The Fourier Transform, the Wave Equation and Crystals

Joe Ferrara, Ph. D.
CSO, Rigaku Americas Corp.
VP XRL, Rigaku Corp.
Vice-Chair, USNC/Cr

LONDON: G. BELL AND SONS, LTD.,
PORTUGAL ST., LINCOLN'S INN, W.C.
NEW YORK: THE MACMILLAN CO.
BOMBAY: A. H. WHEELER & CO.

X RAYS
AND
CRYSTAL STRUCTURE

BY

W. H. BRAGG, M.A., D.Sc., F.R.S.

CAVENDISH PROFESSOR OF PHYSICS, UNIVERSITY OF LEEDS

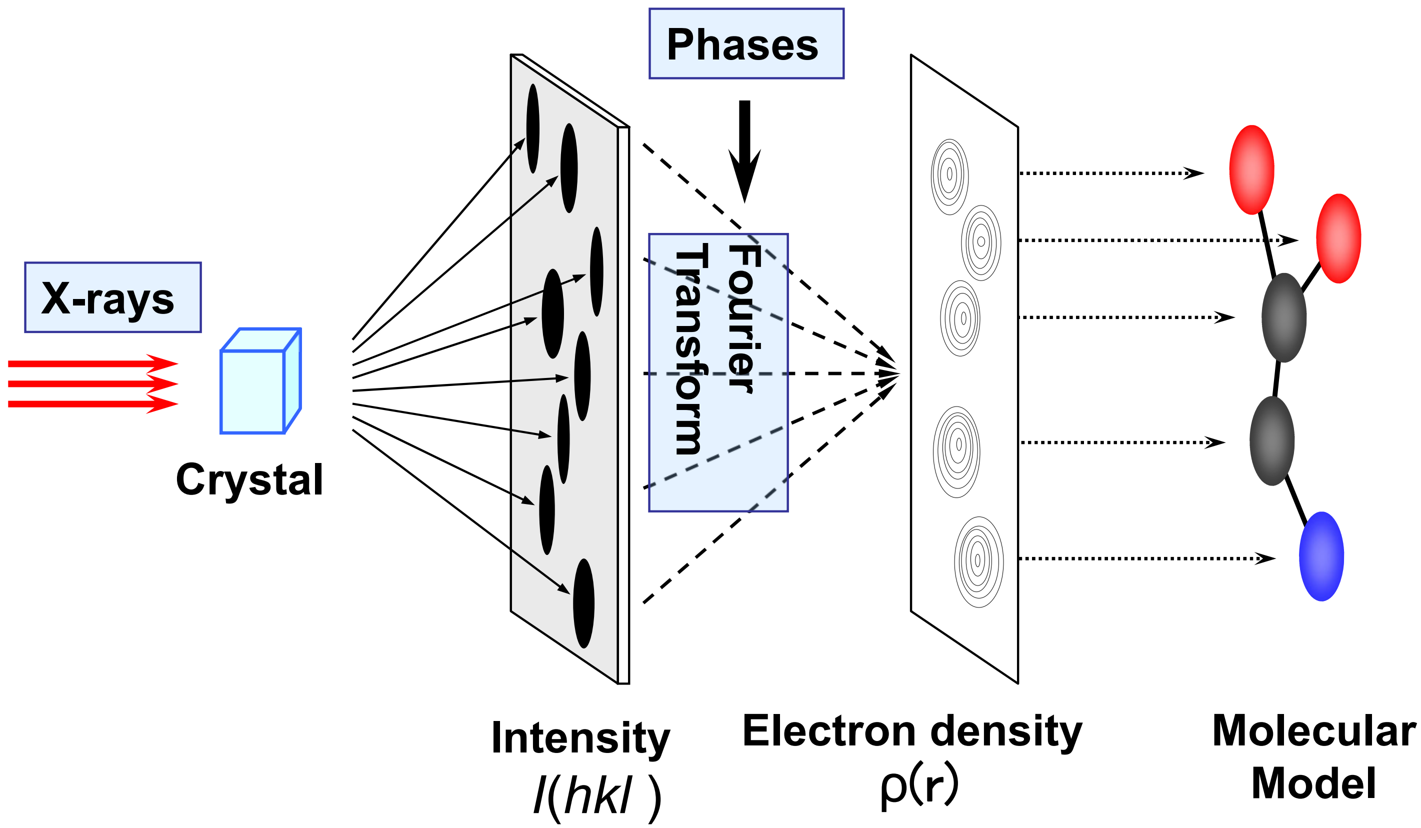
AND

W. L. BRAGG, B.A.

FELLOW OF TRINITY COLLEGE, CAMBRIDGE

LONDON
G. BELL AND SONS, LTD.
1915

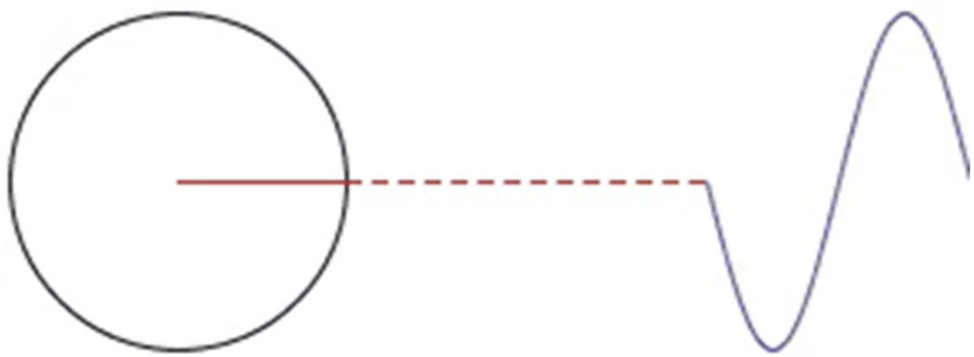
35000 ft view of X-ray Structure Analysis



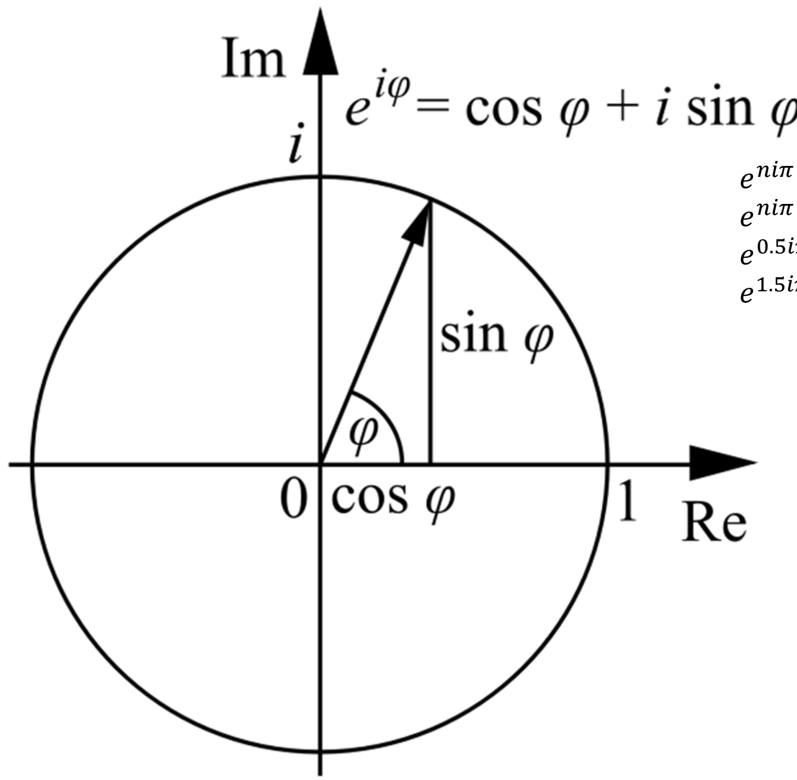
CCCW

Fourier Theory

- Originally proposed by Jean-Bapiste Joseph Fourier in 1822 in *The Analytical Theory of Heat*
- Described discrete functions as the infinite sum of sines



What is a circle?



$e^{ni\pi} = e^{-ni\pi} = -1$ for n odd
$e^{ni\pi} = e^{-ni\pi} = 1$ for n even
$e^{0.5i\pi} = i$
$e^{1.5i\pi} = -i$

http://en.wikipedia.org/wiki/Euler's_formula

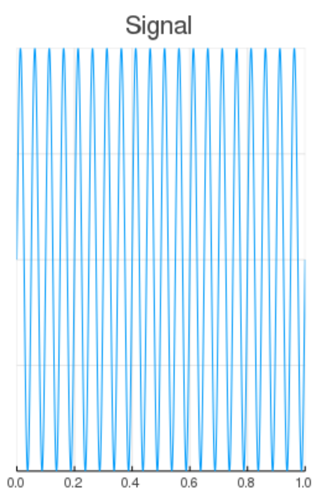
The Fourier Transform

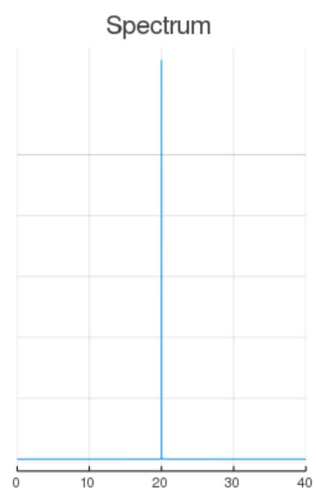
$$F(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx$$

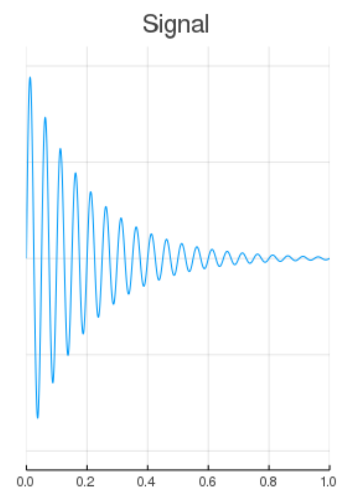
$$F(k) = Tf(x)$$

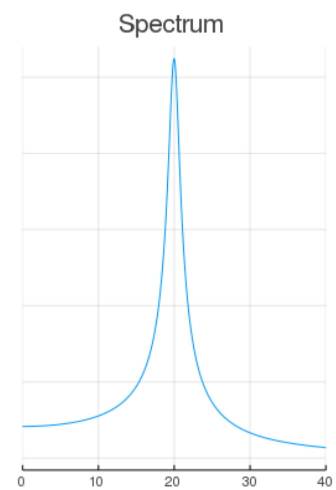
In three dimensions this is generalized to:

$$F(\mathbf{k}) = \int_{\mathbf{r}} f(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} = Tf(\mathbf{r})$$





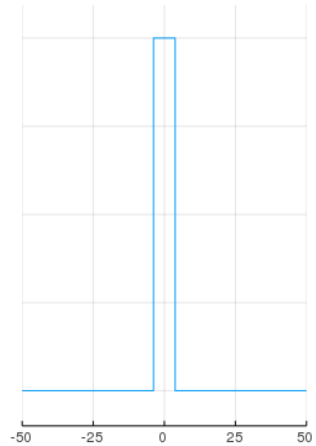




The Fourier Transform

Let's look at an example:

$$\begin{array}{ll} -\infty < x < -X_0, & f(x) = 0 \\ -X_0 \le x \le X_0, & f(x) = h \\ X_0 < x < \infty, & f(x) = 0 \end{array}$$



$$F(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx$$

$$F(k) = h \int_{-X_0}^{X_0} e^{ikx} dx$$

$$F(k) = h \left[\frac{e^{ikx}}{ik} \right]_{-X_0}^{X_0} = h \frac{e^{ikX_0} - e^{ik(-X_0)}}{ik}$$

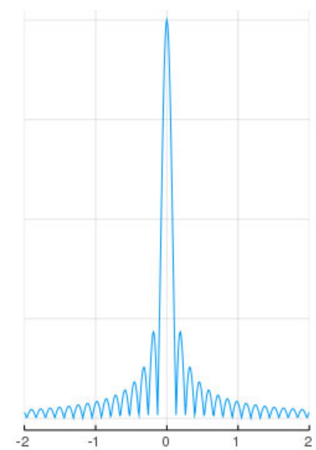
$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}, \qquad \theta = kX_0$$

$$F(k) = 2h \frac{\sin k X_0}{k} = 2X_0 h \frac{\sin k X_0}{kX_0}$$

$$\sin k X_0 = 0$$

$$kX_0 = \pm\pi$$

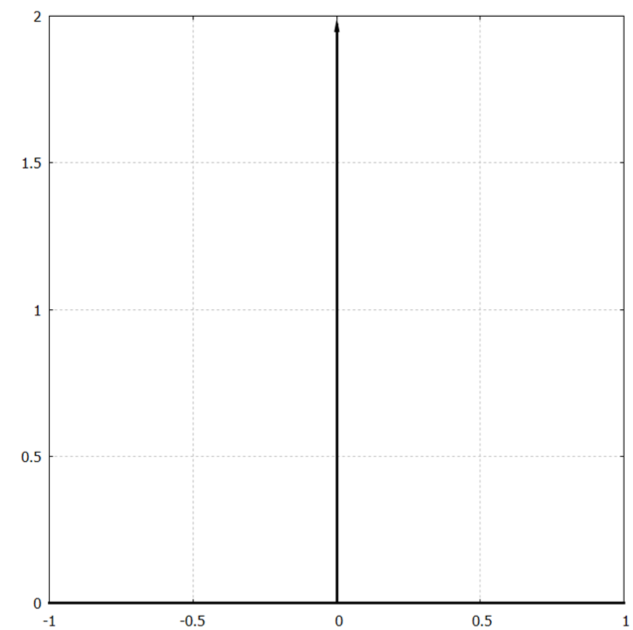
$$k = \pm \frac{\pi}{X_0}$$



The Dirac δ function

$$\delta(x - x_0) \begin{cases} +\infty, (x - x_0) = 0 \\ 0, (x - x_0) \neq 0 \end{cases}$$

$$\int_{-\infty}^{\infty} \delta(x - x_0)dx = 1$$



An important property of the δ function is that acts as a sieve:

$$\int_{-\infty}^{\infty} f(x)\delta(x - x_0)dx = f(x_0) \int_{-\infty}^{\infty} \delta(x - x_0)dx = f(x_0)$$

