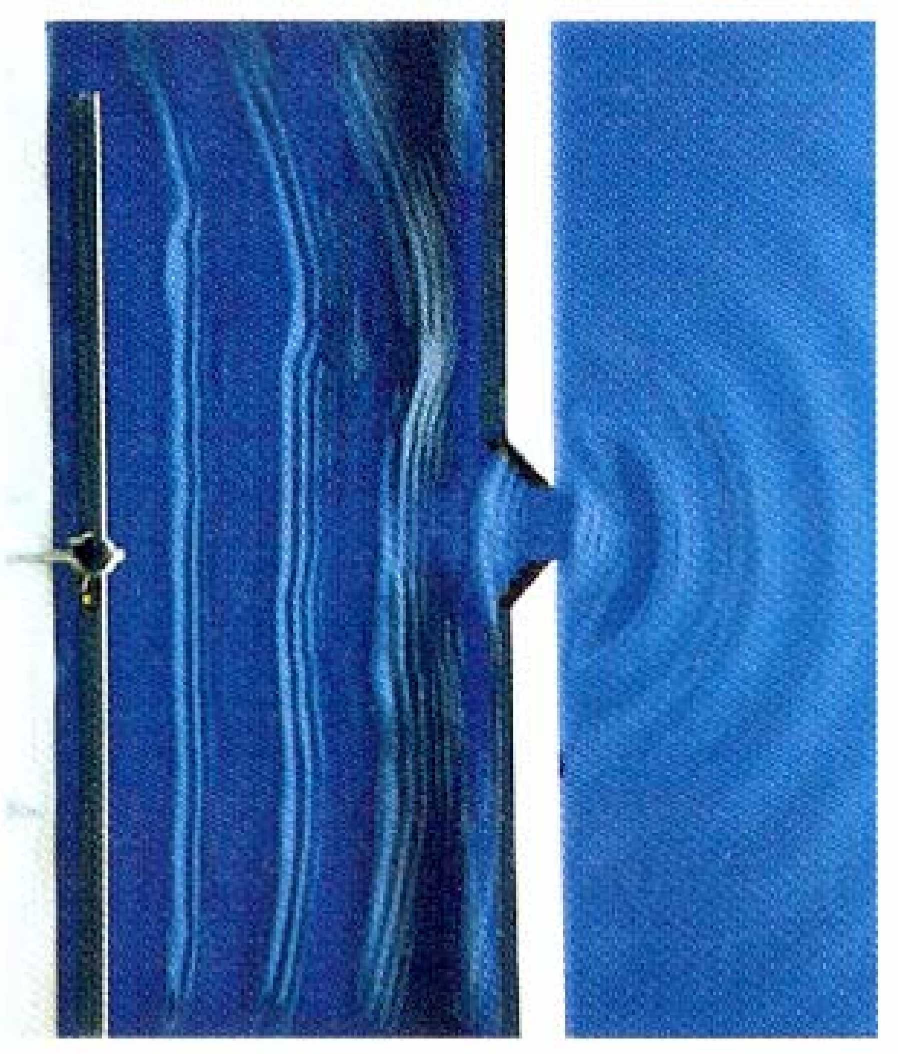


D. Sherwood, Crystals, X-rays, and Proteins

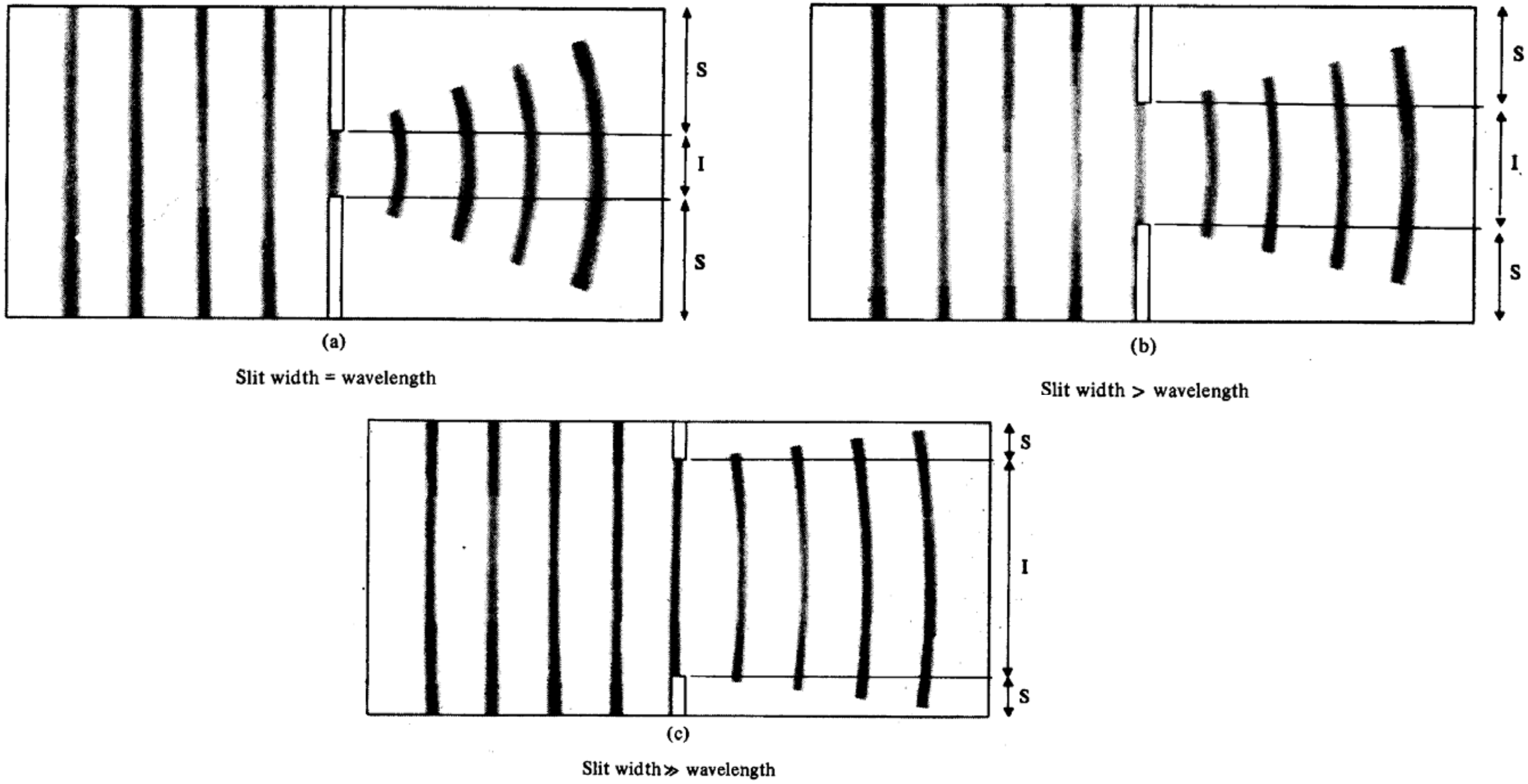
Diffraction of Water Waves



- obstacle- plane wave→curved wave



Diffraction of Water Waves



– when slit width is wide compared to the wavelength of the wave motion, the diffraction effects are masked

Diffraction and Information

- plane wave → obstacle → semi-circular
