III.C CRYSTALS, SYMMETRY AND DIFFRACTION

III.C.6 Diffraction

Diffraction methods provide a powerful way to study molecular structure

X-ray diffraction

Neutron diffraction

Electron diffraction

Optical diffraction

Computed diffraction

Ultimate goal:

Understand the chemical properties of molecules by determining their atomic structure

Types of chemical bonds (ionic, covalent, or hydrogen)

Bond lengths and angles

Van der Waals radii

Rotations about single bonds

etc.

III.C.6 Diffraction

Presently, only **X-ray** and **neutron** diffraction techniques are **routinely** capable of revealing the arrangement of **atoms** in molecular structures

In 1912 von Laue predicted that X-rays should diffract from crystals like light from a diffraction grating (later verified experimentally by Friedrich and Knipping)

W. L. Bragg: developed concept of diffraction from **crystal planes** and that the diffraction pattern could be used to reveal atomic positions in crystals

Physical principles of X-ray diffraction form the fundamental basis of **Fourier image processing** techniques

III.C.6 Diffraction

III.C.6.a Introduction to Diffraction Theory

Diffraction: **non-linear** propagation of electromagnetic radiation

- Occurs when an object **scatters** the incident radiation

- Radiation scattered from different portions of the object **interfere** both **constructively and destructively**, producing a diffraction pattern which can be recorded on a photographic emulsion

Recall:

Electrons (in a TEM) are scattered both by the electrons (inelastic scatter) and nuclei (elastic scatter) of specimen atoms

III.C.6 Diffraction

III.C.6.a Introduction to Diffraction Theory

A characteristic of diffraction: (**remember this!**)

Each point in the diffraction pattern arises from interference of rays scattered from ***all irradiated portions*** of the object

III.C.6 Diffraction

III.C.6.a Introduction to Diffraction Theory

Structure determination by diffraction methods:

- Involves measuring or calculating the **structure factor** (*F*) at many or all points of the diffraction pattern

- Each *F* is described by two quantities, an **amplitude** and a **phase**

Amplitude:

Strength of interference at a particular point

Phase:

Relative time of arrival of scattered radiation (wave) at a particular point

III.C.6 Diffraction

III.C.6.a Introduction to Diffraction Theory

Diffraction facts:

Amplitude is proportional to the square root of the **intensity** in the recorded pattern

$$Amplitude \propto \sqrt{Intensity}$$

Photographic film does **not** record the scattered amplitude, but rather the **intensity** which is proportional to the amplitude squared: *i.e.* $Intensity \propto (Amplitude)^2$

III.C.6 Diffraction

III.C.6.a Introduction to Diffraction Theory

More Diffraction facts:

- **Phase** information is **lost** when the diffraction pattern is recorded

- Phases **cannot** be measured directly from X-ray diffraction photographs

The "Phase Problem"

- Major concern of structure determination using X-ray crystallography

- Necessitates use of *e.g.* heavy atom, isomorphous replacement, molecular replacement etc. methods

III.C.6 Diffraction

III.C.6.a Introduction to Diffraction Theory

X-ray phases could be obtained **if** it were possible to rediffract (focus) scattered X-rays with a lens to form an image

We **can** **directly visualize** objects in **electron and light microscopes** because **electrons and visible** photons scattered by specimens **can be focused** with lenses to form images

III.C.6 Diffraction

III.C.6.a Introduction to Diffraction Theory

In the absence of "noise", an image might be considered to contain structural information (amplitudes and phases) in **directly** interpretable form

Major advantage of image processing:

Provides an **objective means** to extract **reliable** structural information from noisy images

Fourier Transforms

III.C.6 Diffraction

III.C.6.b The Fourier Transform

Mathematically describes the **distribution of amplitude and phase** in different directions, for **all possible** directions of the beam incident on the object

Fourier transform of an object is a particular kind of **weighted integral** of the object

In one-dimension:

$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

III.C.6 Diffraction

III.C.6.b The Fourier Transform

The Fourier transform in 1-D:

$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

F*(X)* = the scattering function (diffraction pattern)

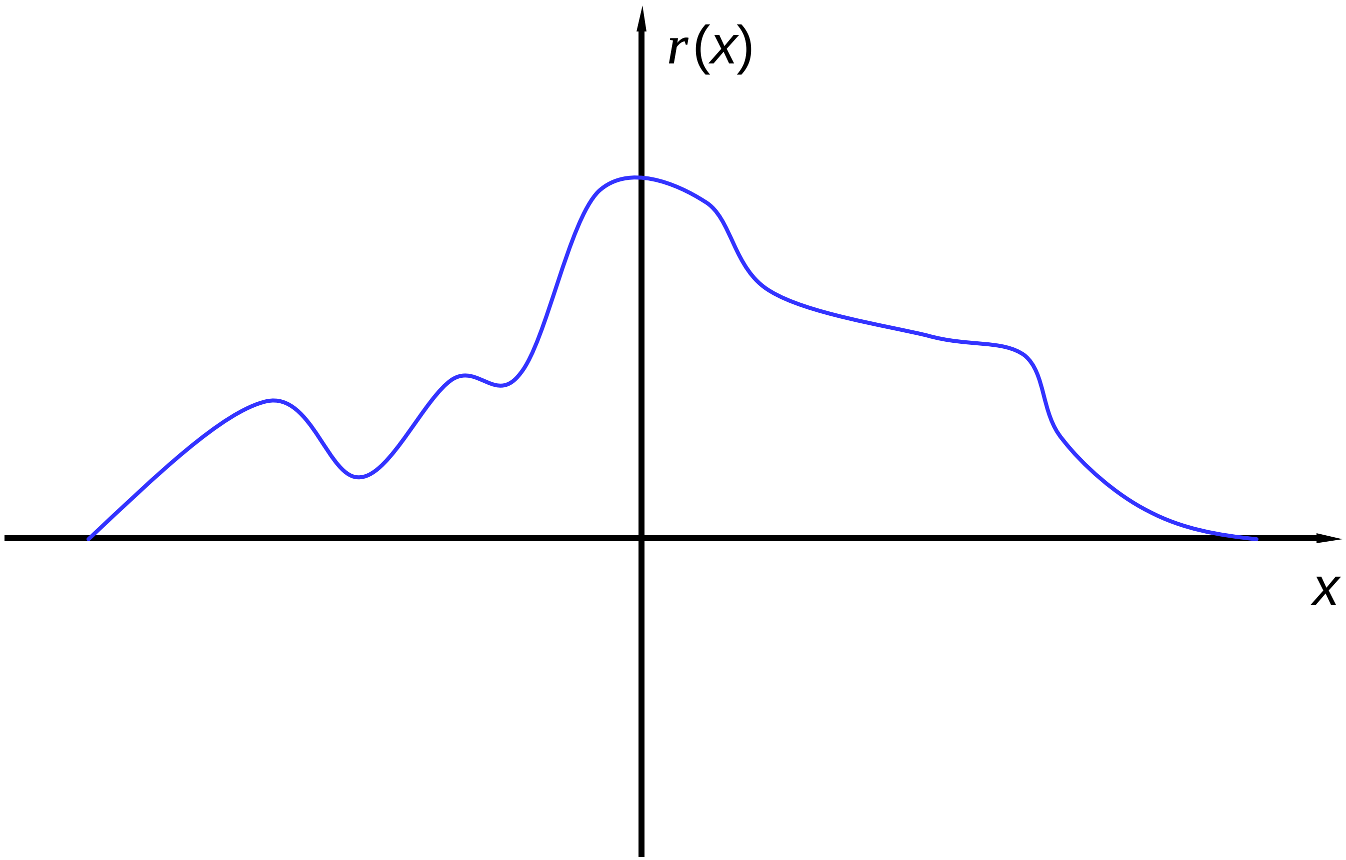
r(x) = the electron density function (object)

Integration is over **all** density values in the structure

III.C.6 Diffraction

III.C.6.b The Fourier Transform

$r(x)$: the object



III.C.6 Diffraction

III.C.6.b The Fourier Transform

The Fourier transform in 1-D:

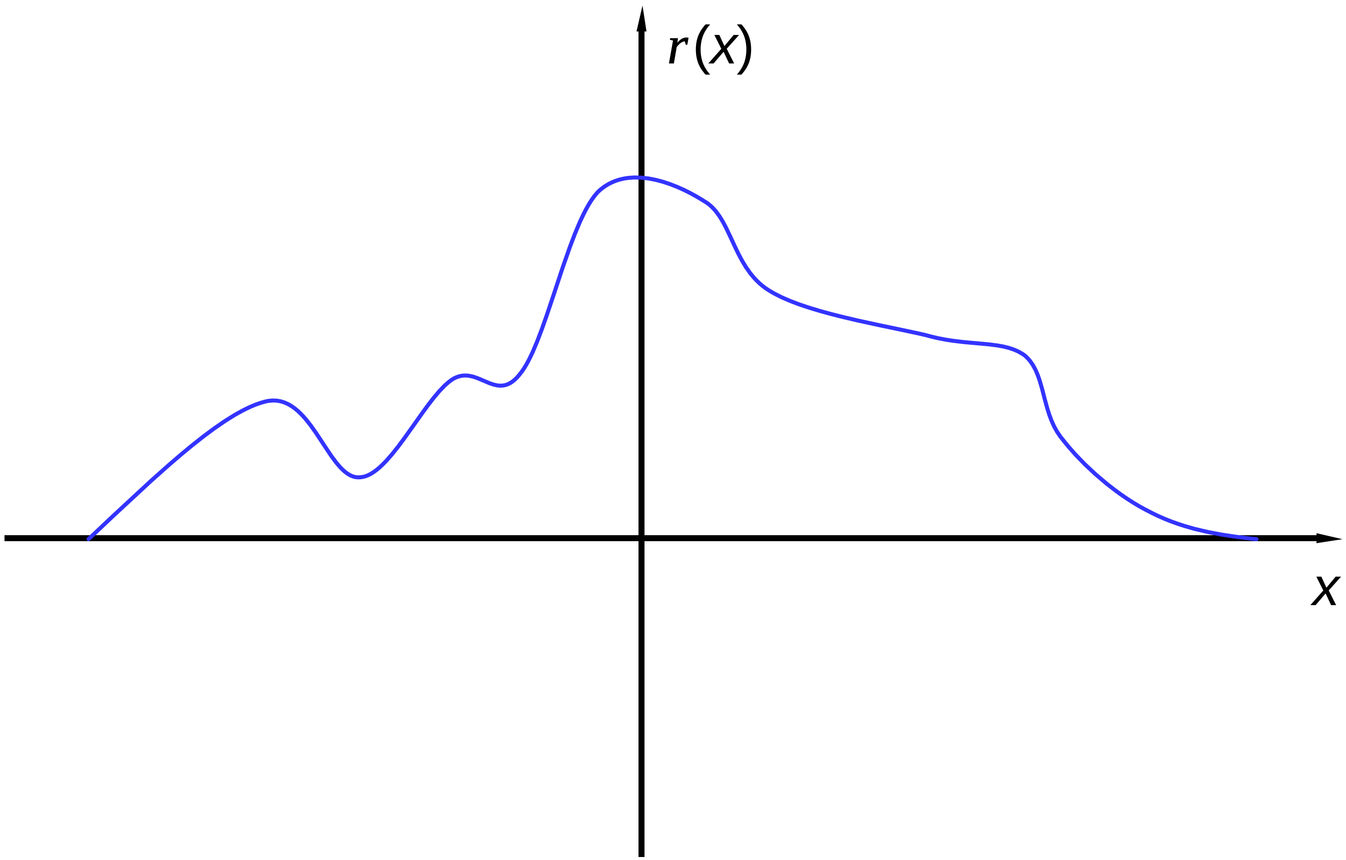
$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

For **sampled** (**discrete**) data:

$$F(X) = \sum_{x} r(x) e^{(2pixX)}$$

III.C.6.b The Fourier Transform

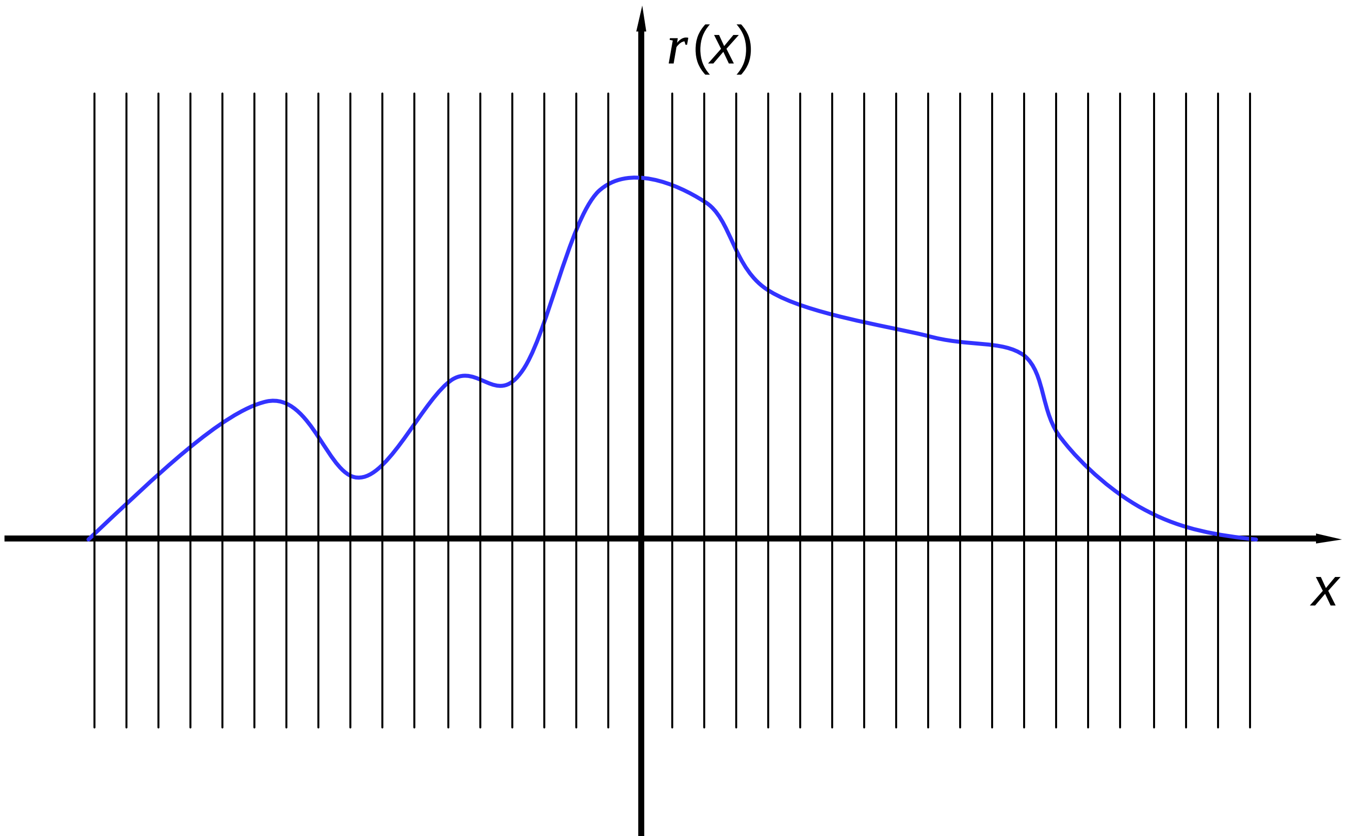
$r(x)$: the object



III.C.6 Diffraction

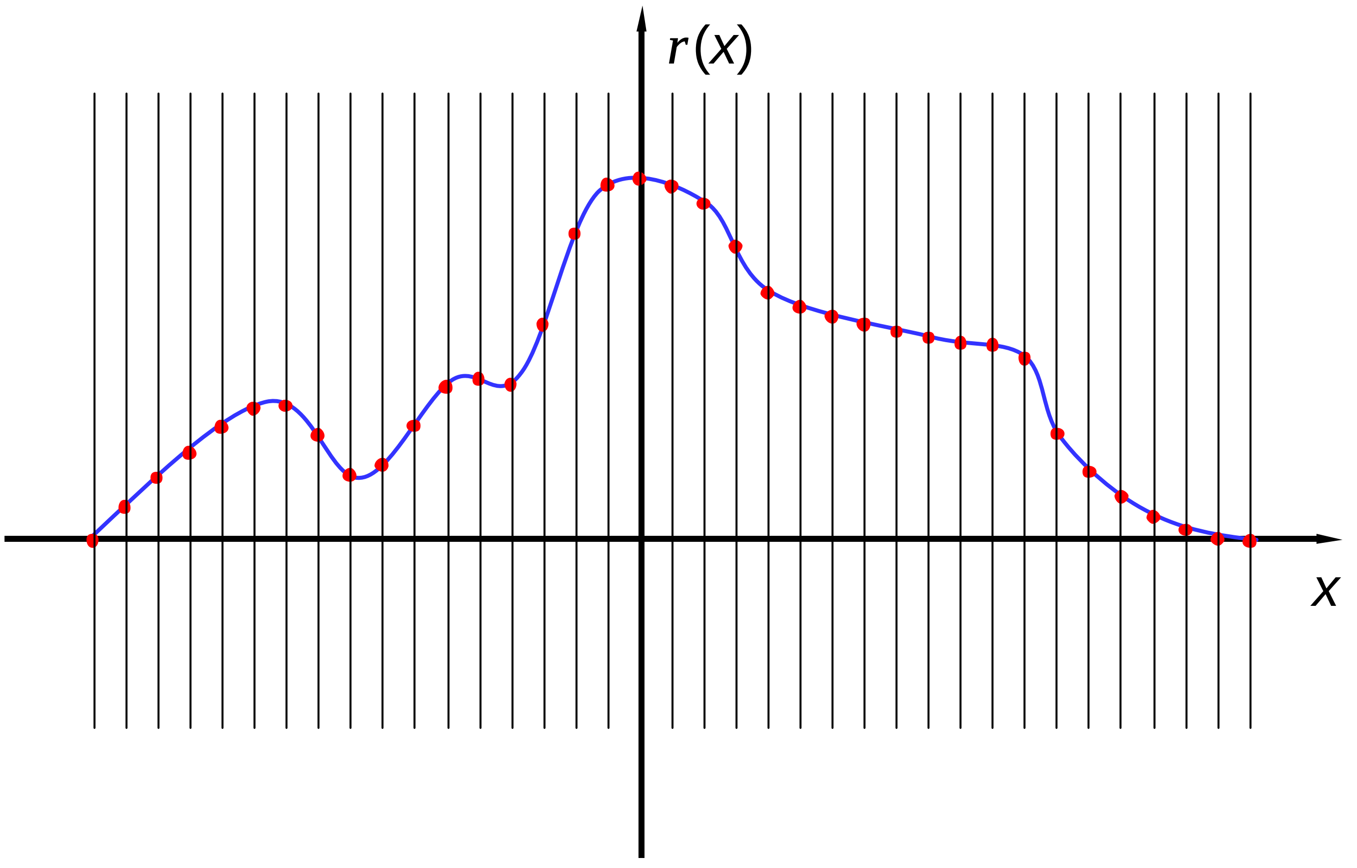
III.C.6.b The Fourier Transform

$r(x)$: the object sampled



III.C.6.b The Fourier Transform

$r(x)$: the object   sampled



III.C.6.b The Fourier Transform

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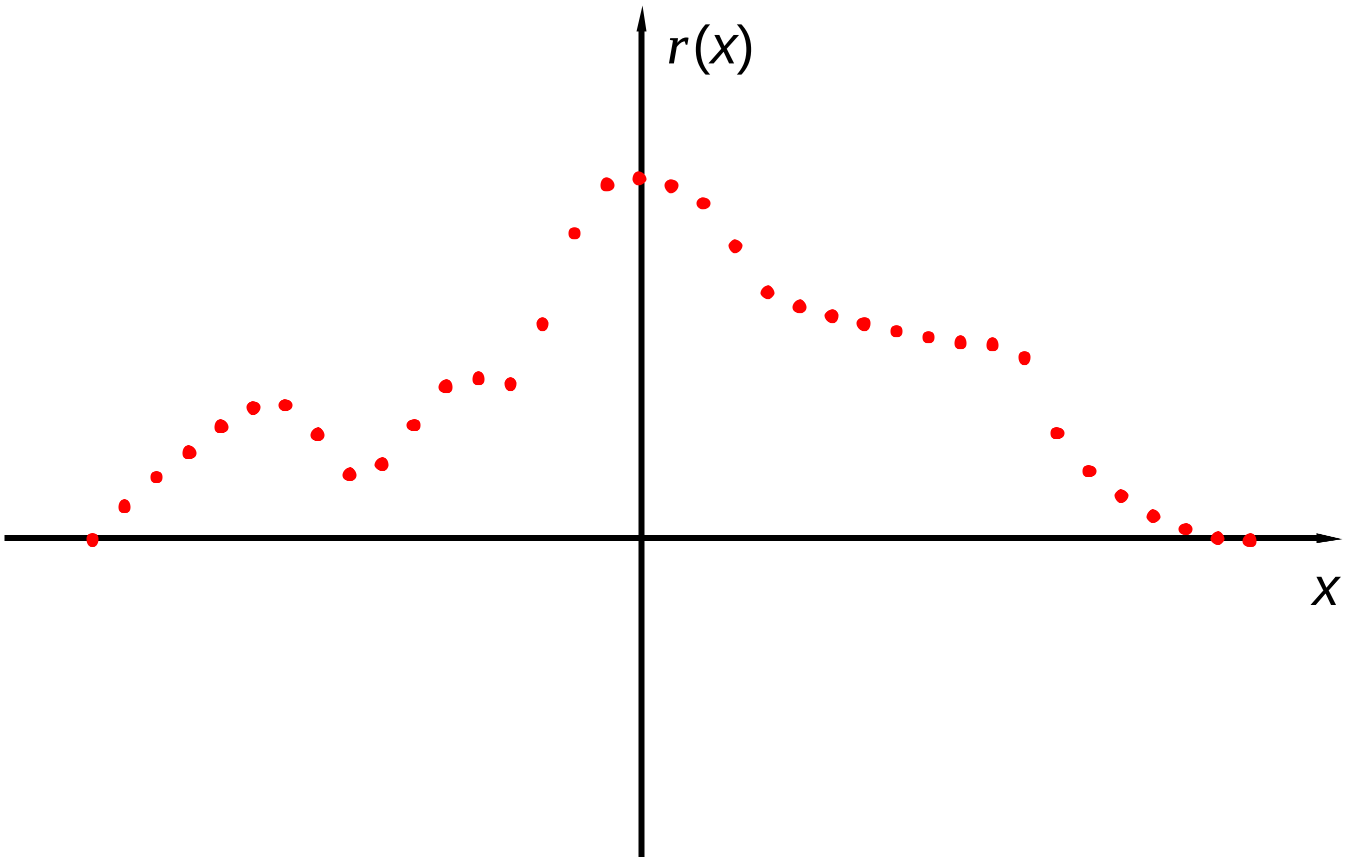

III.C.6 Diffraction

III.C.6.b The Fourier Transform

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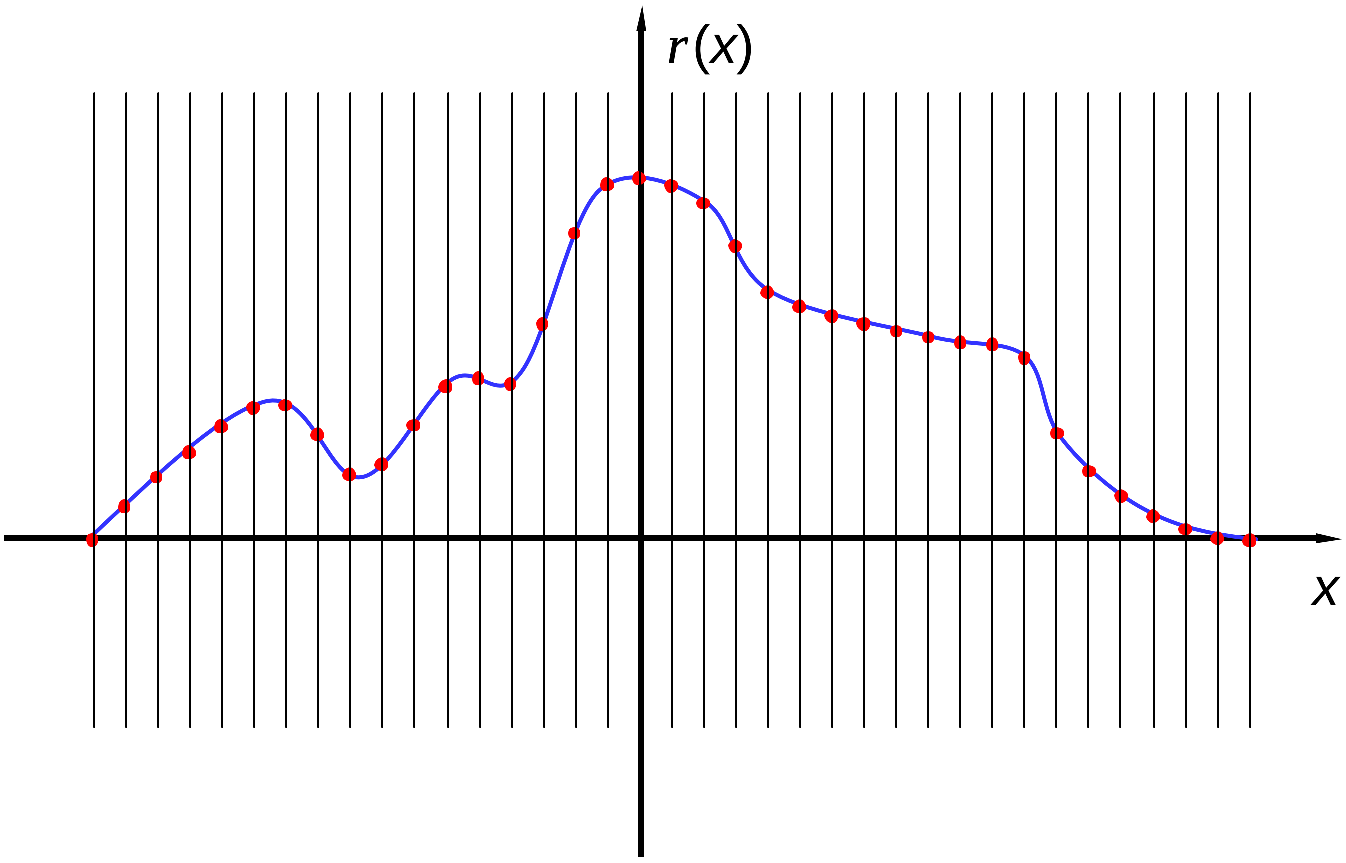

III.C.6 Diffraction

III.C.6.b The Fourier Transform

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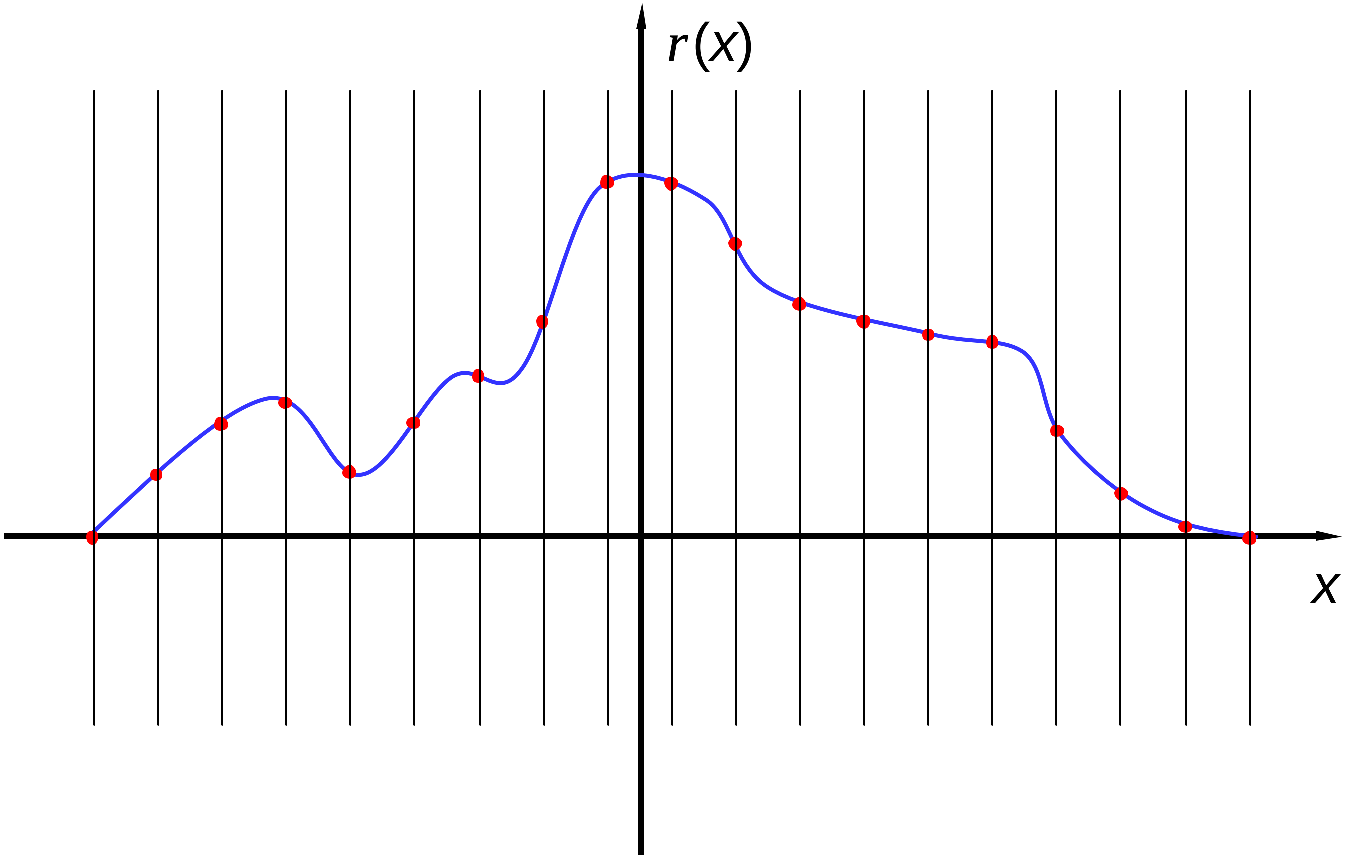

III.C.6.b The Fourier Transform

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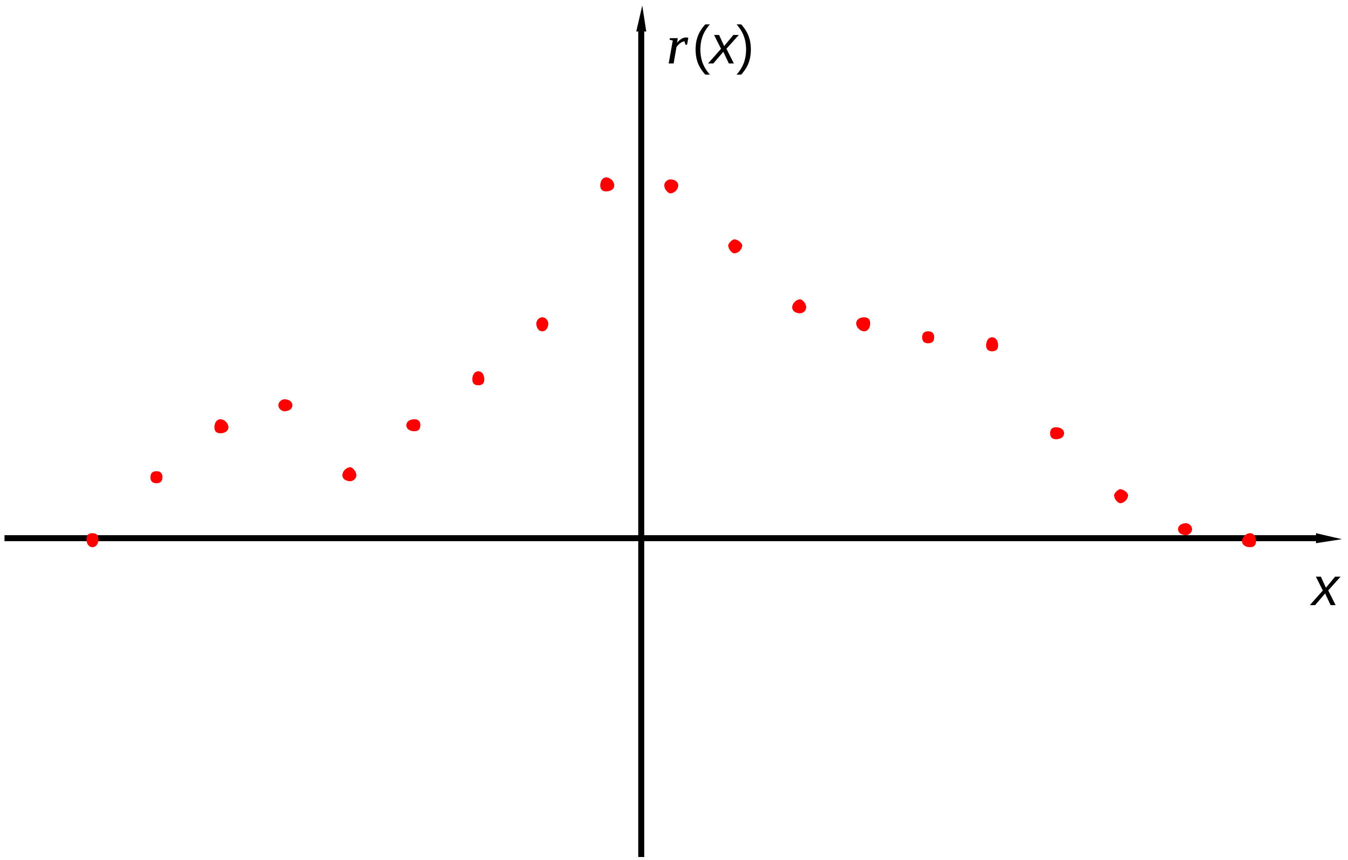

III.C.6.b The Fourier Transform

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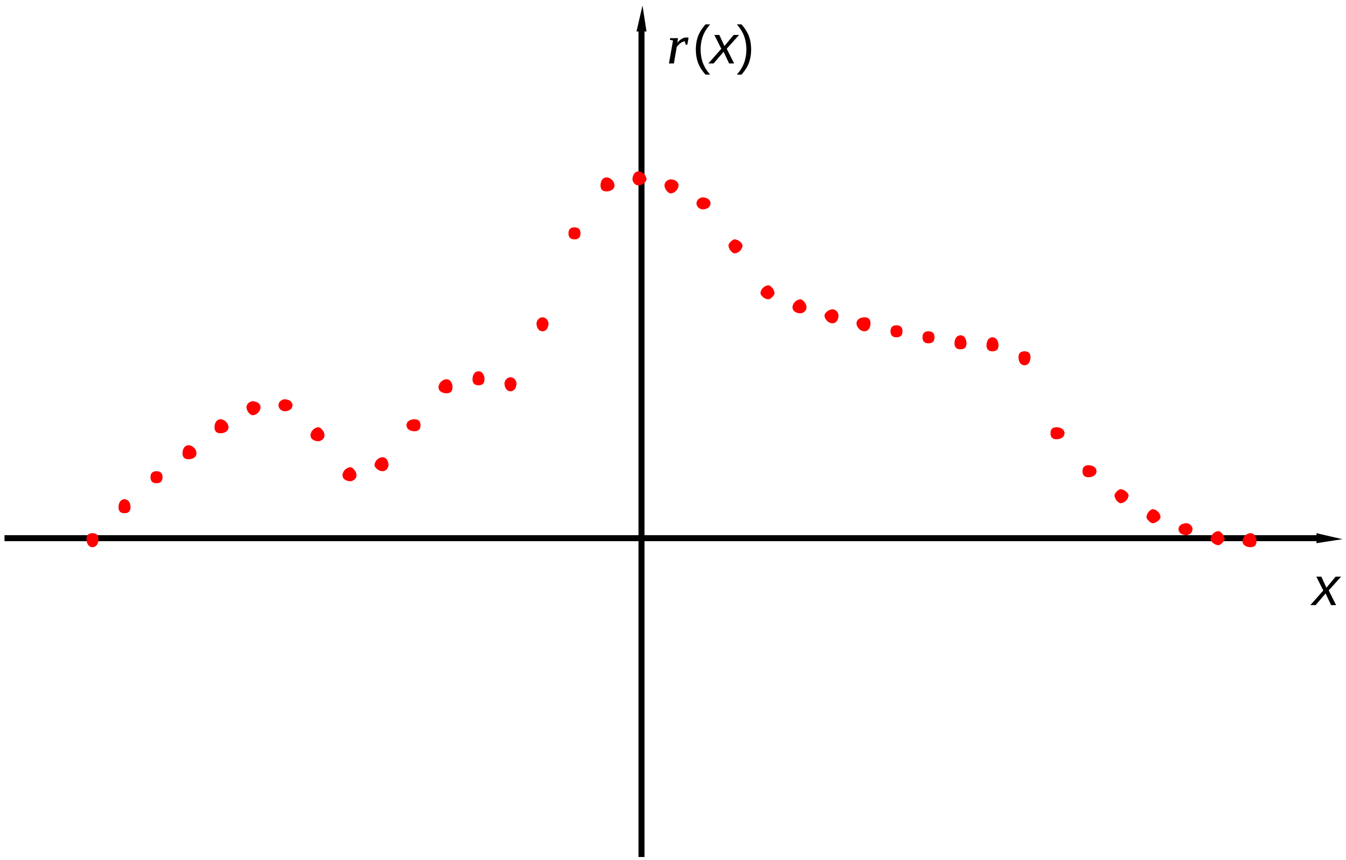