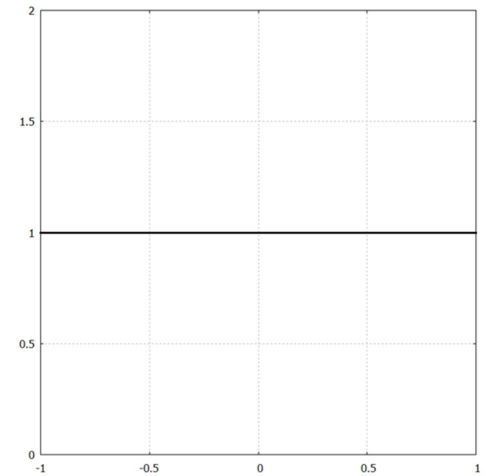
In three dimensions:

$$\int_{-\infty}^{\infty} f(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}_0)d\mathbf{r} = f(\mathbf{r}_0)$$

Fourier transforms and δ functions

One δ function:

$$F(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx = \int_{-\infty}^{\infty} \delta(x) e^{ikx} dx = \left[e^{ikx}\right]_{x=0} = e^0 = 1$$



Two δ functions:

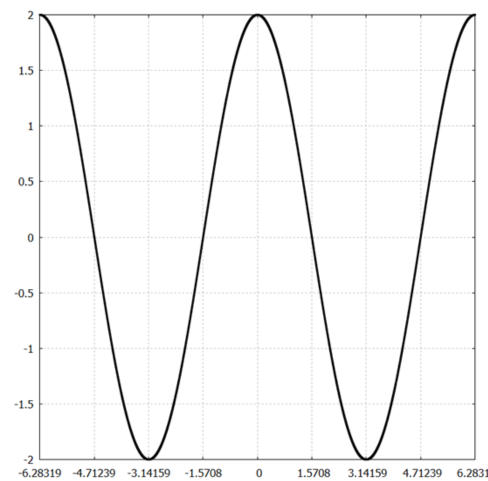
$$f(x) = \delta(x + x_0) + \delta(x - x_0)$$

$$F(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx$$

$$= \int_{-\infty}^{\infty} \delta(x + x_0) e^{ikx} dx + \int_{-\infty}^{\infty} \delta(x - x_0) e^{ikx} dx = e^{-ikx_0} + e^{ikx_0}$$

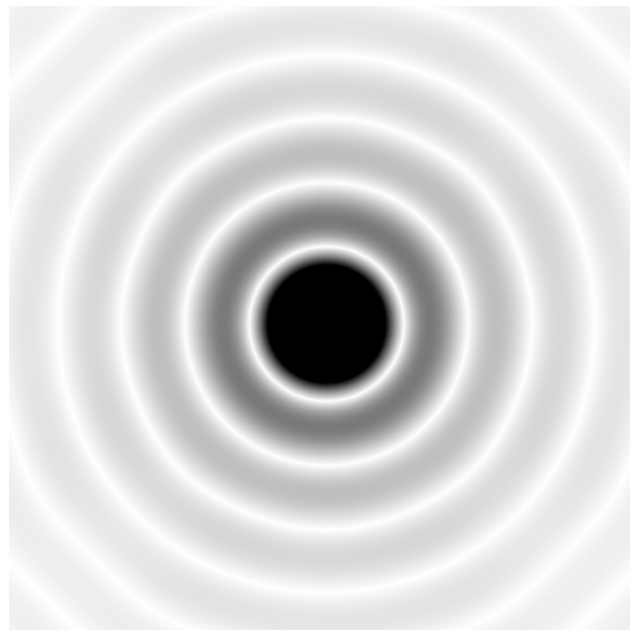
$$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}, \qquad \theta = \mathrm{kx}_0$$

$$F(k) = 2\cos k\, x_0$$



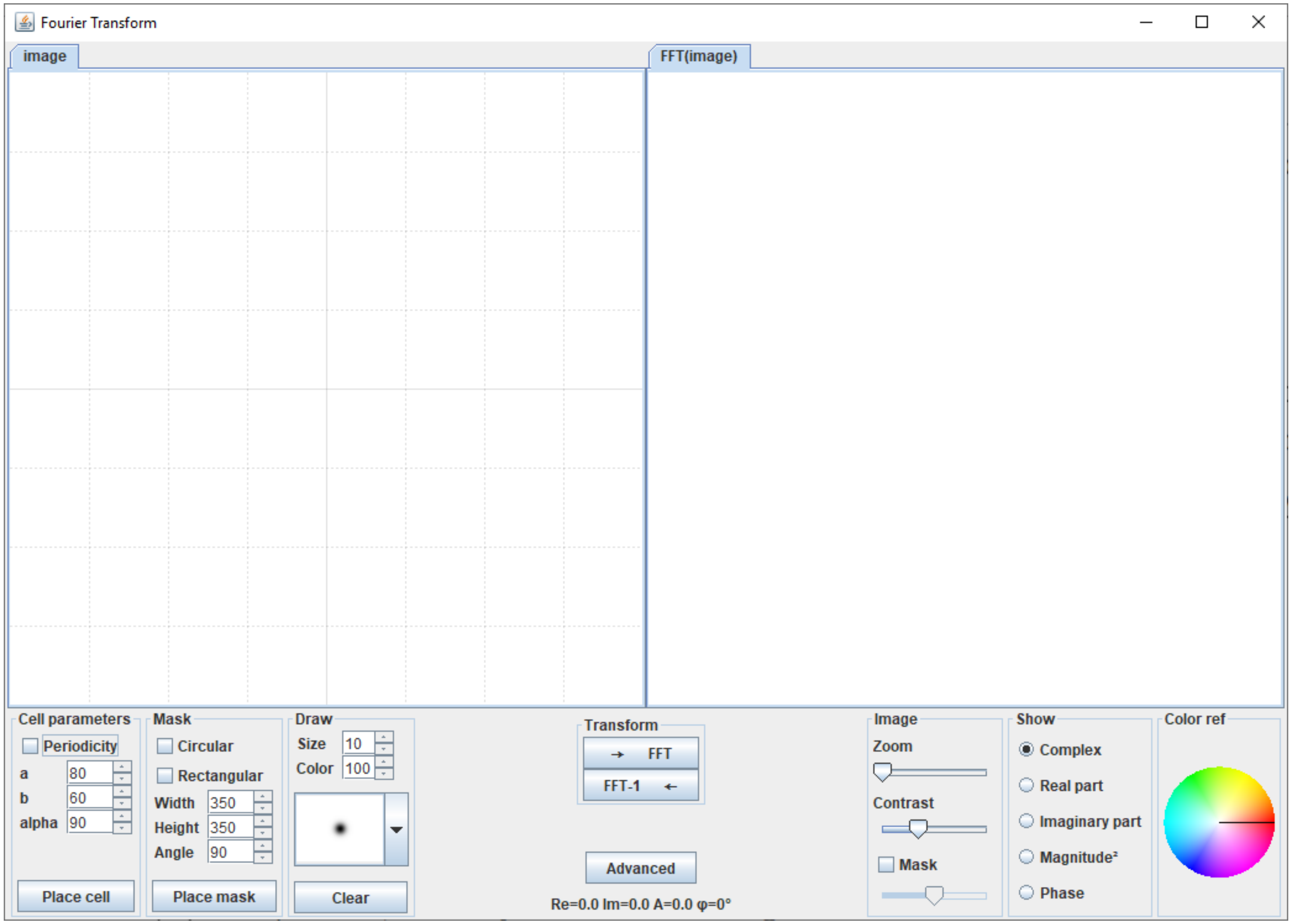
The Fourier Transform

$$F(\mathbf{k}) = \int_{\text{all } \mathbf{r}} f(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{r} = Tf(\mathbf{r})$$



The Fourier Transform

$$F(\mathbf{k}) = \int_{\text{all } \mathbf{r}} f(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}\, d\mathbf{r} = Tf(\mathbf{r})$$

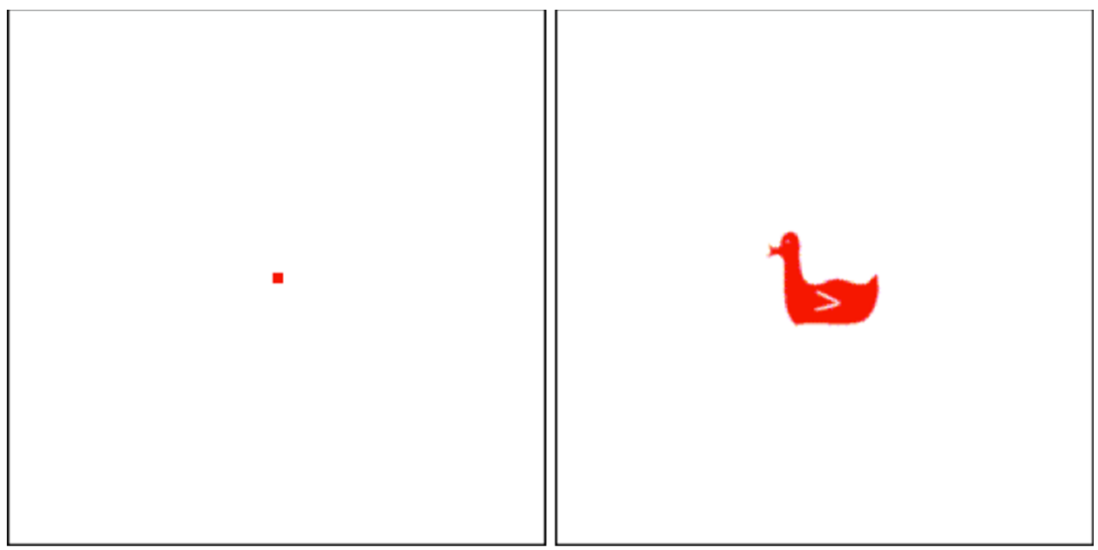

Fourier Transform
image
FFT(image)
Cell parameters
Periodicity
a 80
b 60
alpha 90
Place cell
Mask
Circular
Rectangular
Width 350
Height 350
Angle 90
Place mask
Draw
Size 10
Color 100
Clear
Transform
FFT
FFT-1
Advanced
Re=0.0 Im=0.0 A=0.0 φ=0°
Image
Zoom
Contrast
Mask
Show
Complex
Real part
Imaginary part
Magnitude²
Phase
Color ref

Convolutions

$$c(\mathbf{u}) = \int_{\text{all } \mathbf{r}} f(\mathbf{r}) g(\mathbf{u}-\mathbf{r})\, d\mathbf{r}$$

$$c(\mathbf{u}) = f(\mathbf{r}) * g(\mathbf{r}) = \int_{\text{all } \mathbf{r}} f(\mathbf{r}) g(\mathbf{u}-\mathbf{r})\, d\mathbf{r}$$

$$f(\mathbf{r}) * g(\mathbf{r}) = \int_{\text{all } \mathbf{r}} f(\mathbf{r}) g(\mathbf{u}-\mathbf{r})\, d\mathbf{r} = \int_{\text{all } \mathbf{r}} f(\mathbf{u}-\mathbf{r}) g(\mathbf{r})\, d\mathbf{r}$$

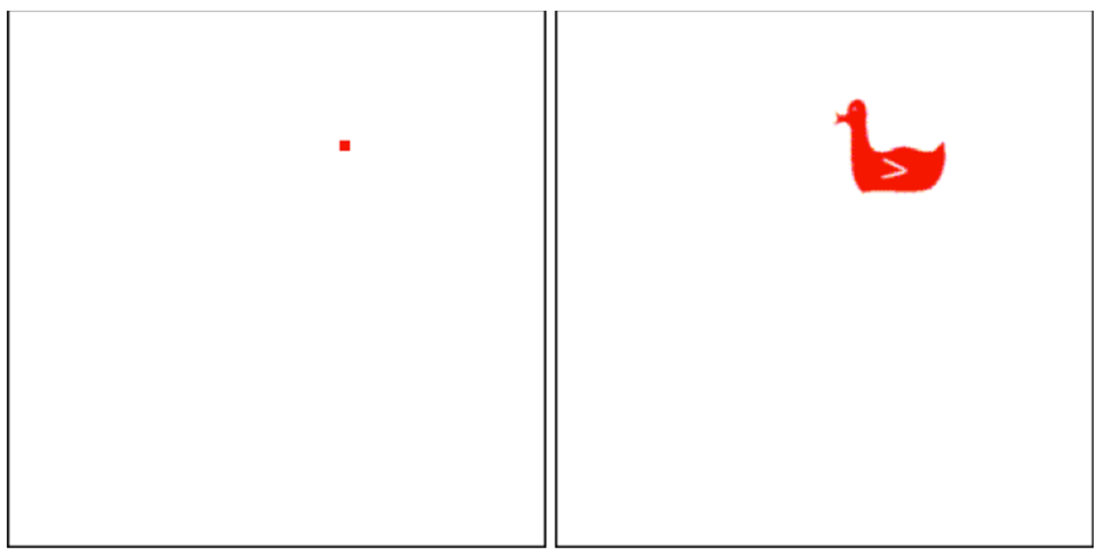


Convolutions

$$c(\mathbf{u}) = \int\limits_{\text{all }\mathbf{r}} f(\mathbf{r})g(\mathbf{u}-\mathbf{r})\,d\mathbf{r}$$

$$c(\mathbf{u}) = f(\mathbf{r}) * g(\mathbf{r}) = \int\limits_{\text{all }\mathbf{r}} f(\mathbf{r})g(\mathbf{u}-\mathbf{r})\,d\mathbf{r}$$

$$f(\mathbf{r}) * g(\mathbf{r}) = \int\limits_{\text{all }\mathbf{r}} f(\mathbf{r})g(\mathbf{u}-\mathbf{r})\,d\mathbf{r} = \int\limits_{\text{all }\mathbf{r}} f(\mathbf{u}-\mathbf{r})g(\mathbf{r})\,d\mathbf{r}$$