  diffracted wave contains additional information about obstacle

- When a wave interacts with an obstacle, diffraction occurs. The detailed behavior depends solely on the diffracting obstacles, and so the diffracted waves may be regarded as containing information on the structure of the obstacles.

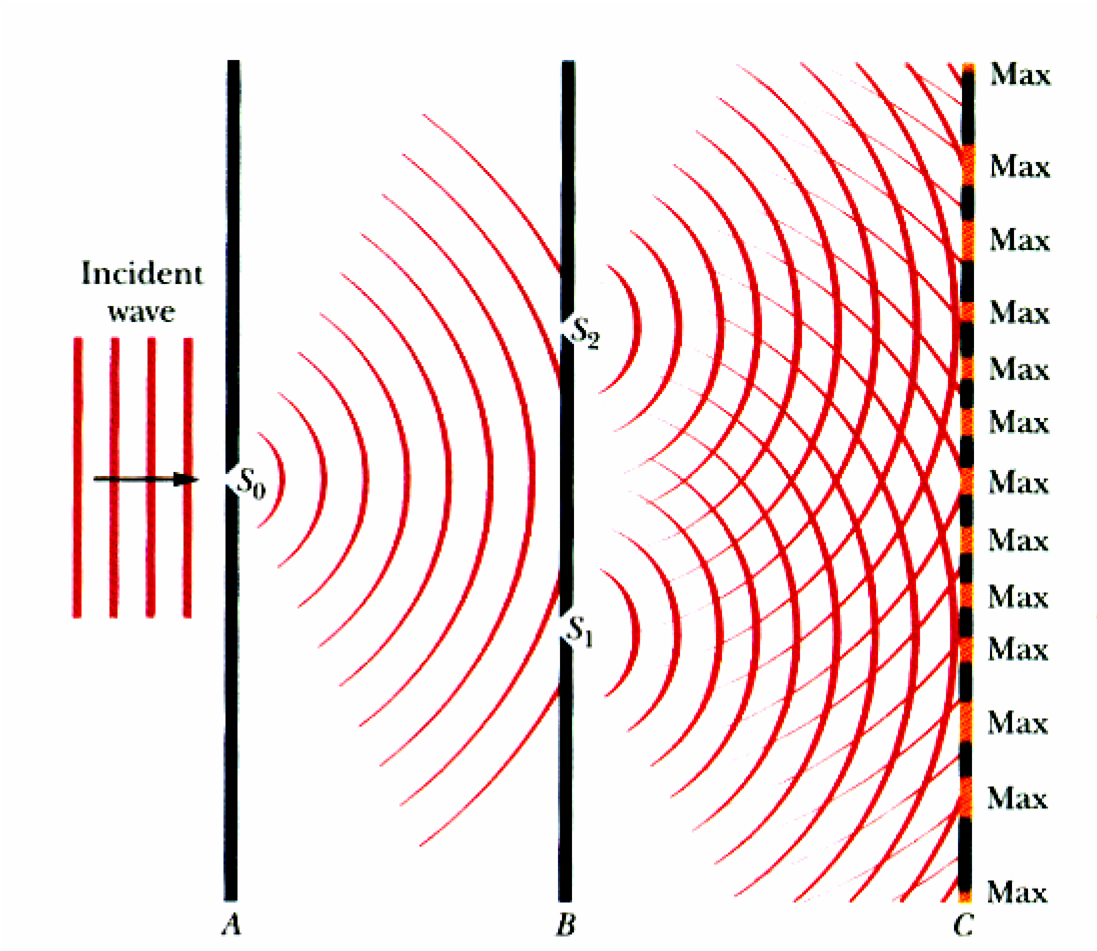
- ex) X-ray → crystal → diffracted pattern