III.C.6 Diffraction

III.C.6.b The Fourier Transform

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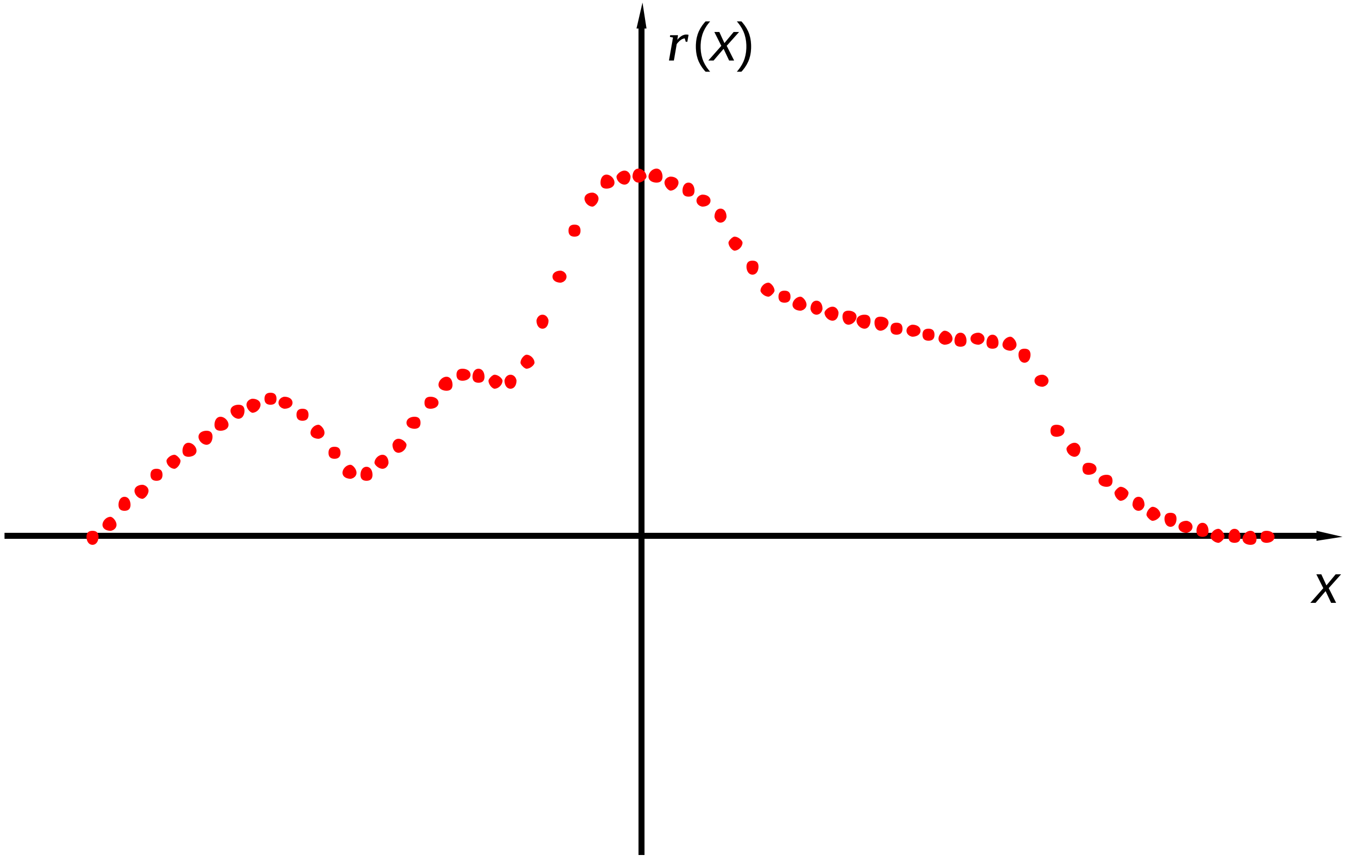


III.C CRYSTALS, SYMMETRY AND DIFFRACTION

III.C.6 Diffraction

KEY CONCEPTS:

- **Diffraction methods** provide a powerful means to study and determine structure

- First goal of diffraction methods is to determine **structure factor amplitudes and phases**; from these we can **reconstruct** structure

- The Fourier transform is just a **different way to represent** an object

- **Any <u>periodic</u> object** can be represented mathematically as a **summation of sinusoidal waves** (Fourier synthesis)

- Image formation is considered a **double diffraction** process

And some more KEY CONCEPTS:

- **Bragg's Law:** visualizes diffraction as arising from **reflection** of radiation from **planes** in crystals

- Structure factors are **complex** numbers

- Concepts of **convolution and multiplication** (sampling) help us understand fundamental properties of Fourier transforms

III.C.6 Diffraction

III.C.6.b The Fourier Transform

In one-dimension:

$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

For sampled (discrete) data:

$$F(X) = \sum_{x} r(x) e^{(2pixX)}$$

III.C.6.b The Fourier Transform

Shorthand Notations:

F = Fourier transform of r

T = Forward Fourier transform operation

F = $T(r)$

III.C.6.b The Fourier Transform

Inverse relationship: (property of FTs)

Recall:

$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

F(X) is the **forward transform** of *r(x)*

$$r(x) = \int_{-\infty}^{\infty} F(X) e^{(-2pixX)} dX$$

thus *r* is the **inverse transform** of *F*

III.C.6.b The Fourier Transform

Inverse relationship: (property of FTs)

$$r(x) = \int_{-\infty}^{\infty} F(X) e^{(-2pixX)} dX$$

r is the **inverse transform** of *F*

In shorthand notation:

$$r = T^{-1}(F) = T^{-1}(T(r))$$

T^{-1} = inverse (reverse, back) Fourier transform operation

III.C.6 Diffraction

III.C.6.b The Fourier Transform

Inversion theorem:

The Fourier transform of the Fourier transform of an object is the original object

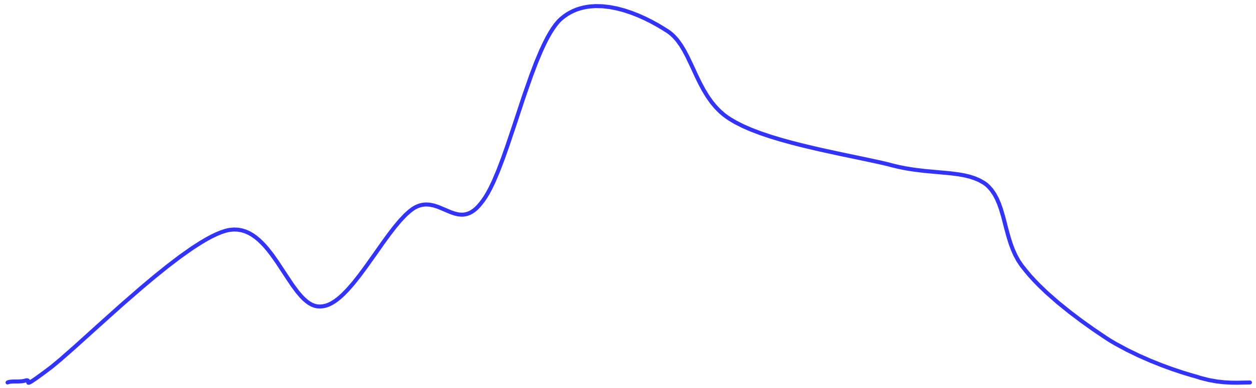
Theorem is analogous to Abbe's treatment of **image formation** which is considered to be a **double-diffraction process**

We will return to this idea a bit later…

III.C.6 Diffraction

III.C.6.c Fourier Synthesis

Any periodic function may be **mathematically** represented by a **summation** of a **series of sinusoidal waves**



III.C.6 Diffraction

III.C.6.c Fourier Synthesis

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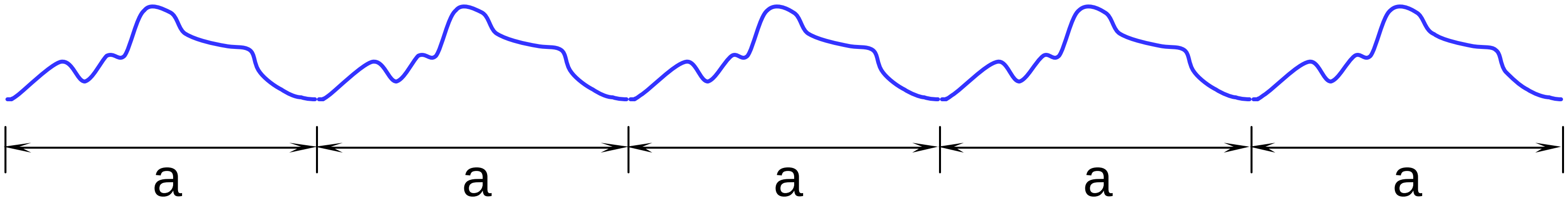

III.C.6 Diffraction

III.C.6.c Fourier Synthesis

Any <u>periodic</u> function may be **mathematically** represented by a **summation** of a **series of sinusoidal waves**

In one-dimension, the Fourier synthesis can be expressed:

$$r(x) = \sum_{n=-\infty}^{\infty} A_n \cos(2pnx/a)$$

III.C.6 Diffraction

III.C.6.c Fourier Synthesis

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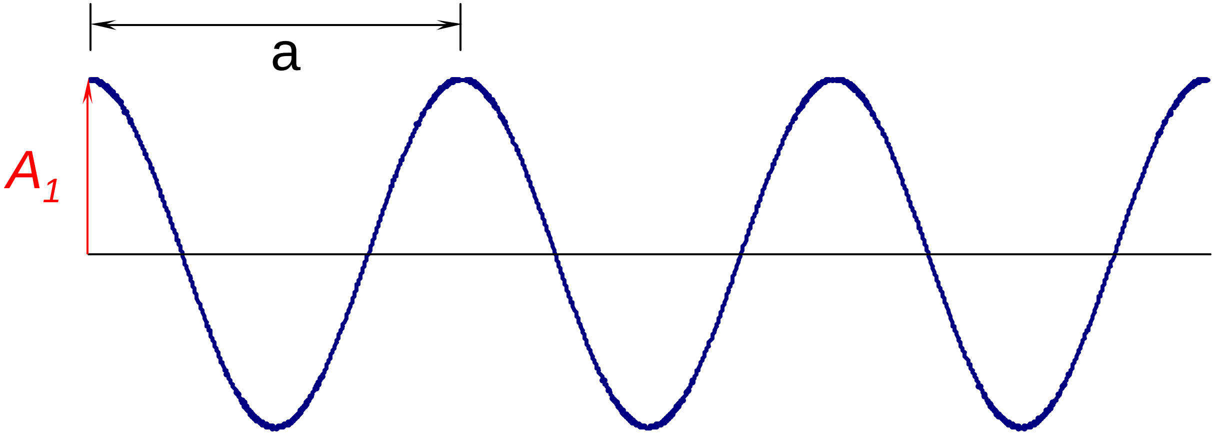

III.C.6 Diffraction

III.C.6.c Fourier Synthesis

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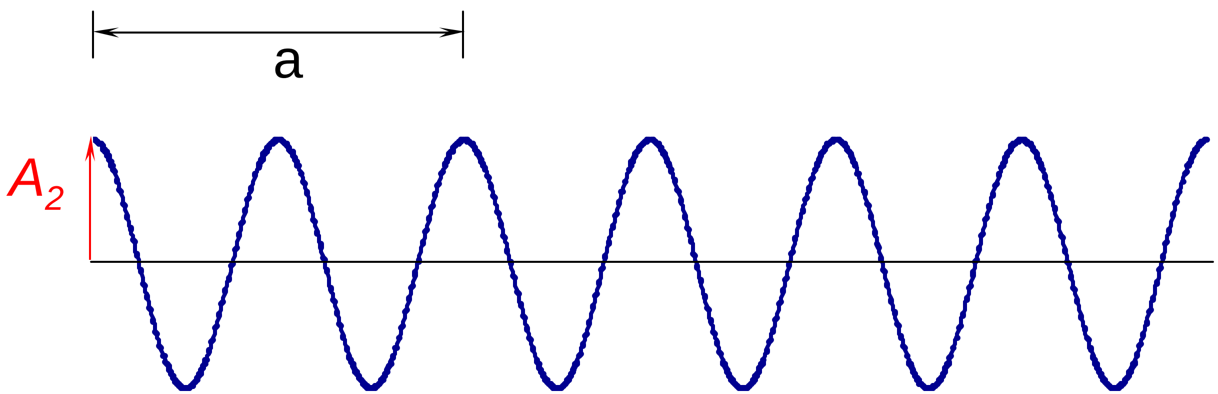


III.C.6 Diffraction

III.C.6.c Fourier Synthesis

$$r(x) = \sum_{n=-\infty}^{\infty} A_n \cos(2pnx/a)$$

$r(x)$	= 1-D density function (object)
x	= coordinate of a point in the object
a	= repeat distance of 1-D periodic object
A_n	= **Fourier coefficient** (amplitude term) for wave number n
n	= wave number (frequency) or cycles per repeat distance a
$(2\pi nx/a)$	= **phase term** (position of wave with respect to a fixed origin point in the repeating structure)

III.C.6 Diffraction

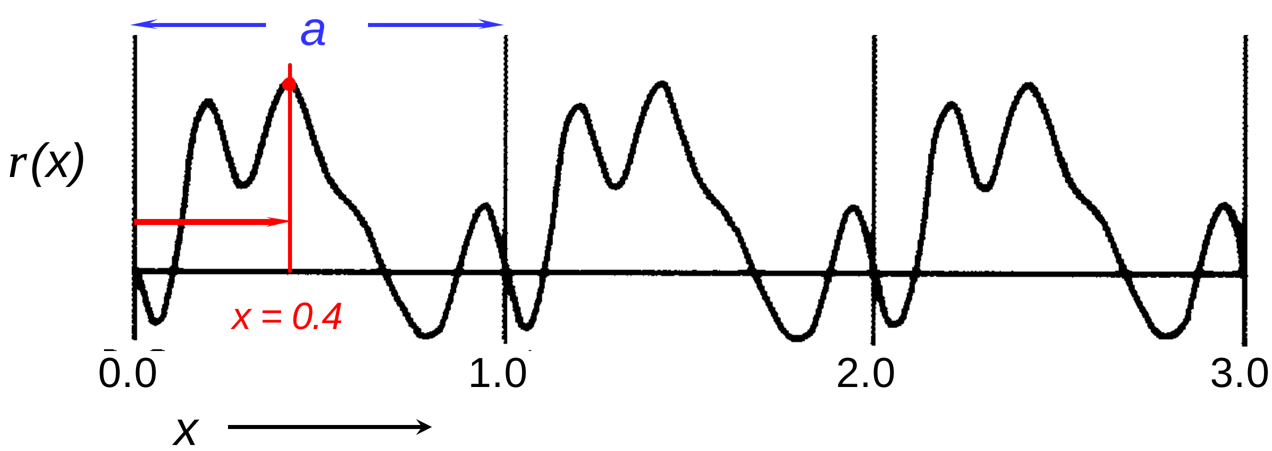
III.C.6.c Fourier Synthesis

$$r(x)=\sum_{n=-\infty}^{\infty} A_n \cos(2pnx/a)$$

r(x) = object

x = coordinate of point in object

a = repeat distance of 1-D periodic object



From Eisenberg & Crothers, Fig. 17-14, p.828

III.C.6 Diffraction

III.C.6.c Fourier Synthesis

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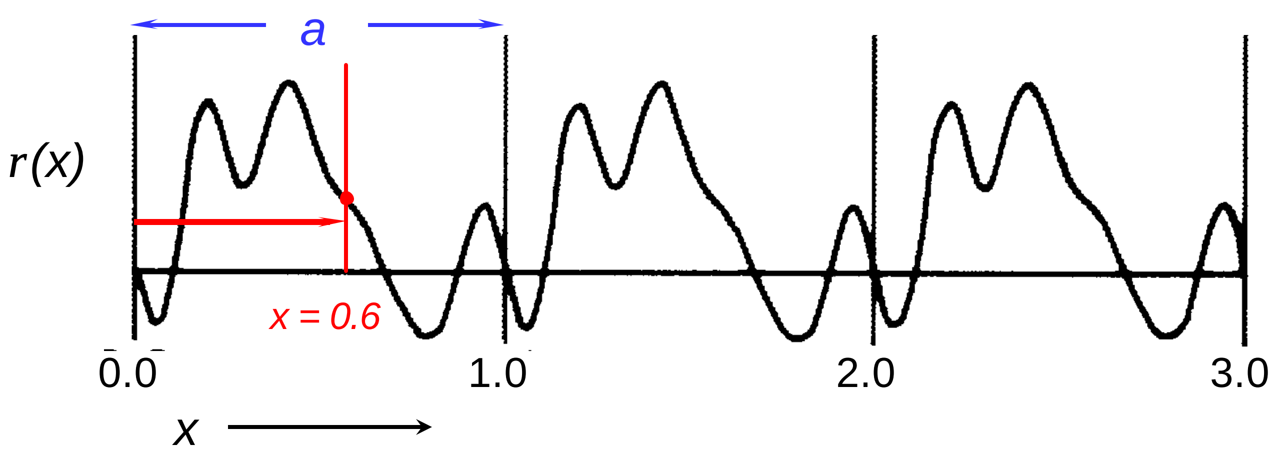

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III.C.6 Diffraction

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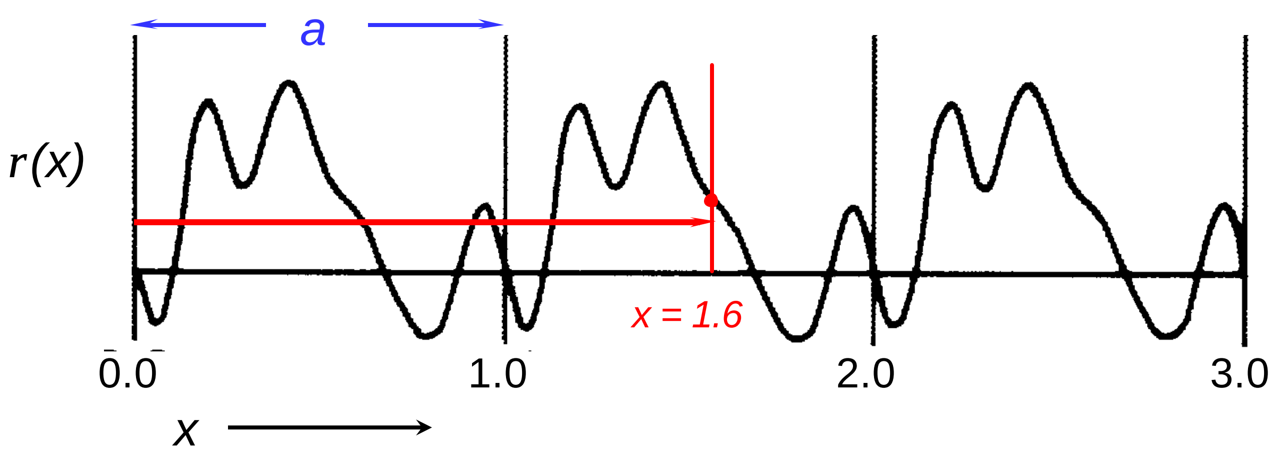

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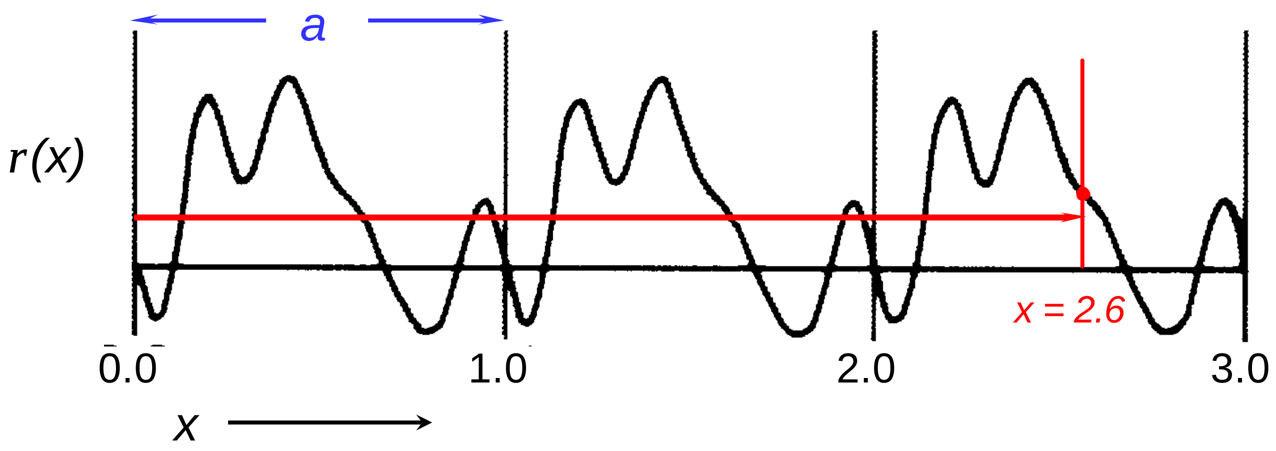

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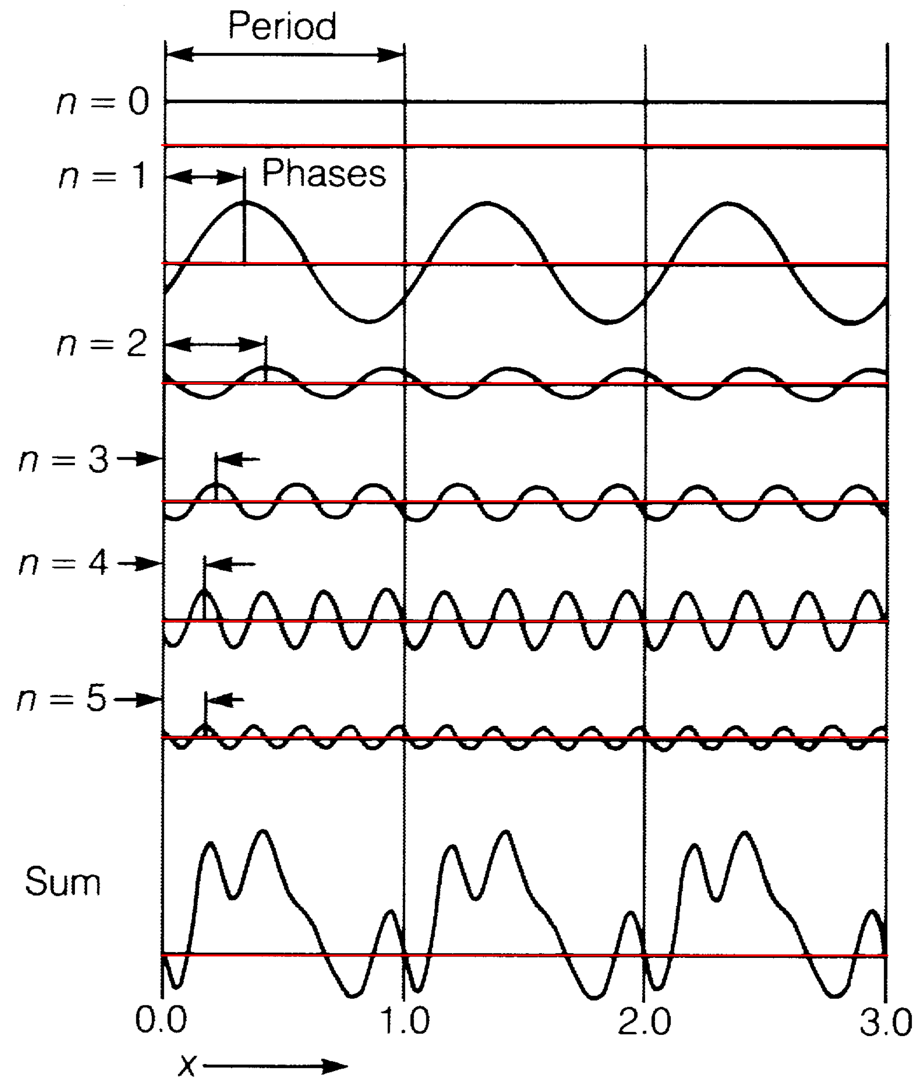


From Eisenberg & Crothers, Fig. 17-14, p.828

III.C.6 Diffraction

III.C.6.c Fourier Synthesis

Fourier Synthesis:

- Mathematical **combination of the waves** to produce the periodic function

Fourier Analysis:

- Opposite process
- **Decomposition** of the periodic function **into its component waves**
- **Example:** analyzing the sound wave harmonics of a musical instrument

III.C.6.c Fourier Synthesis

Analogy between Music and Structure

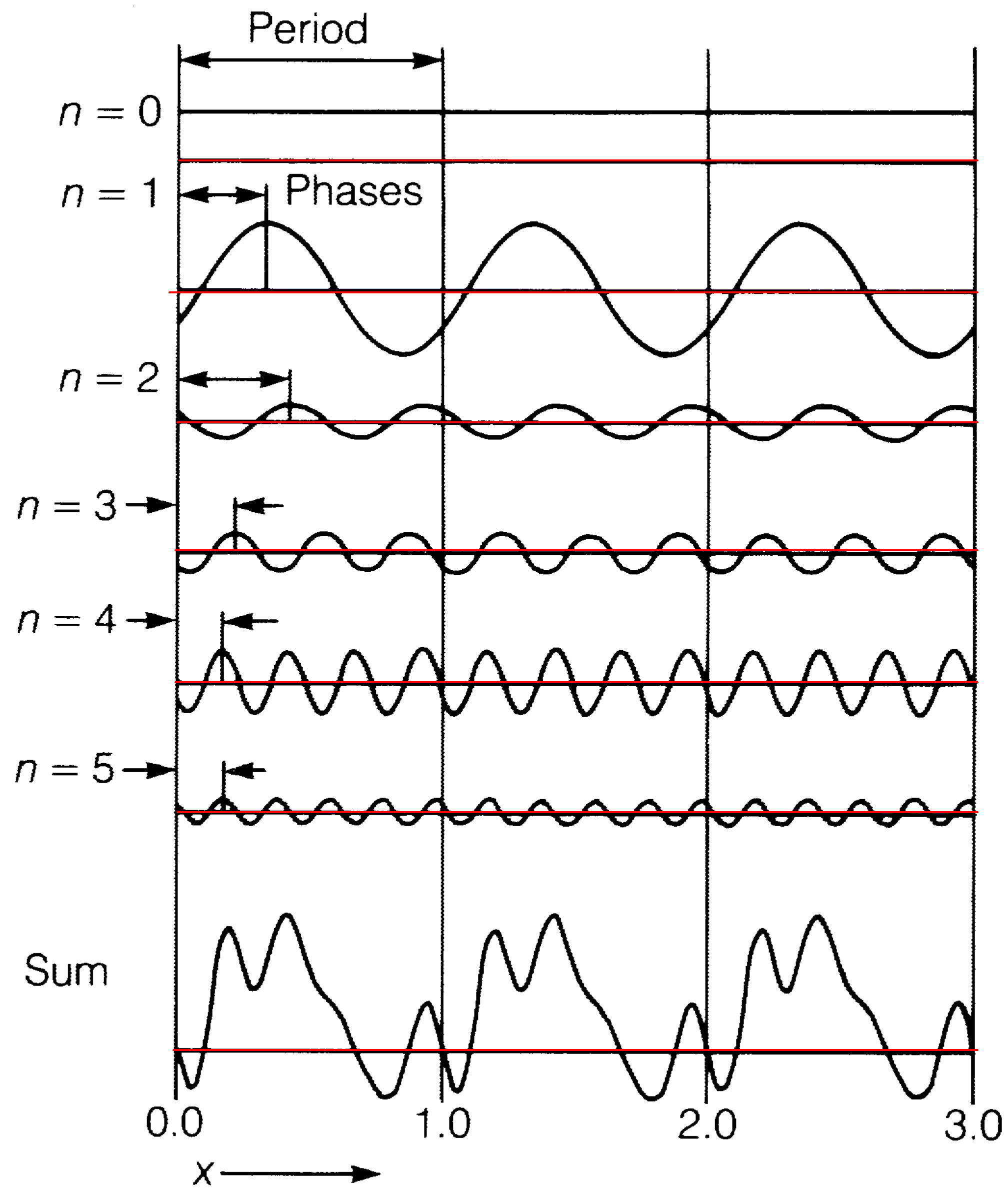
tone = Σ harmonics

structure = Σ structure factors

III.C.6 Diffraction

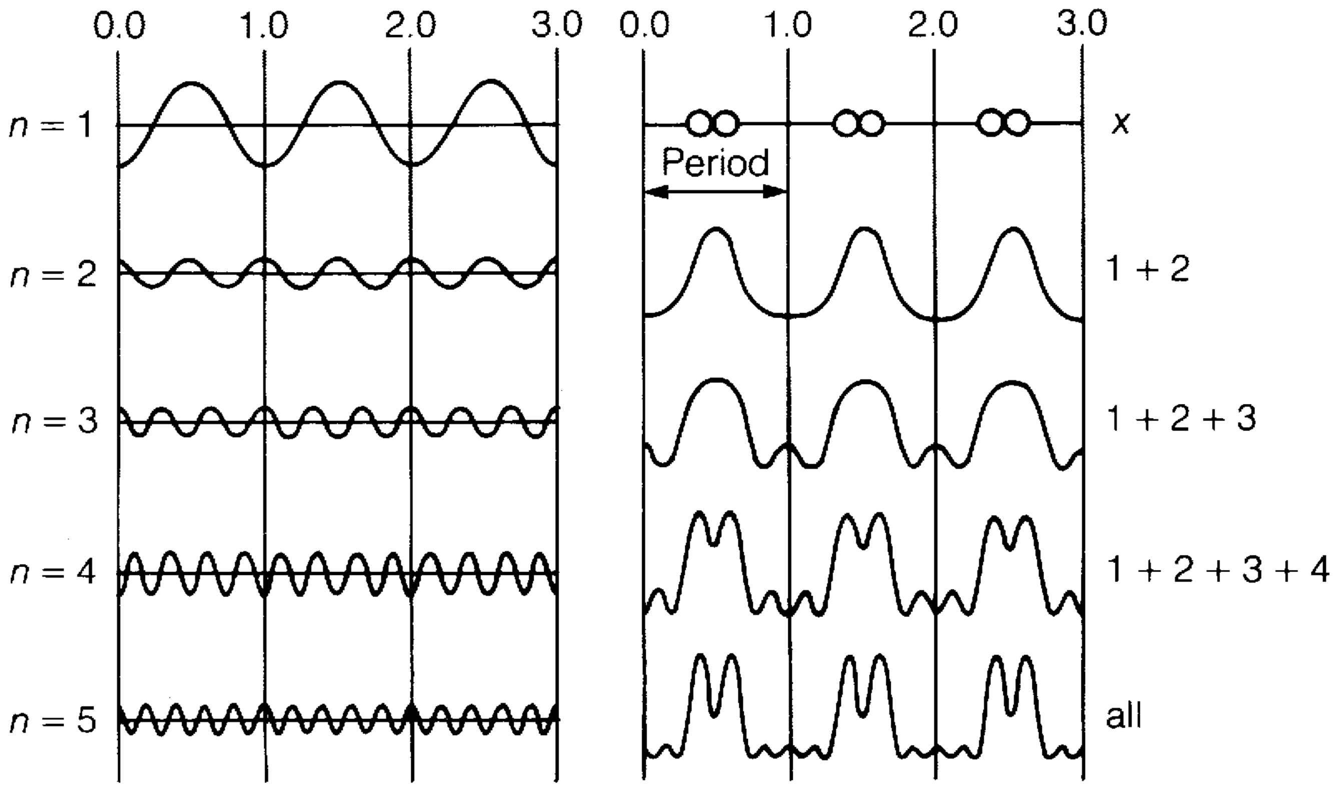
III.C.6.c Fourier Synthesis

Fourier Synthesis of 1-D Periodic Object



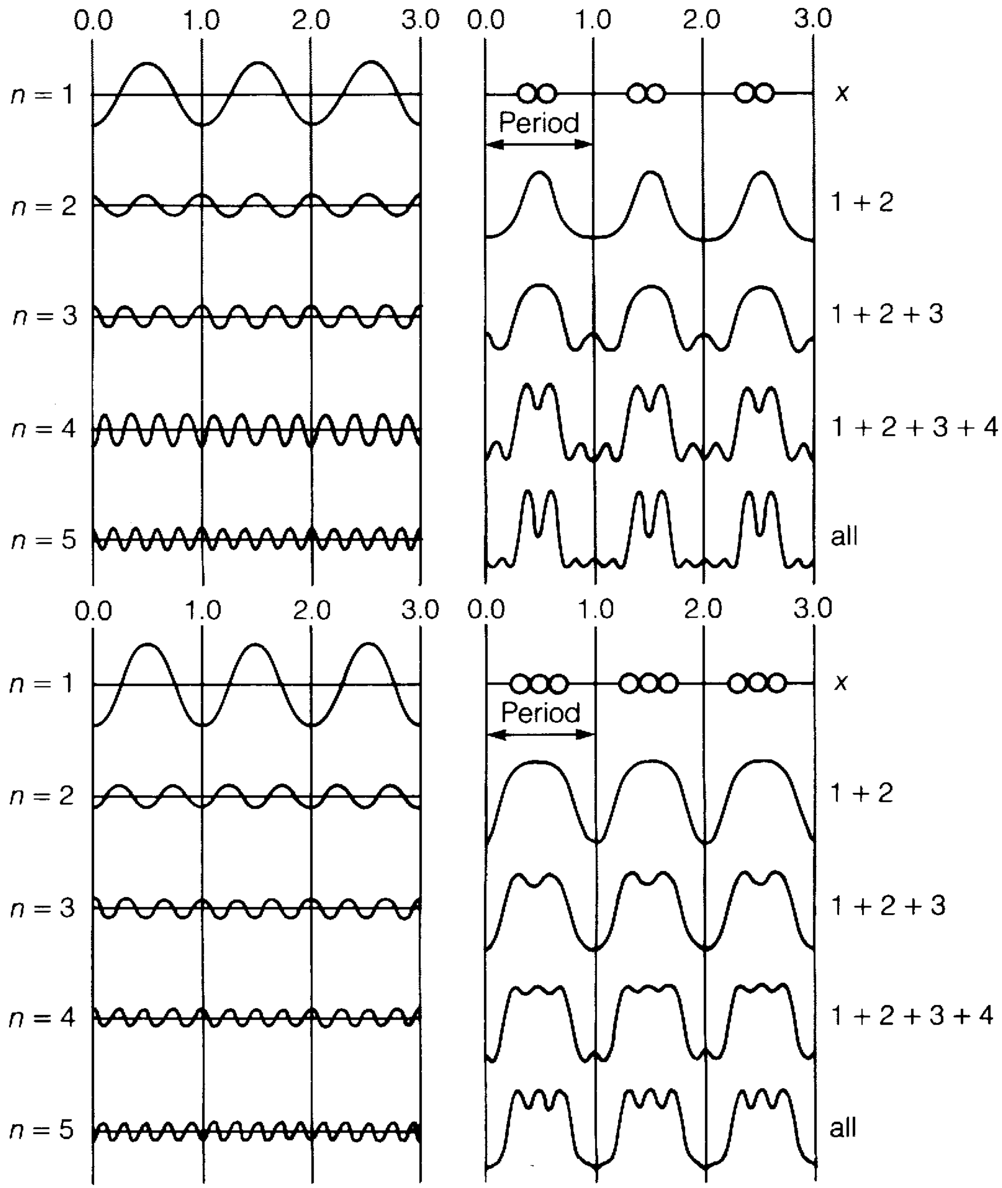
From Eisenberg & Crothers, Fig. 17-14, p.828

Superposition of Waves to Represent 1-D "Crystal"