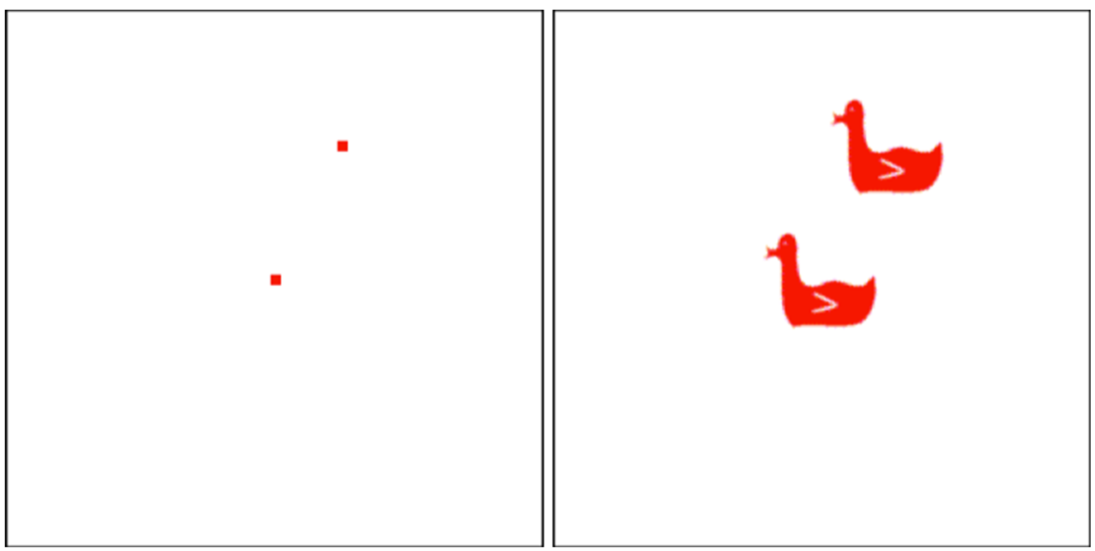


Convolutions

$$c(\mathbf{u}) = \int\limits_{\text{all } \mathbf{r}} f(\mathbf{r}) g(\mathbf{u}-\mathbf{r})\, d\mathbf{r}$$

$$c(\mathbf{u}) = f(\mathbf{r}) * g(\mathbf{r}) = \int\limits_{\text{all } \mathbf{r}} f(\mathbf{r}) g(\mathbf{u}-\mathbf{r})\, d\mathbf{r}$$

$$f(\mathbf{r}) * g(\mathbf{r}) = \int\limits_{\text{all } \mathbf{r}} f(\mathbf{r}) g(\mathbf{u}-\mathbf{r})\, d\mathbf{r} = \int\limits_{\text{all } \mathbf{r}} f(\mathbf{u}-\mathbf{r}) g(\mathbf{r})\, d\mathbf{r}$$



Fourier Transform of a Convolution

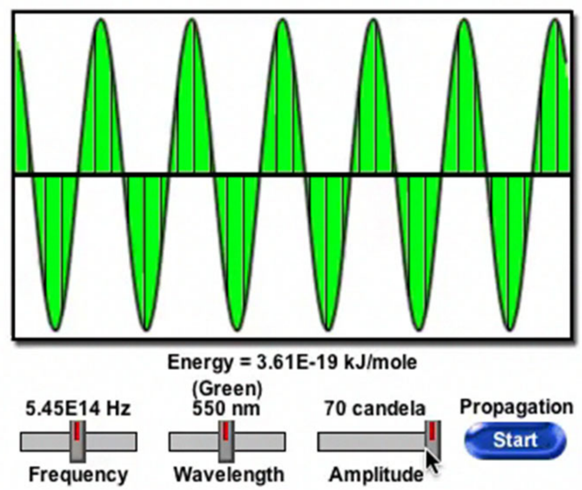
$$F(\mathbf{k}) = T[f(\mathbf{r}) * g(\mathbf{r})]$$

$$T[f(\mathbf{r}) * g(\mathbf{r})] = T[f(\mathbf{r})] \cdot T[g(\mathbf{r})]$$

$$T[f(\mathbf{r}) \cdot g(\mathbf{r})] = T[f(\mathbf{r})] * T[g(\mathbf{r})]$$

Waves and Electromagnetic Radiation

- What is a wave?
  - Direction of propagation
  - Amplitude
    - Wave crest
    - Wave trough
  - Wavelength
    - Period
    - Frequency



http://www.olympusmicro.com/primer/java/wavebasics/index.html

Waves and Electromagnetic Radiation

- What is a wave?
  - Direction of propagation
  - Amplitude
    - Wave crest
    - Wave trough
  - Wavelength
    - Period
    - Frequency

$$\psi(x,0) = \psi_0 \cos 2\pi \frac{x}{\lambda}$$

$$\psi(0,t) = \psi_0 \cos 2\pi \frac{t}{\tau}$$

$$\psi(x,t) = \psi_0 \cos\left(2\pi \frac{x}{\lambda} - 2\pi \frac{t}{\tau}\right)$$

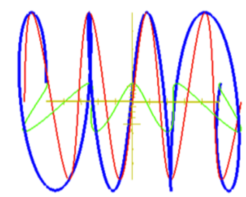
$$k = \frac{2\pi}{\lambda}$$

$$\omega = \frac{2\pi}{\tau}$$

$$\psi(x,t) = \psi_0 \cos(kx - \omega t)$$

$$\frac{\Delta x}{\Delta t} = \frac{k}{\omega} = \mathrm{v}$$

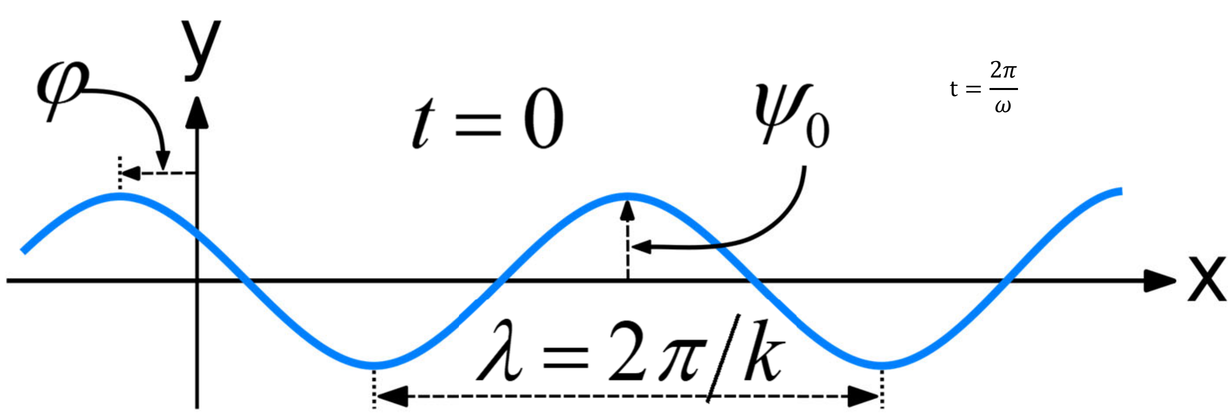
$$\frac{\partial^2\psi(x,y,z,t)}{\partial x^2}+\frac{\partial^2\psi(x,y,z,t)}{\partial y^2}+\frac{\partial^2\psi(x,y,z,t)}{\partial z^2}=\frac{1}{v^2}\frac{\partial^2\psi(x,y,z,t)}{\partial t^2}$$



$$\psi(x,y,z,t)=\psi_0\cos(\,k_x x+k_y y+k_z z-\omega t)$$
$$k_x^2+k_y^2+k_z^2=\frac{\omega^2}{v^2}$$
$$\mathbf{r}=(x,y,z)$$
$$\mathbf{k}=(k_x,k_y,k_z)$$
$$\mathbf{k}\cdot\mathbf{r}=(k_x x+k_y y+k_z z)$$

$$\psi(\mathbf{r},t)=\psi_0\cos(\,\mathbf{k}\cdot\mathbf{r}-\omega t)$$
$$\psi(\mathbf{r},t)=\psi_0\cos(\,\mathbf{k}\cdot\mathbf{r}-\omega t+\phi)$$
$$\boxed{\psi(\mathbf{r},t)=\psi_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi)}}$$

$$I=|\psi(\mathbf{r},t)|^2$$



$t=\frac{2\pi}{\omega}$

Diffraction

- Diffraction by one dimensional objects
- Diffraction by two dimensional objects
- Diffraction by three dimensional objects

Diffraction by a One-dimensional Object

$$\mathbf{k} = (k_x, 0, k_z)$$

$$\mathbf{k}\cdot\mathbf{r} = (k_x, 0, k_z)\cdot(x, 0, 0)$$

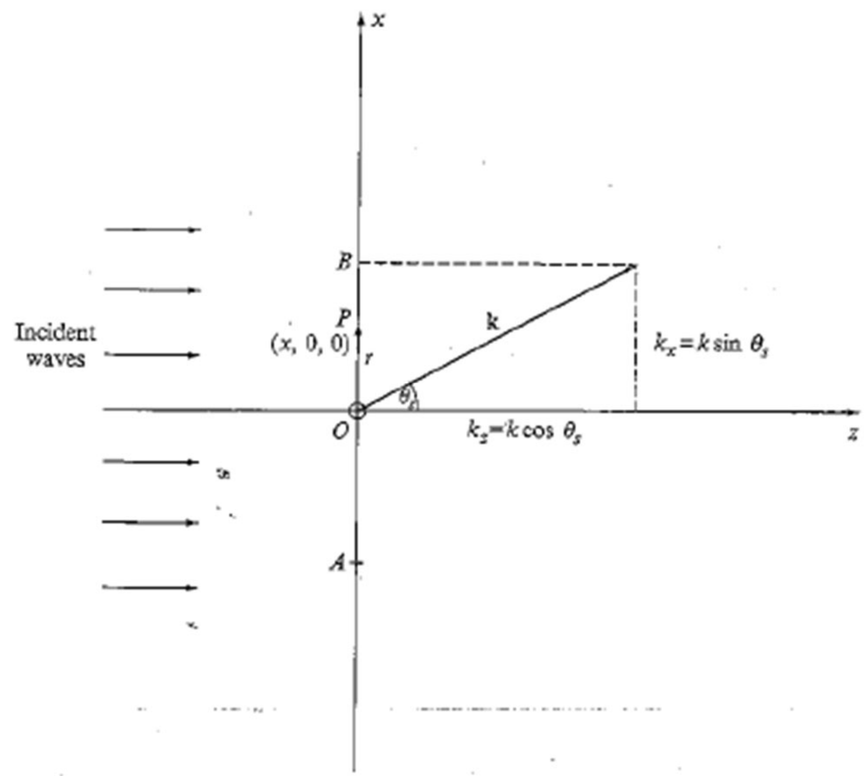
$$\mathbf{k}\cdot\mathbf{r} = k_x x$$

$$k_x = k\sin\theta_s$$

$$\mathbf{k}\cdot\mathbf{r} = kx\sin\theta_s$$

$$F(\mathbf{k}) = \int_{-\infty}^{\infty} f(x)e^{ikx\sin\theta_s}\,dx$$

$$F(\sin\theta_s) = \int_{-\infty}^{\infty} f(x)e^{ikx\sin\theta_s}\,dx$$



Diffraction by One Narrow slit

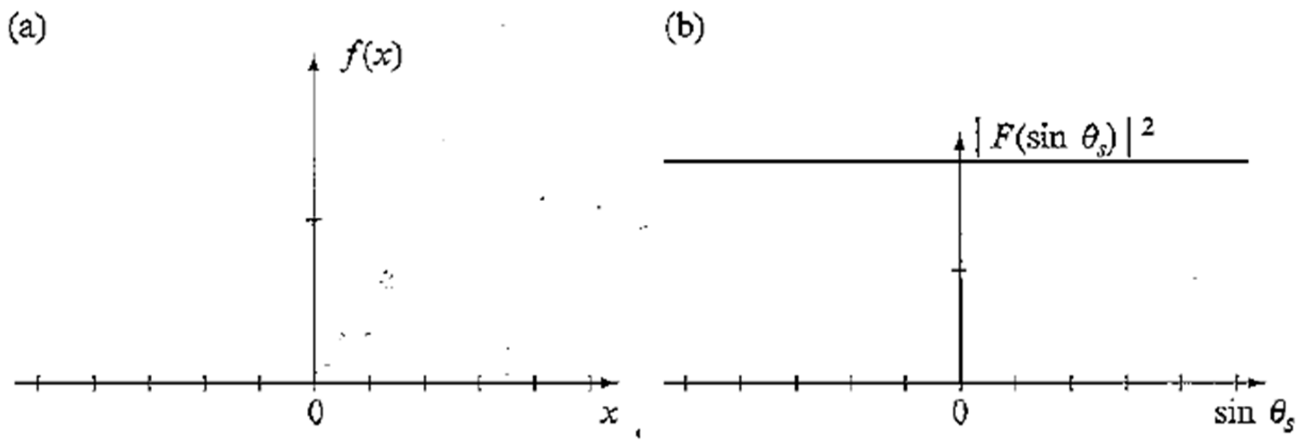
A narrow slit is defined by:

$f(x) = \delta(x)$ and $\delta(0) = +\infty$

$$F(\sin\theta_s) = \int_{-\infty}^{\infty} \delta(x) e^{ikx\sin\theta_s} dx = \int_{-\infty}^{\infty} \delta(x) dx = 1$$

$$F(\sin\theta_s) = 1$$

$$|F(\sin\theta_s)|^2 = 1$$

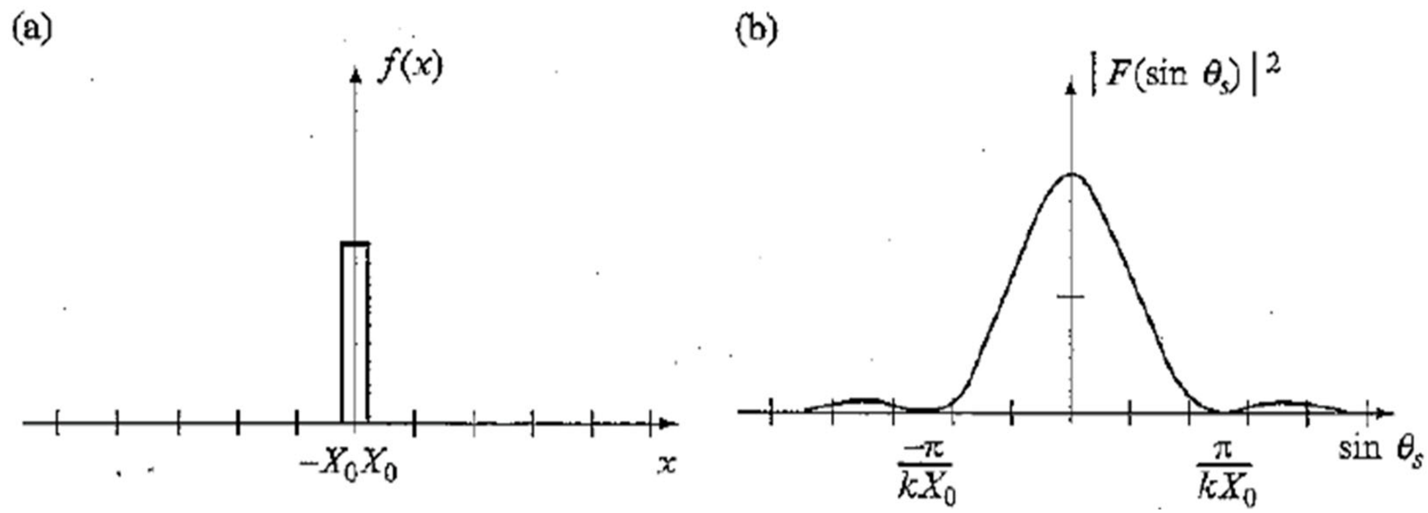


Diffraction by one wide slit

$$f(x) = 0 \text{ if } -\infty < x < -X_0$$
$$f(x) = 1 \text{ if } -X_0 < x < X_0$$
$$f(x) = 0 \text{ if } \quad X_0 < x < \infty$$

$$F(\sin\theta_s) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta_s}\, dx = \int_{-X_0}^{X_0} e^{ikx\sin\theta_s}\, dx = \left[\frac{e^{ikx\sin\theta_s}}{ikx\sin\theta_s}\right]_{-X_0}^{X_0} = \frac{e^{ikX_0\sin\theta_s} - e^{-ikX_0\sin\theta_s}}{ikX_0\sin\theta_s} = 2X_0 \frac{\sin(kX_0\sin\theta_s)}{kX_0\sin\theta_s}$$

$$\left|F(\sin\theta_s)\right|^2 = 4X_0^2 \frac{\sin^2(kX_0\sin\theta_s)}{\left(kX_0\sin\theta_s\right)^2}$$



Diffraction by two narrow slits

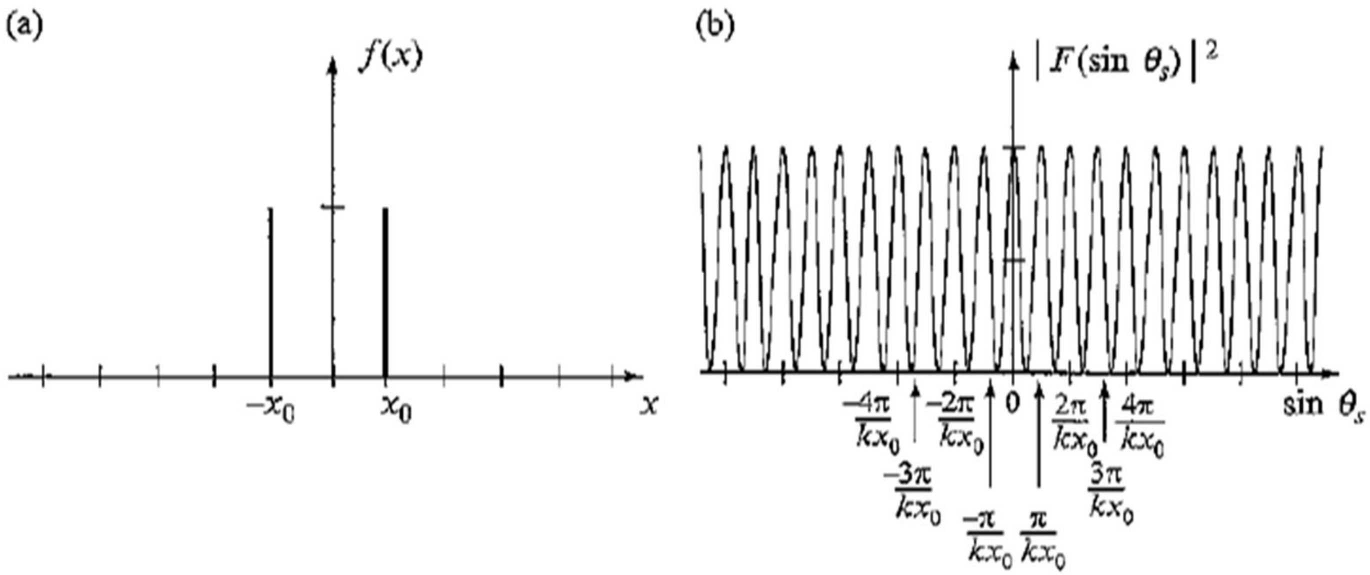
Two narrow slits are defined by:

$$f(x) = \delta(x + x_0) + \delta(x - x_0) \text{ and } \delta(x_0) = +\infty \text{ and } \delta(-x_0) = +\infty$$

$$F(\sin\theta_s) = \int_{-\infty}^{\infty} f(x) e^{ikx \sin\theta_s} dx = 2\cos(kx_0 \sin\theta_s)$$

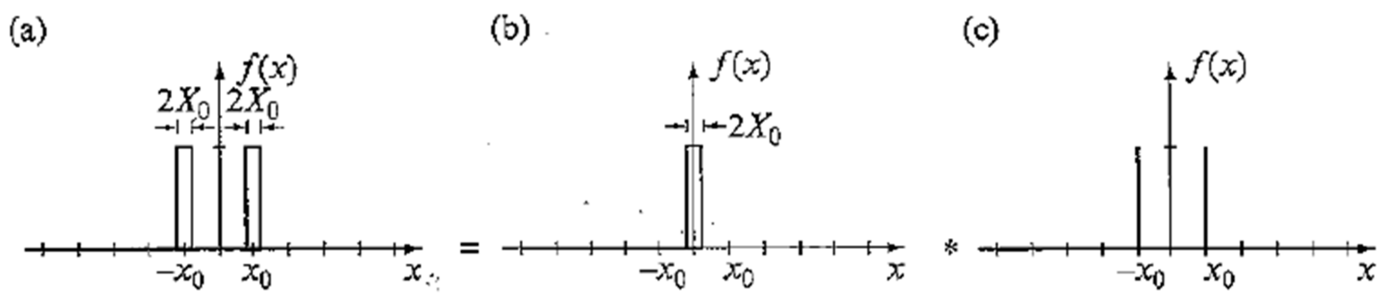
$$F(\sin\theta_s) = 2\cos(kx_0 \sin\theta_s)$$

$$|F(\sin\theta_s)|^2 = 4\cos^2(kx_0 \sin\theta_s)$$

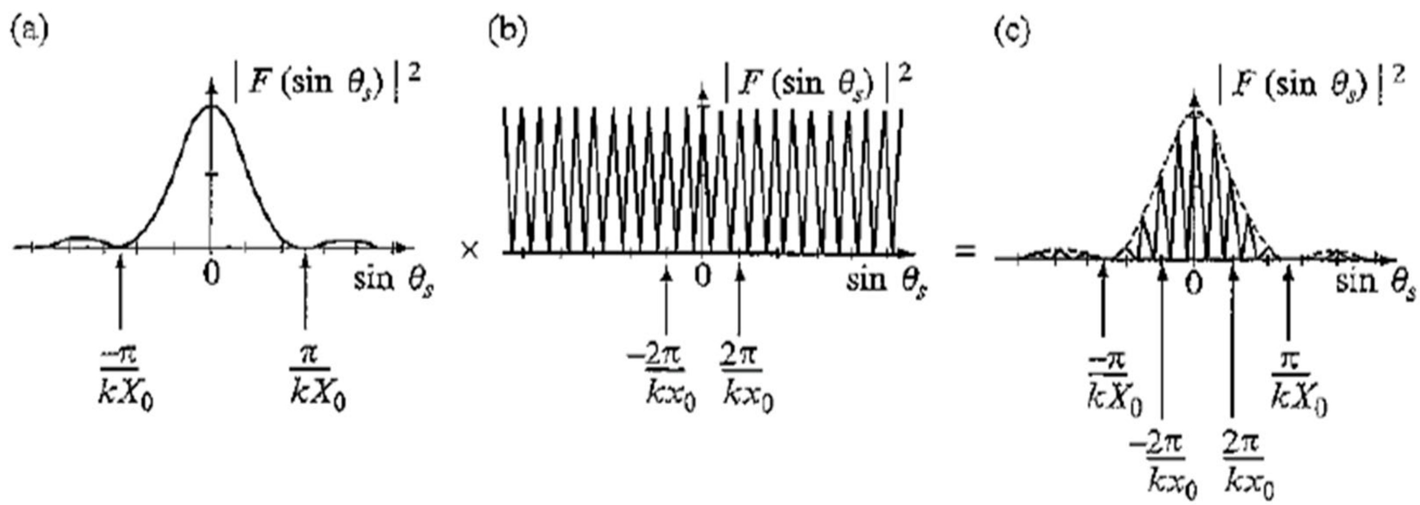


Diffraction by Two Wide Slits

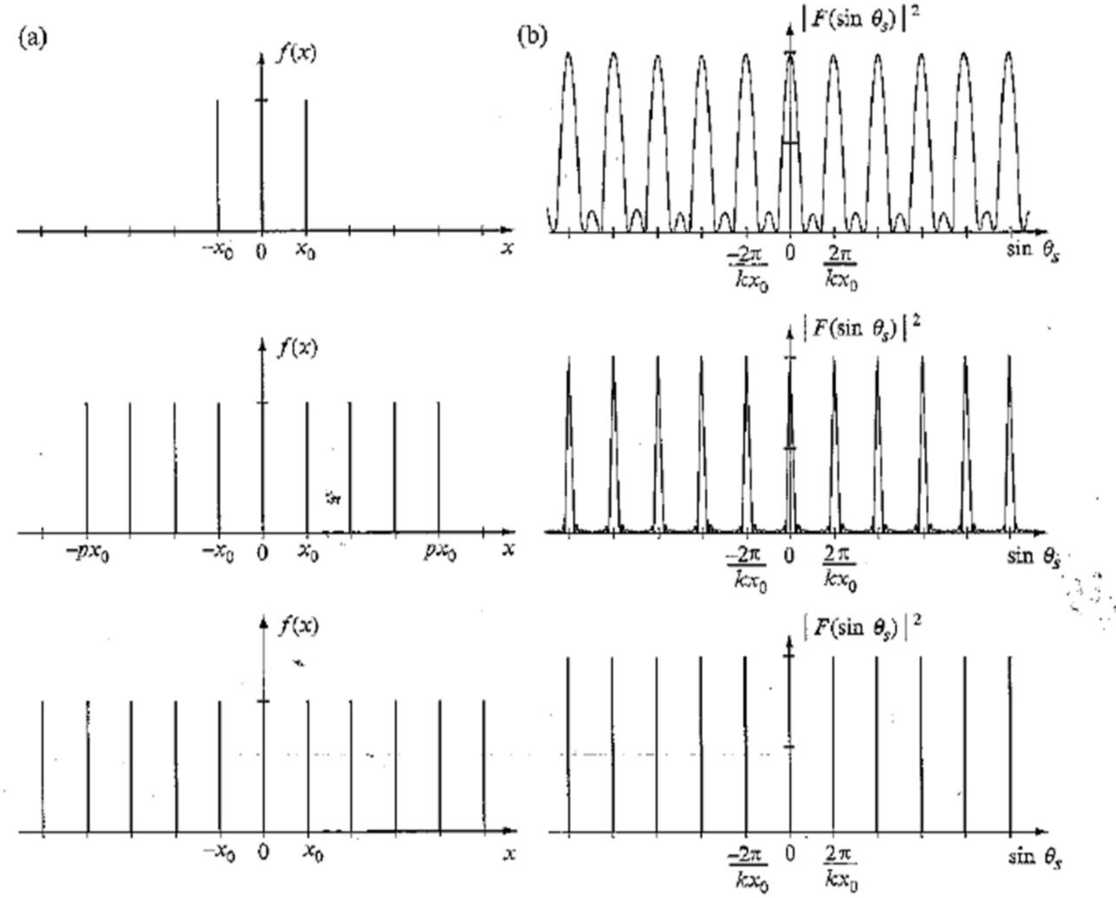
$$f(x) = 0 \text{ if } -\infty < x < -(x_0 + X_0)$$
$$f(x) = 1 \text{ if } -(x_0 + X_0) \le x \le -(x_0 - X_0)$$
$$f(x) = 0 \text{ if } -(x_0 - X_0) < x < (x_0 - X_0)$$
$$f(x) = 1 \text{ if } (x_0 - X_0) \le x \le (x_0 + X_0)$$
$$f(x) = 0 \text{ if } (x_0 + X_0) < x < \infty$$
$$f(\text{two wide slits}) = f(\text{one wide slit}) * f(\text{two narrow slits})$$