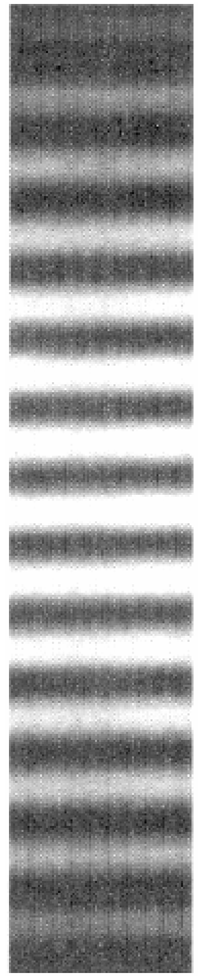
  ↓

  information about nature of molecules and the way they are packed

  ← reconstruct obstacle

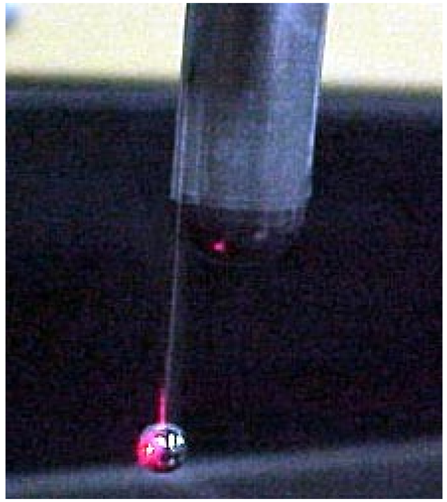
Diffraction of Light

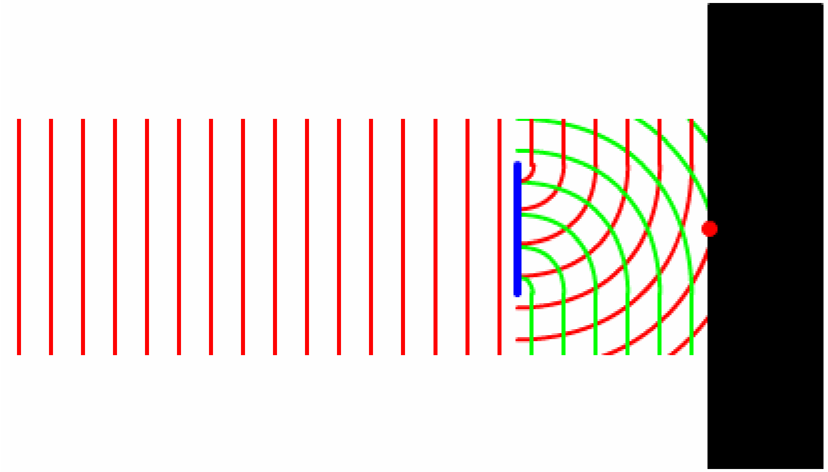


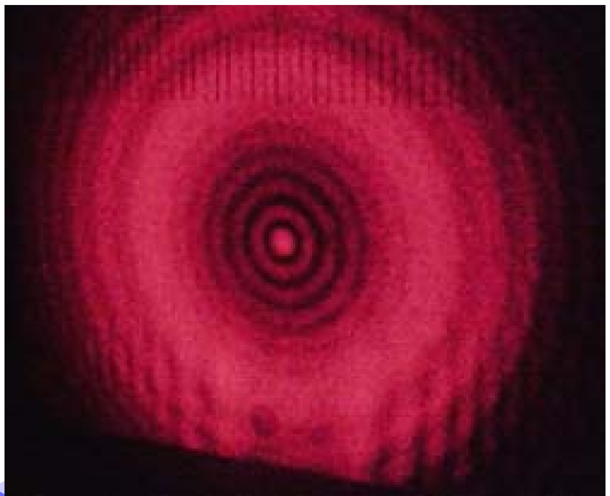


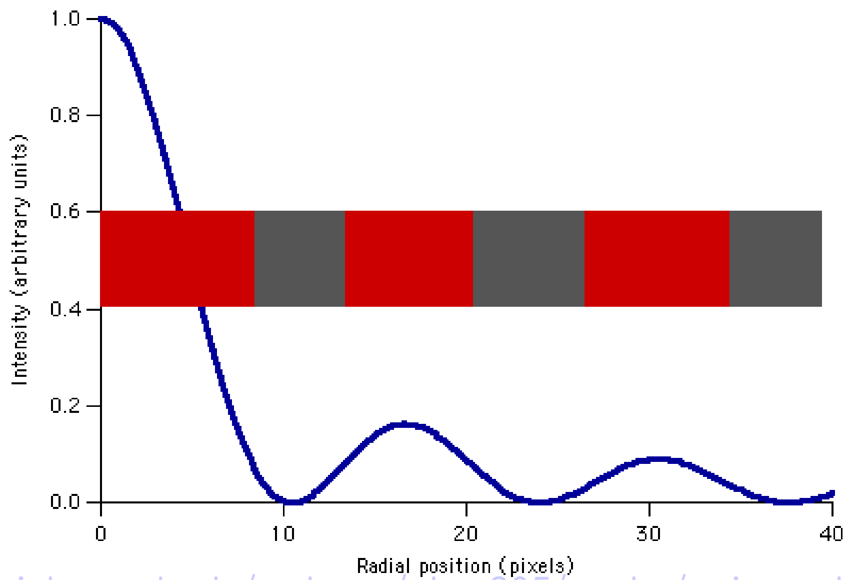
D. Halliday, Fundamentals of Physics

Poisson's Bright Spot



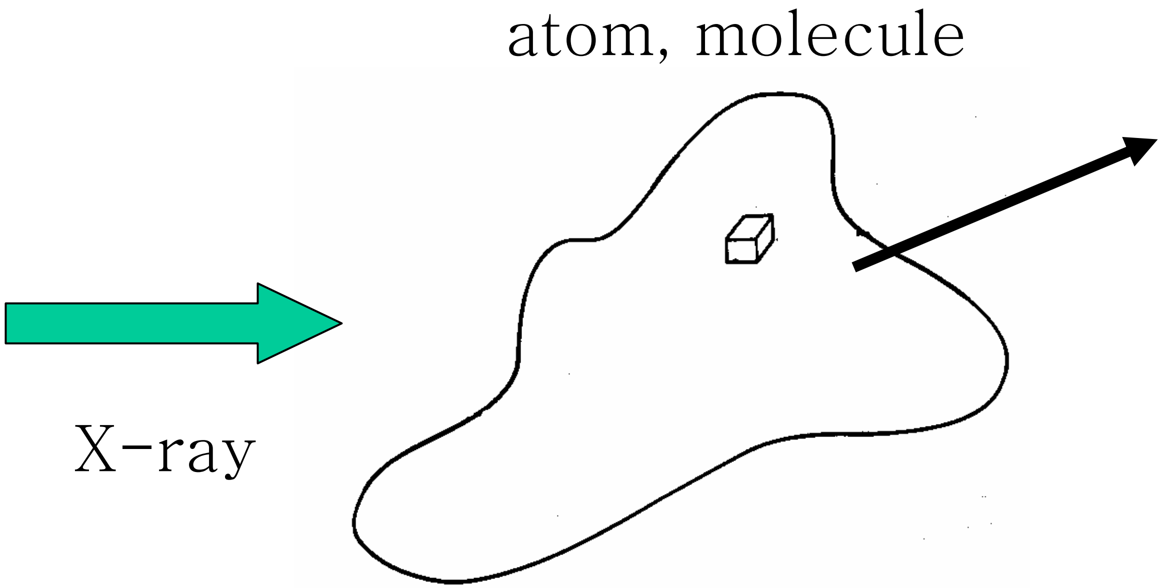






http://www.richmond.edu/~ebunn/phys205/cache/poisson.html