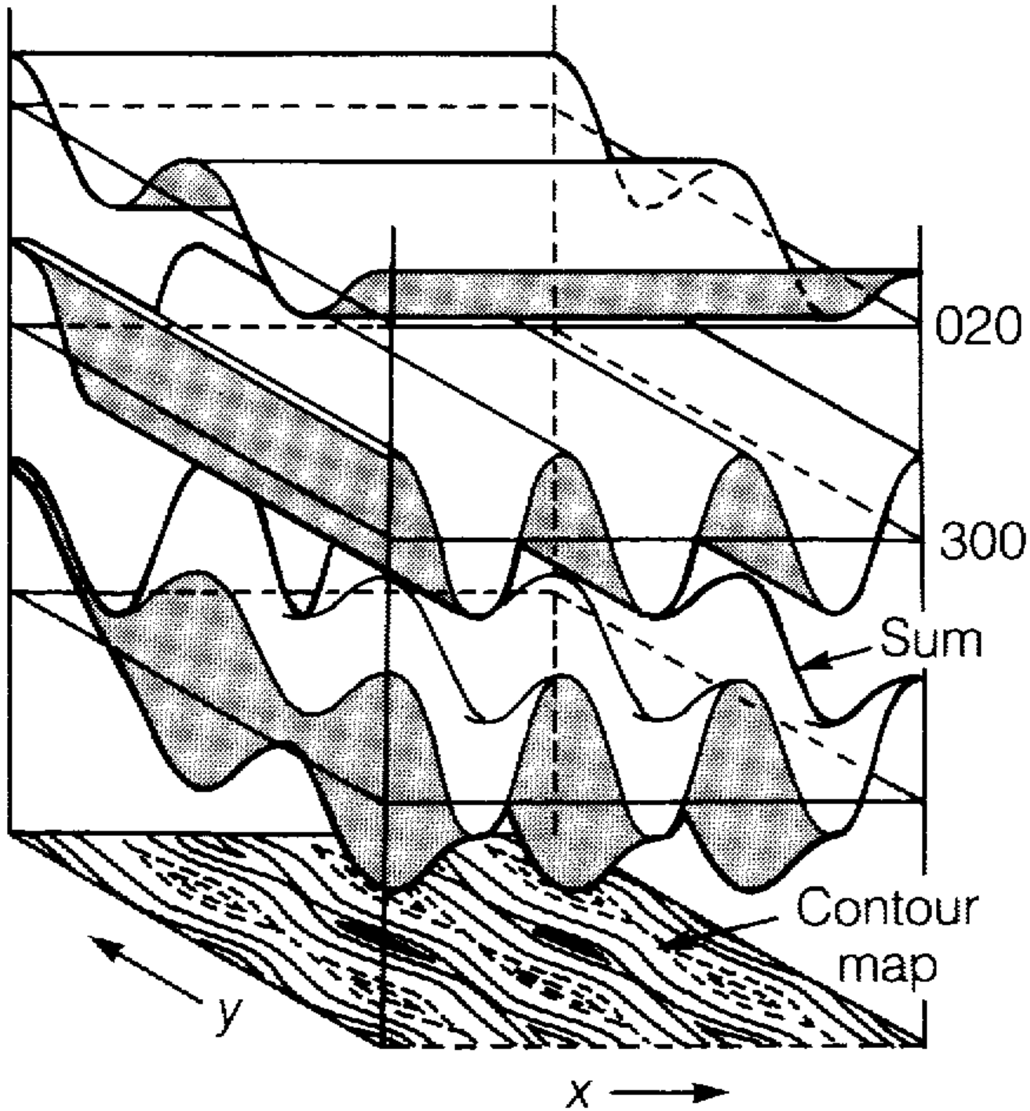
From Eisenberg & Crothers, Fig. 17-15, p.829

Superposition of Waves to Represent 1-D "Crystal"



From Eisenberg & Crothers, Fig. 17-15, p.829

Summation of 2D Waves to Produce 2D "Electron Density"



From Eisenberg & Crothers, Fig. 17-15c, p.830

3-11-04

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

Structure determination by diffraction methods:

- Involves measuring or calculating the **structure factor** (*F*) at many or all points of the diffraction pattern

- Each *F* is described by an **amplitude** and a **phase**

Amplitude:

Strength of interference at a particular point

Phase:

Relative time of arrival of scattered radiation (wave) at a particular point

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

The Fourier Transform

Mathematically describes the **distribution of amplitude and phase** in different directions, for **all possible** directions of the beam incident on the object

Fourier transform of an object is a particular kind of **weighted integral** of the object

In one-dimension:

$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

The Fourier Transform

The Fourier transform in 1-D:

$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

F*(X)* = the scattering function (diffraction pattern)

r(x) = the electron density function (object)

Integration is over **all** density values in the structure

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

The Fourier Transform

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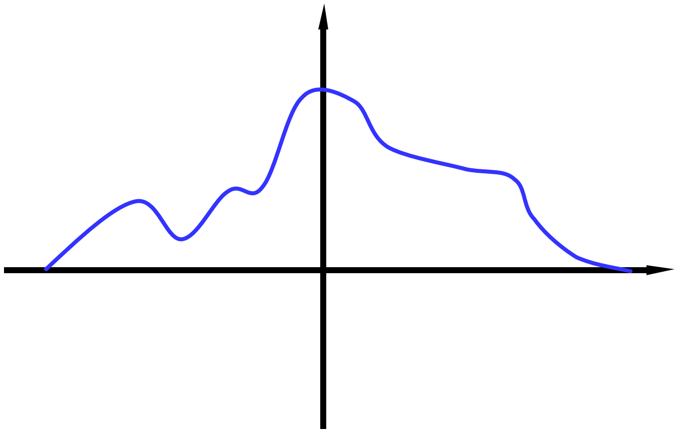
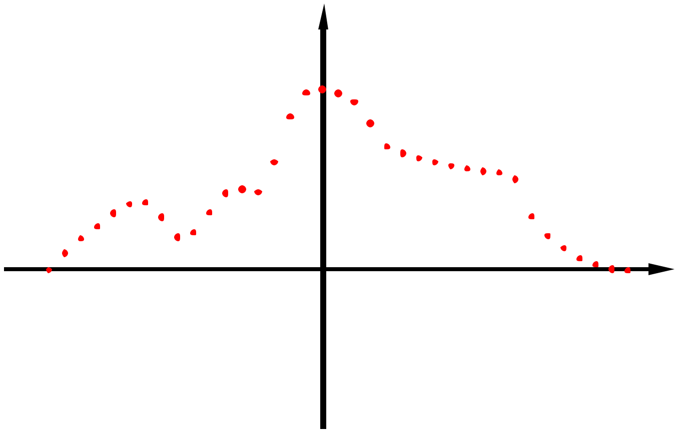


For **sampled** (**discrete**) data:

$$F(X) = \sum_{x} r(x) e^{(2pixX)}$$



III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

The Fourier Transform

- Goal of diffraction methods: determine **structure factor amplitudes and phases**; from these we can **reconstruct** structure

- The Fourier transform is just a **different way to represent** an object

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

Inverse relationship: (property of FTs)

$$F(X) = \int_{-\infty}^{\infty} r(x) e^{(2pixX)} dx$$

F(X) is the **forward transform** of *r(x)*

$$r(x) = \int_{-\infty}^{\infty} F(X) e^{(-2pixX)} dX$$

thus *r* is the **inverse transform** of *F*

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

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r is the **inverse transform** of *F*

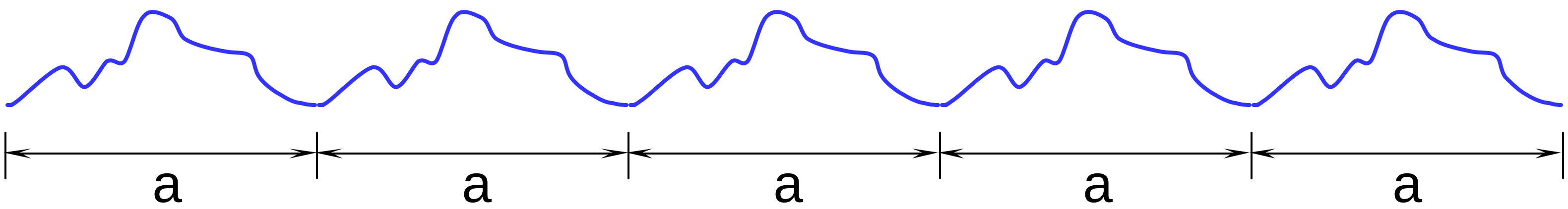
$$r = T^{-1}(F) = T^{-1}(T(r))$$

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

Fourier Synthesis

- **Any <u>periodic</u> object** can be represented mathematically as a **summation of sinusoidal waves**



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III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

Fourier Synthesis

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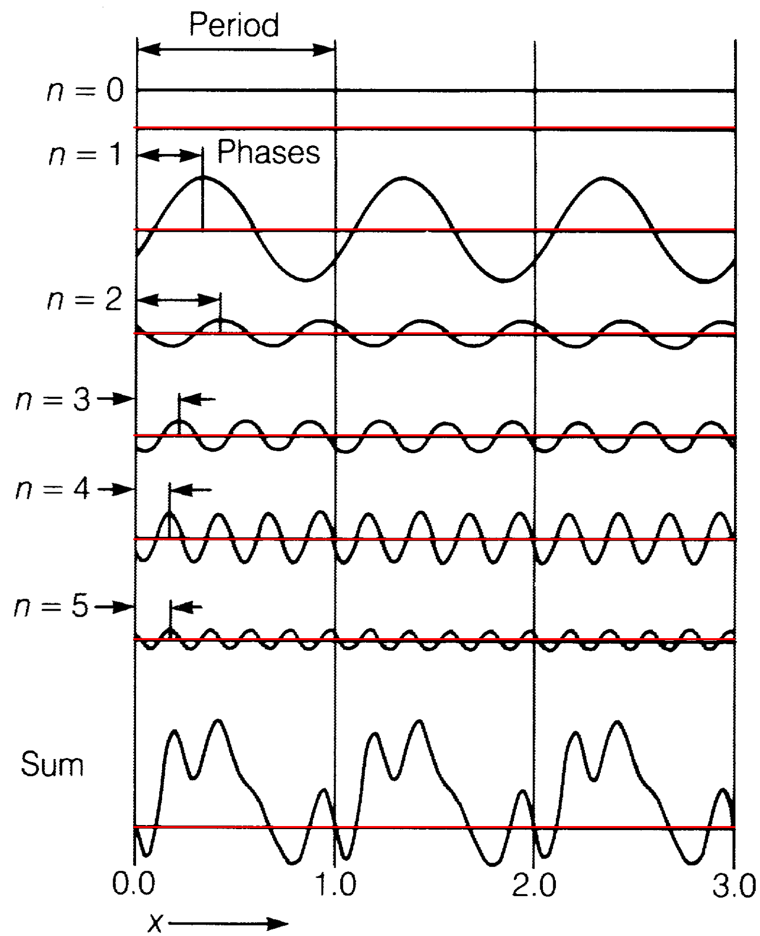


From Eisenberg & Crothers, Fig. 17-14, p.828

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW

Fourier Synthesis:

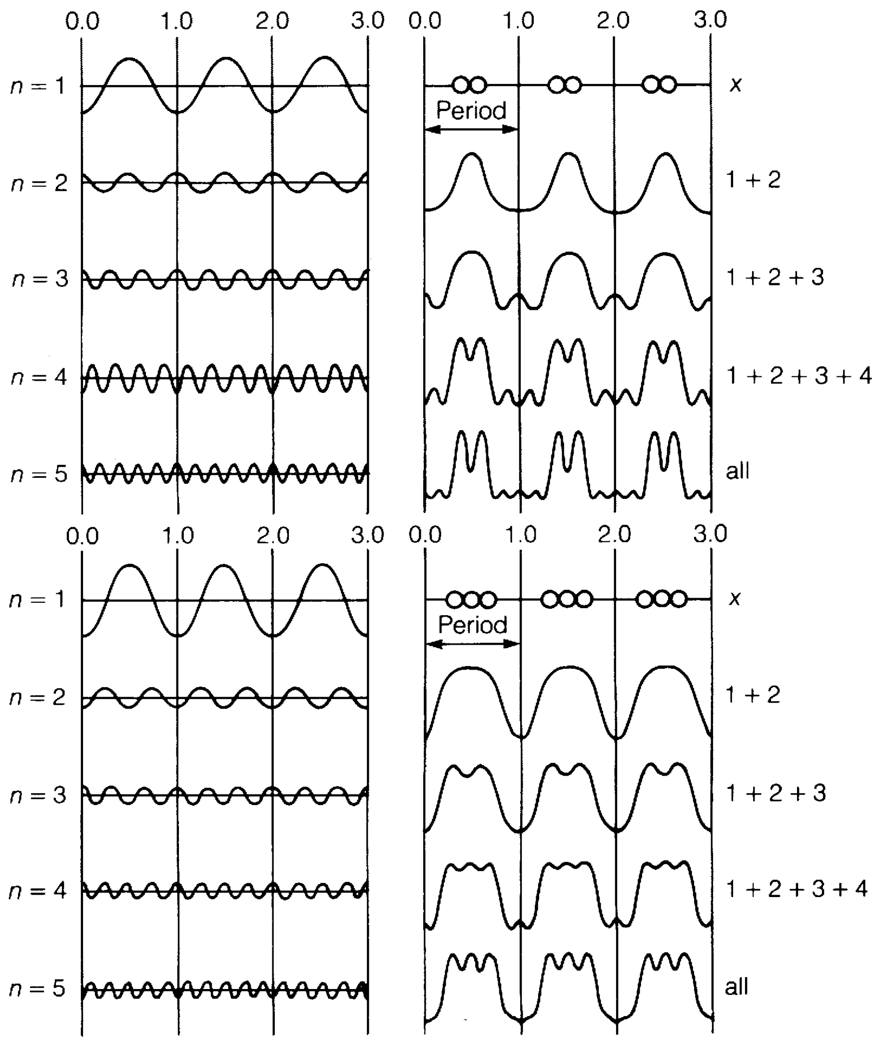
- Mathematical **combination of the waves** to produce the periodic function

Fourier Analysis:

- Opposite process
- **Decomposition** of the periodic function **into its component waves**

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

REVIEW



From Eisenberg & Crothers, Fig. 17-15, p.829

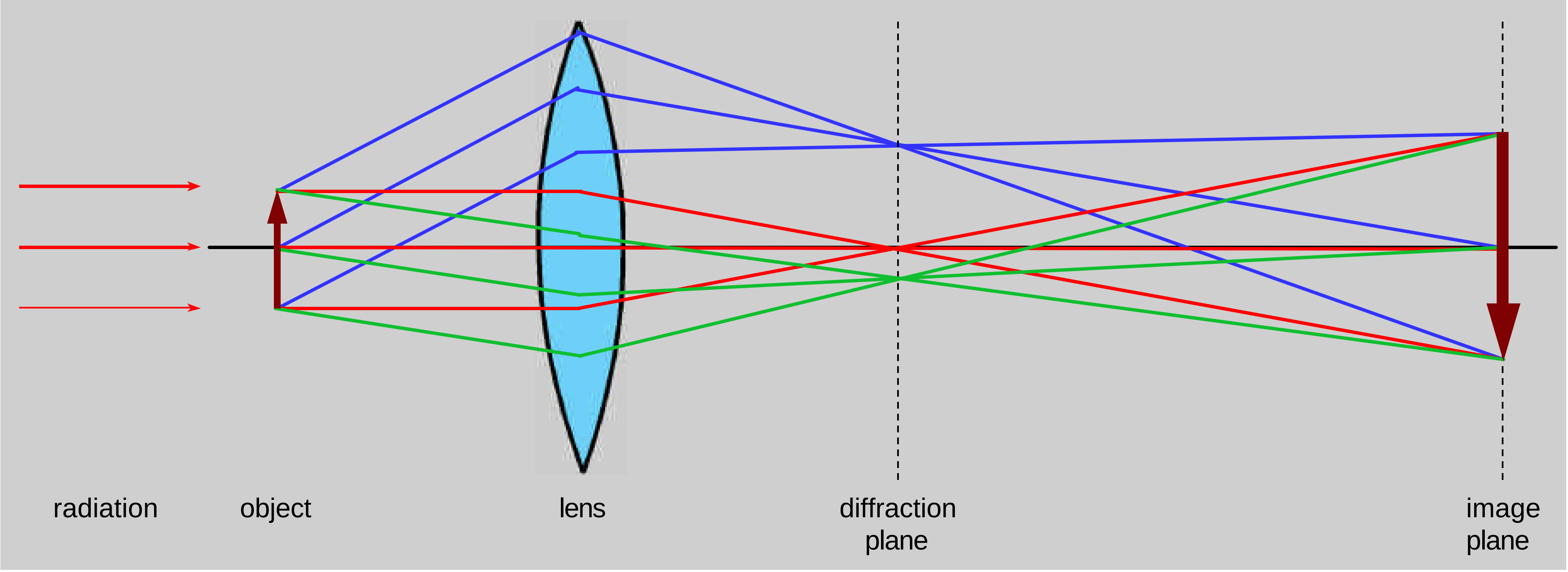
REVIEW

OK, that's enough review

III.C.6 Diffraction

III.C.6.d Image Formation as a Double Diffraction Process

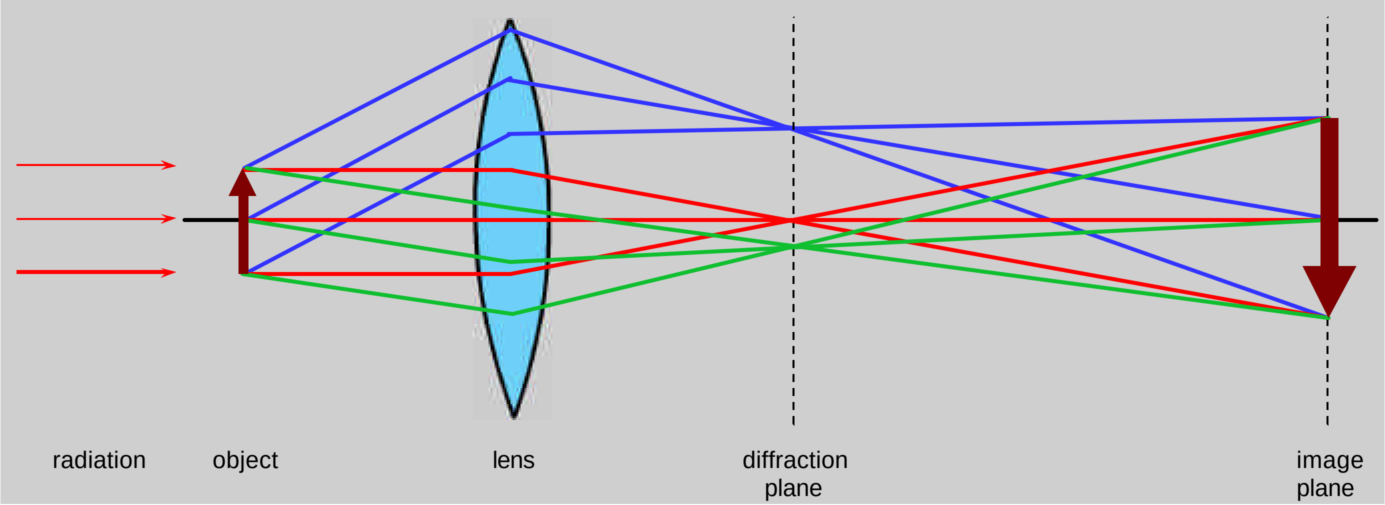
According to Abbe's theory, image formation is a two-stage, **double-diffraction** process



An **image** is the **diffraction pattern of the diffraction pattern** of an **object**

III.C.6 Diffraction

III.C.6.d Image Formation as a Double Diffraction Process

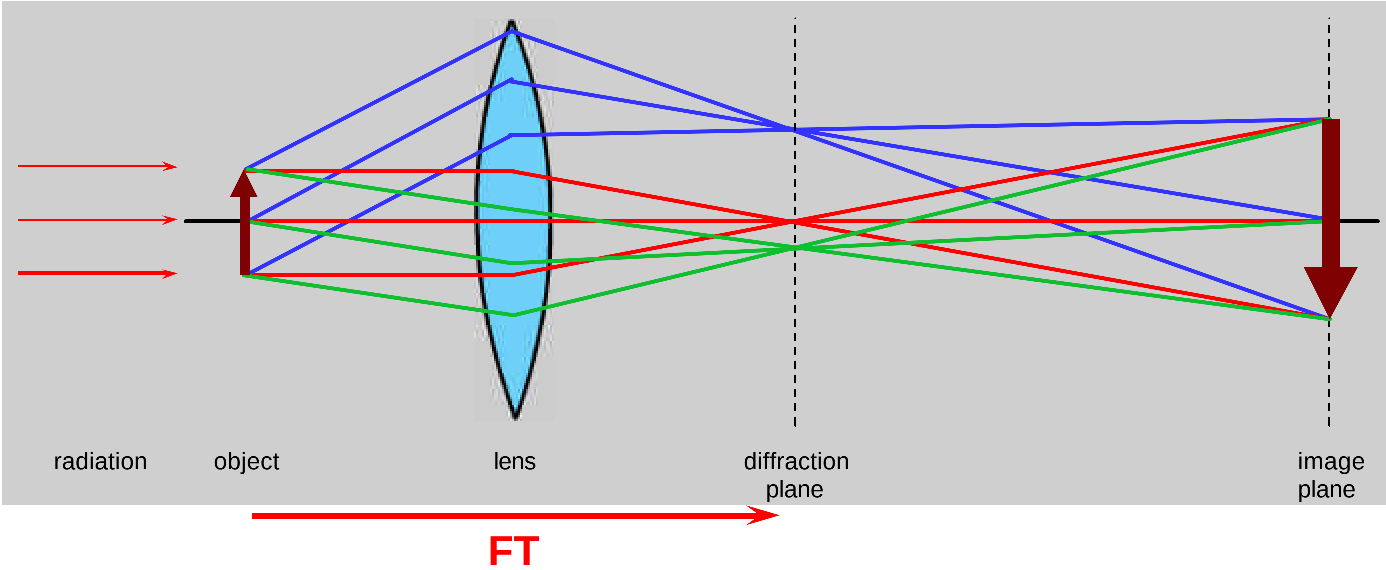


1st stage of image formation

Collimated (parallel) beam of rays incident on the object is scattered and the interference pattern (**Fraunhofer diffraction pattern**) is brought to focus at the **back focal plane** of the lens

III.C.6 Diffraction

III.C.6.d Image Formation as a Double Diffraction Process



1st stage of image formation

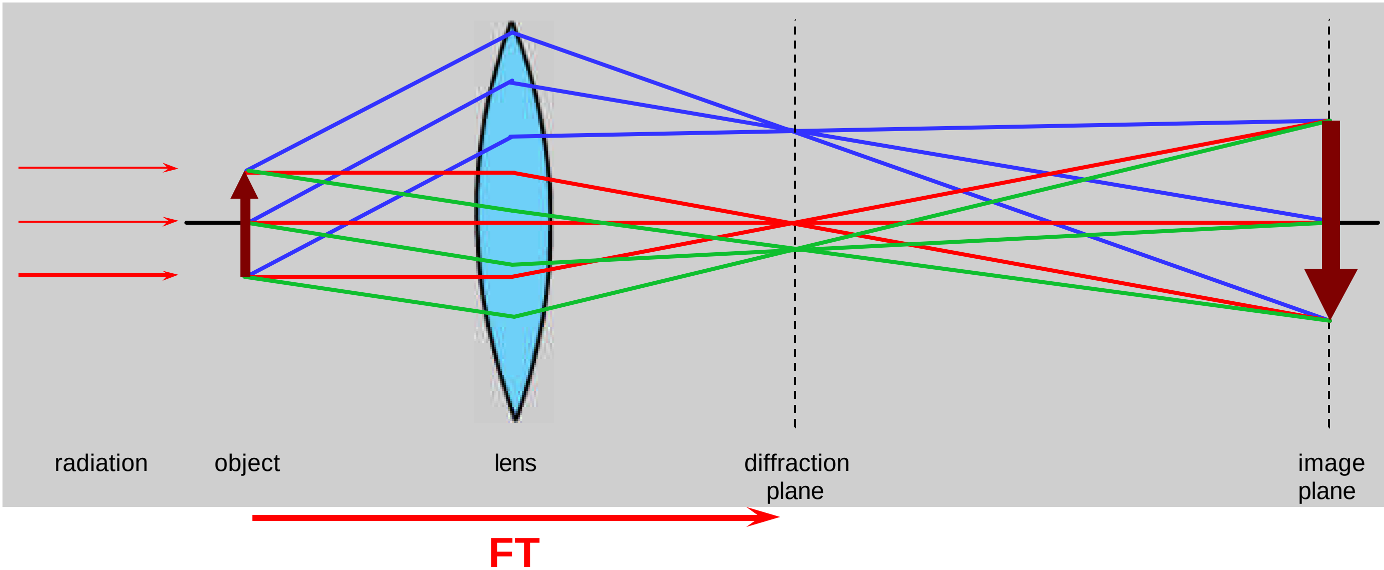
1st stage sometimes referred to as the **forward Fourier transformation**

Intensity distribution of the **recorded diffraction pattern** of an object is proportional to the **square of the Fourier transform** of the object

Terms “transform” and “diffraction pattern” are often used interchangeably, but strictly speaking they are **not** equivalent

III.C.6 Diffraction

III.C.6.d Image Formation as a Double Diffraction Process



1st stage of image formation

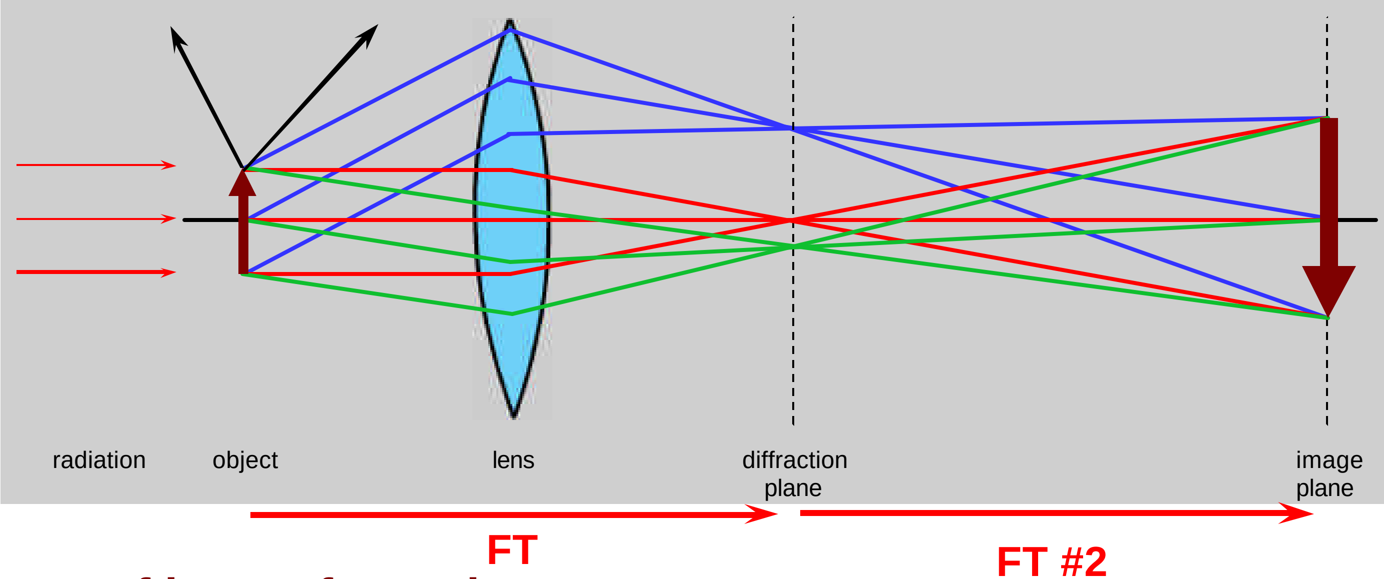
A lens (essential for image formation) focuses the diffraction pattern at a **finite** distance from the object (at back focal plane of lens)

If remove lens, no image forms, but instead **Fresnel** diffraction patterns form at finite distances from the object and the **Fraunhofer** diffraction pattern forms at **infinity** (large distance relative to the object size or wavelength of radiation used)

In X-ray diffraction experiments, there is no lens to focus the X-rays

III.C.6 Diffraction

III.C.6.d Image Formation as a Double Diffraction Process



2nd stage of image formation

Occurs when the **scattered radiation** passes beyond the back focal plane of the lens and **interferes** (recombines) to form an image

Called **back or inverse Fourier transformation stage**

Recall: **Image cannot <u>exactly</u> represent the object** because some scattered rays **never enter the lens** and cannot be focused at the image plane

III.C.6 Diffraction

III.C.6.d Image Formation as a Double Diffraction Process

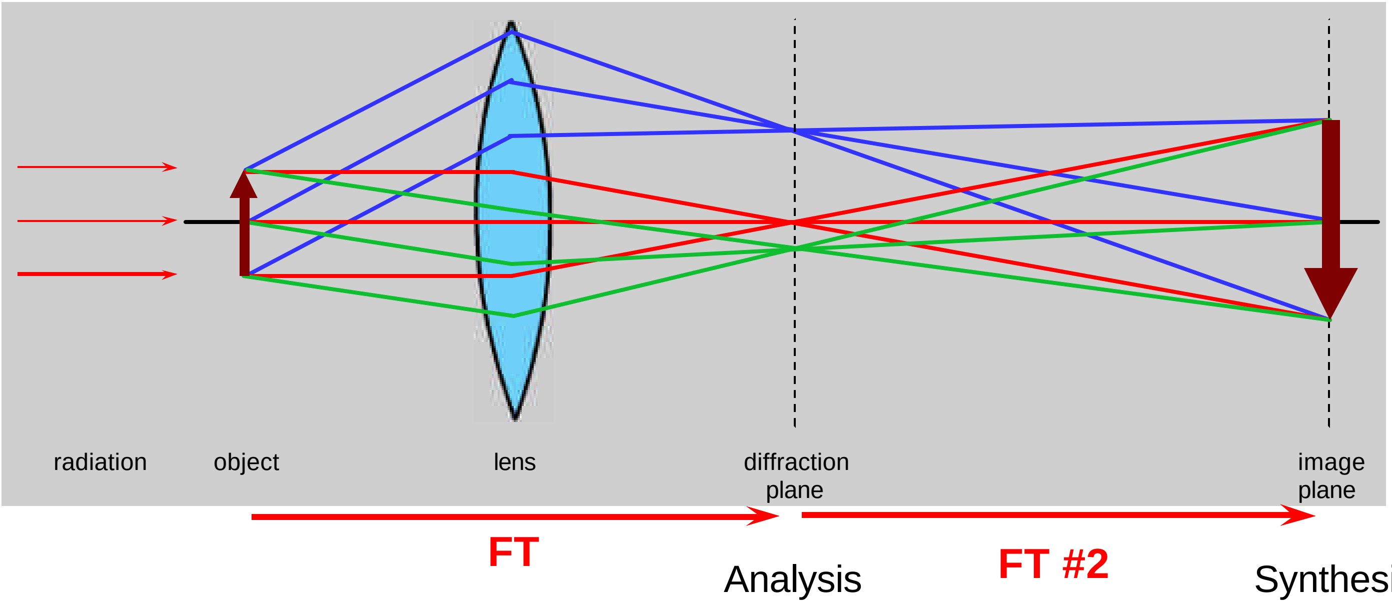


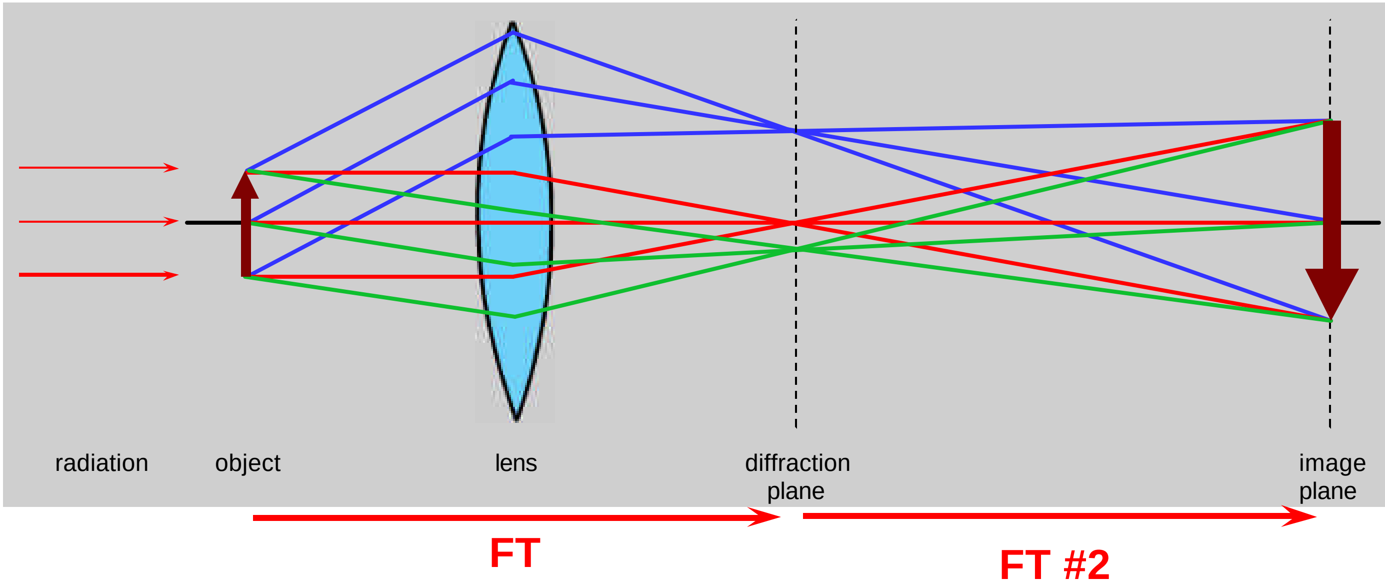
Image formation analogous to:

Fourier analysis in first stage

Fourier synthesis in second stage

III.C.6 Diffraction

III.C.6.d Image Formation as a Double Diffraction Process



Fourier image analysis is a powerful method for analyzing a wide variety of periodic specimens because:

- Separates processing of electron micrograph images into **two stages**

- Formation of diffraction pattern in 1st stage **reveals structural information in a straightforward manner** and **conveniently and objectively separates most of the signal and noise components** in the image

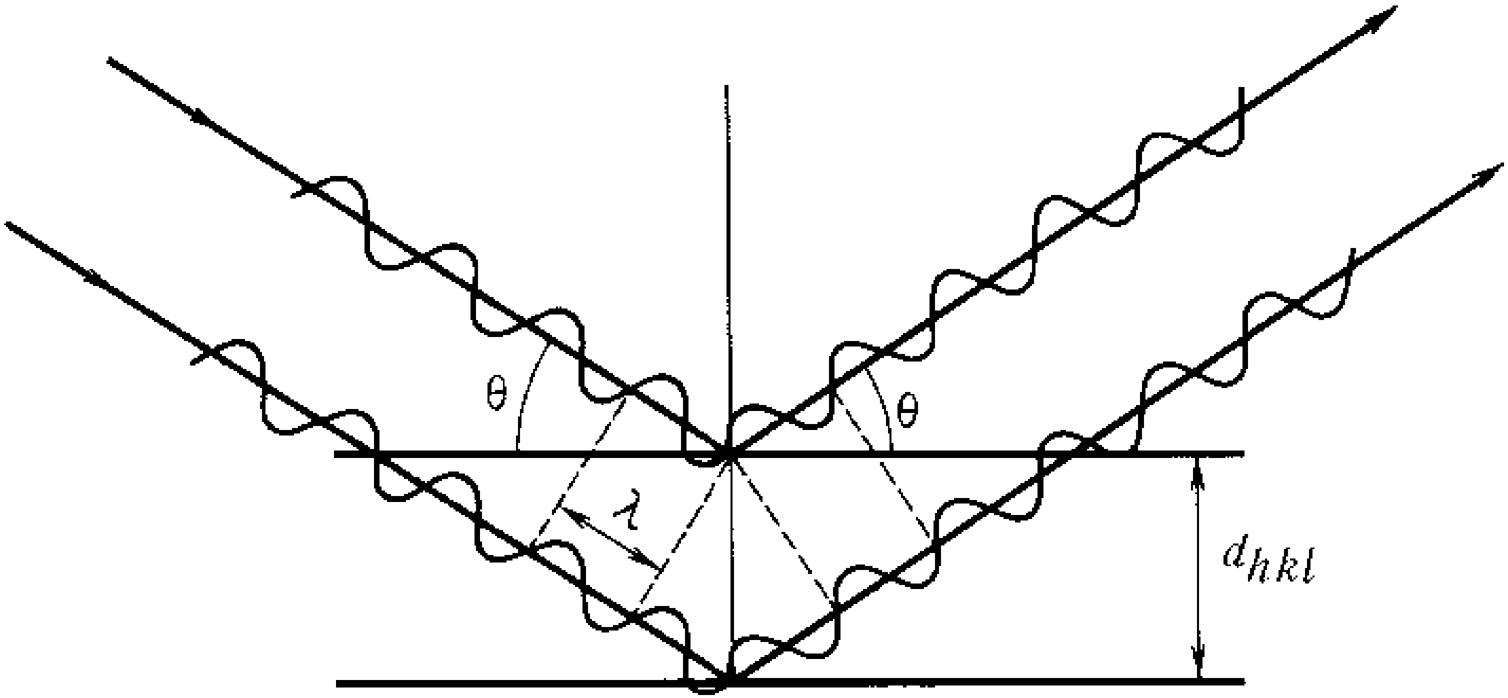
-Transform may then be **manipulated** and **subsequently back-transformed** in 2nd stage to produce a **noise-filtered, reconstructed image**