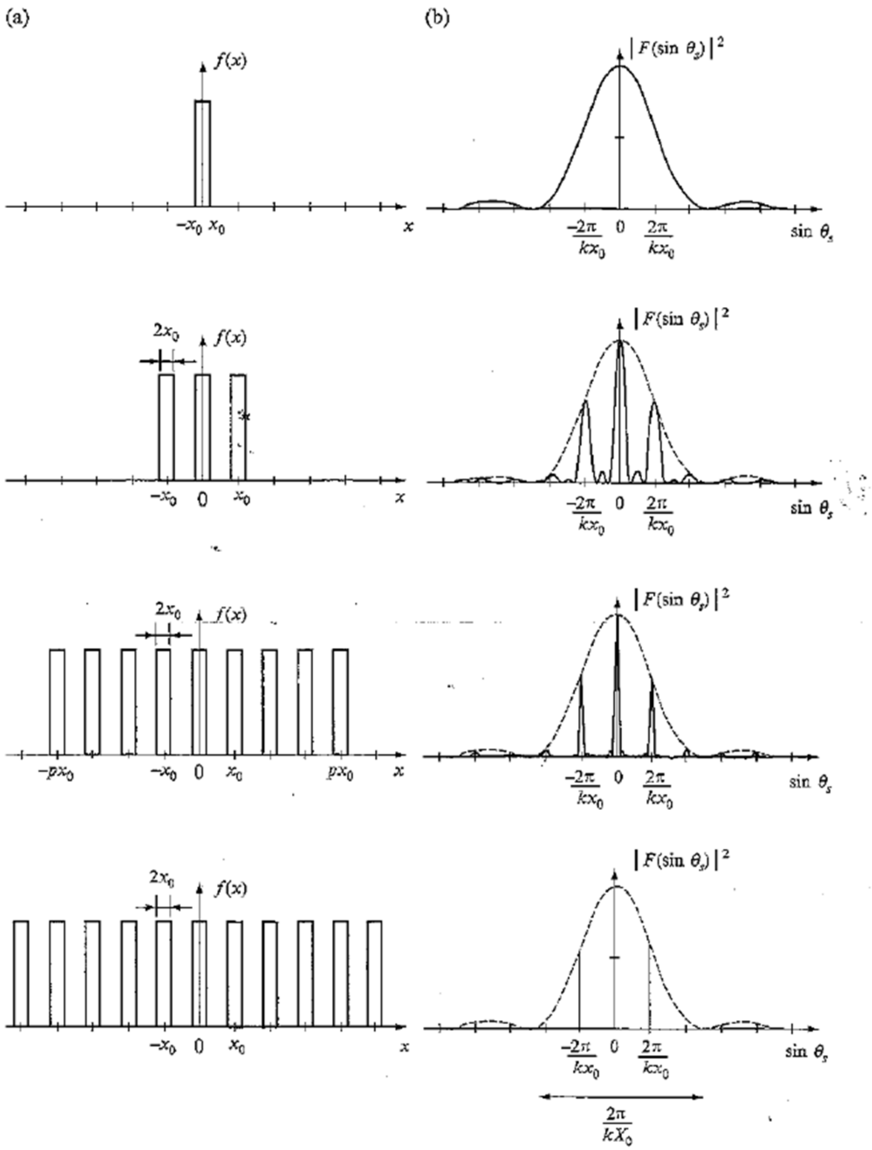


Diffraction by Two Wide Slits



Diffraction by N Narrow Slits





- The position of the main peaks in a diffraction pattern is determined solely by the lattice spacing of the object
- The shape of each main peak is determined by the overall shape of the object.
- The effect of the object is to alter the intensity of each main peak, but the positions of the main peaks remain unchanged.

Diffraction by a 3D Lattice

$$\mathbf{r} = p\mathbf{a} + q\mathbf{b} + r\mathbf{c}$$

$$f(\mathbf{r}) = \sum_{\text{all } p,q,r} \delta(\mathbf{r} - [p\mathbf{a} + q\mathbf{b} + r\mathbf{c}])$$

$$F(\Delta\mathbf{k}) = \int_{\text{all } \mathbf{r}} f(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}$$

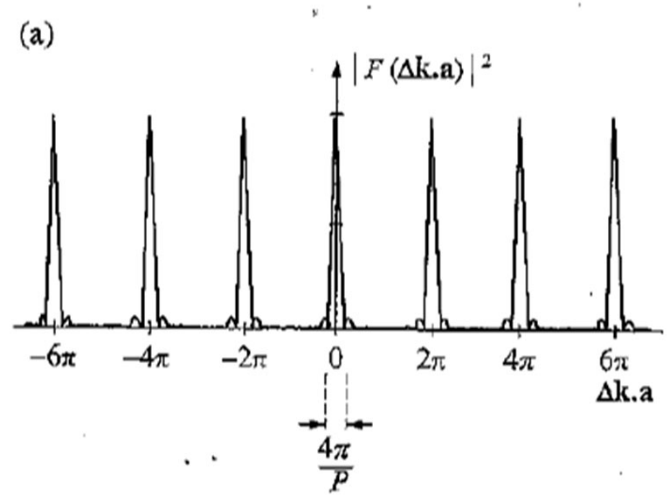
$$F(\Delta\mathbf{k}) = \int_{\text{all } \mathbf{r}} \sum_{\text{all } p,q,r} \delta(\mathbf{r} - [p\mathbf{a} + q\mathbf{b} + r\mathbf{c}]) e^{i\Delta\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}$$

$$F(\Delta\mathbf{k}) = \sum_{\text{all } p,q,r} e^{i\Delta\mathbf{k}\cdot(p\mathbf{a}+q\mathbf{b}+r\mathbf{c})} = \sum_{\text{all } p,q,r} e^{ip\Delta\mathbf{k}\cdot\mathbf{a}} \cdot e^{iq\Delta\mathbf{k}\cdot\mathbf{b}} \cdot e^{ir\Delta\mathbf{k}\cdot r}$$

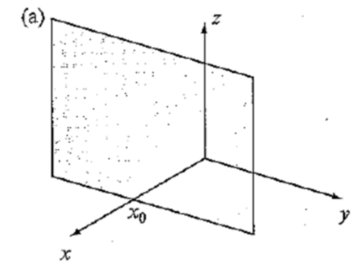
$$F(\Delta\mathbf{k}) = \sum_{\text{all } p} e^{ip\Delta\mathbf{k}\cdot\mathbf{a}} \cdot \sum_{\text{all } q} e^{iq\Delta\mathbf{k}\cdot\mathbf{b}} \cdot \sum_{\text{all } r} e^{ir\Delta\mathbf{k}\cdot r}$$

$$|F(\Delta\mathbf{k})|^2 = \frac{\sin^2 \frac{P\Delta\mathbf{k}\cdot\mathbf{a}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{a}}{2}} \cdot \frac{\sin^2 \frac{Q\Delta\mathbf{k}\cdot\mathbf{b}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{b}}{2}} \cdot \frac{\sin^2 \frac{R\Delta\mathbf{k}\cdot\mathbf{c}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{c}}{2}}$$

Maxima are seen at $\Delta\mathbf{k}\cdot\mathbf{a} = 2h\pi$ where h is a positive or negative integer



$$|F(\Delta\mathbf{k})|^2 = \frac{\sin^2\frac{P\Delta\mathbf{k}\cdot\mathbf{a}}{2}}{\sin^2\frac{\Delta\mathbf{k}\cdot\mathbf{a}}{2}} \cdot \frac{\sin^2\frac{Q\Delta\mathbf{k}\cdot\mathbf{b}}{2}}{\sin^2\frac{\Delta\mathbf{k}\cdot\mathbf{b}}{2}} \cdot \frac{\sin^2\frac{R\Delta\mathbf{k}\cdot\mathbf{c}}{2}}{\sin^2\frac{\Delta\mathbf{k}\cdot\mathbf{c}}{2}}$$



We see maxima when

$\Delta\mathbf{k}\cdot\mathbf{a} = 2h\pi$ where h is a positive or negative integer

The first zero occurs at:

$P\frac{\Delta\mathbf{k}\cdot\mathbf{a}}{2} = \pm\pi$ and the peak width is $\Delta(\Delta\mathbf{k}\cdot\mathbf{a}) = \frac{4\pi}{P}$

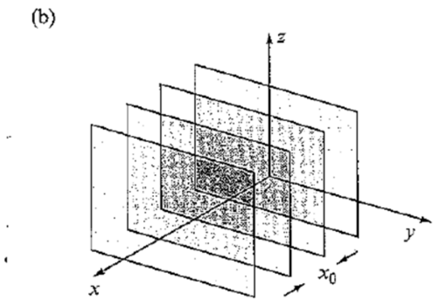
As P, Q and R tend to infinity the functions become δ functions:

$$|F(\Delta\mathbf{k})|^2 = \left[\sum_{\text{all } h} \delta(\Delta\mathbf{k}\cdot\mathbf{a} - 2h\pi)\right]^2 \cdot \left[\sum_{\text{all } k} \delta(\Delta\mathbf{k}\cdot\mathbf{b} - 2k\pi)\right]^2 \cdot \left[\sum_{\text{all } l} \delta(\Delta\mathbf{k}\cdot\mathbf{c} - 2l\pi)\right]^2$$

Each term $\delta(\Delta\mathbf{k}\cdot\mathbf{a} - 2h\pi)$ represents a plane and each summation represents a series of planes.

All three summations thus represents three sets of parallel planes with each intersection of three planes representing a lattice point.

$$|F(\Delta\mathbf{k})|^2 = \frac{\sin^2 \frac{P\Delta\mathbf{k}\cdot\mathbf{a}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{a}}{2}} \cdot \frac{\sin^2 \frac{Q\Delta\mathbf{k}\cdot\mathbf{b}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{b}}{2}} \cdot \frac{\sin^2 \frac{R\Delta\mathbf{k}\cdot\mathbf{c}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{c}}{2}}$$



We see maxima when

$\Delta\mathbf{k}\cdot\mathbf{a} = 2h\pi$ where h is a positive or negative integer

The first zero occurs at:

$P\dfrac{\Delta\mathbf{k}\cdot\mathbf{a}}{2} = \pm\pi$ and the peak width is $\Delta(\Delta\mathbf{k}\cdot\mathbf{a}) = \dfrac{4\pi}{P}$

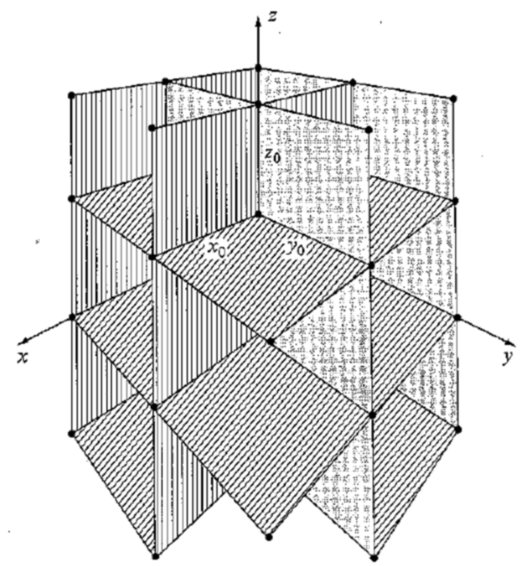
As P, Q and R tend to infinity the functions become δ functions:

$$|F(\Delta\mathbf{k})|^2 = \left[\sum_{\text{all } h} \delta(\Delta\mathbf{k}\cdot\mathbf{a} - 2h\pi)\right]^2 \cdot \left[\sum_{\text{all } k} \delta(\Delta\mathbf{k}\cdot\mathbf{b} - 2k\pi)\right]^2 \cdot \left[\sum_{\text{all } l} \delta(\Delta\mathbf{k}\cdot\mathbf{c} - 2l\pi)\right]^2$$

Each term $\delta(\Delta\mathbf{k}\cdot\mathbf{a} - 2h\pi)$ represents a plane and each summation represents a series of planes.

All three summations thus represents three sets of parallel planes with each intersection of three planes representing a lattice point.

$$|F(\Delta\mathbf{k})|^2 = \frac{\sin^2 \frac{P\Delta\mathbf{k}\cdot\mathbf{a}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{a}}{2}} \cdot \frac{\sin^2 \frac{Q\Delta\mathbf{k}\cdot\mathbf{b}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{b}}{2}} \cdot \frac{\sin^2 \frac{R\Delta\mathbf{k}\cdot\mathbf{c}}{2}}{\sin^2 \frac{\Delta\mathbf{k}\cdot\mathbf{c}}{2}}$$



We see maxima when

$\Delta\mathbf{k}\cdot\mathbf{a} = 2h\pi$ where h is a positive or negative integer

The first zero occurs at:

$P\frac{\Delta\mathbf{k}\cdot\mathbf{a}}{2} = \pm\pi$ and the peak width is $\Delta(\Delta\mathbf{k}\cdot\mathbf{a}) = \frac{4\pi}{P}$

As P, Q and R tend to infinity the functions become δ functions:

$$|F(\Delta\mathbf{k})|^2 = \left[\sum_{\text{all } h} \delta(\Delta\mathbf{k}\cdot\mathbf{a} - 2h\pi)\right]^2 \cdot \left[\sum_{\text{all } k} \delta(\Delta\mathbf{k}\cdot\mathbf{b} - 2k\pi)\right]^2 \cdot \left[\sum_{\text{all } l} \delta(\Delta\mathbf{k}\cdot\mathbf{c} - 2l\pi)\right]^2$$

Each term $\delta(\Delta\mathbf{k}\cdot\mathbf{a} - 2h\pi)$ represents a plane and each summation represents a series of planes.

All three summations thus represents three sets of parallel planes with each intersection of three planes representing a lattice point.