Diffraction of X-rays



crystal: well-defined, 3D ordered array

well-defined phase relationship between scattered waves

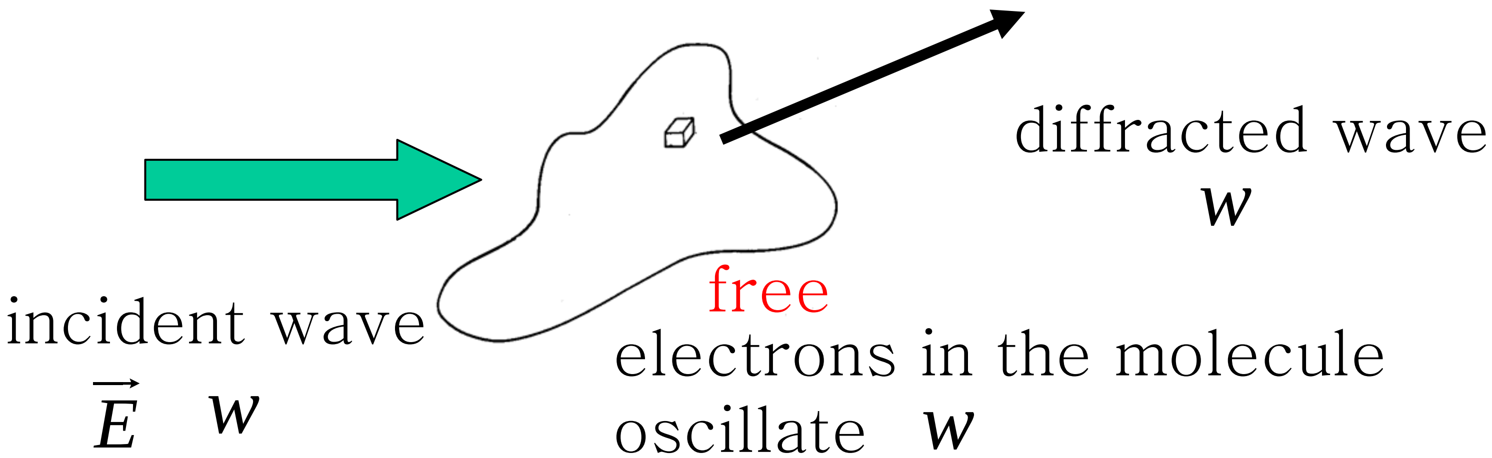
clear and precise diffraction pattern

* liquid- diffuse and imprecise

Mathematics of Diffraction

-assumption-structure and all physical properties of the diffracting obstacle are known.
(diffraction pattern-recipe)
-plane electromagnetic waves of a single frequency w and wavelength λ are incident normally on the obstacle.