Bragg's Law

III.C.6 Diffraction

III.C.6.e Bragg Diffraction

Bragg's Law

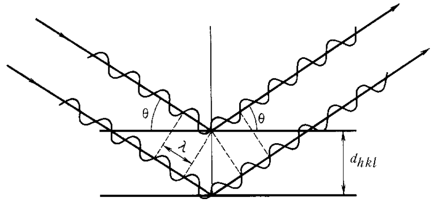


$$n\lambda = 2d_{hkl} \sin q_{???}$$

From Vainshtein, Fig. 4.2, p.224

III.C.6 Diffraction

III.C.6.e Bragg Diffraction



Diffraction can be ***conceptualized*** as arising from the **reflection** of radiation from **planes** of electron density in the 3D crystal (or lines in a 2D crystal)

These planes are **imaginary** parallel planes within crystals

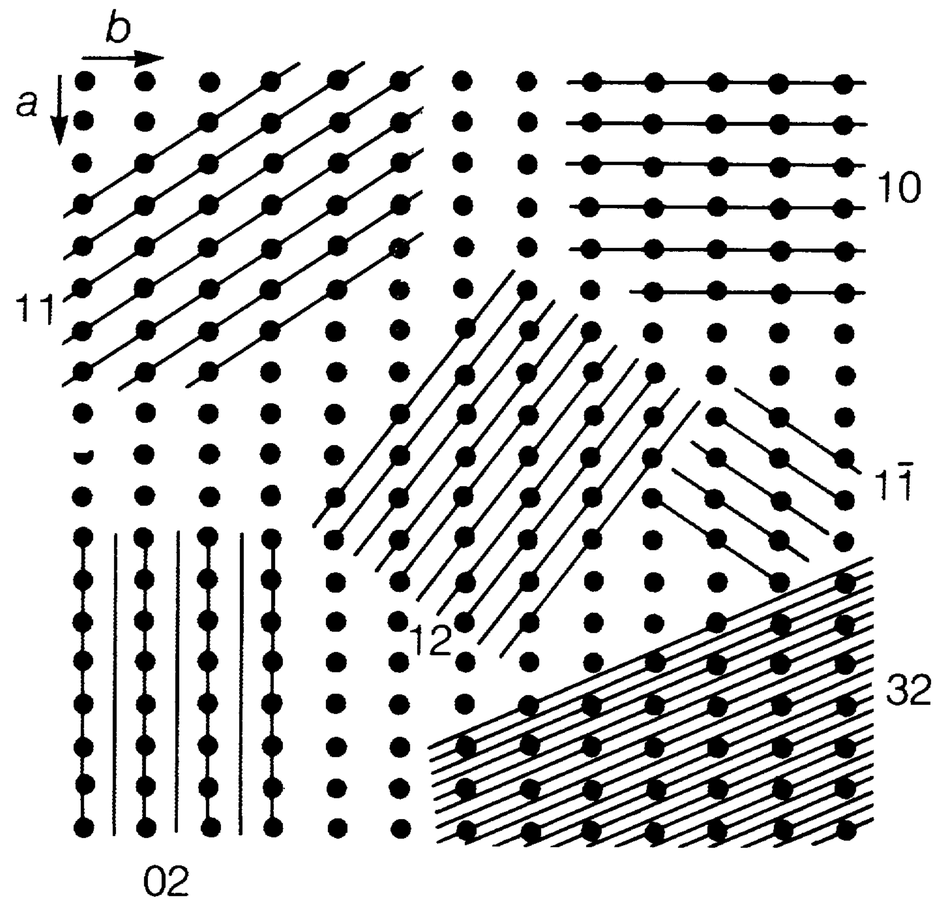
Each set of planes is identified by three **Miller indices**, ***hkl***, which are the reciprocals of the intercepts, in units of cell edge lengths, that the plane makes with the axes of the unit cell

III.C.6 Diffraction

III.C.6.e Bragg Diffraction

Miller Indices of Lattice Planes in a Crystal

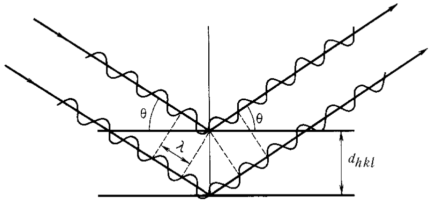
hk(2-D), hkl(3-D):
The reciprocals of the intercepts, in units of cell edge lengths, that the plane/line makes with the axes of the unit cell



From Eisenberg & Crothers, Fig. 17-7, p.811

III.C.6 Diffraction

III.C.6.e Bragg Diffraction



Diffraction from the *hkl* set of planes, separated a distance d_{hkl}, **only occurs for certain orientations of the incident radiation** according to the Bragg relation:

$$n\lambda = 2d_{hkl}\sin q_{???}$$

n = integer

λ = wavelength of incident radiation

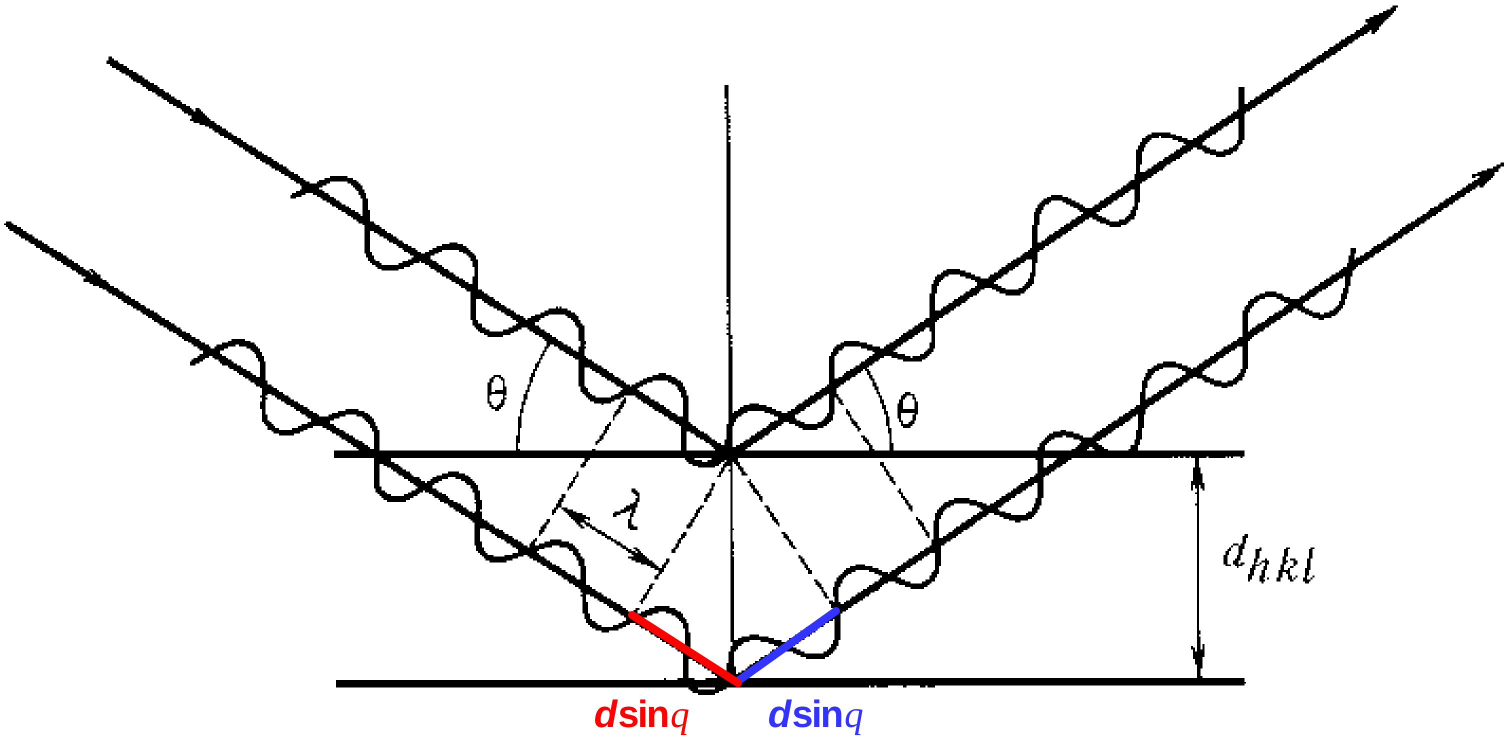
d_{hkl} = crystal lattice spacing between the [*hkl*] set of crystal planes

q_{hkl} = angle of incidence and also of reflection

III.C.6 Diffraction

III.C.6.e Bragg Diffraction

Bragg’s Law



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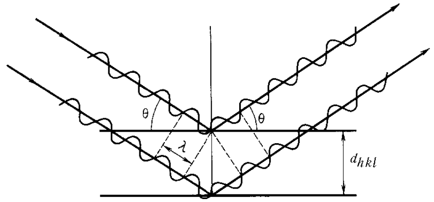
From Vainshtein, Fig. 4.2, p.224

III.C.6 Diffraction

III.C.6.e Bragg Diffraction



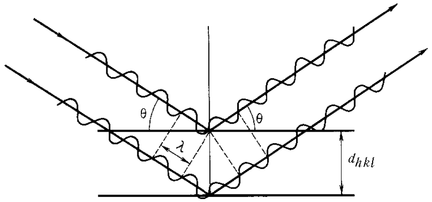
Intensity of each *hkl* reflection is **proportional to the distribution of electron density** in the *hkl* planes

In some planes the density may be **evenly distributed** and the corresponding reflection will be relatively **weak**

In others, where the density is **concentrated** in one region between the planes, the corresponding reflection will be **strong**

III.C.6 Diffraction

III.C.6.e Bragg Diffraction



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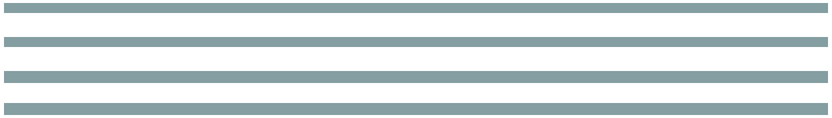
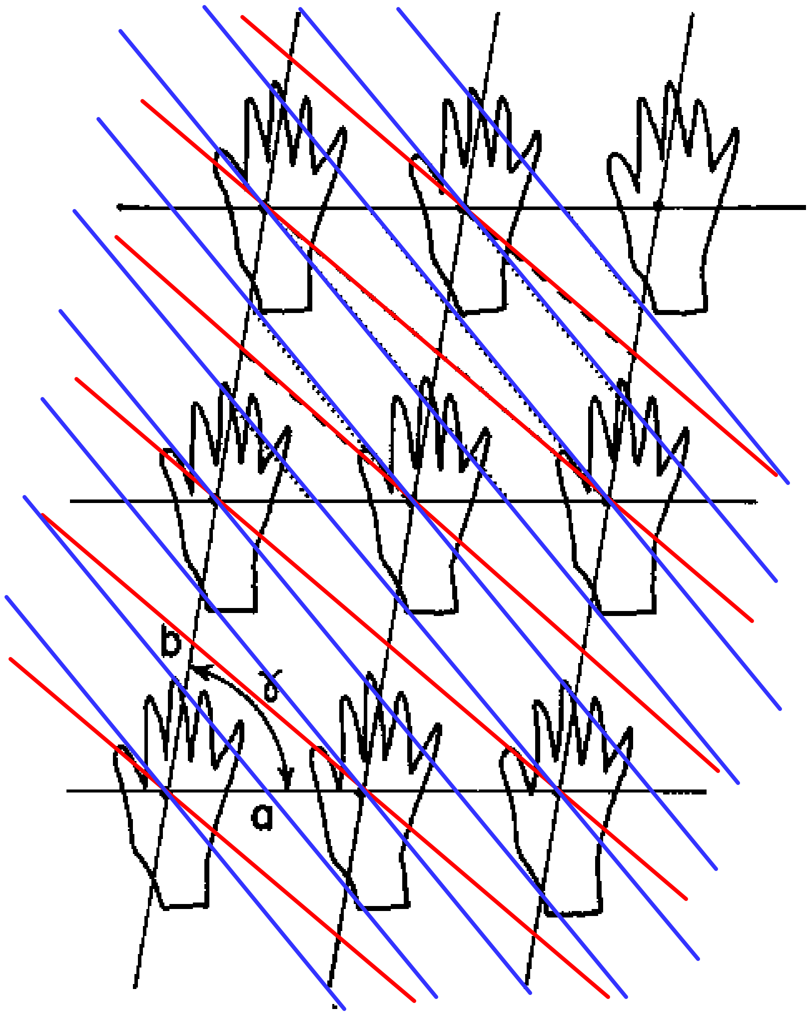


III.C.6 Diffraction

III.C.6.e Bragg Diffraction

2D Crystal of Hands and Corresponding Reciprocal Lattice



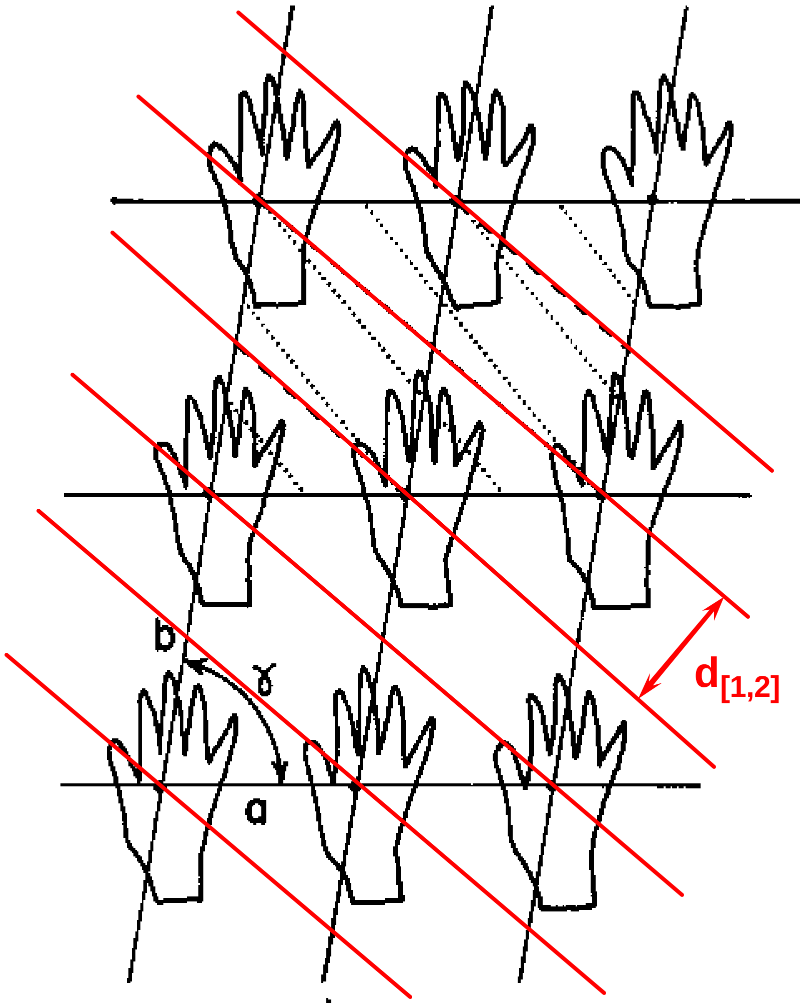
Two Bragg-type “planes” (lines here in 2-D) are depicted in this 2-D crystal of hands

[1,2] and [2,3] are shown

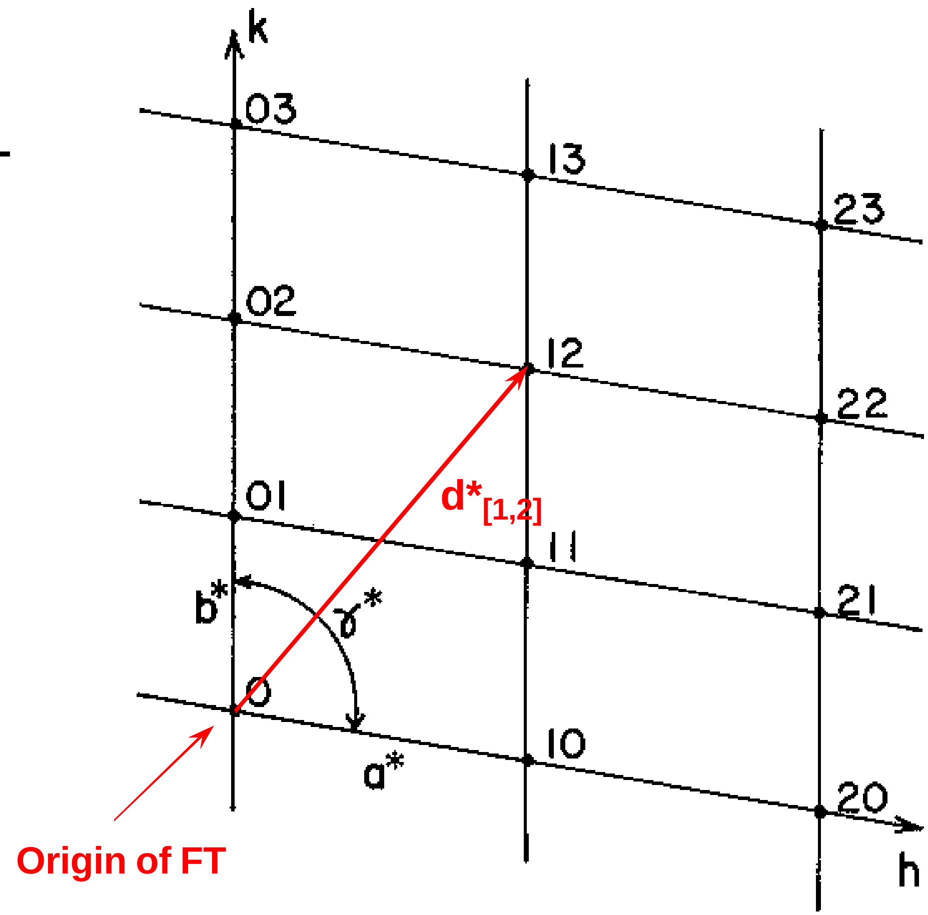
III.C.6 Diffraction

III.C.6.e Bragg Diffraction

2D Crystal of Hands and Corresponding Reciprocal Lattice



real space

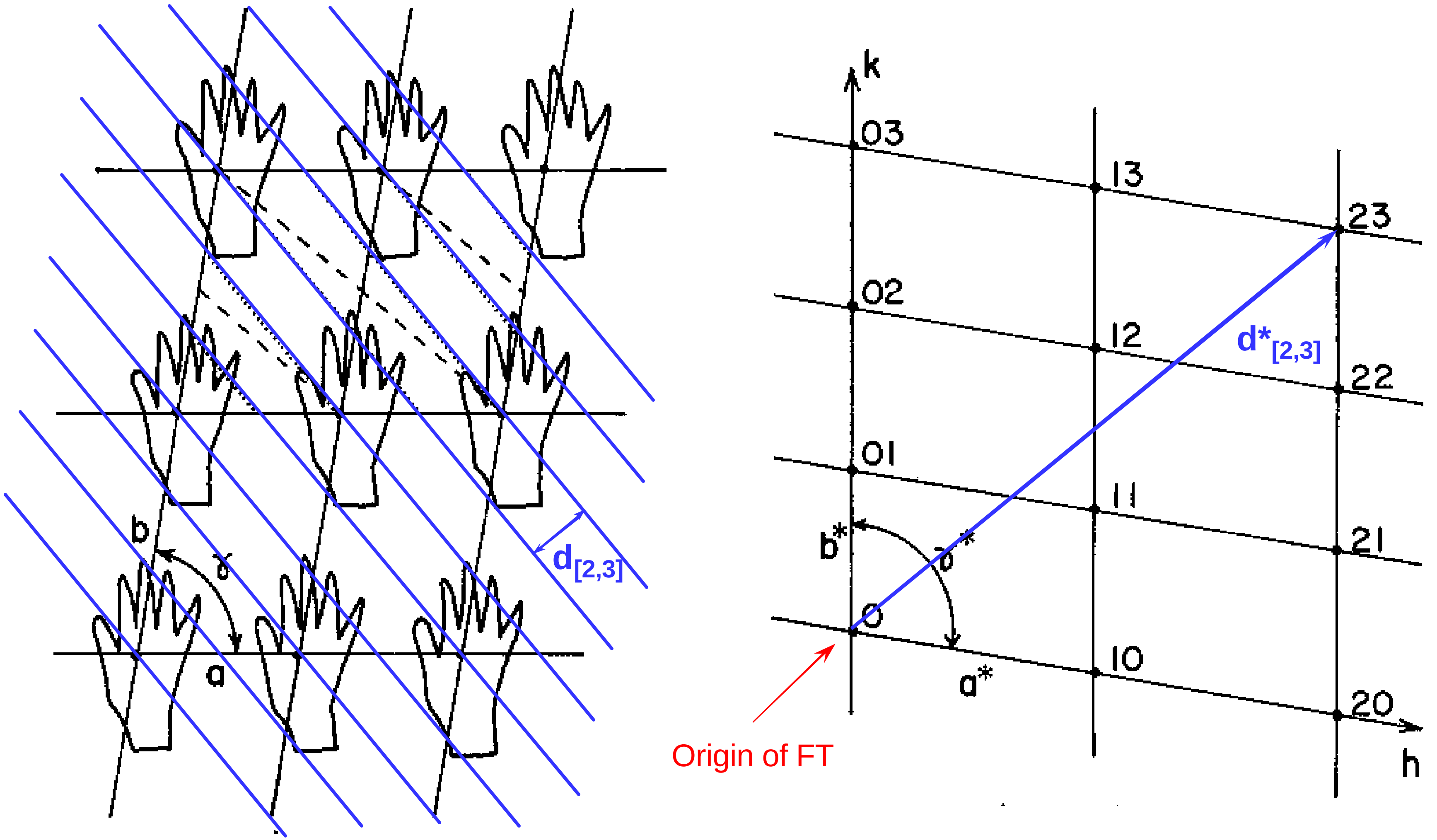


reciprocal space

III.C.6 Diffraction

III.C.6.e Bragg Diffraction

2D Crystal of Hands and Corresponding Reciprocal Lattice



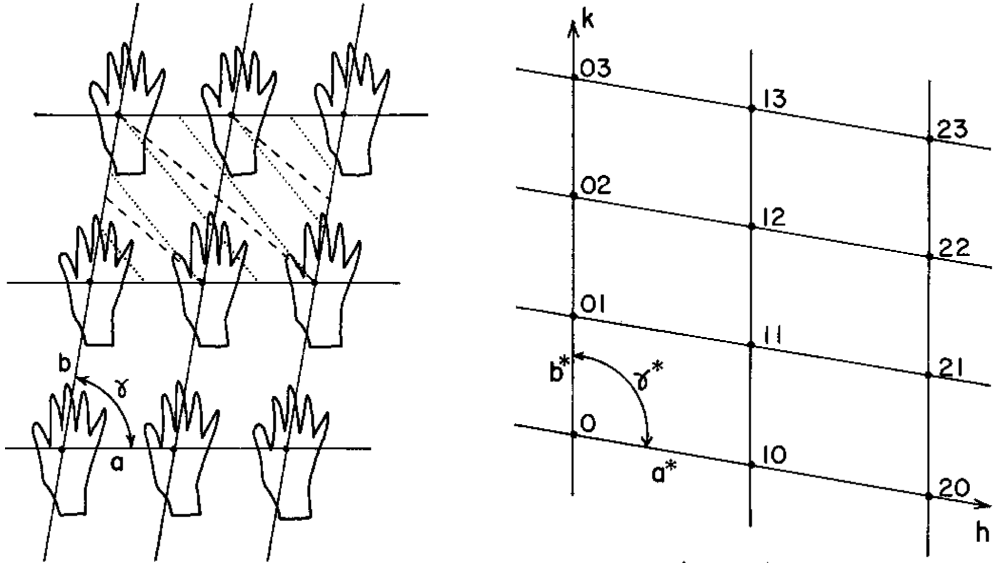
real space

reciprocal space

III.C.6 Diffraction

III.C.6.e Bragg Diffraction

real space



reciprocal space

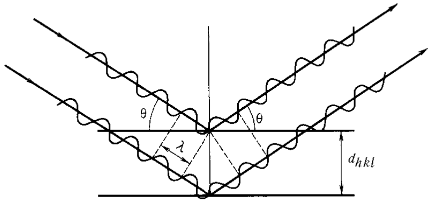
Density that lies between the dashed lines diffract at the reciprocal lattice point labeled [1,2] (and also its **Friedel mate**, [-1,-2], not shown)

Spacing (perpendicular distance) between the lines is **inversely proportional** to the distance of the [1,2] reciprocal lattice point from the origin

Relative to the transform origin (where $\theta_{hkl} = 0°$, which corresponds to direction of **unscattered** radiation), the reciprocal lattice point appears in a direction **normal** to the set of lines

III.C.6 Diffraction

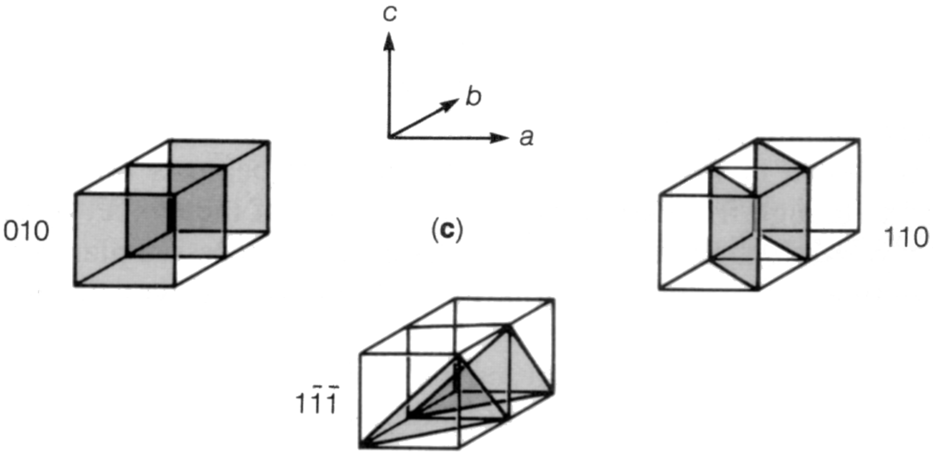
III.C.6.e Bragg Diffraction



For 2D, periodic structures, each **Friedel pair** of spots arises from a set of fringes (sinusoidal density waves) of particular spacing (frequency) and orientation in the crystal

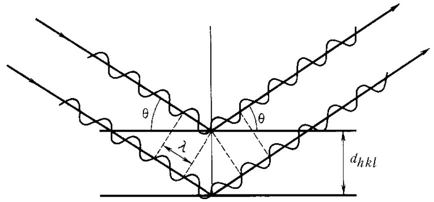
The so-called **Miller index** of each spot corresponds to the two wave numbers (*h* and *k*) which describe the number of wave cycles per repeat in the *a* and *b* directions.

For diffraction from **3D** crystals, the Miller index of each spot is assigned three wave numbers (***h,k,l***) corresponding to the number of wave cycles per repeat in the three unit cell directions (*a,b,c*)



III.C.6 Diffraction

III.C.6.e Bragg Diffraction



Each spot or reflection in the diffraction pattern may be **mathematically represented in real space as a plane wave** whose amplitude is proportional to the square root of the spot intensity and whose phase is measured relative to a particular origin point in the crystal (*e.g.* the unit cell origin).

When the amplitudes and phases (structure factors, F_{hkl}) of all spots in the 3D transform are known, the corresponding real space density waves can be mathematically summed (Fourier synthesis) to reconstruct the 3D object density

In 1D: $$r(x) = \sum_{n=-\infty}^{\infty} A_n \cos(2pnx/a)$$

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

III.C.6 Diffraction

KEY CONCEPTS:

- **Any periodic object** can be represented mathematically as a **summation of sinusoidal waves** (Fourier synthesis)

- Image formation is considered a **double diffraction** process

- **Bragg's Law:** visualizes diffraction as arising from **reflection** of radiation from planes in crystals

- **Structure factors** are **complex** numbers

- Concepts of **convolution and multiplication** (**sampling**) help us understand fundamental properties of Fourier transforms

Structure Factor

III.C.6 Diffraction

III.C.6.f Structure Factor

The **structure factor** describes the scattering from **all** atoms of the unit cell for a **particular** Bragg reflection

Each diffracted ray, or reflection, is described by **one** structure factor, F_{hkl}

F_{hkl} is a **complex number** whose **magnitude** (amplitude) is proportional to the square root of the intensity of the *hkl* reflection

Each structure factor may be regarded as a sum of the contributions of the radiation scattered in the same direction **from all atoms** within the unit cell

III.C.6 Diffraction

III.C.6.f Structure Factor

For **an object with *n* atoms**, the structure factor equation is:

$$F_{hkl} = \sum_{j=1}^{n} f_j \exp\left[2pi\left(hx_j + ky_j + lz_j\right)\right]$$

f_j = atomic scattering factor for atom *j*

= ratio of $\frac{\text{amplitude scattered by the atom}}{\text{amplitude scattered by a single electron}}$

= atomic number at **zero** scattering angle

< atomic number at **larger** scattering angles

hkl = particular set of diffracting planes

x_j, y_j, z_j = fractional unit cell coordinates for atom *j* in the unit cell

III.C.6 Diffraction

III.C.6.f Structure Factor

$$F_{hkl} = \sum_{j=1}^{n} f_j \exp\left[2pi\left(hx_j + ky_j + lz_j\right)\right]$$

Recall: $e^{i\theta} = \cos\theta + i\sin\theta$, so above can be rewritten:

$$F_{hkl} = \sum_{j=1}^{n} f_j \left\{\cos\left[2p\left(hx_j + ky_j + lz_j\right)\right] + i\sin\left[2p\left(hx_j + ky_j + lz_j\right)\right]\right\}$$

$$= \sum_{j=1}^{n} f_j \cos\left[2p\left(hx_j + ky_j + lz_j\right)\right] + i\sum_{j=1}^{n} f_j \sin\left[2p\left(hx_j + ky_j + lz_j\right)\right]$$

$$= A_{hkl} + iB_{hkl}$$

Thus, F_{hkl} is a **complex quantity**, with **real** (A_{hkl}) and **imaginary** (B_{hkl}) parts

III.C.6 Diffraction

III.C.6.f Structure Factor

Argand Diagram

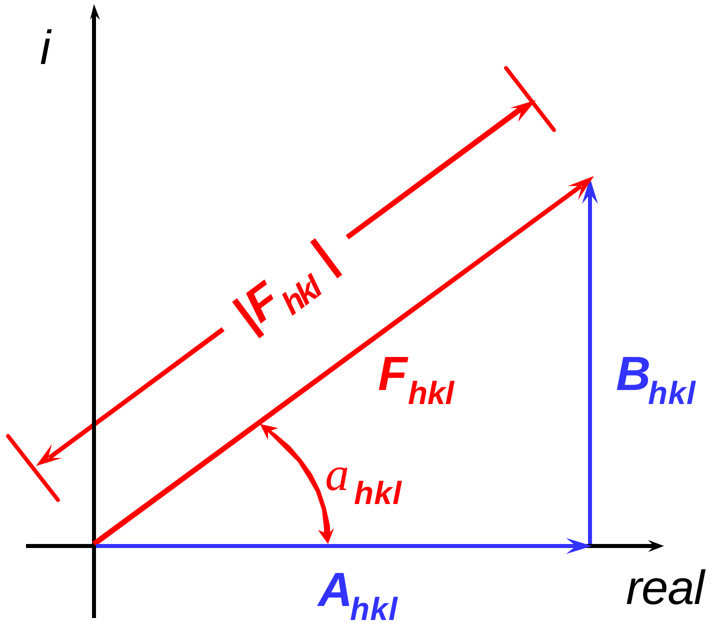
A convenient way to depict F_{hkl}

F_{hkl} is plotted as a **vector quantity** with:

horizontal axis = **real axis**

vertical axis = **imaginary axis**

Vector F_{hkl} makes an **angle** α_{hkl} with respect to real axis



F_{hkl} = vector sum of A_{hkl} (**real** component) and B_{hkl} (**imaginary** component)

Magnitudes of vectors A_{hkl} and B_{hkl} are: $|F_{hkl}|\cos(\alpha_{hkl})$ and $|F_{hkl}|\sin(\alpha_{hkl})$

III.C.6 Diffraction

III.C.6.f Structure Factor

Structure factor amplitude (modulus or magnitude of F_{hkl}): ½$\boldsymbol{F_{hkl}}$½

$$|F_{hkl}| = [(A_{hkl})^2 + (B_{hkl})^2]^{1/2}$$

Structure factor phase: a_{hkl}

Since $F_{hkl} = A_{hkl} + iB_{hkl}$

$$= \underbrace{|F_{hkl}|\cos(a_{hkl})}_{\textbf{real}} + \underbrace{|F_{hkl}|\,i\sin(a_{hkl})}_{\textbf{imaginary}}$$

$$= |F_{hkl}|\exp(i\,a_{hkl})$$

III.C.6 Diffraction

III.C.6.f Structure Factor

For a **3D** structure with **continuous density**, $r(xyz)$, the structure factor equation becomes:

$$F_{hkl} = V \iiint r(xyz) \exp(2pi\,[hx+ky+lz])\; dx\, dy\, dz$$

Integration is over the **entire unit cell volume**, *V*.

Reemphasizes a property of Fourier transforms: **Every point** in the **object** contributes to **every point** in the **diffraction pattern**

III.C.6.g Convolution and Multiplication

- Convolution
- Multiplication

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

These concepts provide a fundamental basis for under-standing diffraction from crystalline objects

According to Holmes and Blow (1965), **convolution** of two functions can be described in the following way:

*"Set down the **origin** of the first function **in every possible position of the second**, **multiply** the value of the first function in each position by the value of the second at that point and take the **sum** of all such possible operations."*

Sounds simple enough…right?