Diffraction

- In this section we will:
  - Learn scattering (diffraction) by a single electron
  - Learn scattering by a group of electrons
  - Define the electron density function
  - Define the structure factor
  - Define the atomic scattering factor
  - Apply a correction for thermal motion
  - Define Friedel's Law and when it fails
  - What the effect of translational symmetry has on the diffraction pattern

Diffraction by a 3D Object

$e^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}$ and $f(\mathbf{r}_1)d\mathbf{r}_1$

diffracted wave from element $d\mathbf{r}_1 = f(\mathbf{r}_1)e^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}d\mathbf{r}_1$

diffracted wave from element $d\mathbf{r}_2 = f(\mathbf{r}_2)e^{i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}d\mathbf{r}_2$

diffracted wave from all elements $d\mathbf{r}_n = \sum_n f(\mathbf{r}_n)e^{i(\mathbf{k}\cdot\mathbf{r}_n-\omega t)}d\mathbf{r}_n$

diffraction pattern $= \int_V f(\mathbf{r})e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\,d\mathbf{r}$

diffraction pattern $= e^{-\omega t}\int_V f(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{r}$

diffraction pattern $= \int_V f(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{r}$

If $\mathbf{r}$ is outside the object, $f(\mathbf{r})=0$

diffraction pattern $= \int_{\text{all }\mathbf{r}} f(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{r} \Rightarrow T[f(\mathbf{r})]$

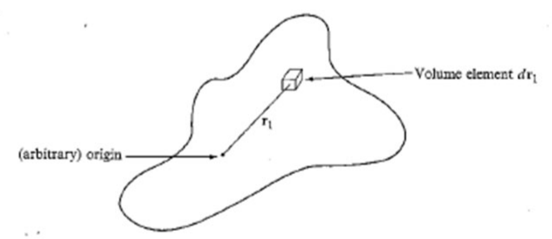


Fig. 6.5 *Diffraction by a volume element.* The volume element $d\mathbf{r}_1$ centred on $\mathbf{r}_1$ affects the waves in a manner which may be represented by the function $f(\mathbf{r})\,d\mathbf{r}_1$. A wave $e^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}$ is propagated, and the mathematical expression for the contribution of the volume element $d\mathbf{r}_1$ to the overall diffraction pattern must be some mathematical combination of $f(\mathbf{r})\,d\mathbf{r}_1$ and $e^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}$.

Thomson Scattering by a Single Electron

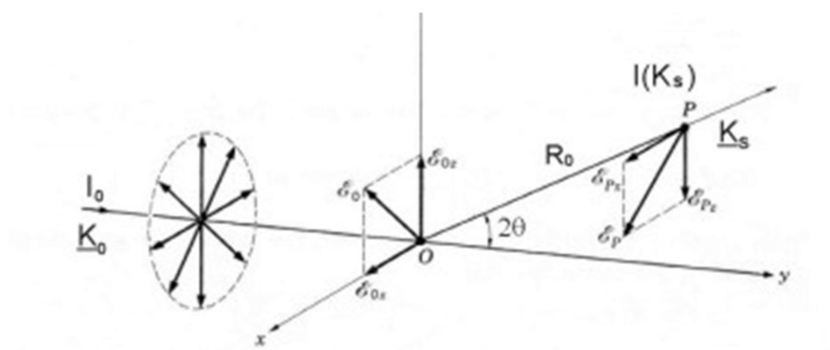
$$\frac{E_{scat}}{E_{in}} = \frac{e^2}{4\pi\varepsilon_0 rmc^2}\sqrt{\frac{1+\cos^2 2\theta}{2}}$$

$$\varepsilon_0 = 8.854\times10^{-12}\ \mathrm{F\cdot m^{-1}}$$

$$c = \text{ speed of light}$$

$$r = \text{ radius of interaction}$$

$$\theta = \text{ Bragg angle}$$



http://www.xtal.iqfr.csic.es/Cristalografia/parte_05-en.html

Thomson Scattering by a Group of Electrons (I)

$$\frac{E_{scat}}{E_{in}} = \frac{e^2}{4\pi\varepsilon_0 rmc^2}\sqrt{\frac{1+\cos^2 2\theta}{2}}$$

$$f_e = \frac{e^2}{4\pi\varepsilon_0 rmc^2}$$

$$\frac{E_{scat}}{E_{in}} = f_e\sqrt{\frac{1+\cos^2 2\theta}{2}}$$

but if the beam is polarized we can write:

$$\frac{E_{scat}}{E_{in}} = f_e p(2\theta)$$

where $p(2\theta)$ is the polarization factor.

For now let's ignore $p(2\theta)$.

Thomson Scattering by a Group of Electrons (II)

$$\left(E_{scat}\right)_A = f_e E_{in}$$

$$\left(E_{scat}\right)_B = f_e E_{in} e^{i\phi}$$

$$\left(E_{scat}\right)_{tot} = \left(E_{scat}\right)_A + \left(E_{scat}\right)_B$$

$$\frac{\left(E_{scat}\right)_{tot}}{E_{in}} = f_e + f_e e^{i\phi}$$

$$\frac{\left(E_{scat}\right)_{tot}}{E_{in}} = \sum_n f_e e^{i\phi_n}$$

Remember

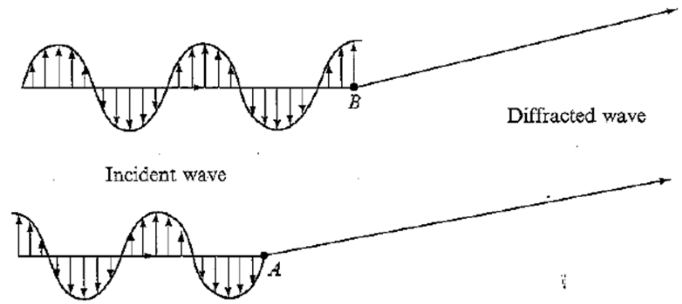
$$\boxed{F(\Delta\mathbf{k}) = \int_{\text{all } r} f(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}}\, d\mathbf{r}}$$

The amplitude function of a group of electrons is

$$f_e \rho(\mathbf{r})$$

Substituting into $F(\Delta\mathbf{k})$ gives

$$F(\Delta\mathbf{k}) = \int_{\text{all } r} f_e \rho(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}}\, d\mathbf{r}$$



Thomson Scattering by a Group of Electrons (III)

$$F(\Delta\mathbf{k}) = \int_{\text{all } r} f_e \rho(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}}\, d\mathbf{r}$$

$$F(\Delta\mathbf{k}) = f_e \int_{\text{unit cell}} \rho(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}}\, d\mathbf{r} \text{ or } F_{rel}(\Delta\mathbf{k}) = \int_{\text{unit cell}} \rho(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}}\, d\mathbf{r}$$

Let's define coordinates of the unit cell as follows:

$$0 \le X \le a,\ 0 \le Y \le b,\ 0 \le Z \le c$$

$$x = \frac{X}{a},\ \mathrm{y} = \frac{Y}{b},\ \mathrm{z} = \frac{Z}{c} \text{ and } 0 \le x \le 1,\ 0 \le y \le 1,\ 0 \le z \le 1$$

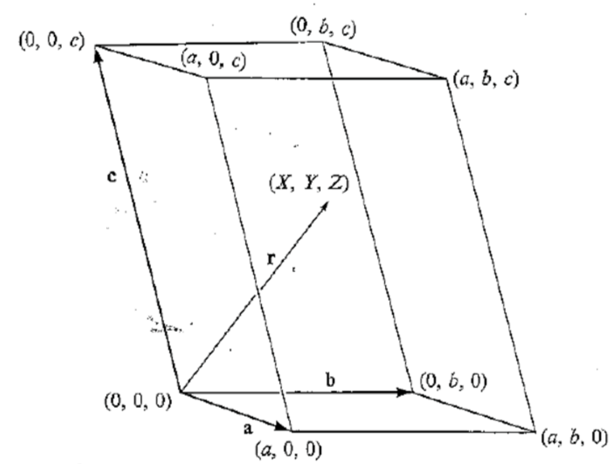
X, Y and Z represent absolute coordinates and

x, y and z represent fractional coordinates.

$$\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$$

$$d\mathbf{r} = dx\ dy\ dz\ \mathbf{a} \cdot \mathbf{b} \wedge \mathbf{c} = V\ dx\ dy\ dz$$

$\rho(\mathbf{r})$ becomes $\rho(x, y, z)$



The Electron Density Function

$$F_{rel}(\Delta\mathbf{k}) = F_{hkl} = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x,y,z) e^{i\Delta\mathbf{k}\cdot(x\mathbf{a}+y\mathbf{b}+z\mathbf{c})} dx\, dy\, dz$$

F_{hkl} is the Fourier transform of $\rho(x,y,z)$

$$\rho(x,y,z) = \frac{1}{V} \int_{\text{all } \Delta\mathbf{k}} F_{rel}(\Delta\mathbf{k}) e^{-i\Delta\mathbf{k}\cdot(x\mathbf{a}+y\mathbf{b}+z\mathbf{c})} d(\Delta\mathbf{k})$$

$$\rho(x,y,z) = \frac{1}{V} \int_{\text{all } \Delta\mathbf{k}} F_{rel}(\Delta\mathbf{k}) e^{-2\pi i(hx+ky+lz)} d(\Delta\mathbf{k})$$

hkl values are discrete so we can rewrite this as:

$$\rho(x,y,z) = \frac{1}{V} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky+lz)}$$

The Structure Factor

$$F_{hkl} = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x,y,z) e^{i\Delta\mathbf{k}\cdot(x\mathbf{a}+y\mathbf{b}+z\mathbf{c})}\, dx\ dy\ dz$$

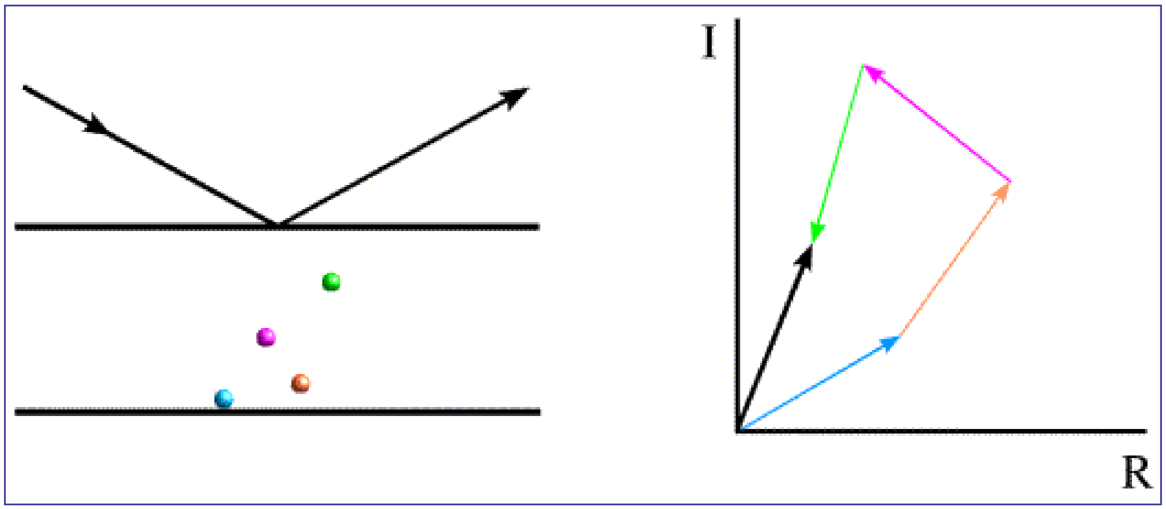
$$F_{hkl} = \sum_j f_j e^{2\pi i(hx_j+ky_j+lz_j)}$$

- In the first equation, the coordinates (x, y, z) refer to any position within the unit cell, whereas (x_j, y_j, z_j) in the second equation define the position of the atoms.
- $\rho(x, y, z)$ is a continuous function describing the overall electron density, f_j, is a property of each atom.
- The first equation requires an integration over the entire unit cell, but the second equation requires a summation over the positions of the atoms within the unit cell.

What does $F_{hkl} = \sum_j f_j e^{2\pi i(hx+ky+lz)} = |F_{hkl}| e^{i\varphi}$ mean?

- All atoms contribute to F_{hkl}
- The amplitude of scattering depends on the number of electrons in each atom.
- The phase depends on the fractional distance it lies from the lattice plane.

Scattering from lattice planes

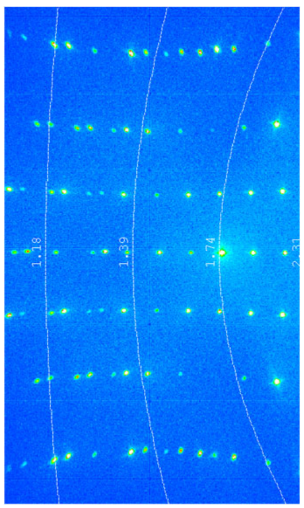


Atomic structure factors add as complex numbers, or vectors.

Randy Read

How Important is the Phase?