(a) frequency and wavelength



Mathematics of Diffraction

(a) frequency and wavelength

in any medium, velocity of electromagnetic radiation is constant→wavelength λ is also unchanged

* diffracted waves have the same frequency and wavelength as the incident waves.
* electrons in the molecules are not really free

$$\text{X-ray}: \lambda = 0.1\ \text{nm},\ w = 10^{19}\ \text{Hz}$$

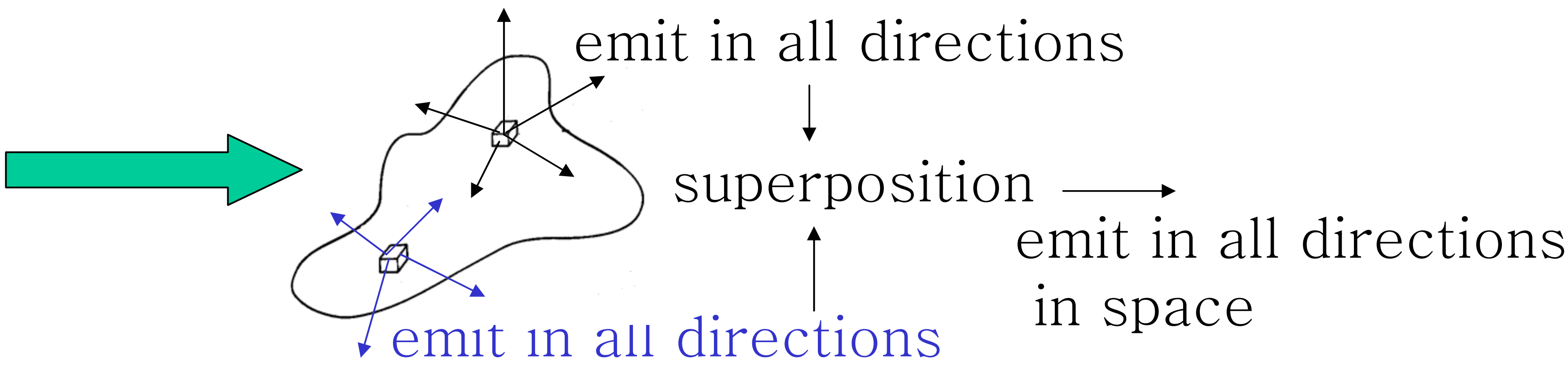
$$\text{orbital motion of an electron: } w = 10^{16}\ \text{Hz}$$

* during one cycle of the X-radiation, the electron has hardly changed its position relative to the nucleus→ electron forget the presence of nucleus → electrons behave as if it were free

Mathematics of Diffraction

(b) spatial consideration

frequency and wavelength unchanged
some other effect



plane wave → spatially different wave
* information of the wave is somehow contained in the way in which they are spread out in space.

Mathematics of Diffraction

(c) significance of the wave vector $\vec{k}$

$$\psi = \psi_o e^{i(\vec{k}\bullet\vec{r}-wt)}$$

magnitude : $k = |\vec{k}| = \dfrac{2\pi}{\lambda}$

direction: normal to the advancing wavefront

$\vec{k} \rightarrow$ spatial information

* total set of diffracted waves may be represented by a set of wave vectors all of which have the same magnitude, equal to that of incident wave, but different directions

Mathematics of Diffraction

(d) mathematical description

- assumption- structure and physical properties known
- phenomenon- (1) waves are propagated through obstacle

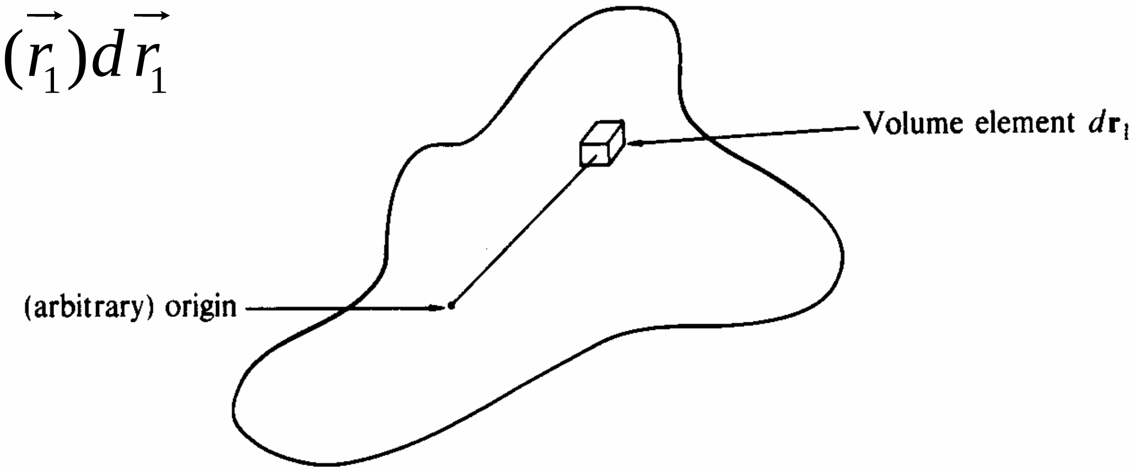
  (2) obstacle perturb these waves

- arbitrary origin, position vector $\vec{r}$,

  infinitesimal volume element centered on $\vec{r}$ by $d\vec{r}$

- volume element $d\vec{r}_1$ centered on $\vec{r}_1 \rightarrow e^{i(\vec{k}\cdot\vec{r}_1 - wt)}$

  perturbing effect $f(\vec{r}_1)d\vec{r}_1$



Mathematics of Diffraction

- two different way of combining $e^{i(\vec{k}\bullet\vec{r}_1 - wt)}$ and $f(\vec{r}_1)d\vec{r}_1$

  diffracted wave from volume element $d\vec{r}_1$

  - $f(\vec{r}_1)d\vec{r}_1 + e^{i(\vec{k}\bullet\vec{r}_1 - wt)}$ or
  - $f(\vec{r}_1)e^{i(\vec{k}\bullet\vec{r}_1 - wt)}d\vec{r}_1$