*Well, sort of…especially if one function is "**simple**"*

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

Mathematical expression for **convolution**:

$$c(u) = \int_{-\infty}^{\infty} f(x)g(u-x)dx$$

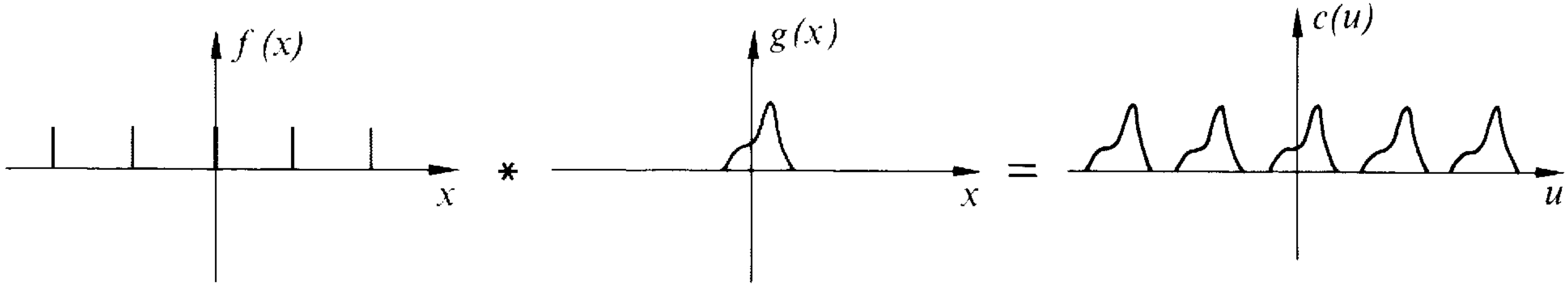
This is known as the convolution of *f(x)* and *g*(*x*), and may be written in shorter form as:

$$c(u) = f(x) * g(x)$$

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

Convolution of *f(x)*, an array of d functions, with *g(x)*, an arbitrary function



From Sherwood, Fig. 5.19, p.173

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

$$c(u) = f(x) * g(x)$$

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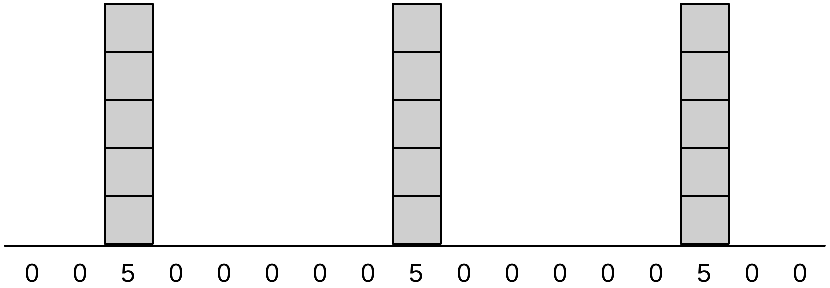
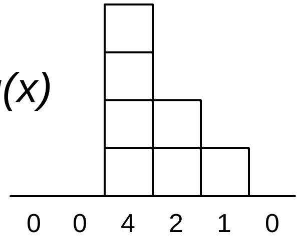
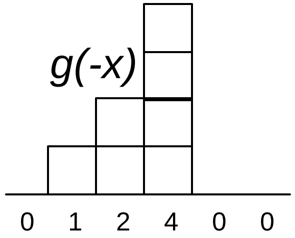
f(x)



g(x)



g(-x)



c(u)

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

$$c(u) = f(x) * g(x)$$

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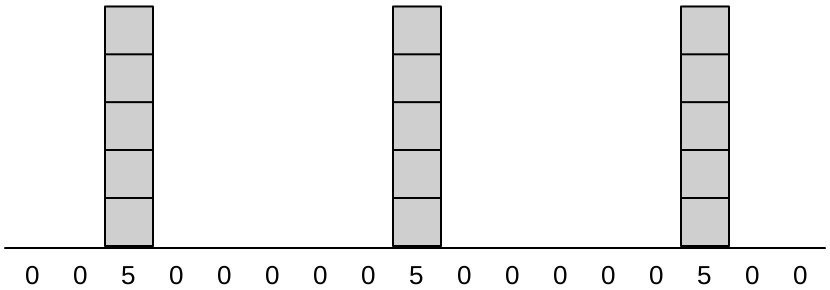

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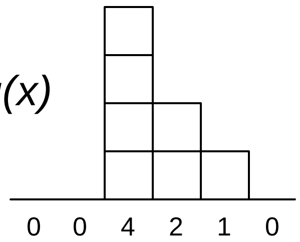

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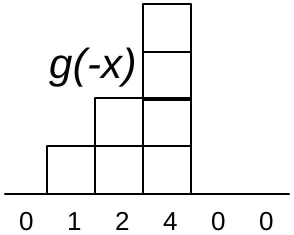

c(u)

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

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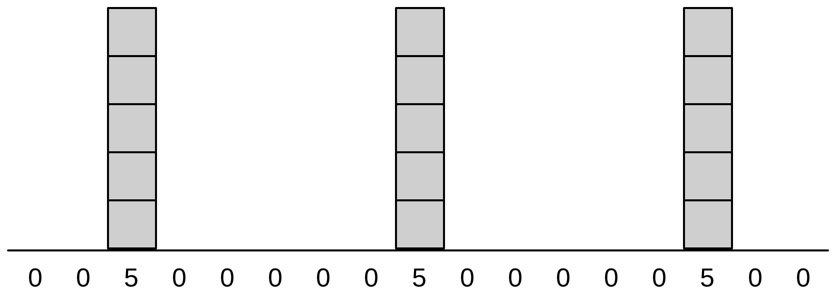
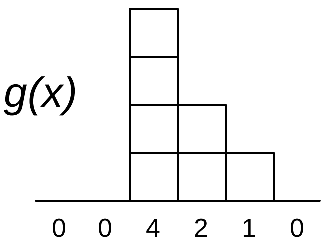


g(x)



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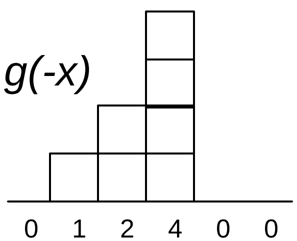
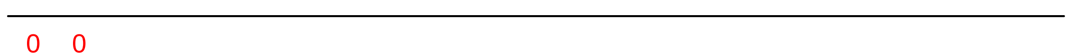


c(u)



III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

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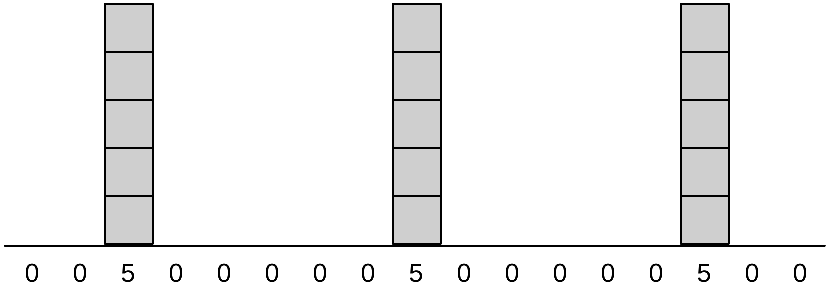
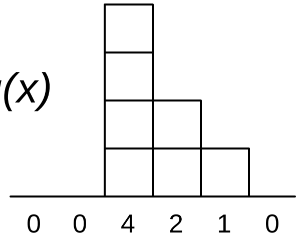
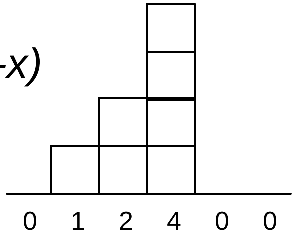
f(x)



g(x)



g(-x)



c(u)

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

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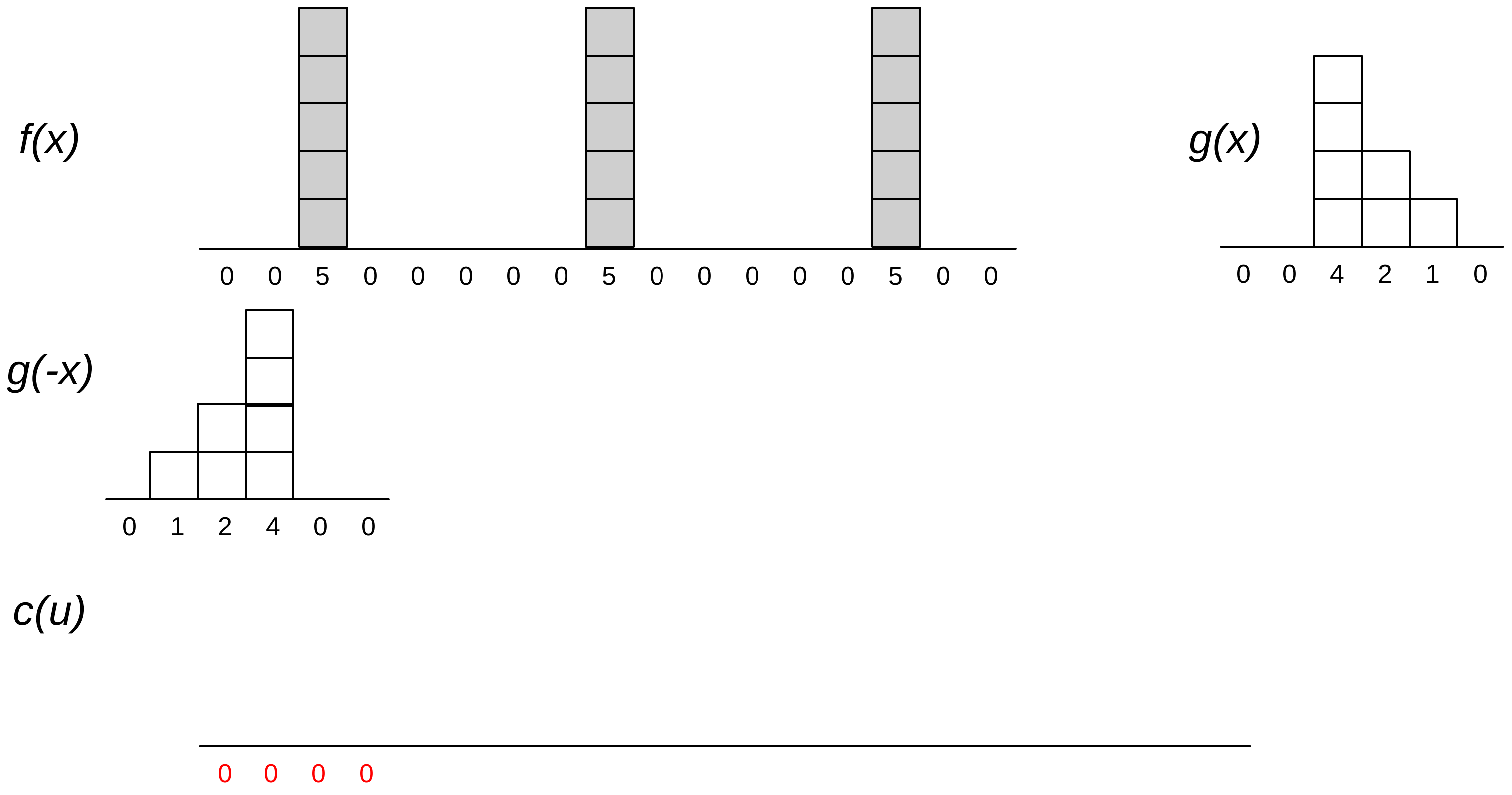

III.C.6 Diffraction

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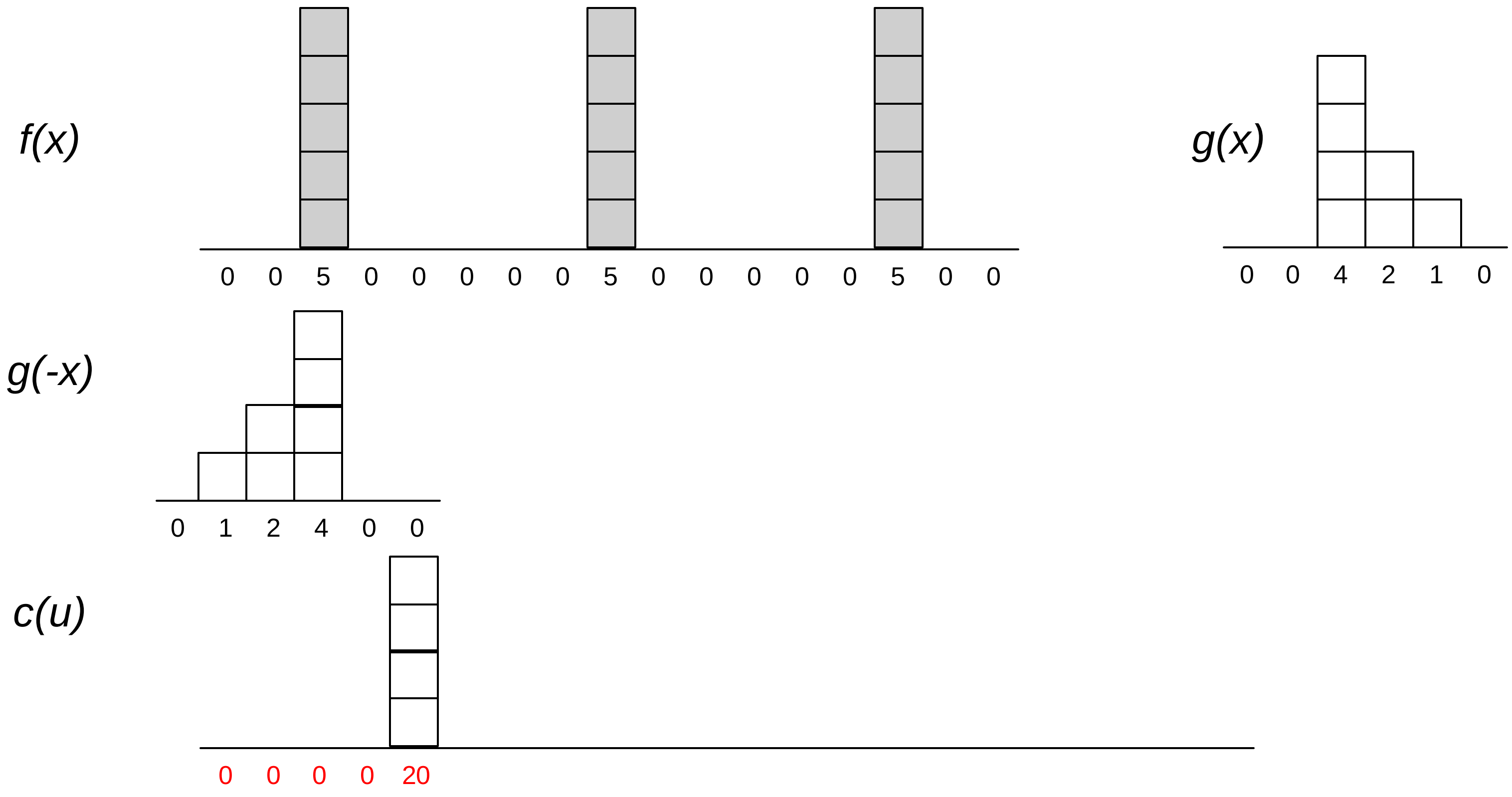

III.C.6 Diffraction

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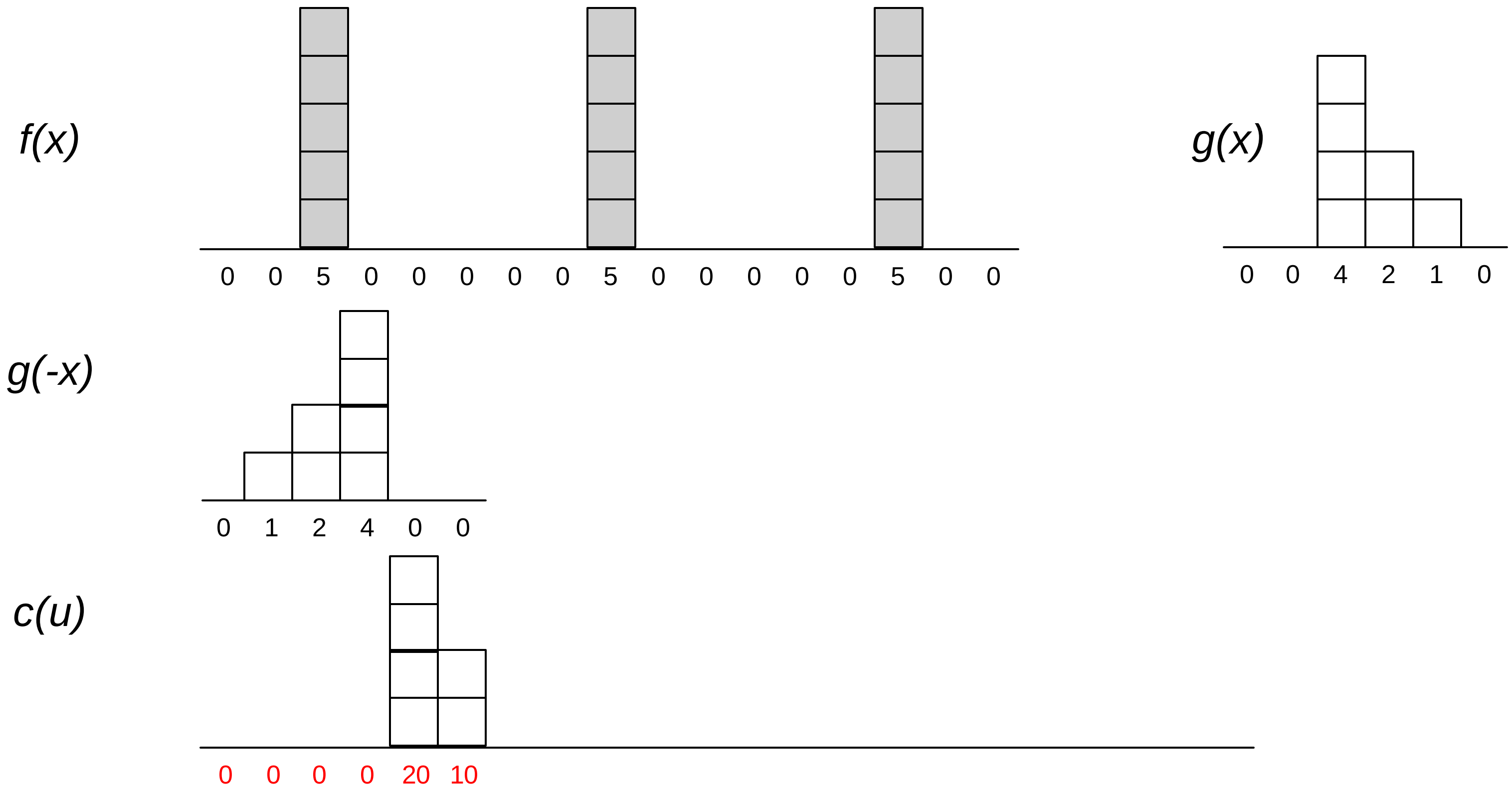

III.C.6 Diffraction

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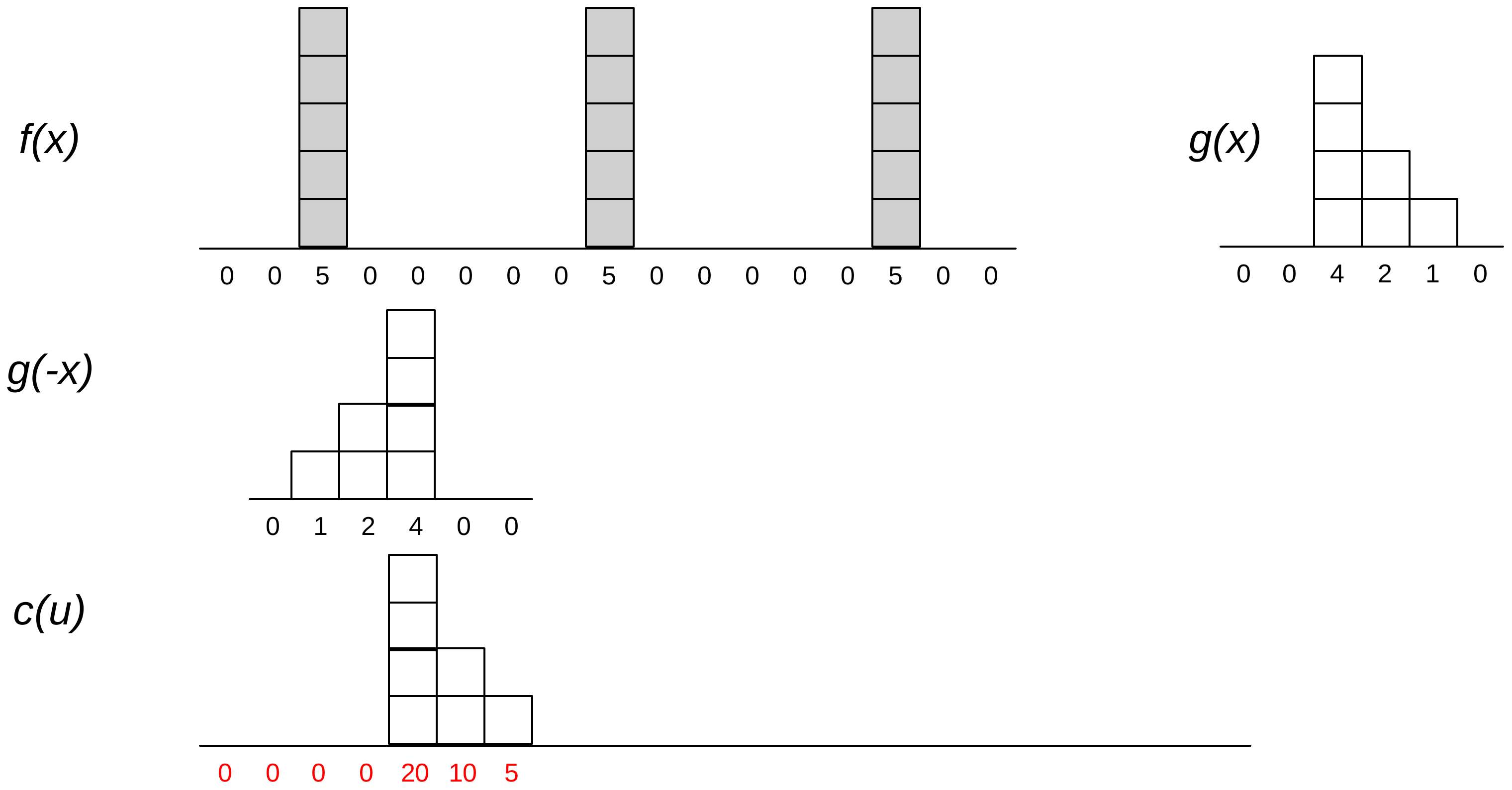

III.C.6 Diffraction

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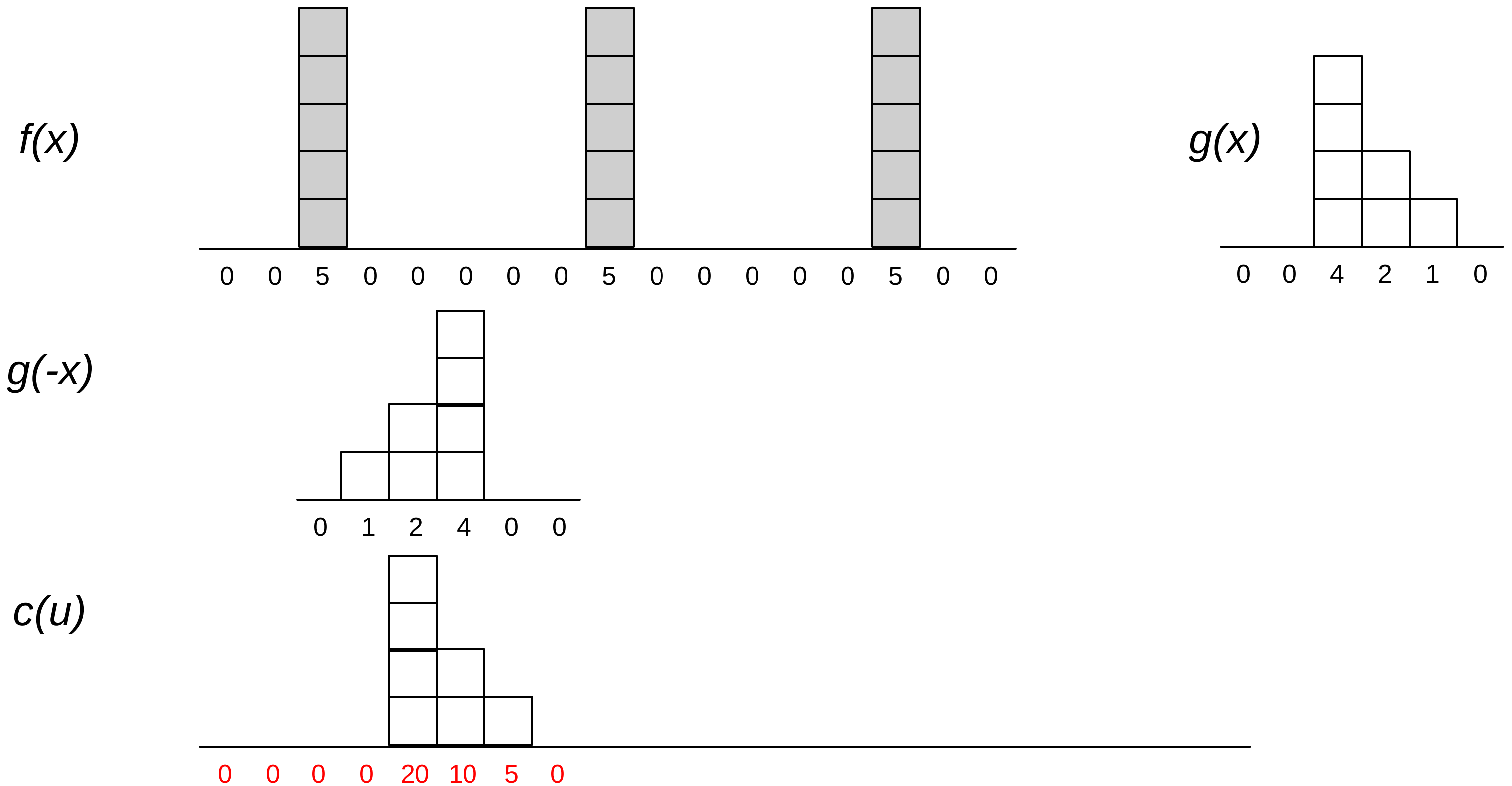
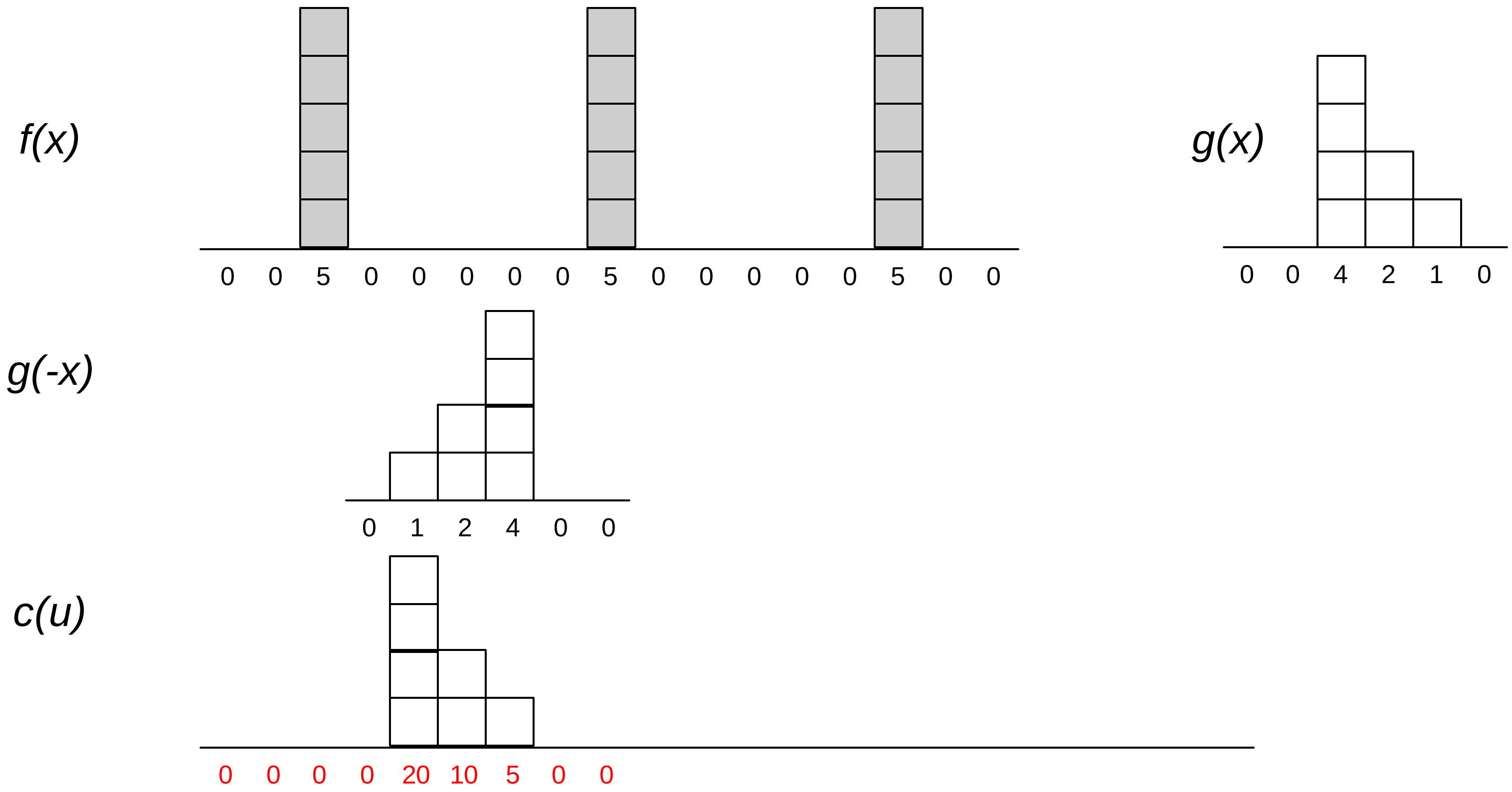


III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

$$c(u) = f(x) * g(x)$$

$$c(u) = \int_{-\infty}^{\infty} f(x)g(u-x)dx$$



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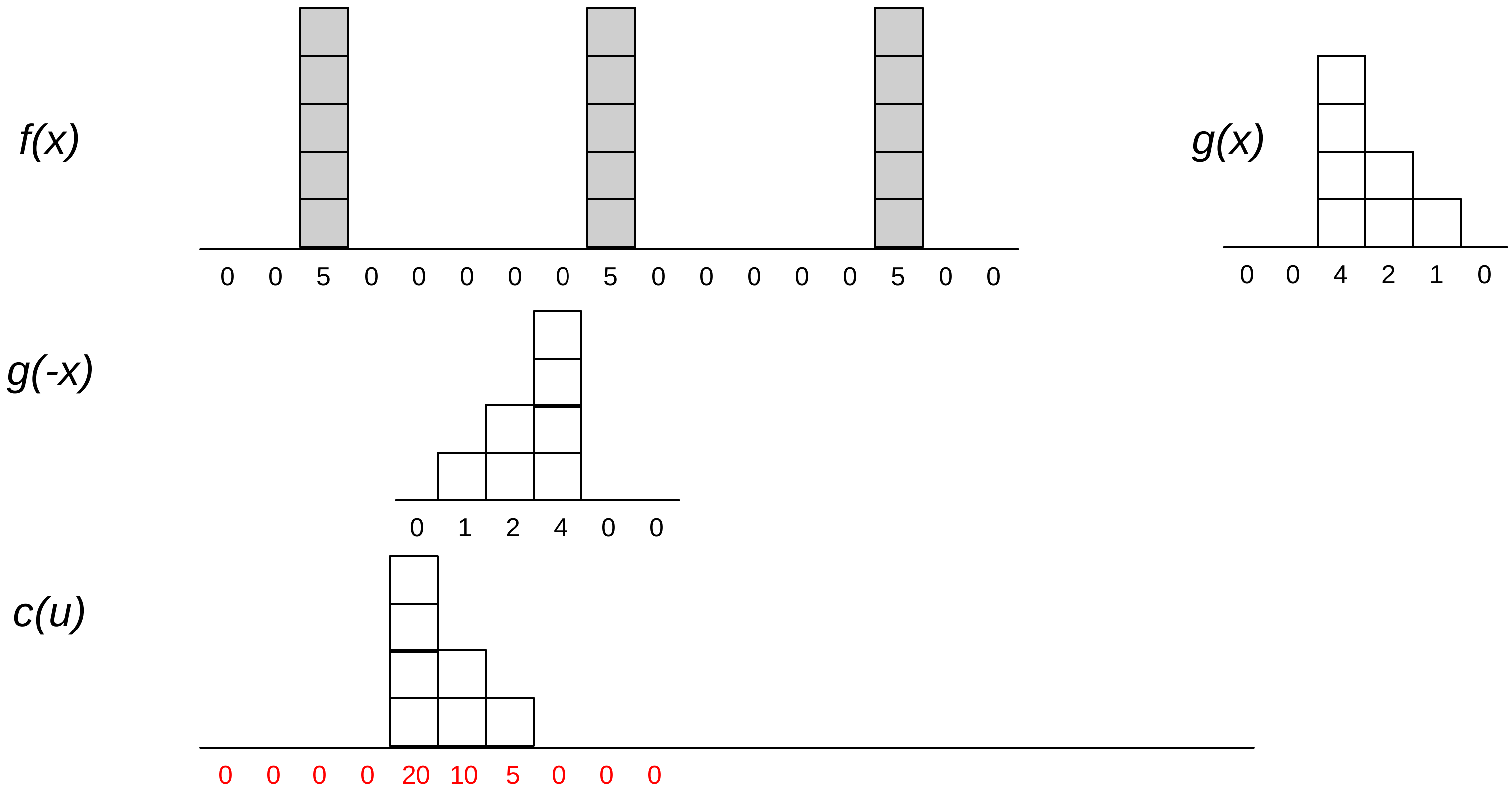

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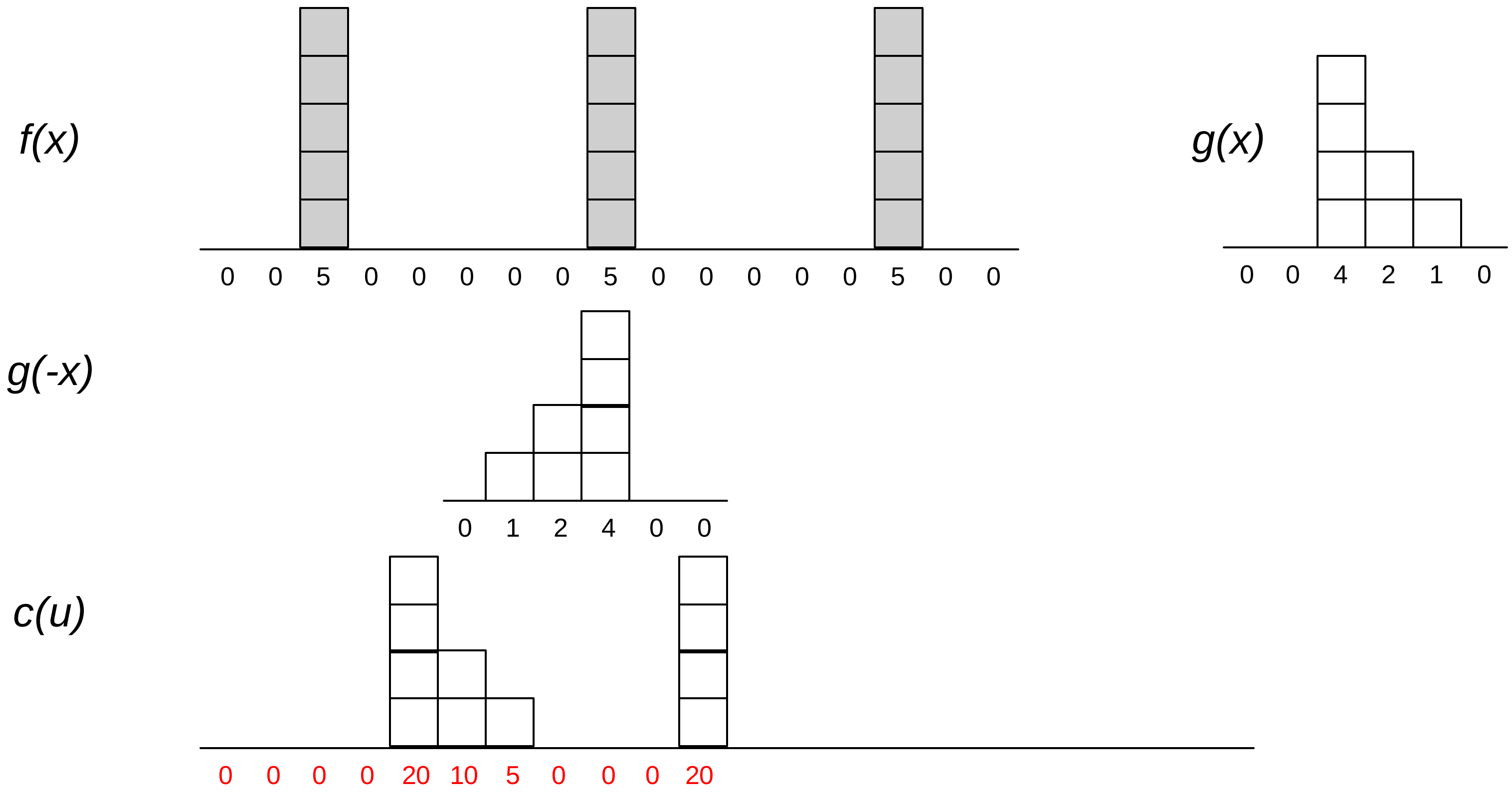