Structure Factor and Intensity



$$F_{hkl} = \sum_j f_j \, e^{2\pi i \left(hx_j + ky_j + lz_j\right)}$$

$$I_{hkl} = \frac{I_0}{\omega} K L_{hkl} p_{hkl} A_{hkl} e_{hkl} \left|\left(F_{hkl}\right)_T\right|^2 V$$

$$K = \left(\frac{q^2}{4\pi\epsilon_0 m_e c^2}\right)^2 N^2 \lambda^3 \qquad L_{hkl} = \frac{1}{\sqrt{(\sin 2\theta)^2 - \xi^2}}$$

$$p_{hkl} = \frac{\left((\cos\epsilon)^2 + (\sin\epsilon)^2(\cos 2\theta)^2\right) + (\sin\epsilon)^2 + (\cos\epsilon)^2}{2}$$

$$\epsilon = \cos^{-1}(\xi \csc 2\theta)$$

$$A_{hkl} = \frac{I_{hkl}}{I_0} = e^{-\mu t}$$

The Atomic Scattering Factor

$$d\mathbf{R} = R^2 \sin\phi \; dR \; d\phi \; d\psi \text{ and } \mathbf{S}_{hkl} \cdot \mathbf{R} = S_{hkl} R \cos\phi$$

$$f_j = \int_{\text{atom}} \rho_j(\mathbf{R}) e^{2\pi i \mathbf{S}_{hkl} \cdot \mathbf{R}} \, d\mathbf{R} = \int_{\text{atom}} \rho_j(R) e^{2\pi i S_{hkl} R \cos\phi} R^2 \sin\phi \; dR \; d\phi \; d\psi$$

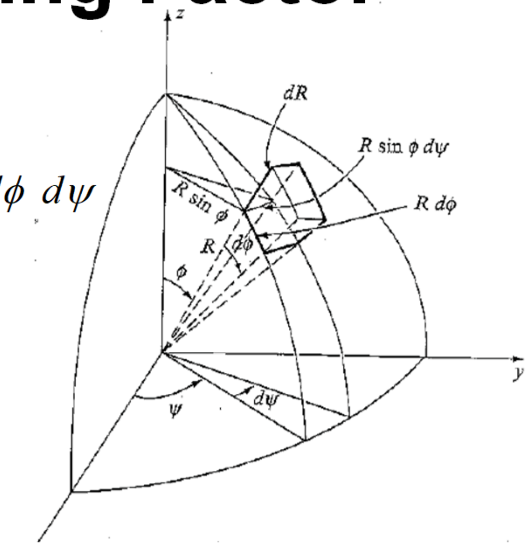
$$f_j = \int_{\psi=0}^{\psi=2\pi} \int_{\phi=0}^{\phi=\pi} \int_{R=0}^{R=\infty} \rho_j(R) e^{2\pi i S_{hkl} R \cos\phi} R^2 \sin\phi \; dR \; d\phi \; d\psi$$

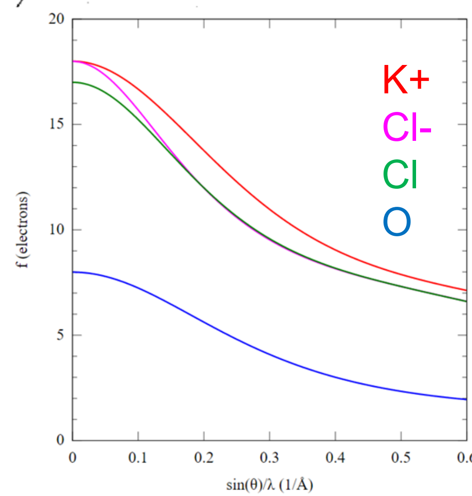
$$f_j = 2\pi \int_0^\infty R^2 \rho_j(R) \left(\frac{e^{2\pi S_{hkl} R} - e^{-2\pi S_{hkl} R}}{2\pi S_{hkl} R} \right) dR$$

$$f_j = 4\pi \int_0^\infty R^2 \rho_j(R) \left(\frac{\sin 2\pi S_{hkl} R}{2\pi S_{hkl} R} \right) dR$$

$$S_{hkl} = \frac{2\sin\theta}{\lambda}$$

$$f_j = 4\pi \int_0^\infty R^2 \rho_j(R) \left(\frac{\sin\left(\dfrac{4\pi \sin\theta}{\lambda} R \right)}{\dfrac{4\pi \sin\theta}{\lambda} R} \right) dR$$





Correction for Thermal Motion (I)

$$F_{hkl} = \sum_j f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

$$F_{hkl} = \sum_j f_j e^{2\pi i \mathbf{S}_{hkl}\cdot\mathbf{r}_j}$$

Consider a small random displacement about $\mathbf{r}_j$

$$F_{hkl} = \sum_j f_j e^{2\pi i \mathbf{S}_{hkl}\cdot(\mathbf{r}_j + \mathbf{u}_j)}$$

$$F_{hkl} = \sum_j f_j e^{2\pi i \mathbf{S}_{hkl}\cdot\mathbf{r}_j} e^{2\pi i \mathbf{S}_{hkl}\cdot\mathbf{u}_j}$$

Let us define $\mathbf{u}_j$ as motion in the direction of $\mathbf{S}_{hkl}$ that is perpendicular to the plane *hkl*:

$\mathbf{S}_{hkl}\cdot\mathbf{u}_j$ becomes $S_{hkl}u_j$ and

$$F_{hkl} = \sum_j f_j e^{2\pi i \mathbf{S}_{hkl}\cdot\mathbf{r}_j} e^{2\pi i S_{hkl}u_j}$$

F_{hkl} is measured over a long time

$$F_{hkl} = \sum_j f_j e^{2\pi i \mathbf{S}_{hkl}\cdot\mathbf{r}_j}\, \overline{e^{2\pi i S_{hkl}u_j}}$$

$$\overline{e^{2\pi i S_{hkl}u_j}} \approx 1 + 2\pi i \overline{S_{hkl}u_j} - 2\pi^2 \overline{\left(S_{hkl}u_j\right)^2}$$

$$\overline{e^{2\pi i S_{hkl}u_j}} \approx 1 + 2\pi i S_{hkl}\overline{u_j} - 2\pi^2 S_{hkl}^2 \overline{u_j^2}$$

$$\overline{e^{2\pi i S_{hkl}u_j}} \approx 1 - 2\pi^2 S_{hkl}^2 \overline{u_j^2}$$

$$\overline{e^{2\pi i S_{hkl}u_j}} \approx e^{2\pi^2 S_{hkl}^2 \overline{u_j^2}}$$

Correction for Thermal Motion (II)

$$-2\pi^2 S_{hkl}^2 \overline{u_j^2} = -2\pi^2 \left(\frac{2\sin\theta}{\lambda}\right)^2 \overline{u_j^2}$$

$$-2\pi^2 S_{hkl}^2 \overline{u_j^2} = -8\pi^2 \left(\frac{\sin\theta}{\lambda}\right)^2 \overline{u_j^2}$$

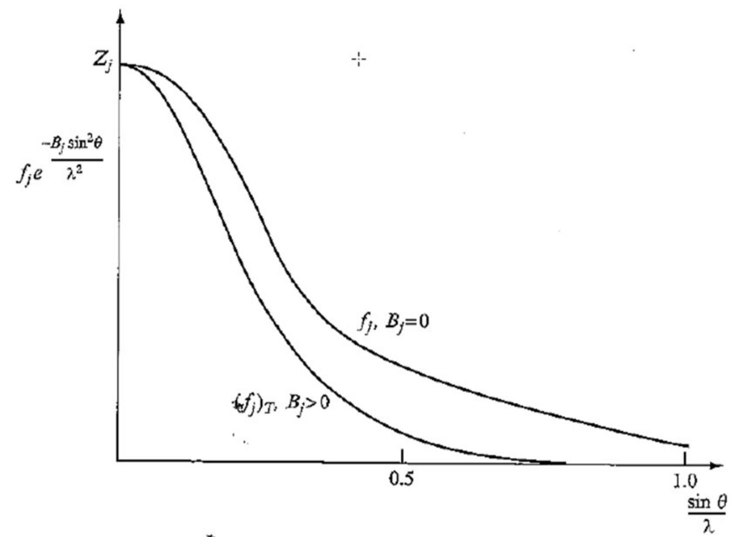
Let us define $B_j = 8\pi^2 \overline{u_j^2}$

$$\overline{e^{2\pi i S_{hkl} u_j}} \approx e^{-B_j (2\sin\theta/\lambda)^2}$$

$$\left(f_j\right)_T = f_j e^{-B_j (2\sin\theta/\lambda)^2}$$

$$\left(F_{hkl}\right)_T = \sum_j \left(f_j\right)_T e^{2\pi i (hx_j + ky_j + lz_j)}$$

$$\left(F_{hkl}\right)_T = \sum_j f_j e^{-B_j (2\sin\theta/\lambda)^2} e^{2\pi i (hx_j + ky_j + lz_j)}$$



Freidel's Law

Let's consider two centrosymmetrically disposed reflections:

$$F_{hkl} = \sum_j f_j e^{2\pi i(hx_j+ky_j+lz_j)}$$

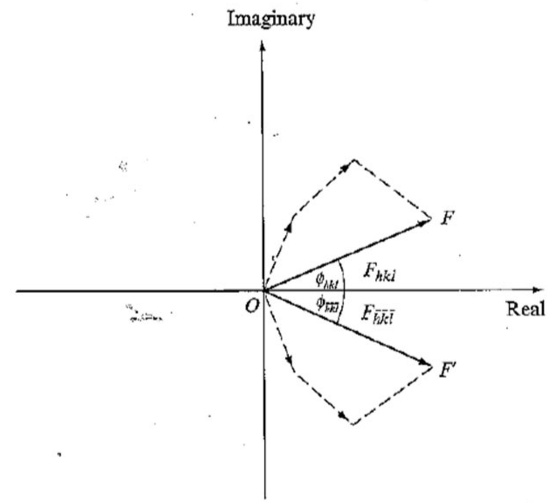
$$F_{\overline{hkl}} = \sum_j f_j e^{2\pi i(\bar{h}x_j+\bar{k}y_j+\bar{l}z_j)} = \sum_j f_j e^{-2\pi i(hx_j+ky_j+lz_j)}$$

$$|F_{hkl}| = \left|F_{\overline{hkl}}\right|$$

$$I_{hkl} = I_{\overline{hkl}} = |F_{hkl}|^2 = \left|F_{\overline{hkl}}\right|^2$$

Furthermore:

$$\phi_{\overline{hkl}} = -\phi_{hkl}$$



Dispersion

- Scattering is the result of an interaction of electromagnetic radiation with an electron.
  - Rayleigh or elastic scattering
  - Compton or inelastic scattering
- Dispersion occurs when electromagnetic radiation interacting with an electron in a shell has nearly the same frequency as the oscillator, ie resonates

$$\frac{d^2\bar{x}_j}{dt^2} + \kappa_j \frac{d\bar{x}_j}{dt} + \omega_j \bar{x}_j = -\frac{\mathrm{e}}{m}\bar{E}_0 e^{i\omega_0 t - i2\pi \bar{k}_0 \cdot \bar{r}_j}$$

$$\bar{x}_j = \frac{\mathrm{e}}{m\omega_0^2} \frac{1}{1 - \frac{\omega_j^2}{\omega_0^2} - i\frac{\kappa_j}{\omega_0}} \bar{E}_0 e^{i\omega_0 t - i2\pi \bar{k}_0 \cdot \bar{r}_j}$$

$$f = \sum_j \frac{\phi_j}{1 - \frac{\omega_j^2}{\omega_0^2} - i\frac{\kappa_j}{\omega_0}} = \sum_j \phi_j \int_{\omega_j}^{\infty} \frac{w_j\, d\omega}{1 - \frac{\omega_j^2}{\omega_0^2} - i\frac{\kappa_j}{\omega_0}} = f^0 + \sum_j \phi_j(\xi_j + i\eta_j) = f^0 + f' + if''$$

Breakdown of Freidel's Law

$$F_{hkl} = \sum_j f_j e^{2\pi i(hx_j+ky_j+lz_j)}$$

$$F_{hkl} = \sum_{j\neq A} f_j e^{2\pi i(hx_j+ky_j+lz_j)} + \left[\left(f_A^0 + f' + if''\right) e^{2\pi i(hx_A+ky_A+lz_A)}\right]$$

$$F_{\overline{hkl}} = \sum_j f_j e^{2\pi i(\bar{h}x_j+\bar{k}y_j+\bar{l}z_j)} + \left[\left(f_A^0 + f' + if''\right) e^{2\pi i(\bar{h}x_A+\bar{k}y_A+\bar{l}z_A)}\right]$$

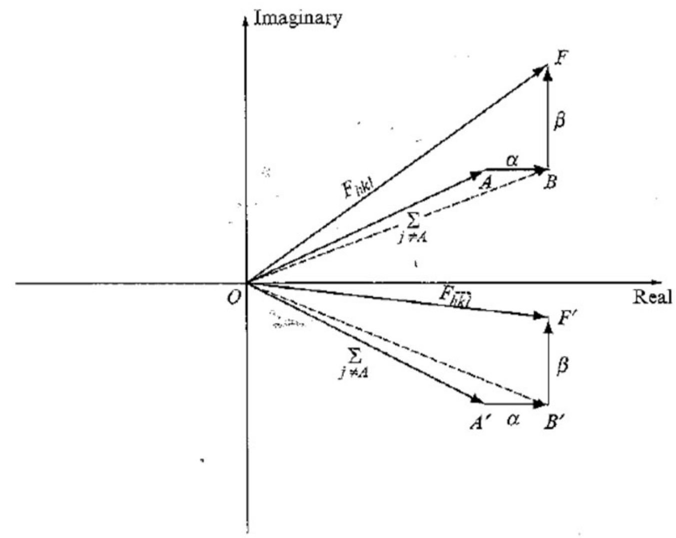
$$F_{\overline{hkl}} = \sum_j f_j e^{-2\pi i(hx_j+ky_j+lz_j)} + \left[\left(f_A^0 + f' + if''\right) e^{-2\pi i(hx_A+ky_A+lz_A)}\right]$$

$F^*_{hkl} \neq F_{\overline{hkl}}$ and thus $\left|F_{hkl}\right| = \left|F^*_{hkl}\right| \neq \left|F_{\overline{hkl}}\right|$

$I_{hkl} \neq I_{\overline{hkl}}$ and $\left|F_{hkl}\right|^2 \neq \left|F_{\overline{hkl}}\right|^2$

Furthrmore:

$\phi_{\overline{hkl}} \neq -\phi_{hkl}$



Absorption

- Absorption is another resonance effect and is related to dispersion by the equation

$$\mu_0 = \frac{4\pi N e^2}{m\omega c} f''$$

Systematic Absences (I)

Consider a body centered lattice. For a given atom at coordinates (x, y, z) there will be a second atom at $(x+1/2, y+1/2, z+1/2)$ and F_{hkl} becomes

$$F_{hkl} = \sum_{j}^{j=N/2} \left(f_j e^{2\pi i(hx_j + ky_j + lz_j)} + f_j e^{2\pi i[h(x_j+1/2)+k(y_j+1/2)+l(z_j+1/2)]} \right)$$

$$F_{hkl} = \sum_{j}^{j=N/2} f_j e^{2\pi i(hx_j + ky_j + lz_j)} \left(1 + e^{\pi i(h+k+l)}\right)$$

If $h+k+l$ is even: $e^{\pi i(h+k+l)} = 1$ but

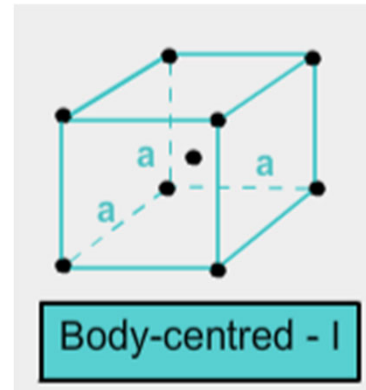
if $h+k+l$ is odd: $e^{\pi i(h+k+l)} = -1$