- consider a perfectly absorbing obstacle $\rightarrow f(\vec{r}) = 0$

  no diffracted wave $\rightarrow$ second equation is correct

- wave diffracted from volume element $d\vec{r}_1 = f(\vec{r}_1)e^{i(\vec{k}\bullet\vec{r}_1 - wt)}d\vec{r}_1$
- wave diffracted from volume element $d\vec{r}_2 = f(\vec{r}_2)e^{i(\vec{k}\bullet\vec{r}_2 - wt)}d\vec{r}_1$

Mathematics of Diffraction

- Principle of superposition

$$\text{diffraction pattern} = f(\vec{r}_1)e^{i(\vec{k}\bullet\vec{r}_1 - wt)}d\vec{r}_1 + f(\vec{r}_2)e^{i(\vec{k}\bullet\vec{r}_2 - wt)}d\vec{r}_1$$

$$f(\vec{r}_3)e^{i(\vec{k}\bullet\vec{r}_3 - wt)}d\vec{r}_3 + \bullet\bullet\bullet$$

$$= \int_V f(\vec{r})e^{i(\vec{k}\bullet\vec{r} - wt)}d\vec{r}$$

$$= e^{-iwt}\int_V f(\vec{r})e^{i\vec{k}\bullet\vec{r}}d\vec{r}$$

- X-ray: λ~0.1 nm, $w \sim 10^{19}$ Hz, one cycle $\vec{E} \sim 10^{-19}$ sec
- no recording device is availabele
- diffraction experiment- time average of the intensity of the diffracted wave

Mathematics of Diffraction

- diffraction pattern = $\int_V f(\vec{r})e^{i\vec{k}\bullet\vec{r}}d\vec{r}$

- limits on the integral

  $f(\vec{r})$: finite $\rightarrow$ mathematically not well behaved

  define $f(\vec{r})$ over an infinite range dividing the values into two domains

  diffraction pattern = $\int_{\text{all } \vec{r}} f(\vec{r})e^{i\vec{k}\bullet\vec{r}}d\vec{r}$

  (Fourier trnasform of $f(\vec{r})$)

  $f(\vec{r})$: amplitude function

- diffraction pattern of any obstacle is the Fourier transform of the amplitude function

Significance of Fourier Transform

- diffraction pattern = $\int_{\text{all } \vec{r}} f(\vec{r}) e^{i\vec{k}\cdot\vec{r}} d\vec{r}$

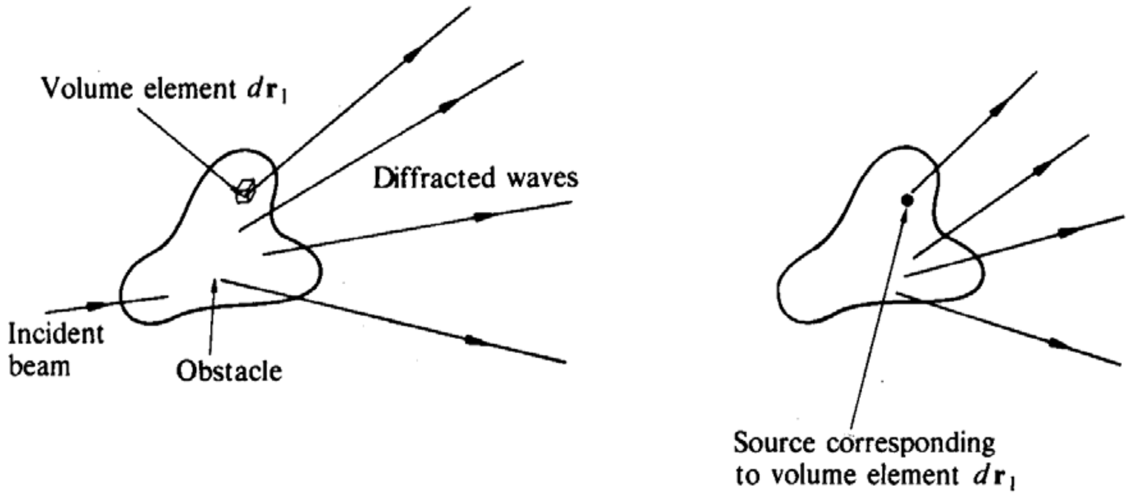
1. integrand - function of $\vec{k}$ and $\vec{r}$, integration - over $\vec{r}$

   diffraction pattern $\rightarrow F(\vec{k})$

   information in the diffraction pattern-spatial $\leftarrow \vec{\text{k}}$

2. $e^{i\vec{k}\cdot\vec{r}}$: wave, $f(\vec{r})$: amplitude type function

   passive scatterer $\rightarrow$ replaced by active source $\rightarrow$ identical