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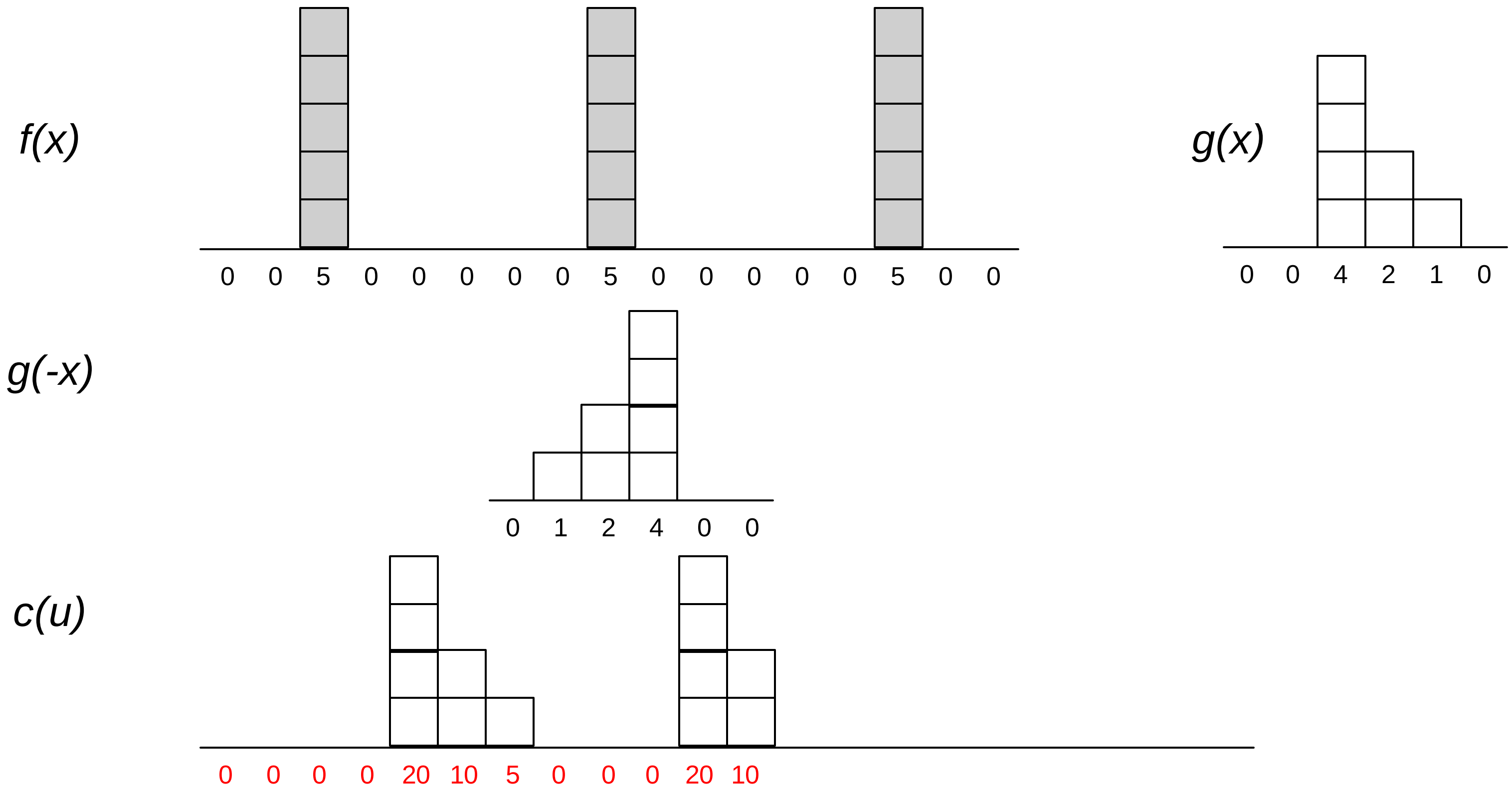

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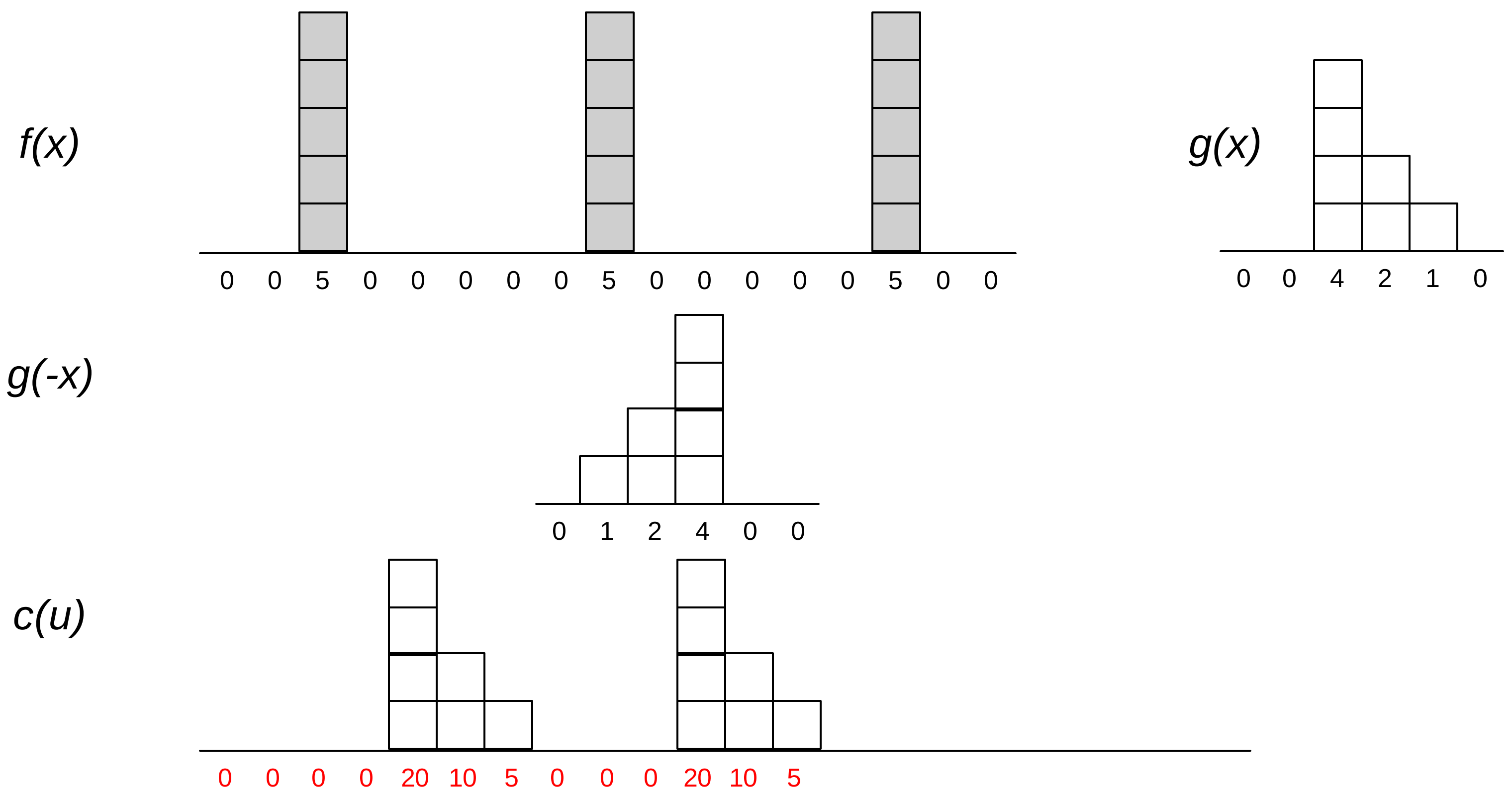

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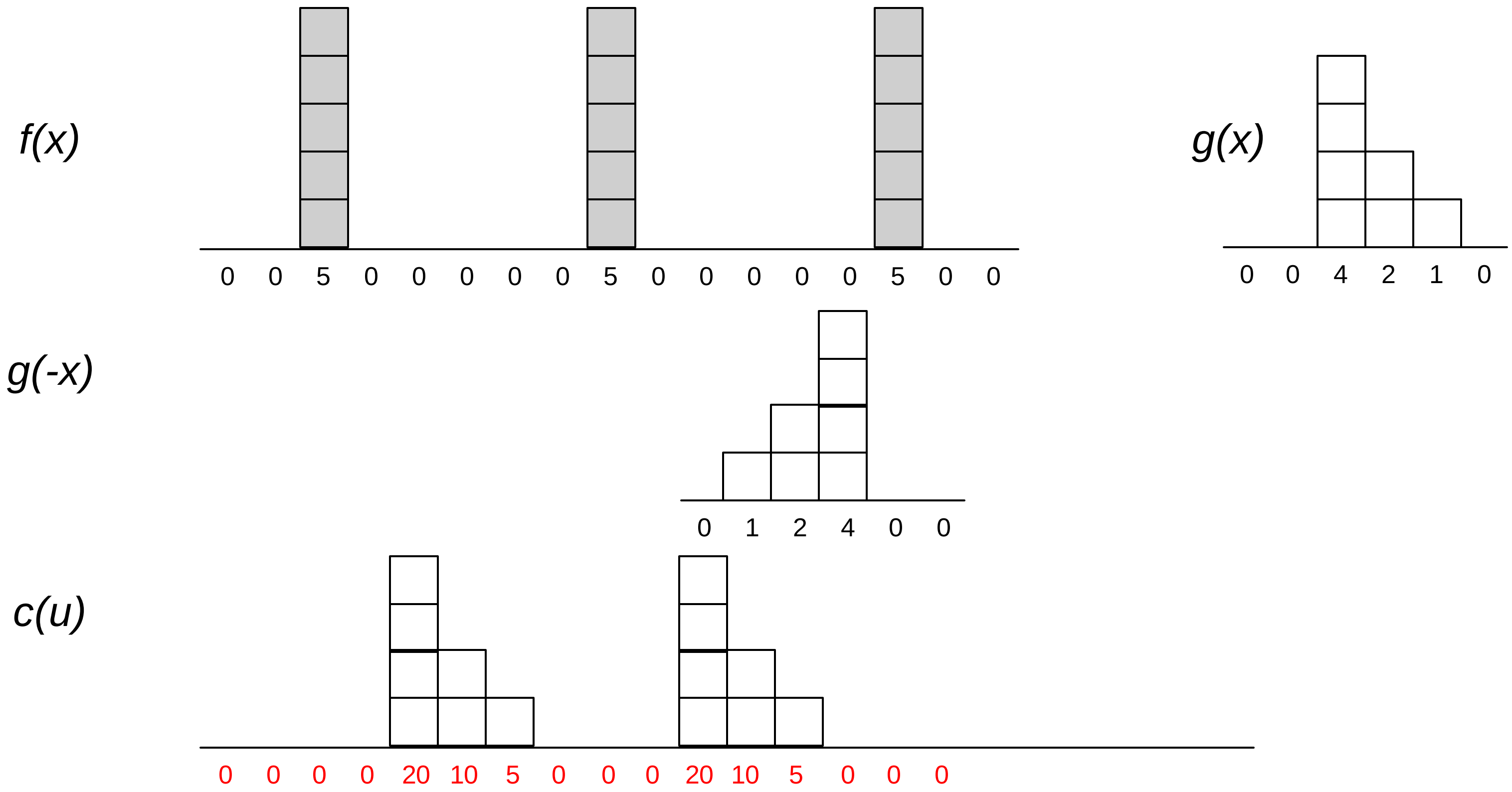

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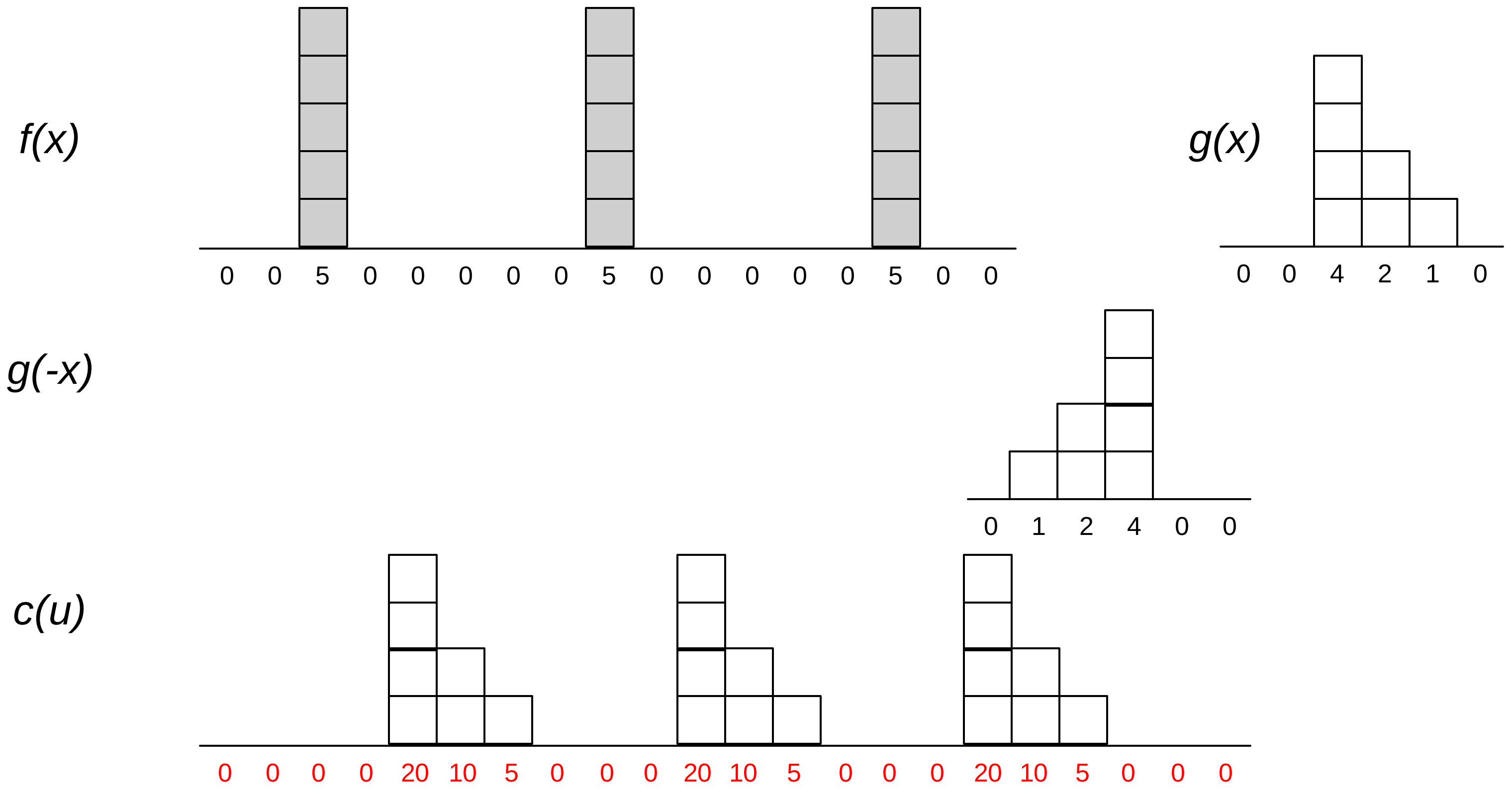

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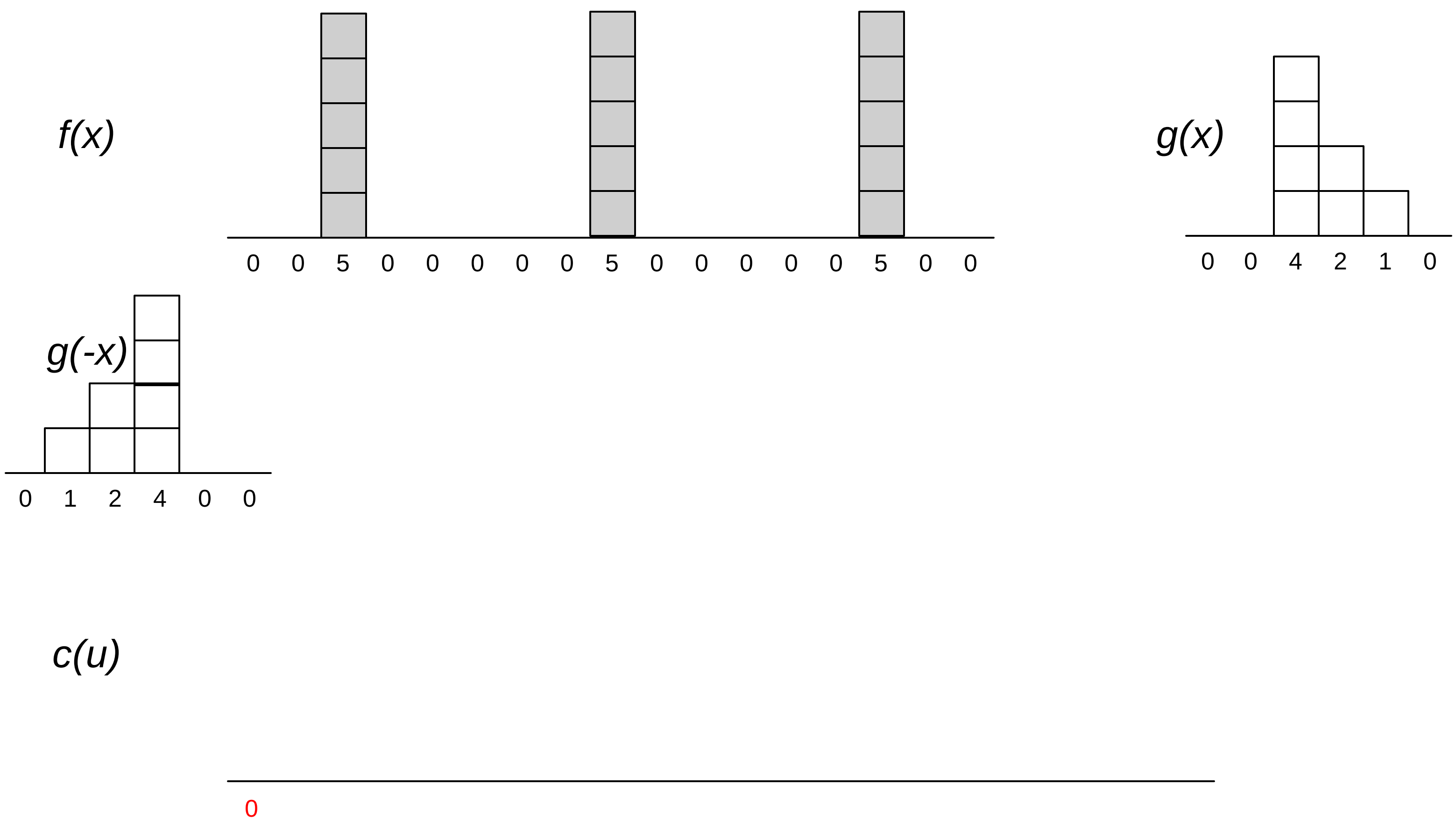

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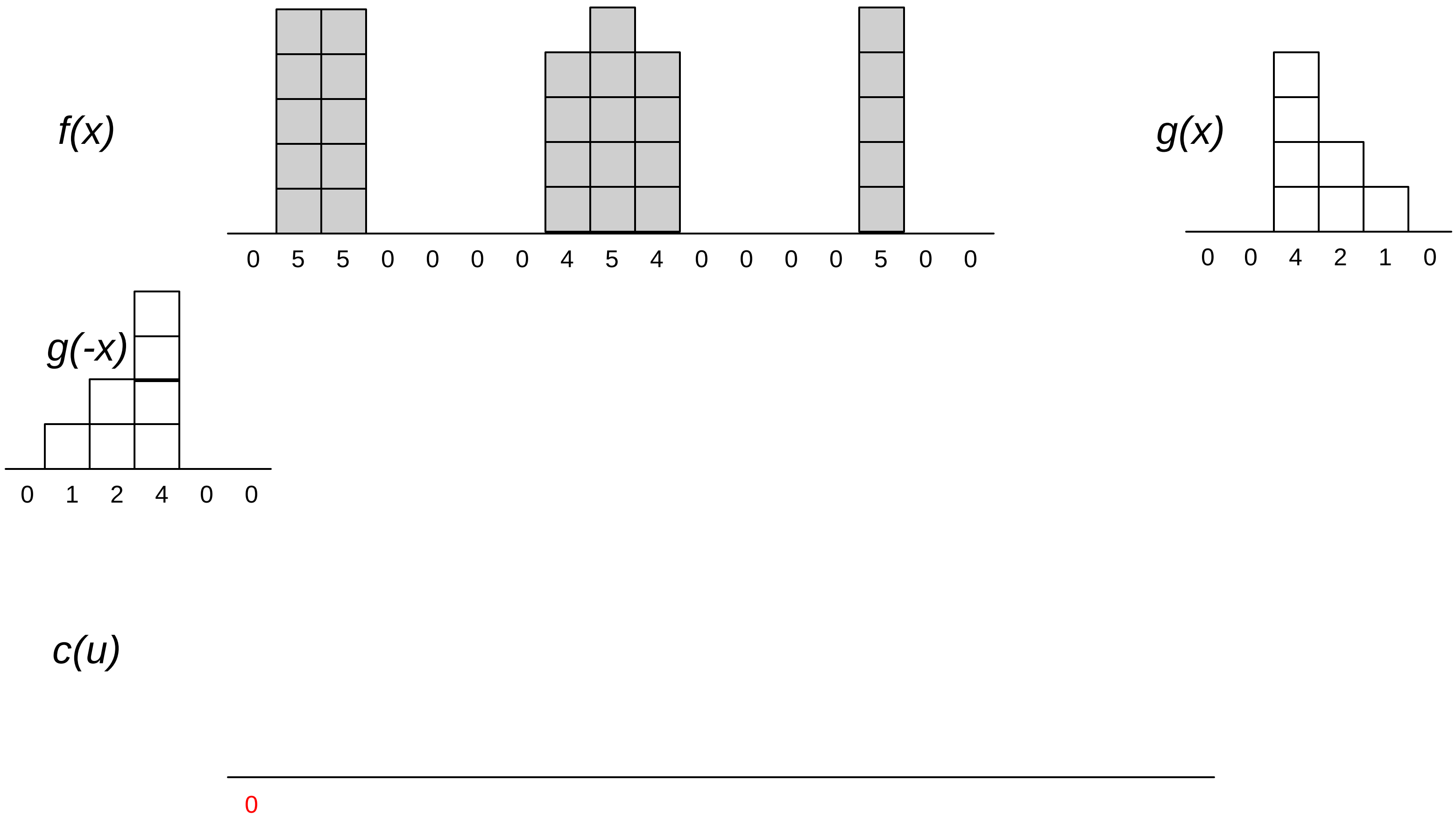

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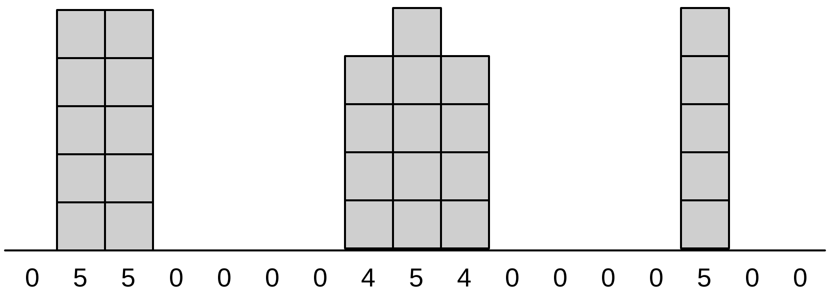
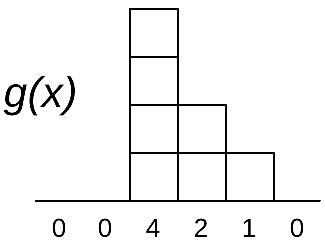
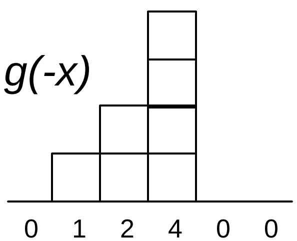
f(x)



g(x)



g(-x)



c(u)

0 0

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

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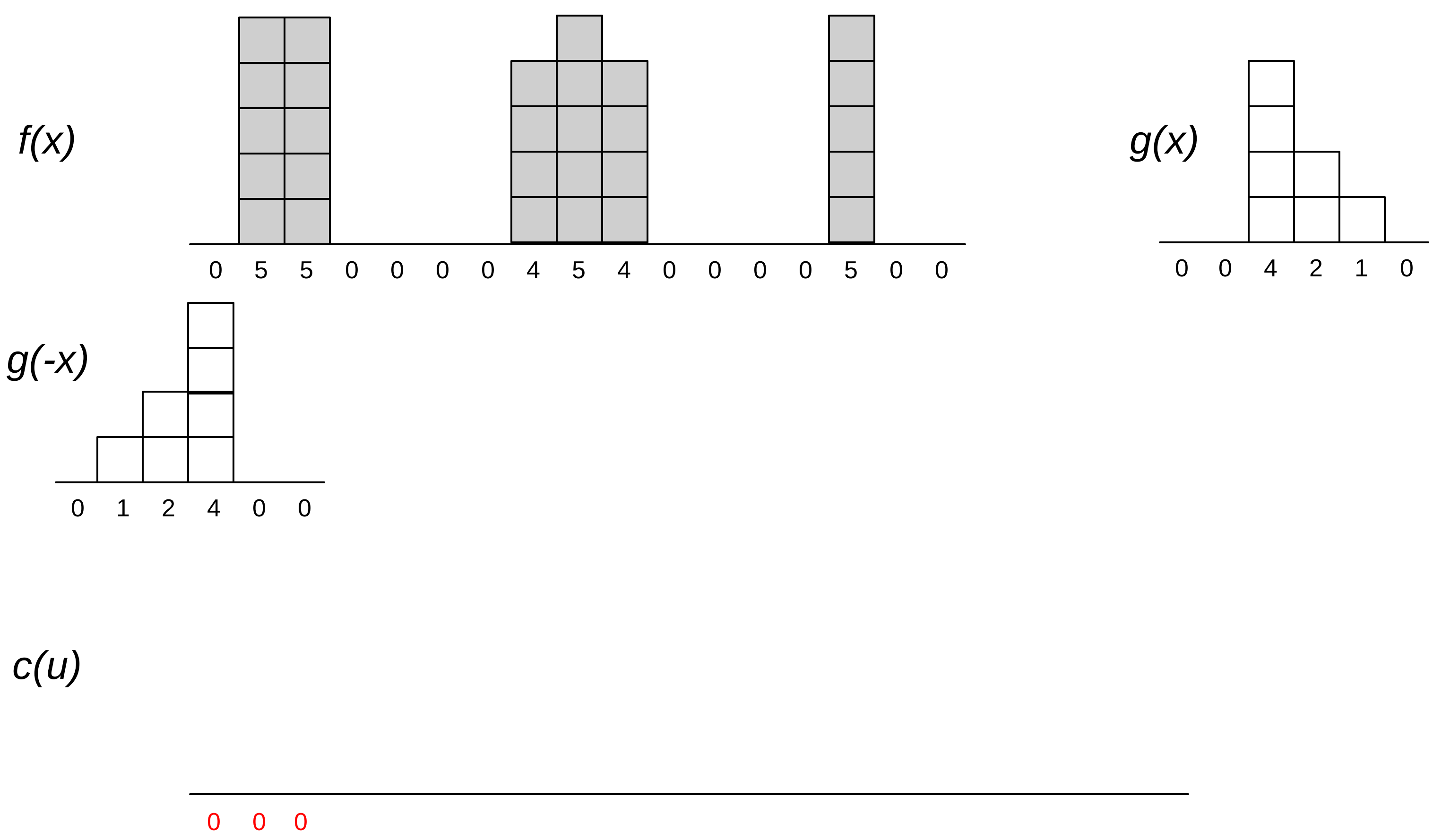

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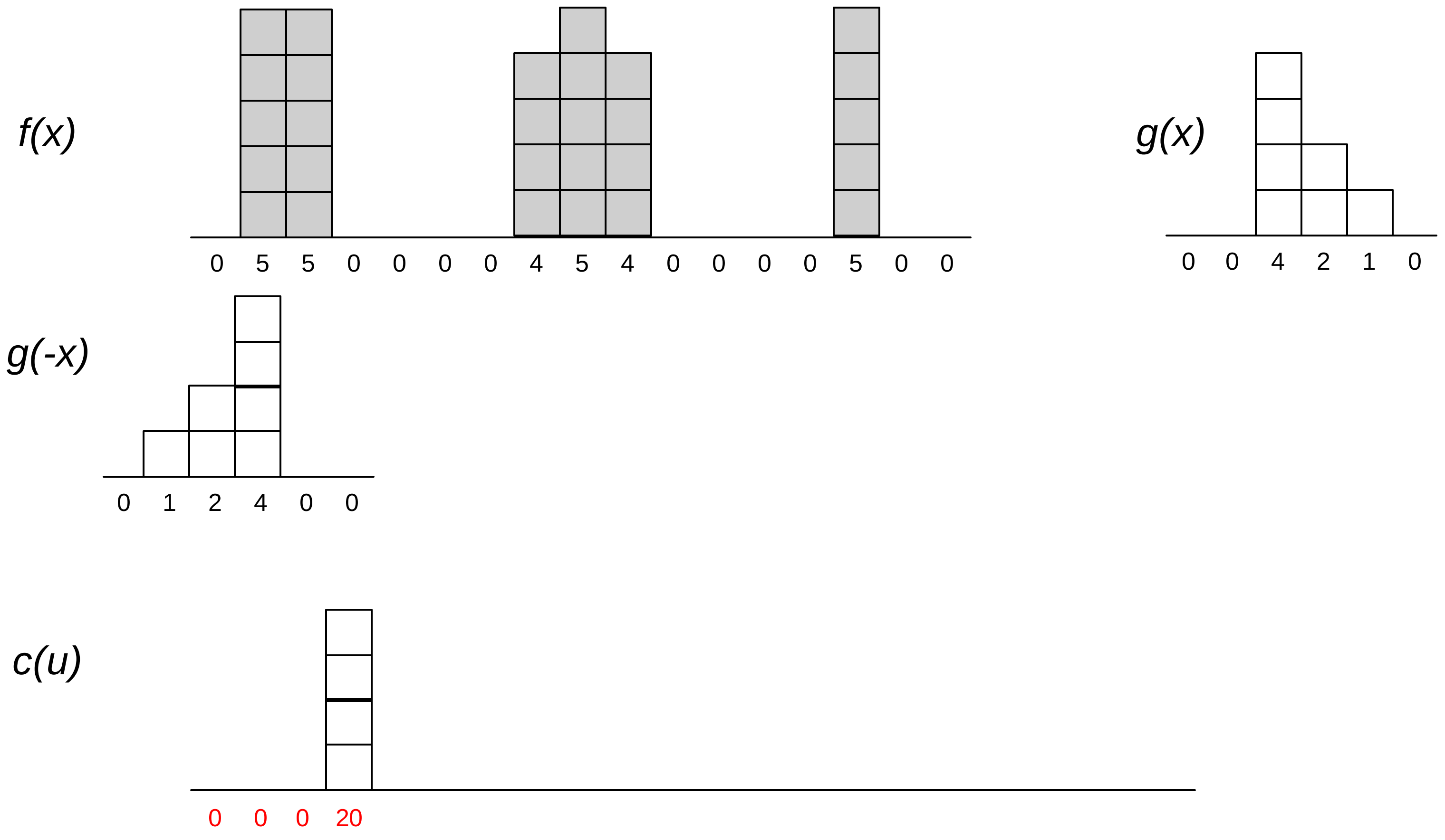

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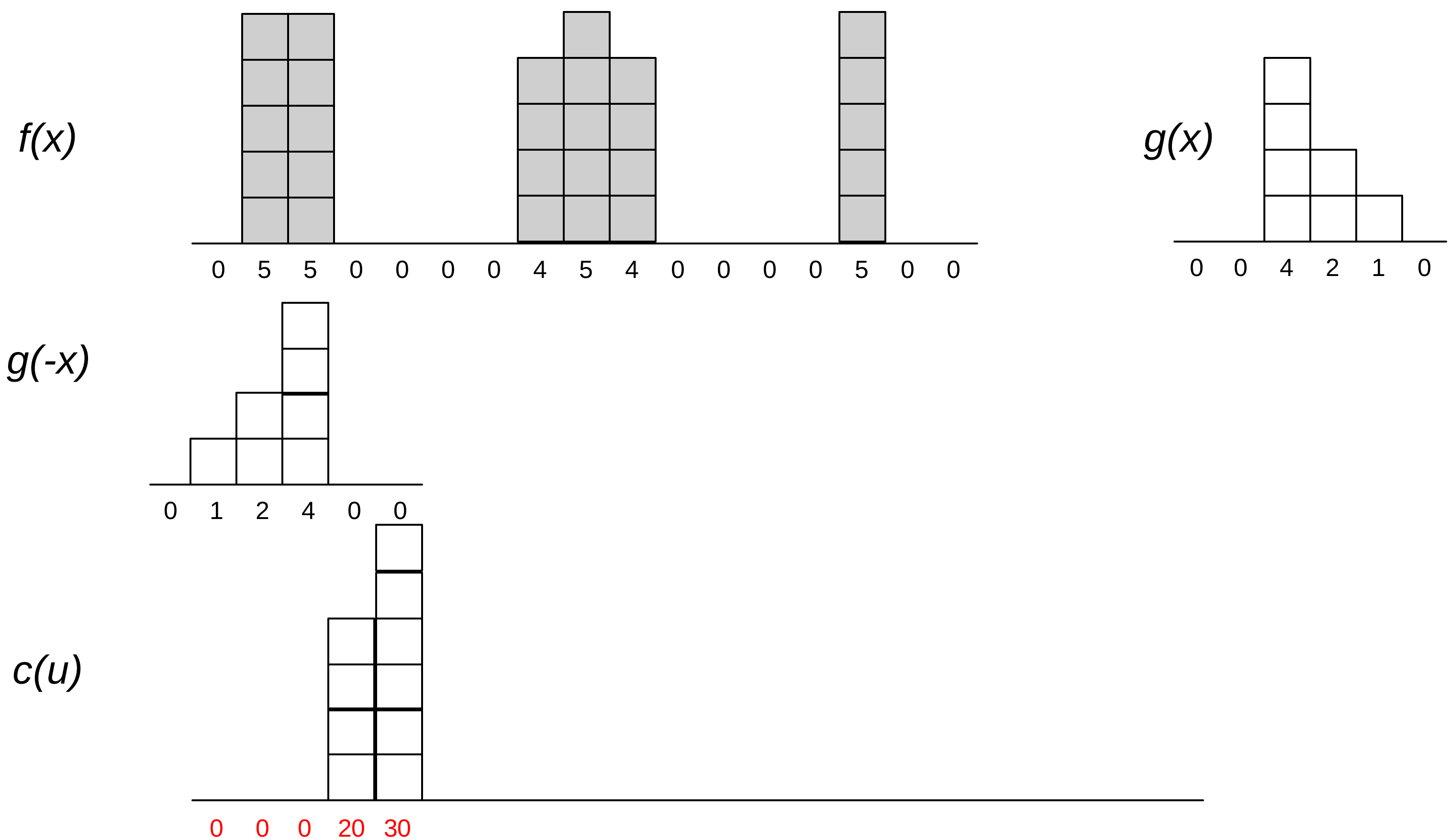

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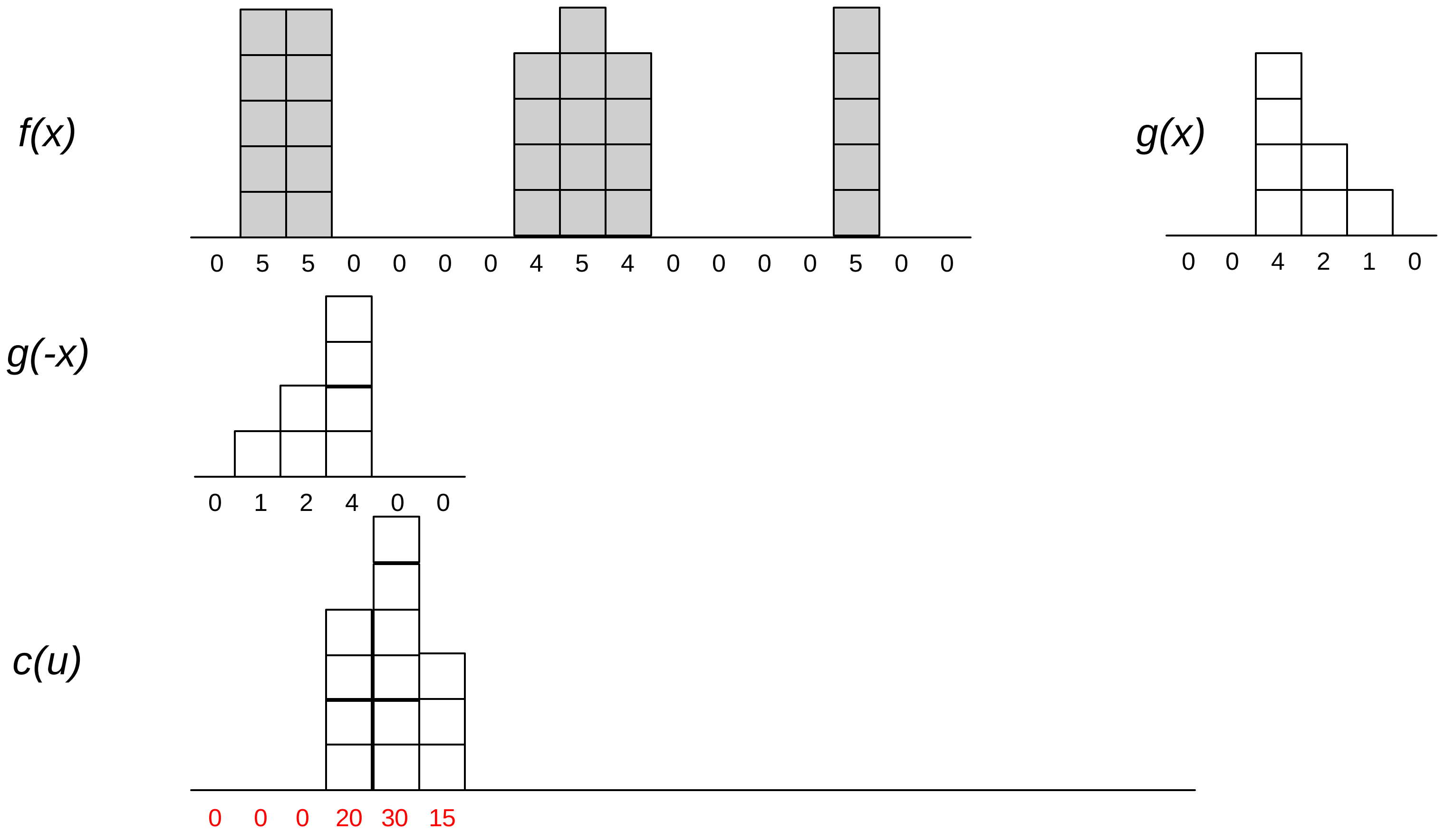