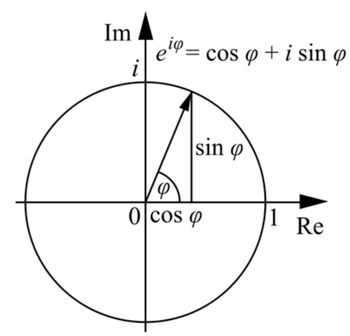
For $h+k+l = 2n$:

$$F_{hkl} = \sum_{j}^{j=N/2} f_j e^{2\pi i(hx_j + ky_j + lz_j)} (1+1) = 2\sum_{j}^{j=N/2} f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

For $h+k+l = 2n+1$:

$$F_{hkl} = \sum_{j}^{j=N/2} f_j e^{2\pi i(hx_j + ky_j lz_j)} \left(1+(-1)\right) = 0$$





Systematic Absences (II)

Let's consider a 2_1 screw axis. For a given atom at coordinates (x, y, z) there will be a second atom at $(-x, y+\frac{1}{2}, -z)$ and F_{hkl} becomes

$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} \left(f_j e^{2\pi i(hx_j+ky_j+lz_j)} + f_j e^{2\pi i[h(-x_j)+k(y_j+\frac{1}{2})+l(-z_j)]} \right)$$

For $h = 0$ and $l = 0$

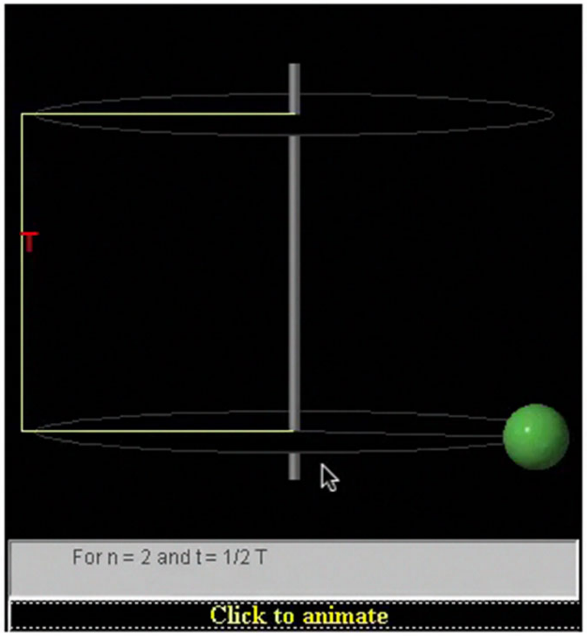
$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i(hx_j+ky_j+lz_j)} \left(1 + e^{\pi ik}\right)$$

When k is even $e^{\pi ik} = 1,$ thus:

$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i(hx_j+ky_jl+z_j)} (1+1) = 2\sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i(hx_j+ky_j+lz_j)}$$

For $h = 0$ and $l = 0,$ when k is odd: $e^{\pi ik} = -1$, thus

$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i(hx_j+ky_j+lz_j)} (1 + (-1)) = 0$$



http://wwwba.ic.cnr.it/sites/default/files/abc/abc/symmetry/restr2.htm

Systematic Absences (III)

Let′s consider a c-glide. For a given atom at coordinates (x, y, z) there will be a second atom at $(x, -y, z + \frac{1}{2})$ and F_{hkl} becomes

$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} \left(f_j e^{2\pi i (hx_j + ky_j + lz_j)} + f_j e^{2\pi i [h(x_j) + k(-y_j) + l(z_j + \frac{1}{2})]} \right)$$

For $k = 0$ and

$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i (hx_j + ky_j + lz_j)} \left(1 + e^{\pi i l}\right)$$

When l is even $e^{\pi i l} = 1,$ thus:

$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i (hx_j + ky_j l + z_j)} (1 + 1) = 2 \sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i (hx_j + ky_j + lz_j)}$$

For $h = 0$ and $k = 0,$ when l is odd: $e^{\pi i l} = -1$, thus

$$F_{hkl} = \sum_{j}^{j=\frac{N}{2}} f_j e^{2\pi i (hx_j + ky_j + lz_j)} (1 + (-1)) = 0$$

No. 7 $P1c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1

Reflection conditions

General:

$h0l$: $l = 2n$
$00l$: $l = 2n$

Textbooks and Resources Used

Crystals, X-rays and Proteins: Comprehensive Protein Crystallography, by D. Sherwood and J. Cooper, Oxford University Press, © 2011

Fundamentals of Crystallography, 2^{nd} Ed., C. Giacovazzo ed. Oxford University Press, © 2002

Understanding Single Crystal X-ray Crystallography, D. Bennett, Wiley-VCH, © 2010

International Tables for Crystallography, Volume A, Space Group Symmetry, T. Hahn, Springer, 2002

Dauter and Jaskolski, *J. Appl. Cryst.* (2010), **43**, 1150-1171

http://escher.epfl.ch/software/

http://www.ysbl.york.ac.uk/~cowtan/sfapplet/sfintro.html

https://see.stanford.edu/Course/EE261

XRayView (theraj.org)

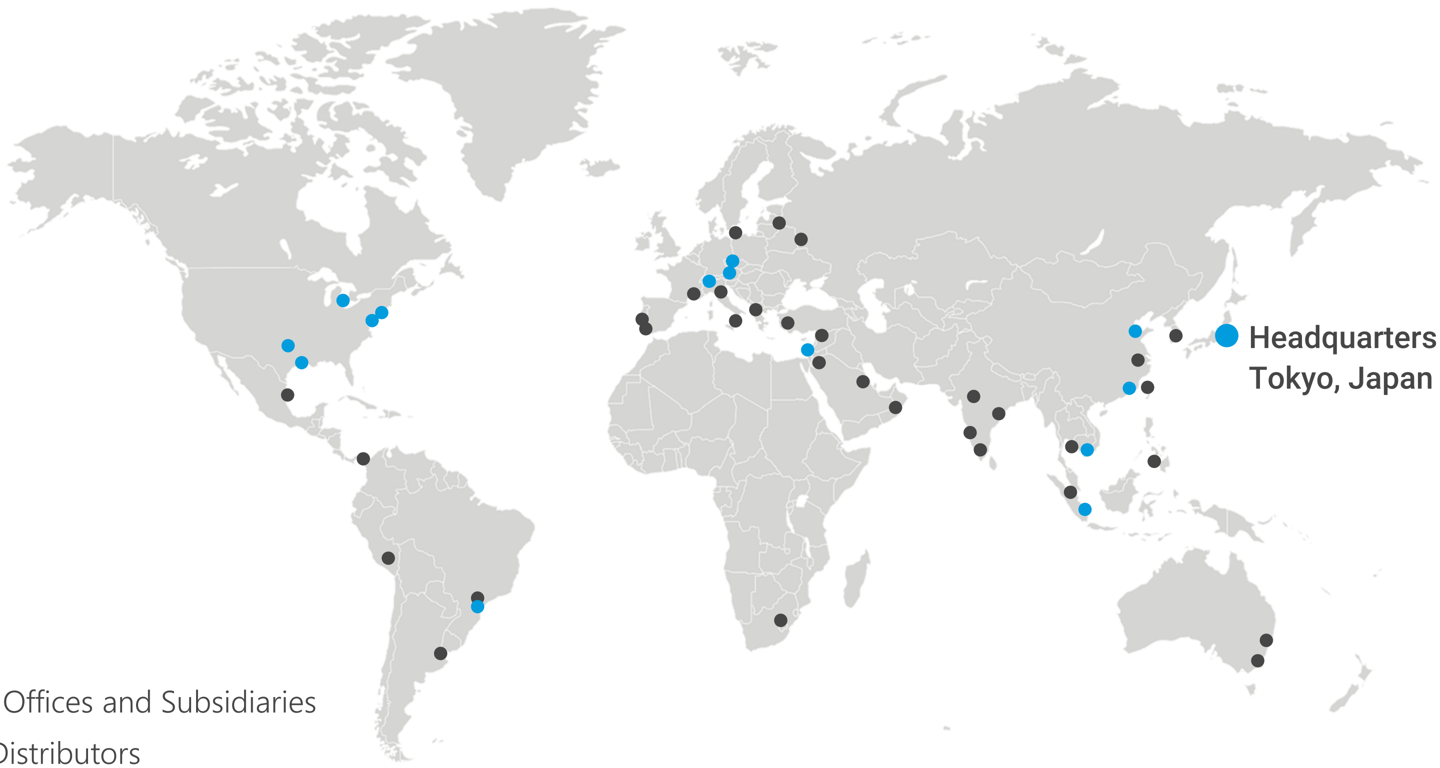
WHO WE ARE

A Brief History

Since its inception in 1951, Rigaku has been at the forefront of analytical and industrial instrumentation technology. Today, with hundreds of major innovations to their credit, the Rigaku group of companies are world leaders in the fields of general X-ray diffraction, thin film analysis, X-ray fluorescence spectrometry, small angle X-ray scattering, protein and small molecule X-ray crystallography, Raman spectroscopy, X-ray optics, semiconductor metrology, X-ray sources, computed tomography, nondestructive testing and thermal analysis.

OUR LOCATIONS

Rigaku Offices, Subsidiaries and Major Distributors

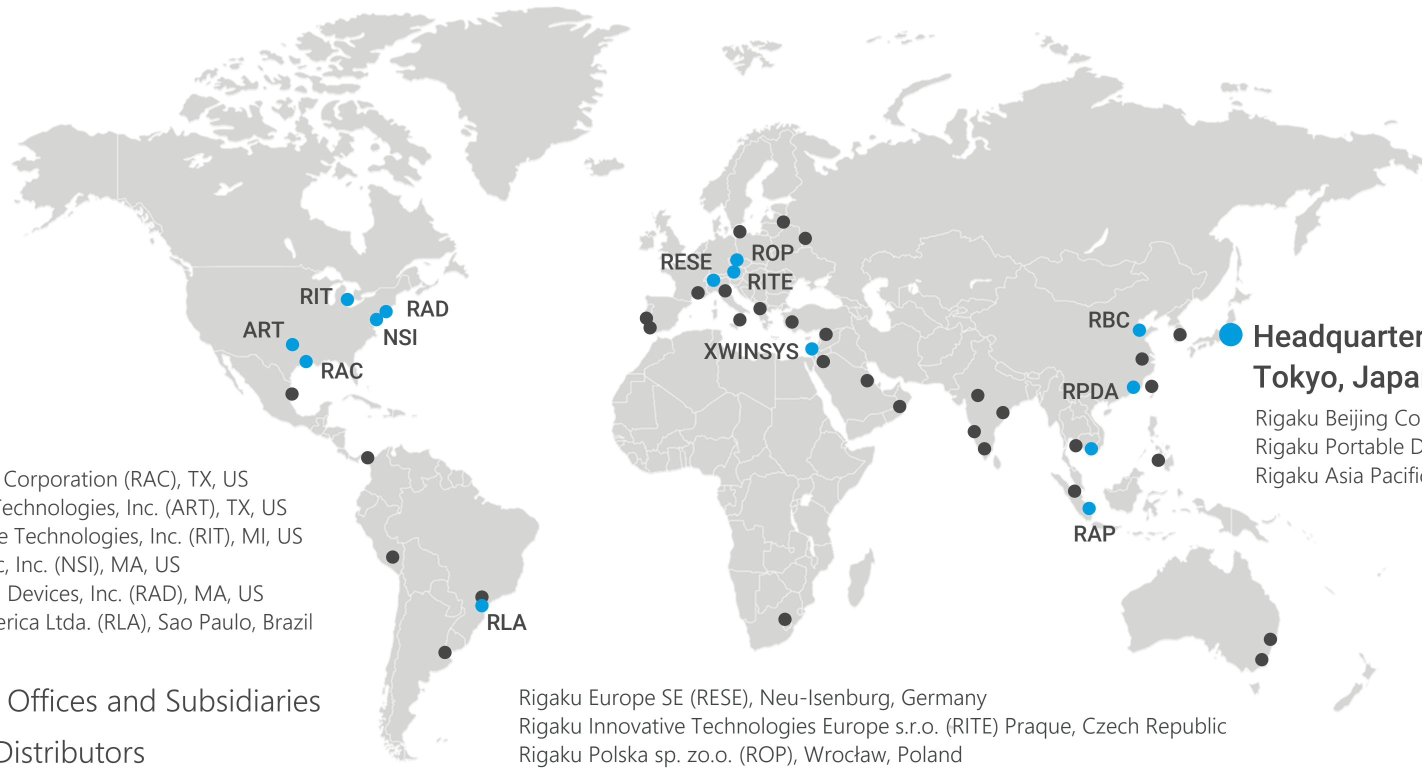


Rigaku Offices and Subsidiaries
Major Distributors

Rigaku

OUR LOCATIONS

Rigaku Offices, Subsidiaries and Major Distributors



Rigaku Beijing Corporation (RBC), Beijing, China
Rigaku Portable Devices Asia Limited (RPDA)
Rigaku Asia Pacific Pte. Ltd. (RAP) Singapore

Rigaku Americas Corporation (RAC), TX, US
Applied Rigaku Technologies, Inc. (ART), TX, US
Rigaku Innovative Technologies, Inc. (RIT), MI, US
Newton Scientific, Inc. (NSI), MA, US
Rigaku Analytical Devices, Inc. (RAD), MA, US
Rigaku Latin America Ltda. (RLA), Sao Paulo, Brazil

- Rigaku Offices and Subsidiaries
- Major Distributors

Rigaku Europe SE (RESE), Neu-Isenburg, Germany
Rigaku Innovative Technologies Europe s.r.o. (RITE) Praque, Czech Republic
Rigaku Polska sp. zo.o. (ROP), Wrocław, Poland
XwinSys Technologies Development Ltd. (XwinSys) Migdal Haemek, Israel

CONTACT US

Rigaku Corporation

+1 (281) 362 2300

info@rigaku.com

rigaku.com