Fourier Transform and Shape

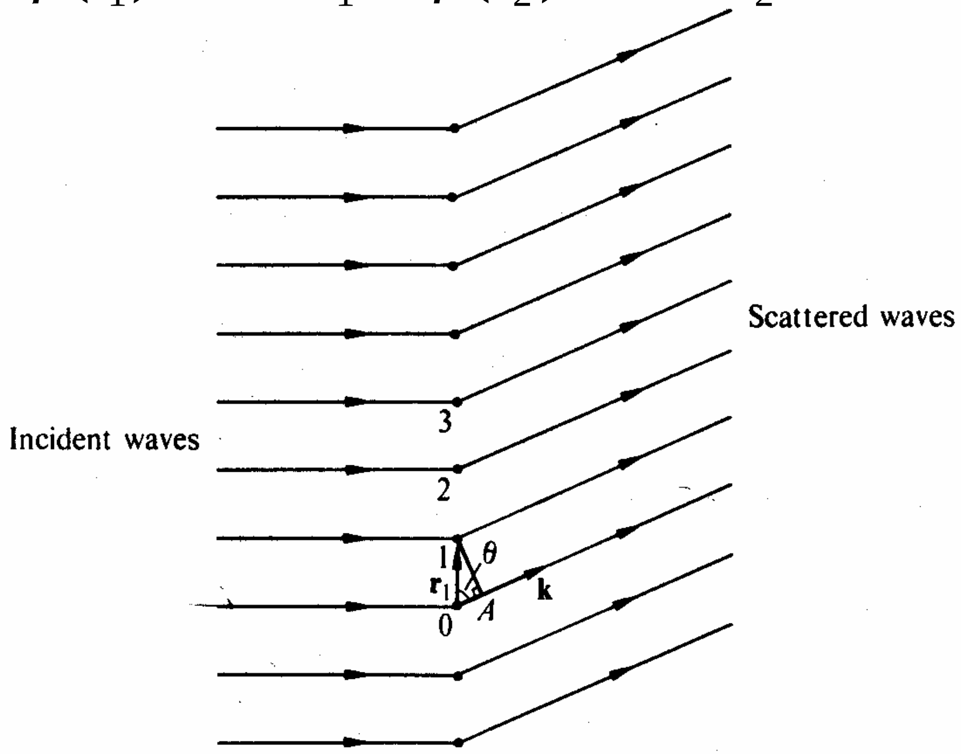
- a linear array of scattering center in an obstacle
- phase at point 0=0

  phase at point 1= $\frac{2\pi}{\lambda}\overline{\text{OA}}(=r_1\cos\theta)=\vec{k}\bullet\vec{r_1}$

- total scattered wave= $f(\vec{r_0})d\vec{r_0}+f(\vec{r_1})e^{i\vec{k}\bullet\vec{r_1}}d\vec{r_1}+f(\vec{r_2})e^{i\vec{k}\bullet\vec{r_2}}d\vec{r_2}+\bullet\bullet\bullet$

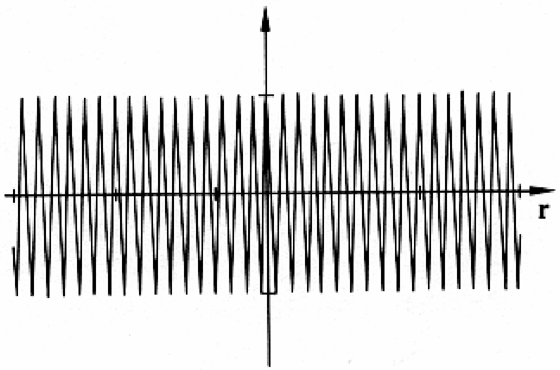
  $$=\int_{obstacle} f(\vec{r})e^{i\vec{k}\bullet\vec{r}}d\vec{r}$$

- exponential term-specifiy phase relationship between scattering centers and an arbitrary origin



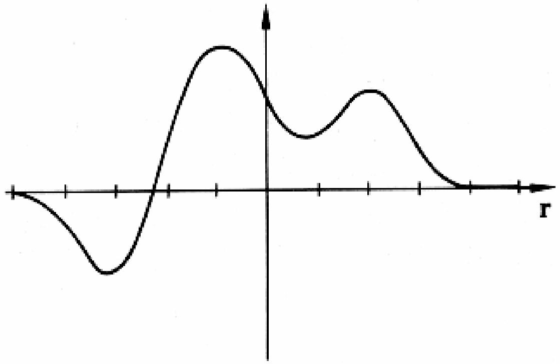
Fourier Transform and Information

- $f(\vec{r})e^{i\vec{k}\bullet\vec{r}}$



$e^{i\vec{k}\bullet\vec{r}}$

(a)



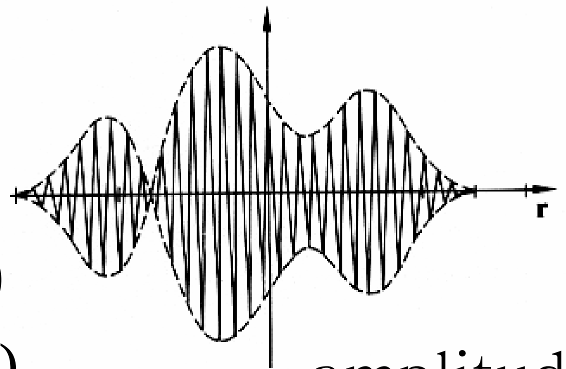
(b)

$f(\vec{r})$

- AM radio

  radio frequency (of order 10^5 Hz)

  audio frequency (of order 500 Hz)



(c) amplitude modulated

Fourier Transform and Information

- diffraction pattern in terms of Fourier transform

(i) the description is, sa required, a function of $\vec{k}$

(ii) the decription agrees with our physical knowledge of the interaction of wave with obstacles

(iii) the description represents a general solution of three-dimensional wave equation

(iv) the description is capable of containing the required information

Inverse Transform

- diffraction pattern $F(\vec{k})$

$$F(\vec{k}) = \int_{\text{all } \vec{r}} f(\vec{r}) e^{i\vec{k}\bullet\vec{r}} d\vec{r}$$