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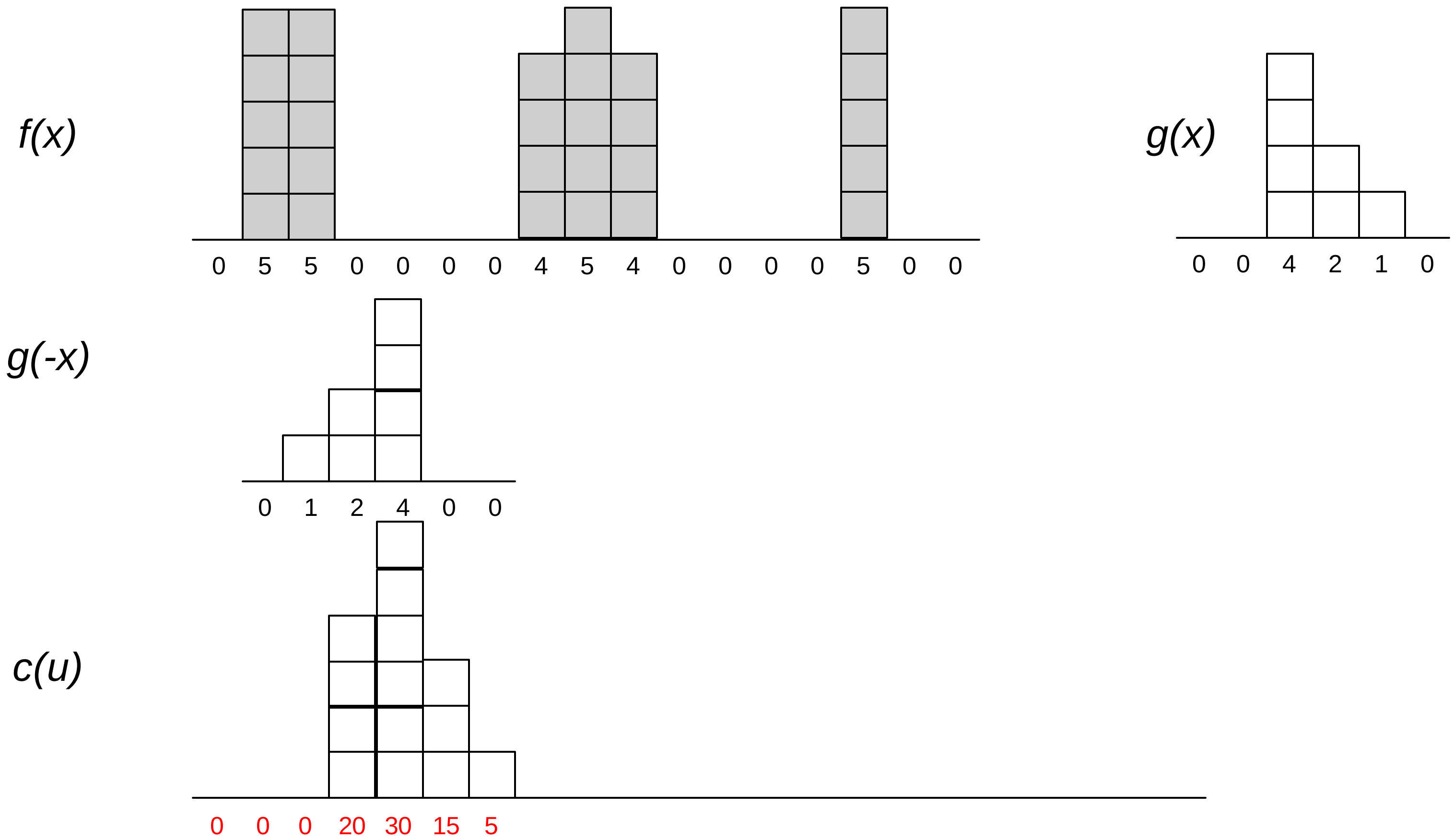

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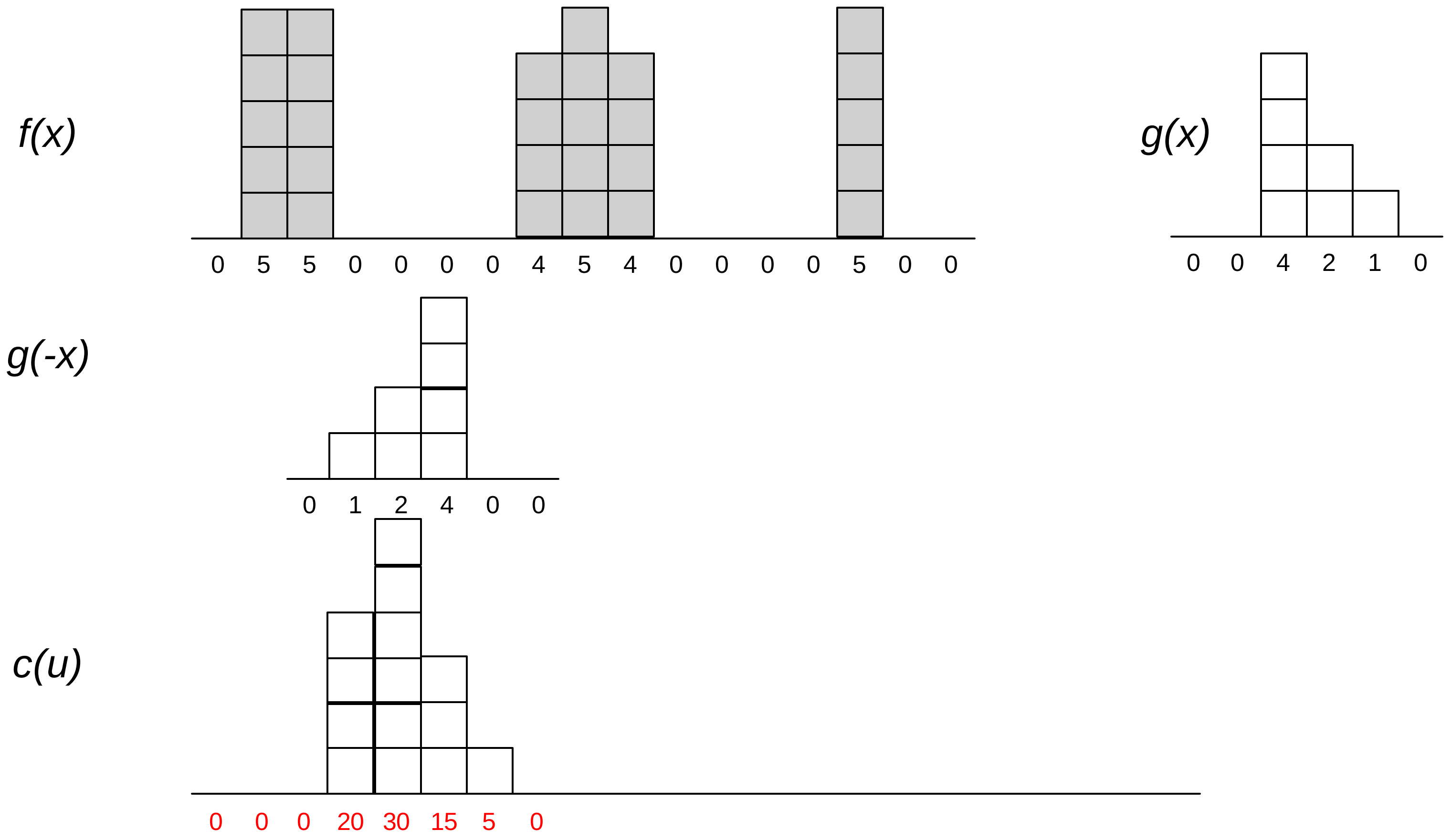

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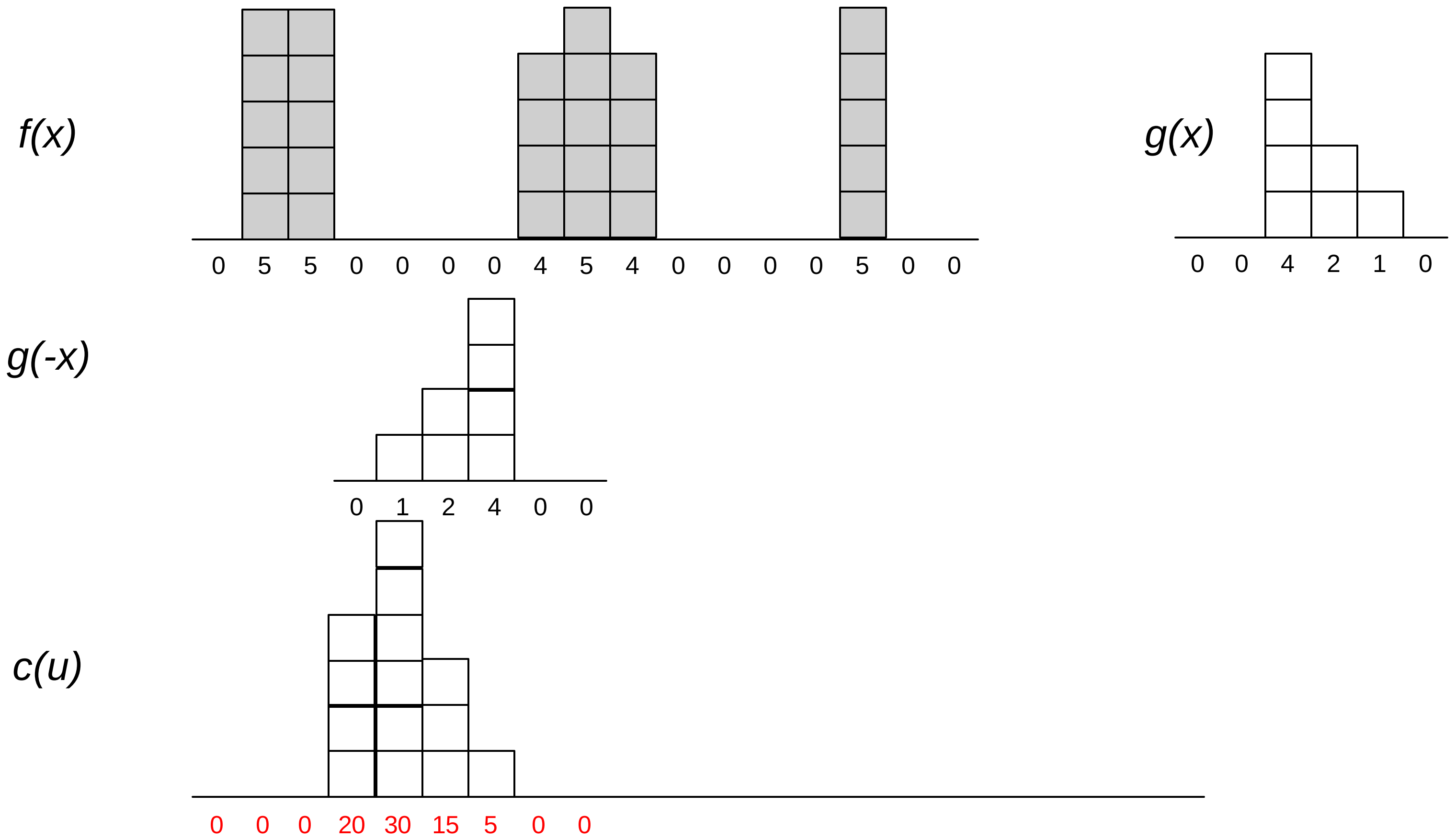

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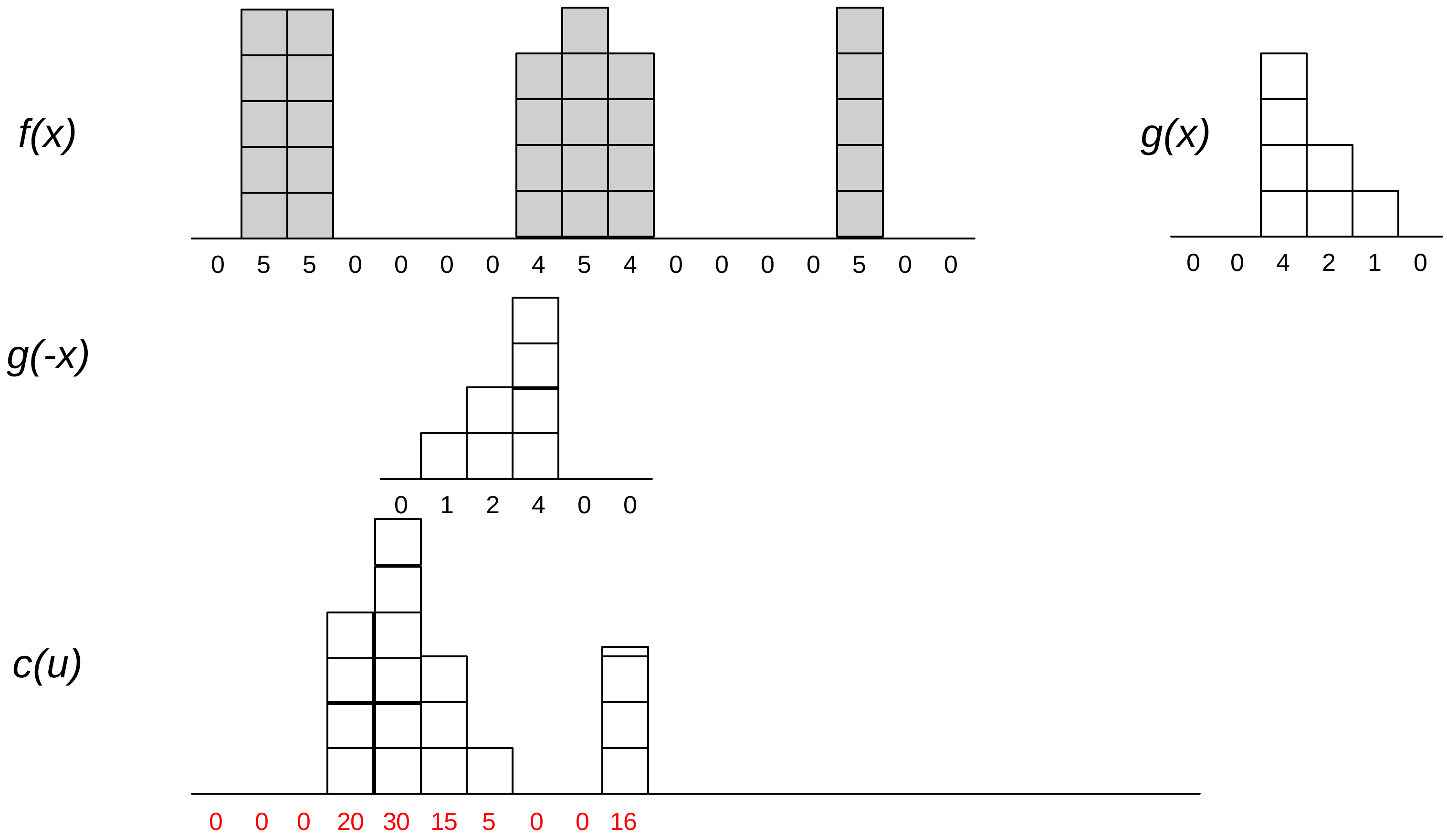

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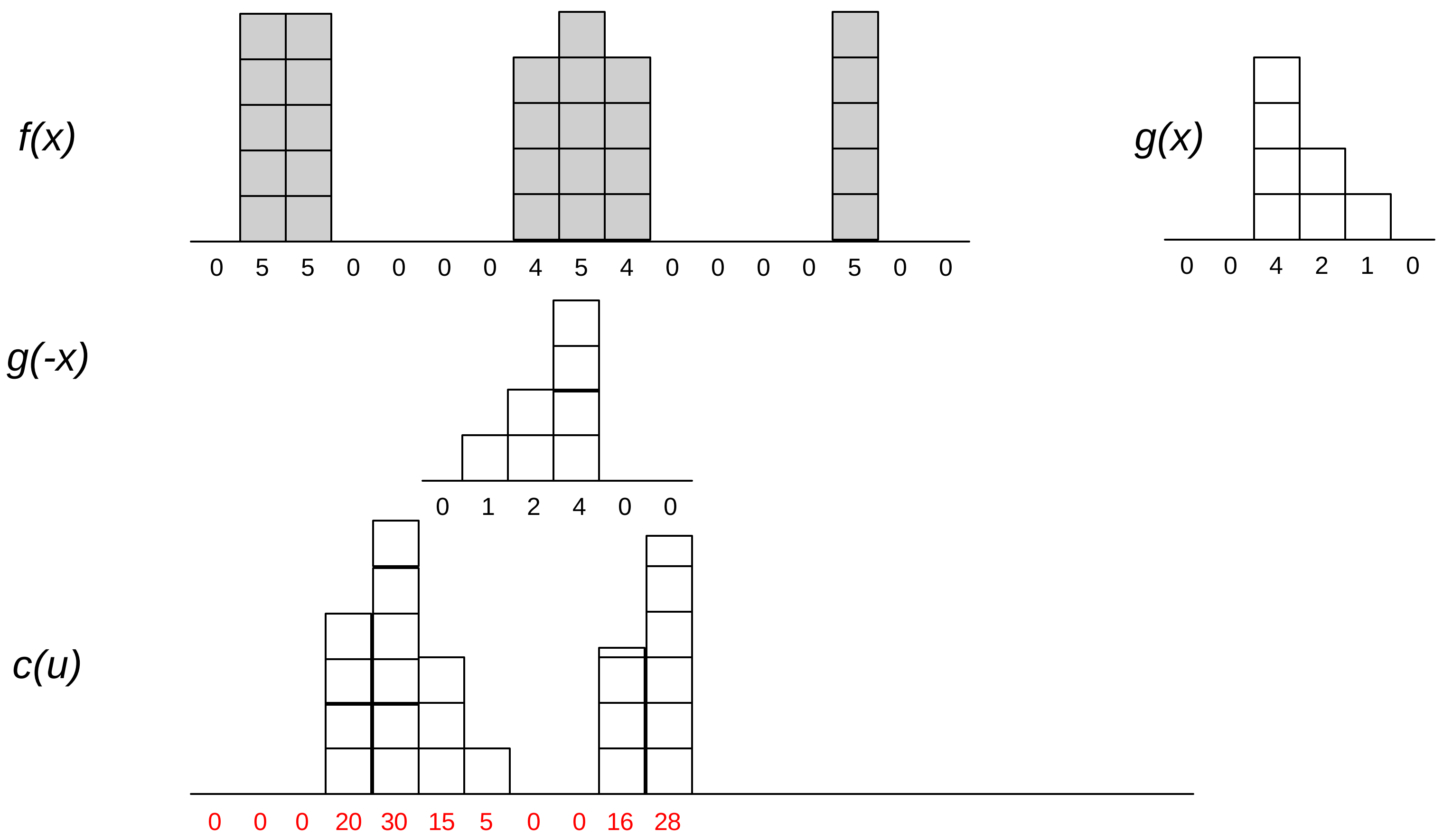

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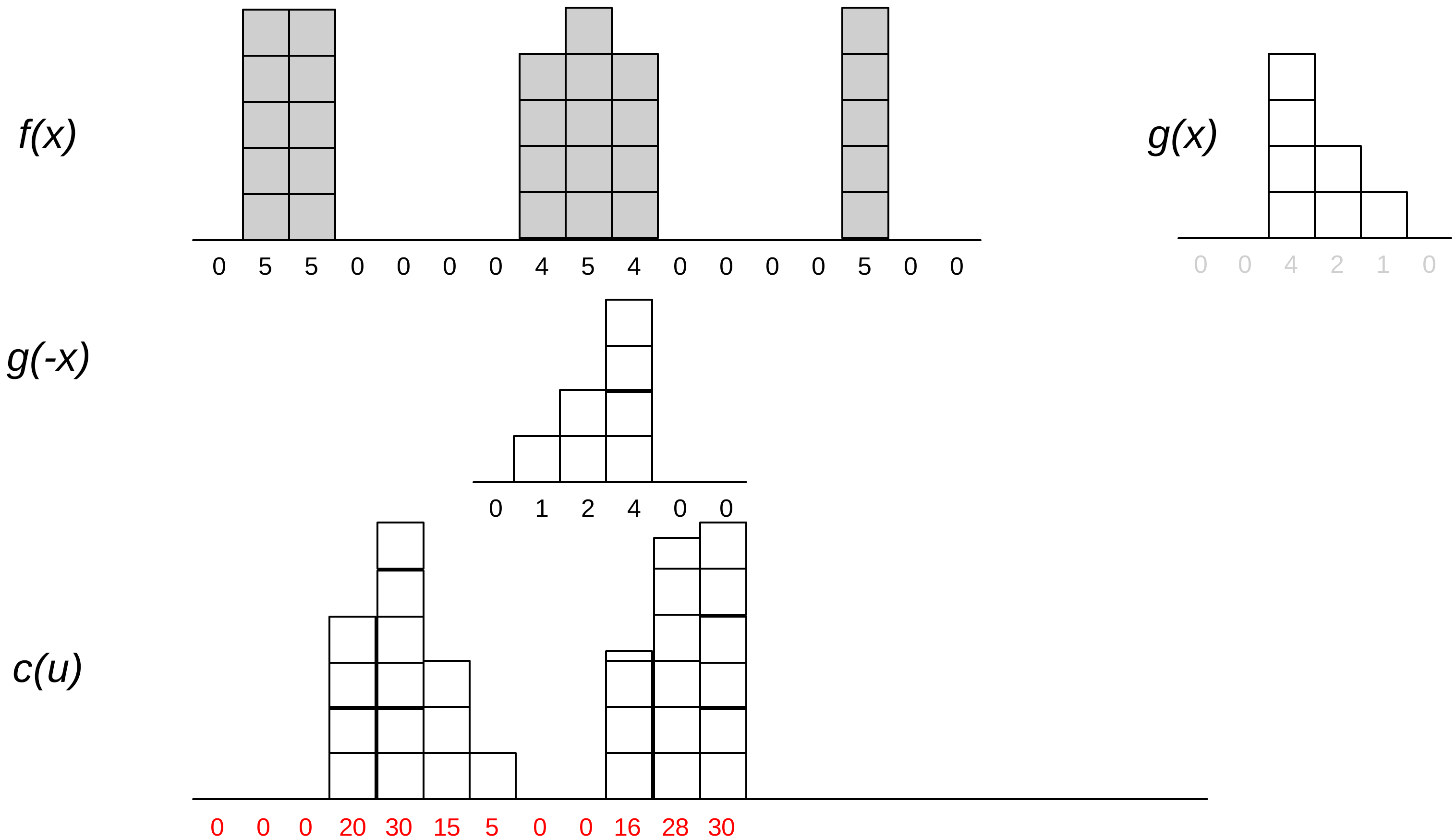

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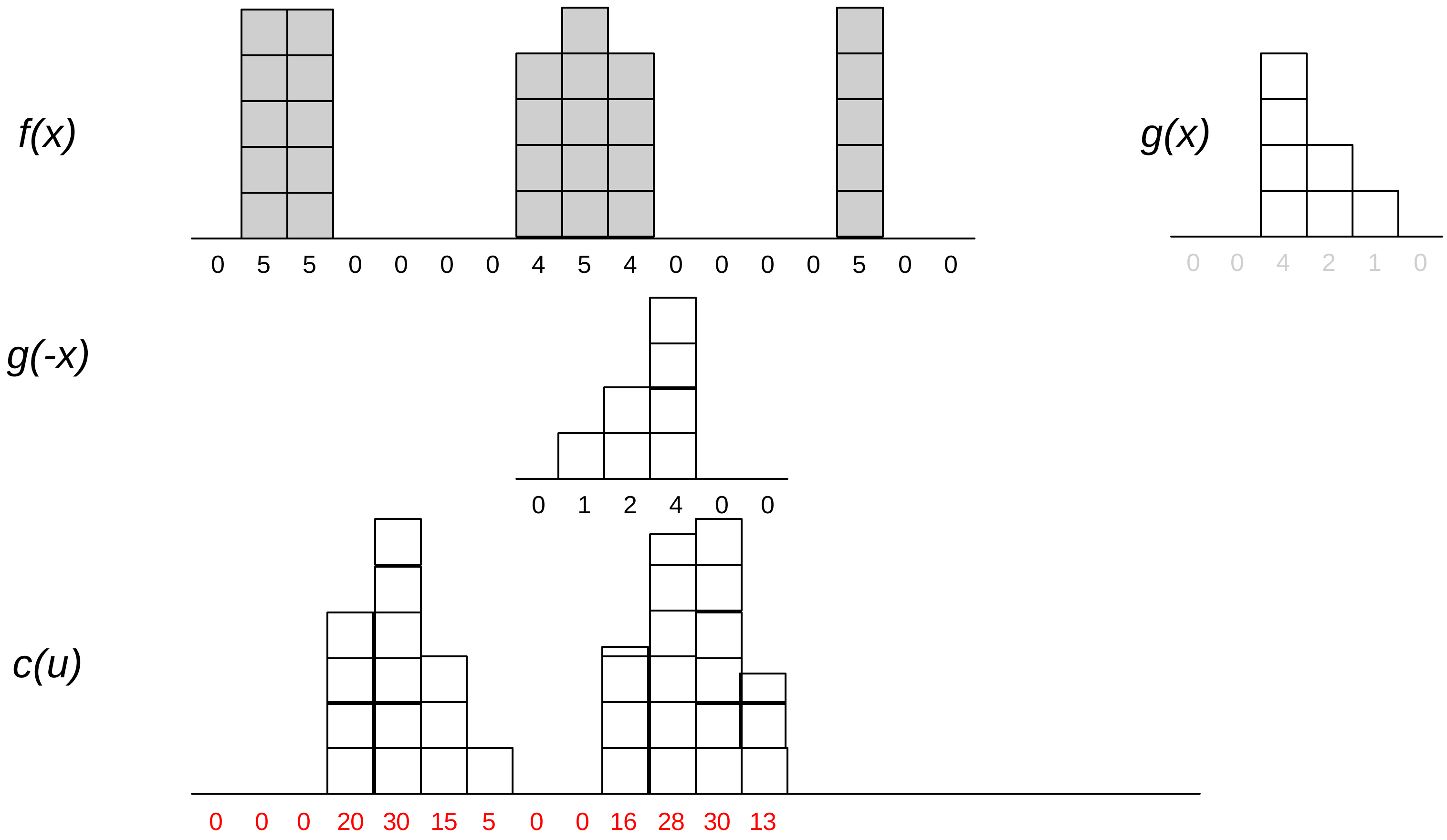

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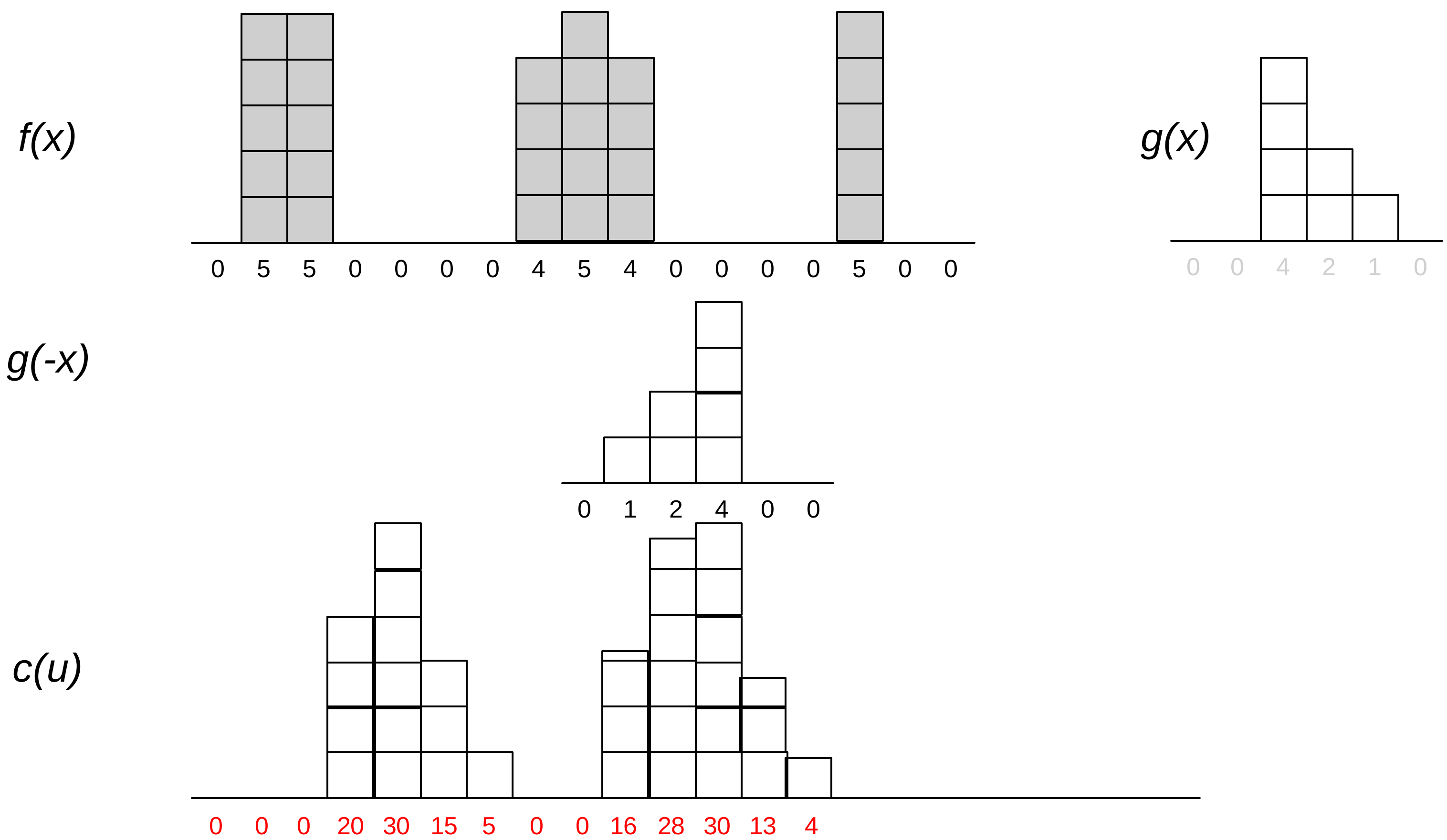

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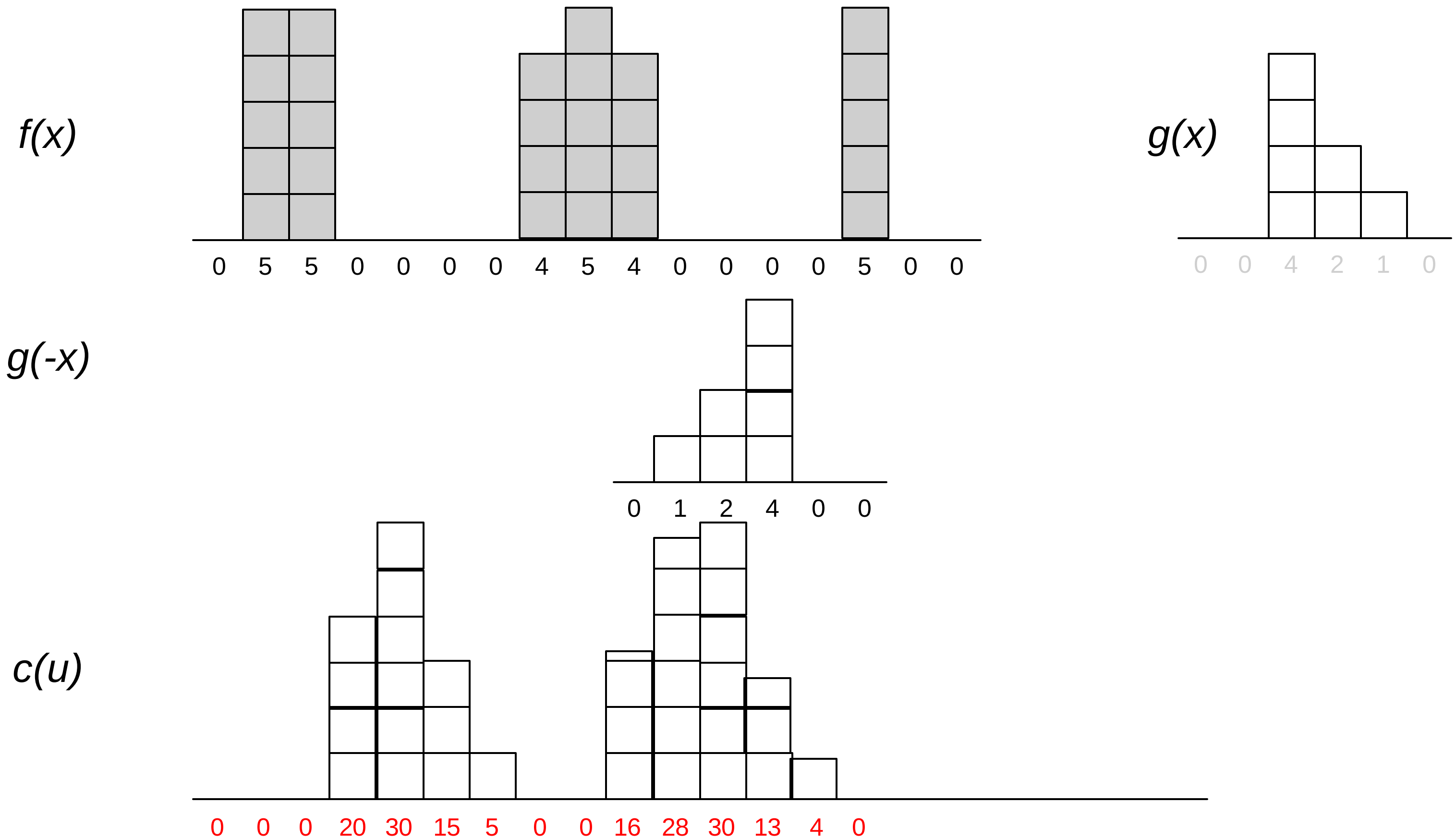