$F(\vec{k})$ is Fourier transform of $f(\vec{r})$

- inverse transform

$$f(\vec{r}) = \int_{\text{all } \vec{k}} F(\vec{k}) e^{-i\vec{k}\bullet\vec{r}} d\vec{k}$$

- $F(\vec{k})$: diffraction pattern function- information on spatial distribution of diffraction pattern

$f(\vec{r})$: information on the structure of obstacle

- diffraction experiment $\rightarrow$ intensity $\propto \left|F(\vec{k})\right|^2 \rightarrow F(\vec{k}) \rightarrow f(\vec{r})$

Microscope

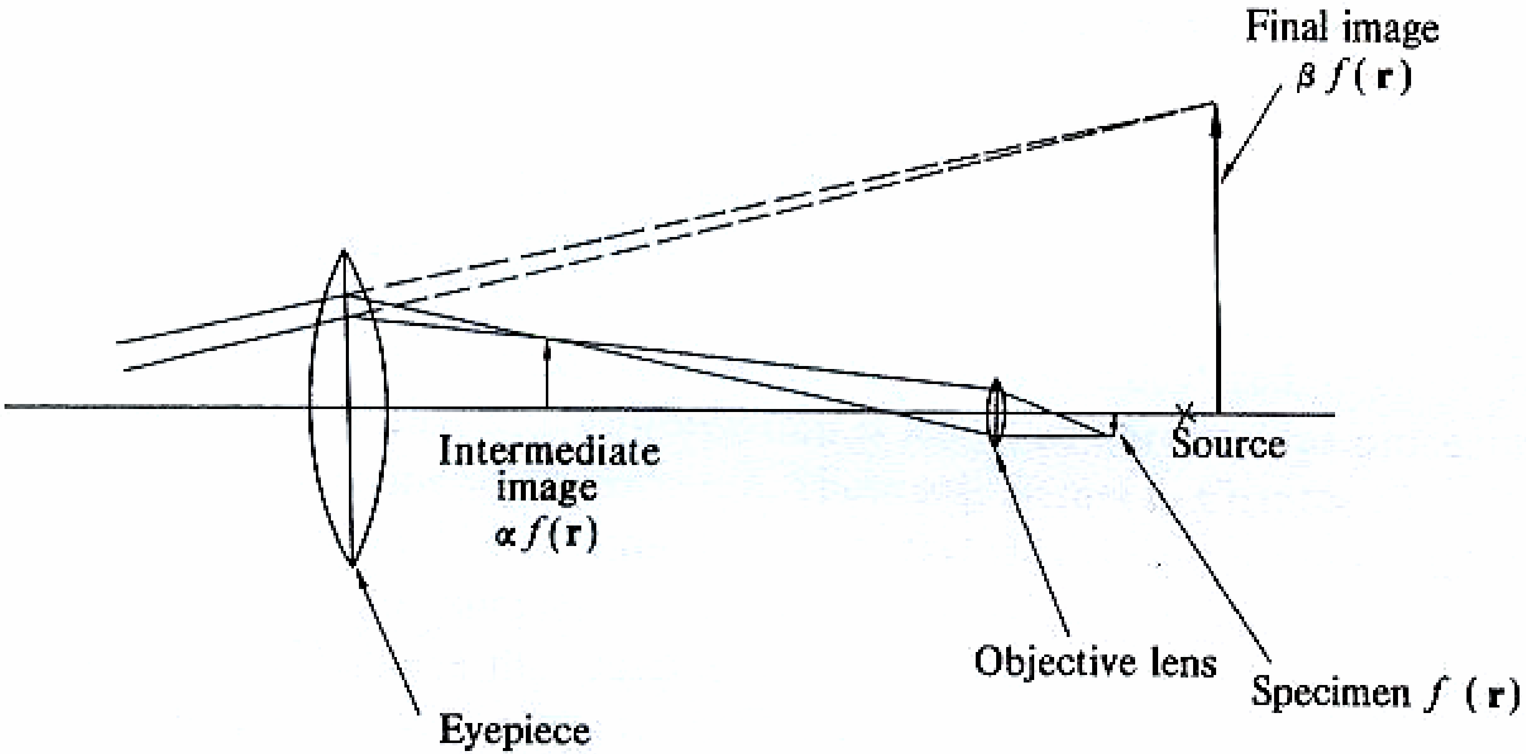


Fig. 6.12. *Schematic representation of a microscope*. The light diffracted by the specimen $f(\mathbf{r})$ is caught by the objective lens which acts to take the Fourier transform of the diffraction pattern, thereby throwing an intermediate image $\alpha f(\mathbf{r})$, where α is a magnifying factor. The intermediate image now acts as an object for the eyepiece, which forms the final image $\beta f(\mathbf{r})$, β being the overall magnification. Ideally, all the information is transferred without distortion, and so the images are identical in form to the specimen, and magnified.

Experimental Limitation

- diffraction pattern $F(\vec{k})$

$$F(\vec{k}) = \int_{\text{all } \vec{r}} f(\vec{r}) e^{i\vec{k}\bullet\vec{r}} d\vec{r}$$

- information contained in all space

  physically impossible to scan all space to collect

  some information lost

- phase problem

  measure only the intensity not the complex amplitude of diffraction pattern

$$F(\vec{k}) = \left|F(\vec{k})\right| e^{i\delta}$$

observe $\left|F(\vec{k})\right|^2 \rightarrow$ lost information on δ