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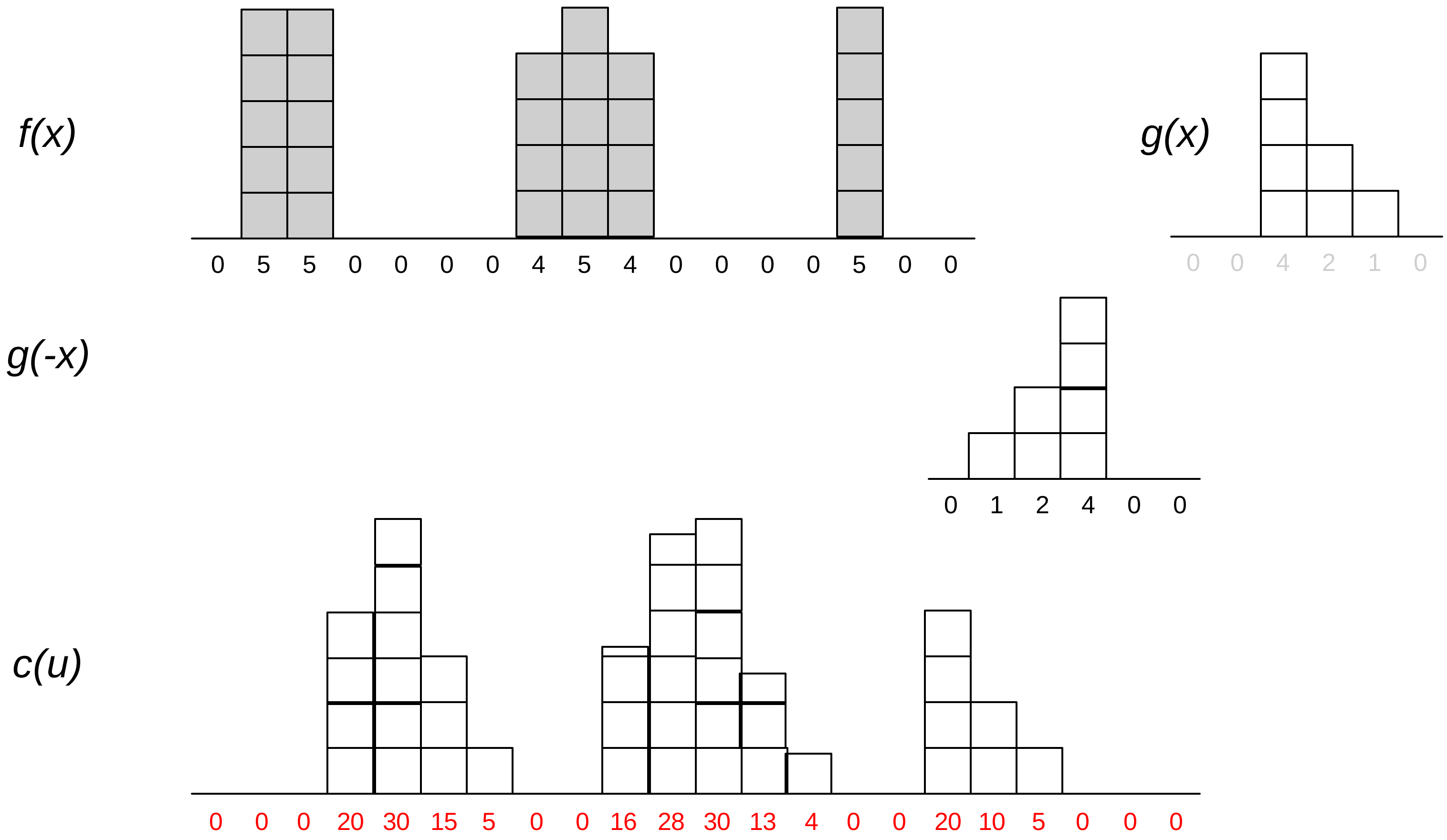
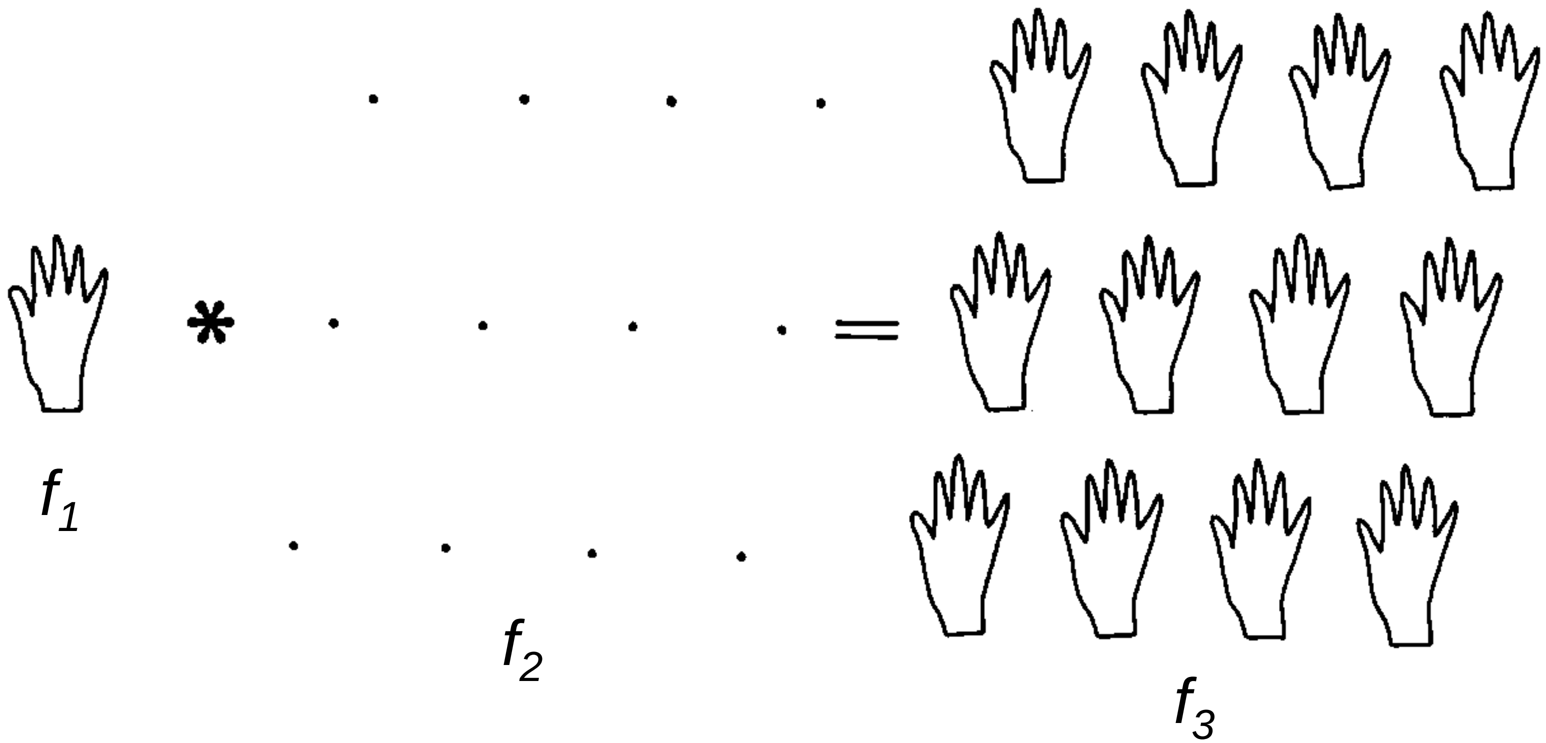


III.C.6.g Convolution and Multiplication

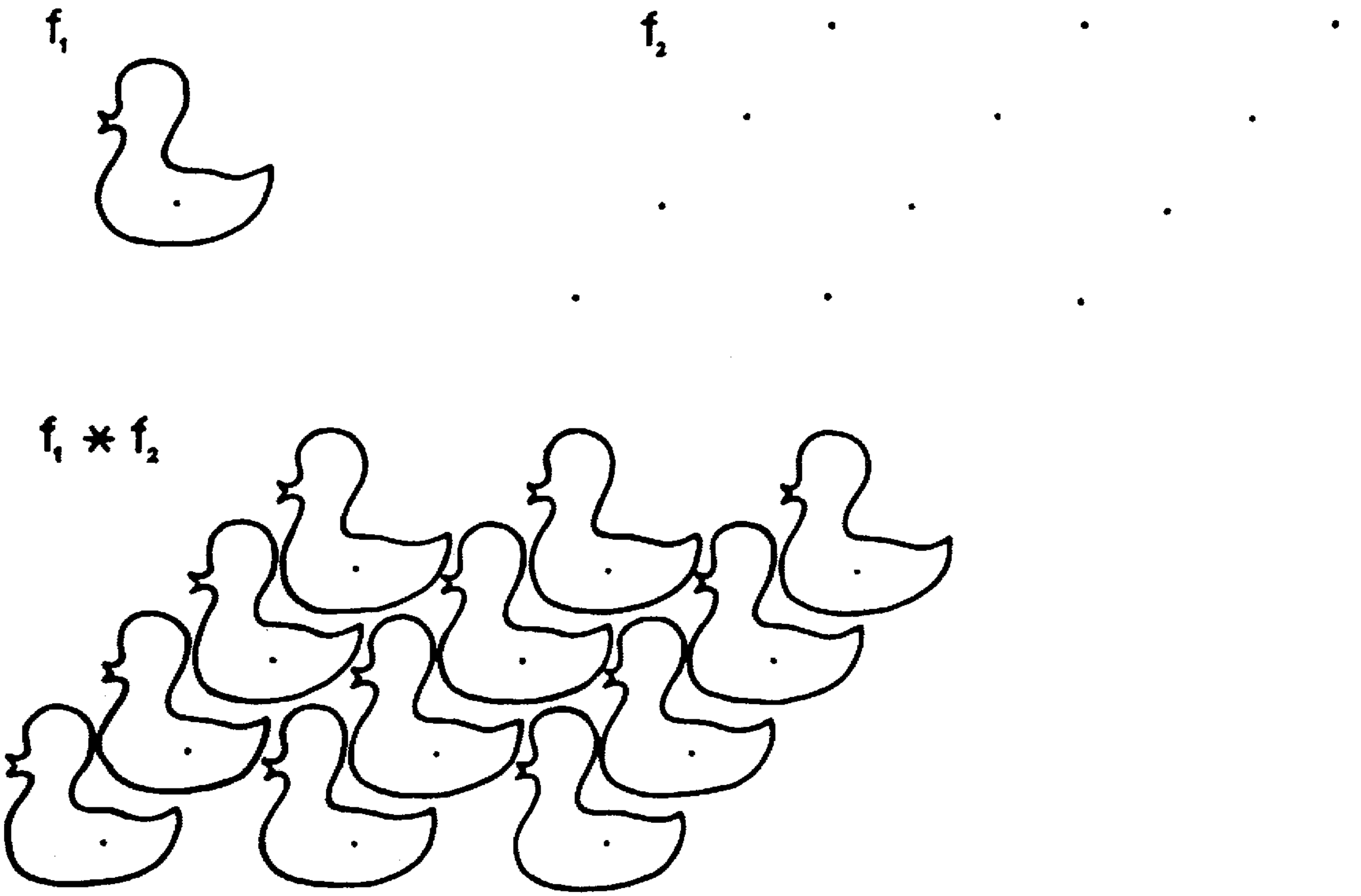
Convolution of hand and 2D lattice produces 2D crystal of hands



III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

Convolution of Duck and 2D Lattice Produces 2D Crystal of Ducks



From Holmes and Blow, Fig. 4, p.123

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

Convolution Theorem:

Provides a precise way to describe the relationship between objects (real space) and transforms (reciprocal space)

The Fourier transform of the **convolution** of two functions is the **product** of their Fourier transforms

$$T(f * g) = F \times G$$

Symbols: $*$ = **convolution** operation

X = **multiplication** operation

f and *g* represent two separate functions

F and *G* are the respective Fourier transforms

III.C.6.g Convolution and Multiplication

Convolution Theorem:

The Fourier transform of the **convolution** of two functions is the **product** of their Fourier transforms

$$T(f \ast g) = F \times G$$

The **converse** relationship also holds:

The Fourier transform of the **product** of two functions is equal to the **convolution** of the transforms of the individual functions

$$T(f \times g) = F \ast G$$

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

Crystal Structure: (real space) $f_3 = f_1 * f_2$ (f_1 = unit cell contents; f_2 = real space lattice)

Equivalent to the convolution of the **contents** of the unit cell (f_1) with a **finite lattice** (f_2)

The above equation can also be written as:

$$f_3 = T^{-1}(F_3)$$

$$f_3 = T^{-1}(F_1 \times F_2)$$

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

Transform of Crystal Structure: (reciprocal space)

$$F_3 = F_1 \times F_2$$

$$= T(f_3)$$

$$= T(f_1 * f_2)$$

Equivalent to the transform of the unit cell **contents**, F_1, multiplied (sampled) by the transform of the crystal lattice, F_2 (**reciprocal lattice**)

These examples are easy to conceptualize because, in each case, one of the functions (f_2 or F_2) is **"simple"** (*i.e.* an array of points or a lattice)

III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

In the reciprocal lattice, the **sampling interval** is **reciprocally related** to the real space lattice repeat

F_1, the transform of the contents of the unit cell, is a **continuous function**

F_3, the transform of the crystal, is **discrete** (because F_2 is discrete)

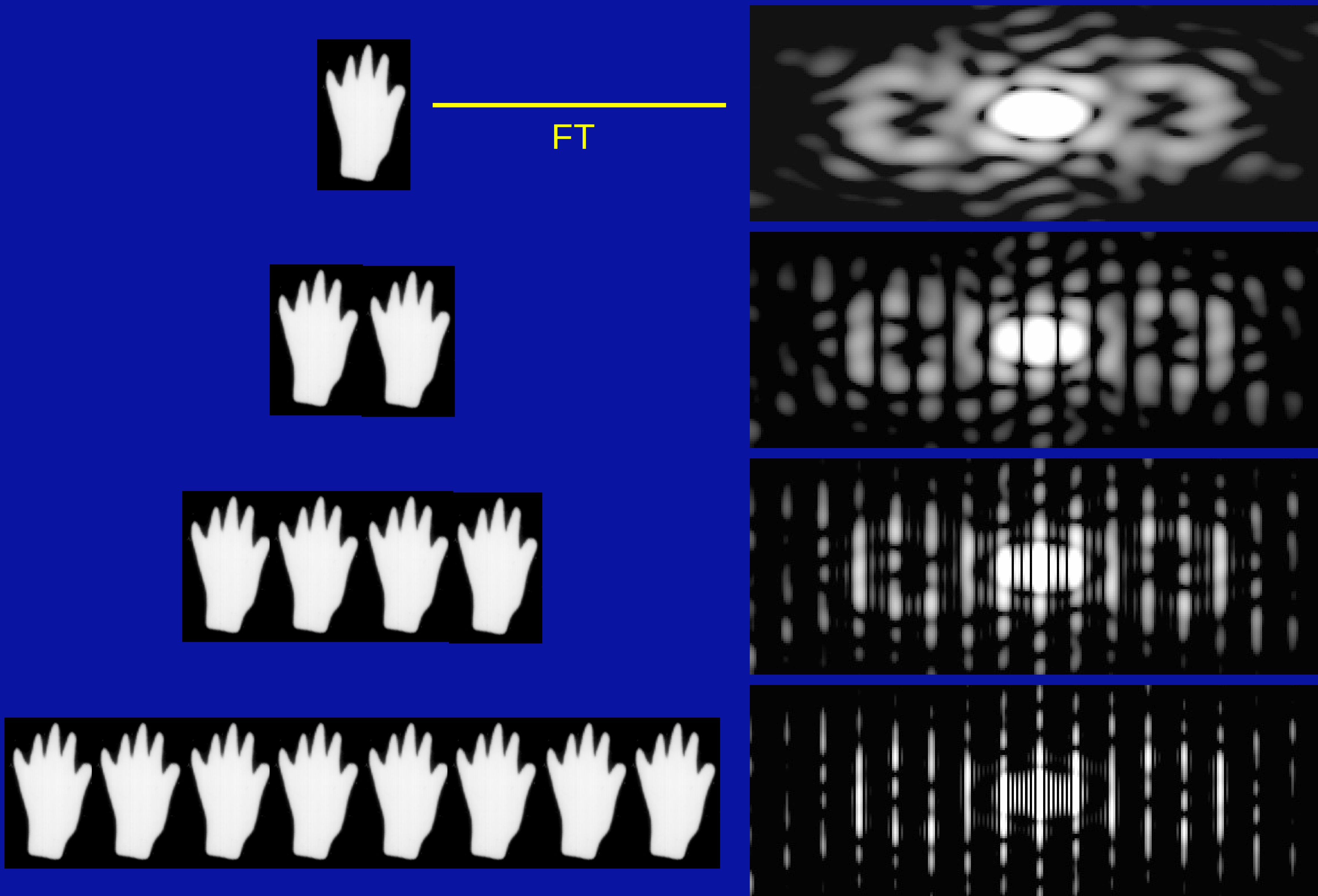
The **crystal** transform (F_3) is the transform of the single unit cell **"sampled"** at the reciprocal lattice points

Values of the Fourier transform at the reciprocal lattice points are called the **structure factors (F_{hkl})**

III.C.6.g Convolution and Multiplication

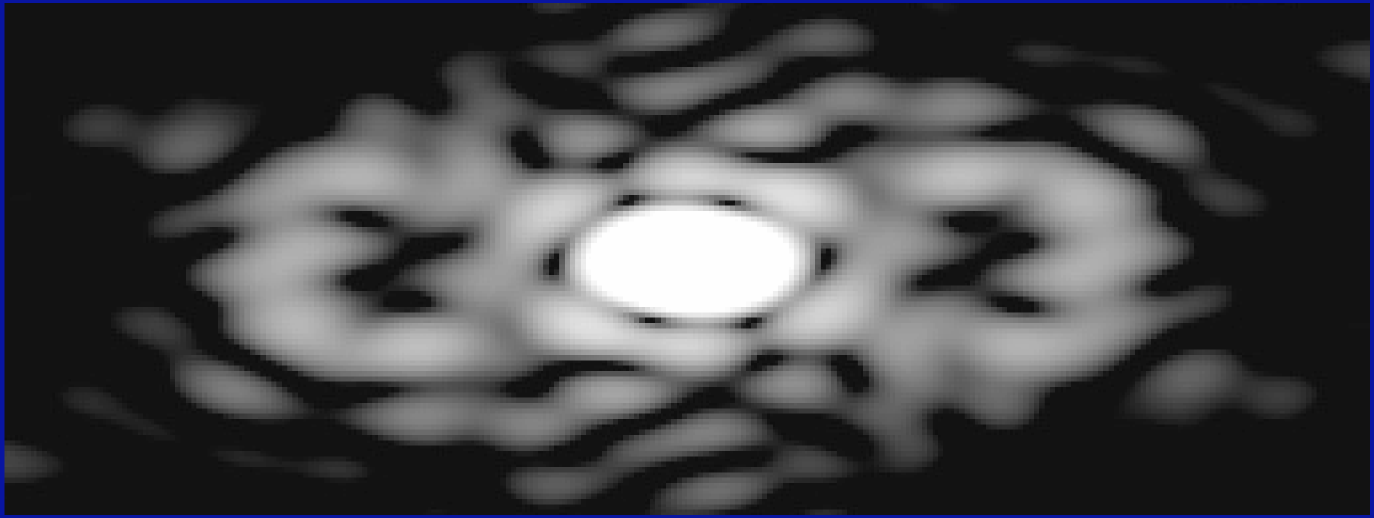
1-D lattices give rise to transforms sampled in only one direction

Effect of Crystal Lattice on Transform
(Transform Sampling)



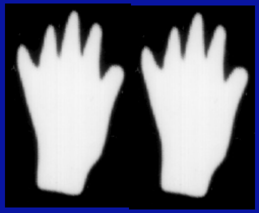
Effect of Crystal Lattice on Transform (Transform Sampling)

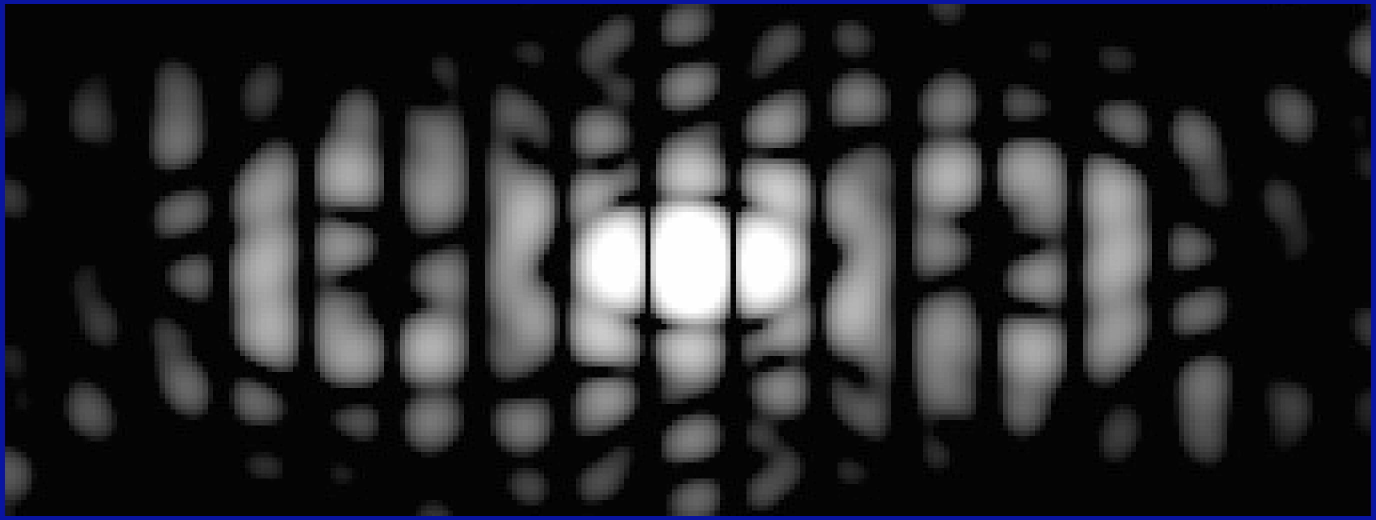
1 hand



Effect of Crystal Lattice on Transform (Transform Sampling)

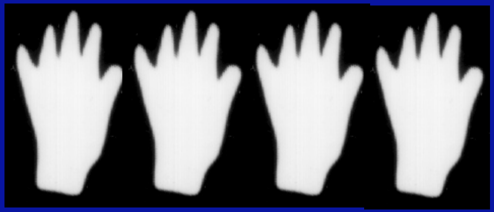
2 hands

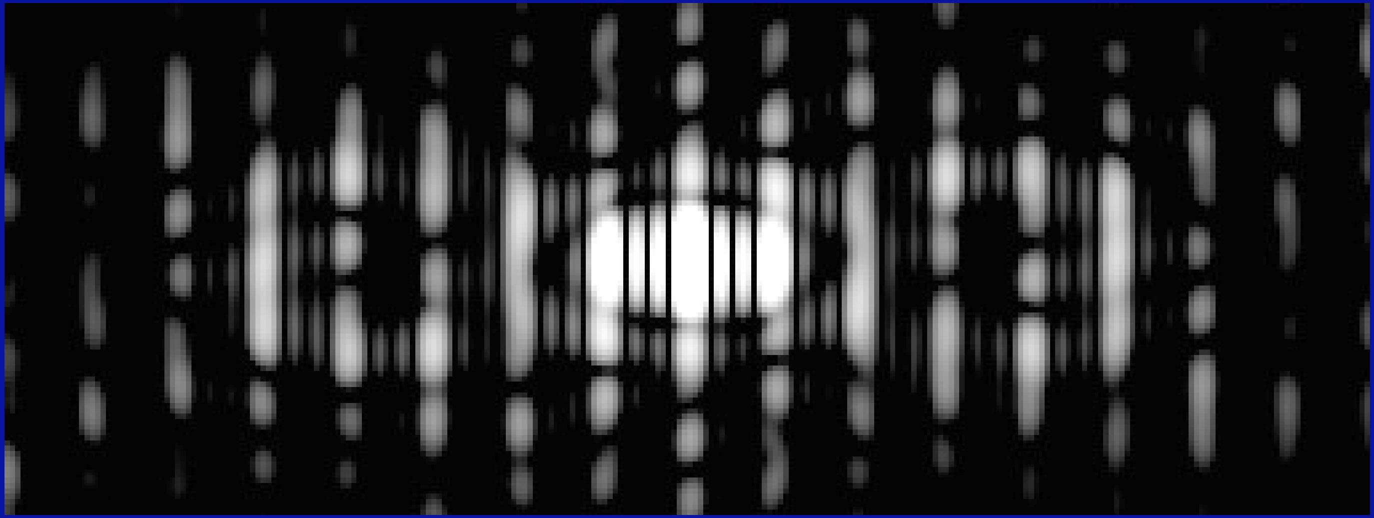




Effect of Crystal Lattice on Transform (Transform Sampling)

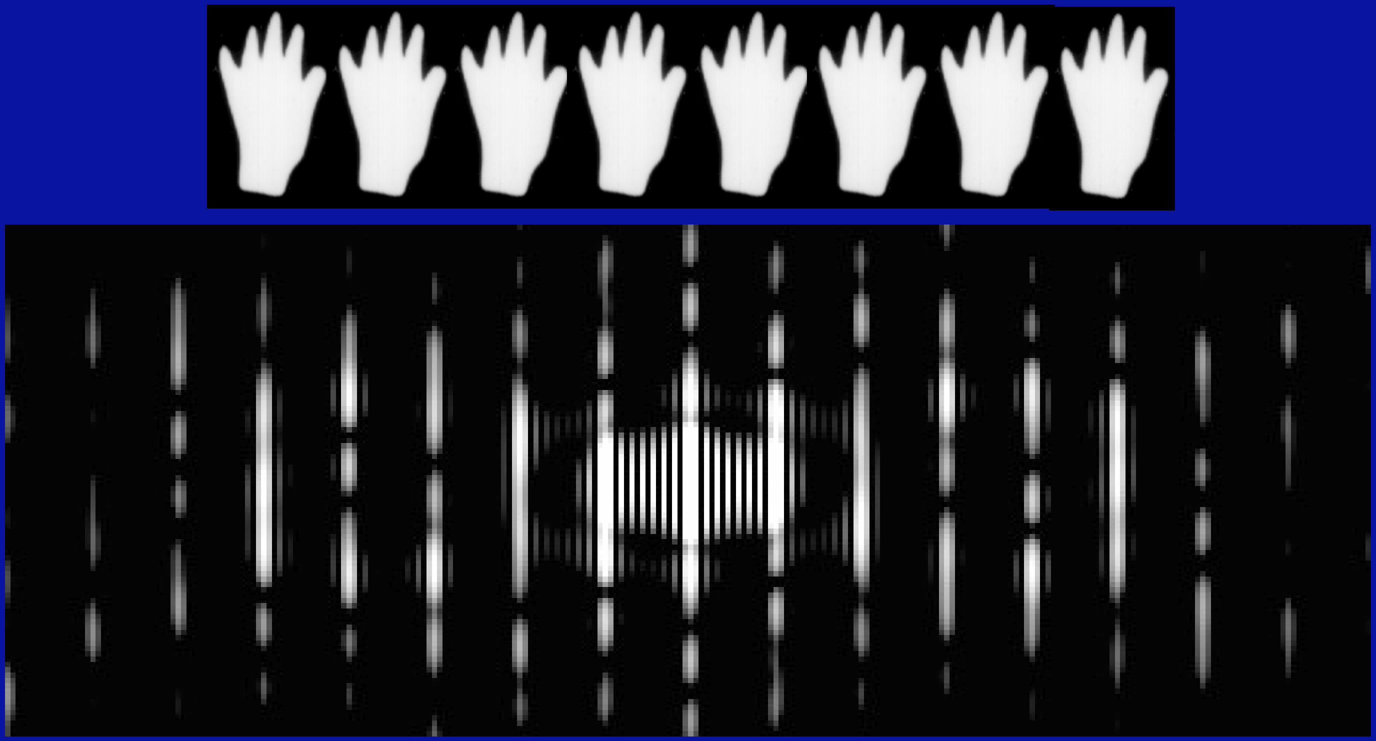
4 hands





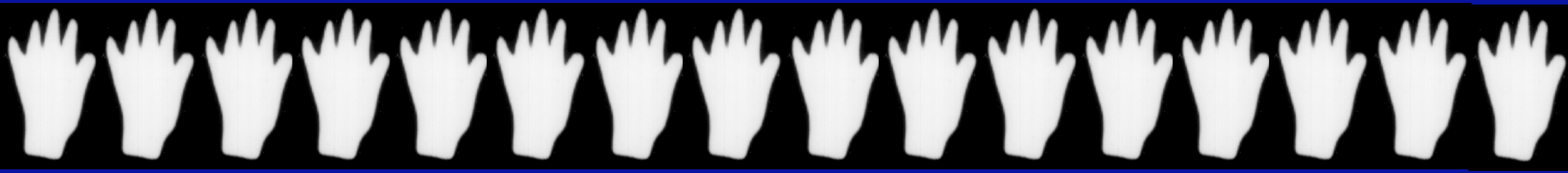
Effect of Crystal Lattice on Transform (Transform Sampling)

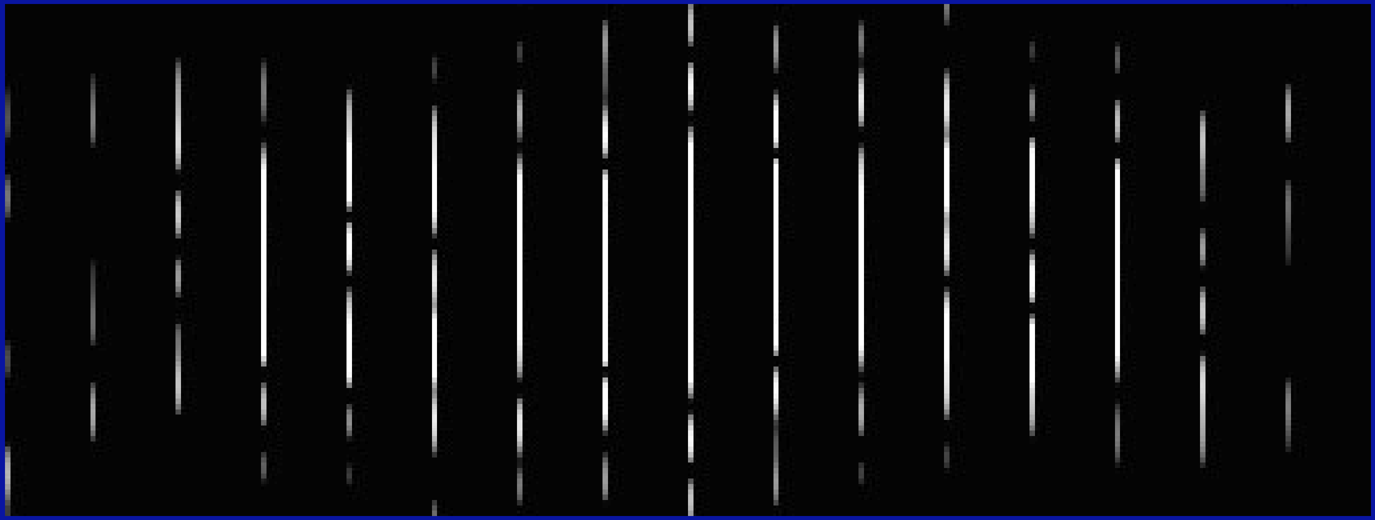
8 hands



Effect of Crystal Lattice on Transform
(Transform Sampling)

16 hands





III.C.6 Diffraction

III.C.6.g Convolution and Multiplication

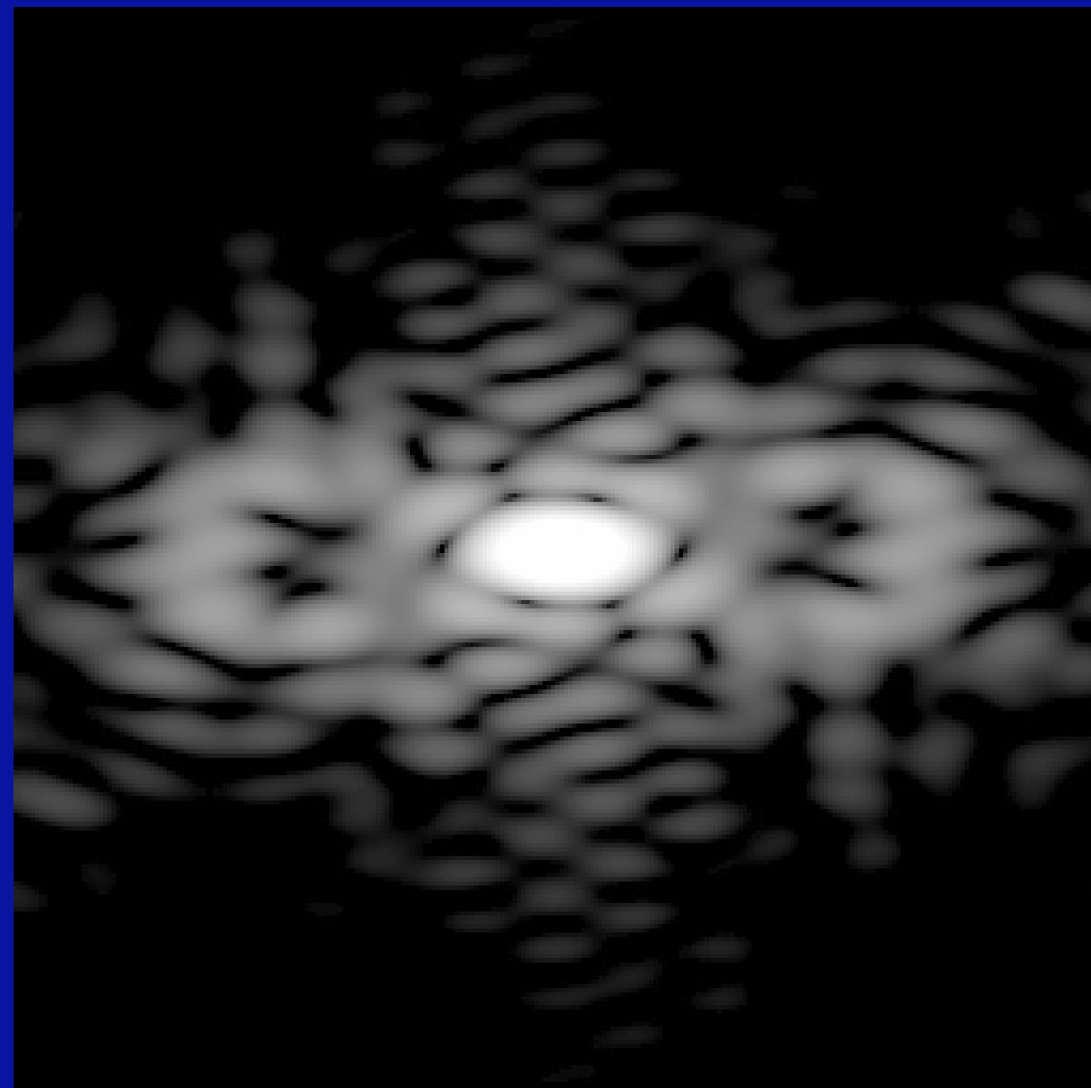
1-D lattices give rise to transforms sampled in only one direction

2-D lattices produce sampling on a 2-D grid or reciprocal lattice

Example 1: Orthogonal 2-D lattice

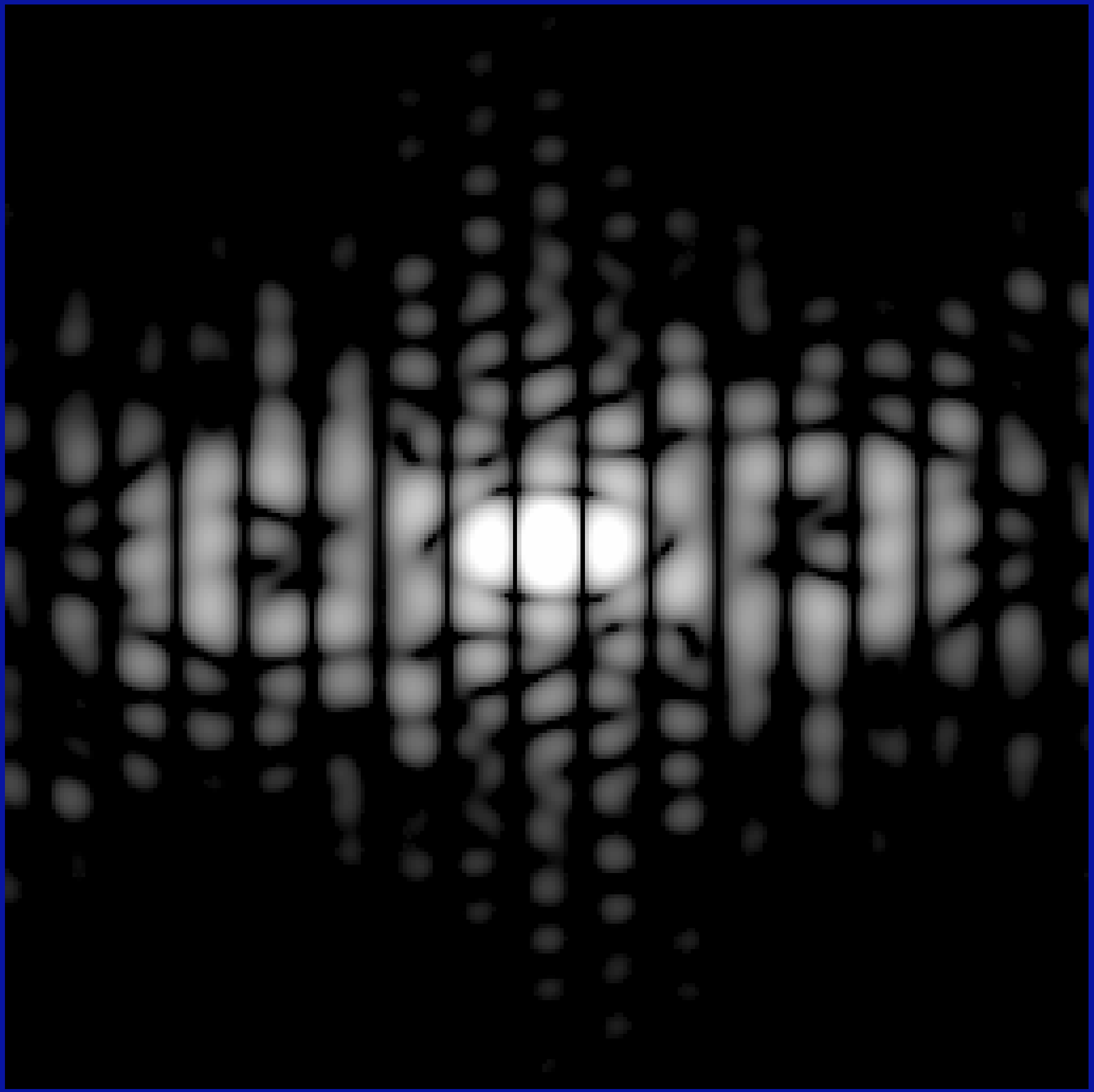
Effect of 2-D Crystal Lattice on Transform
(Transform Sampling)

1 hand



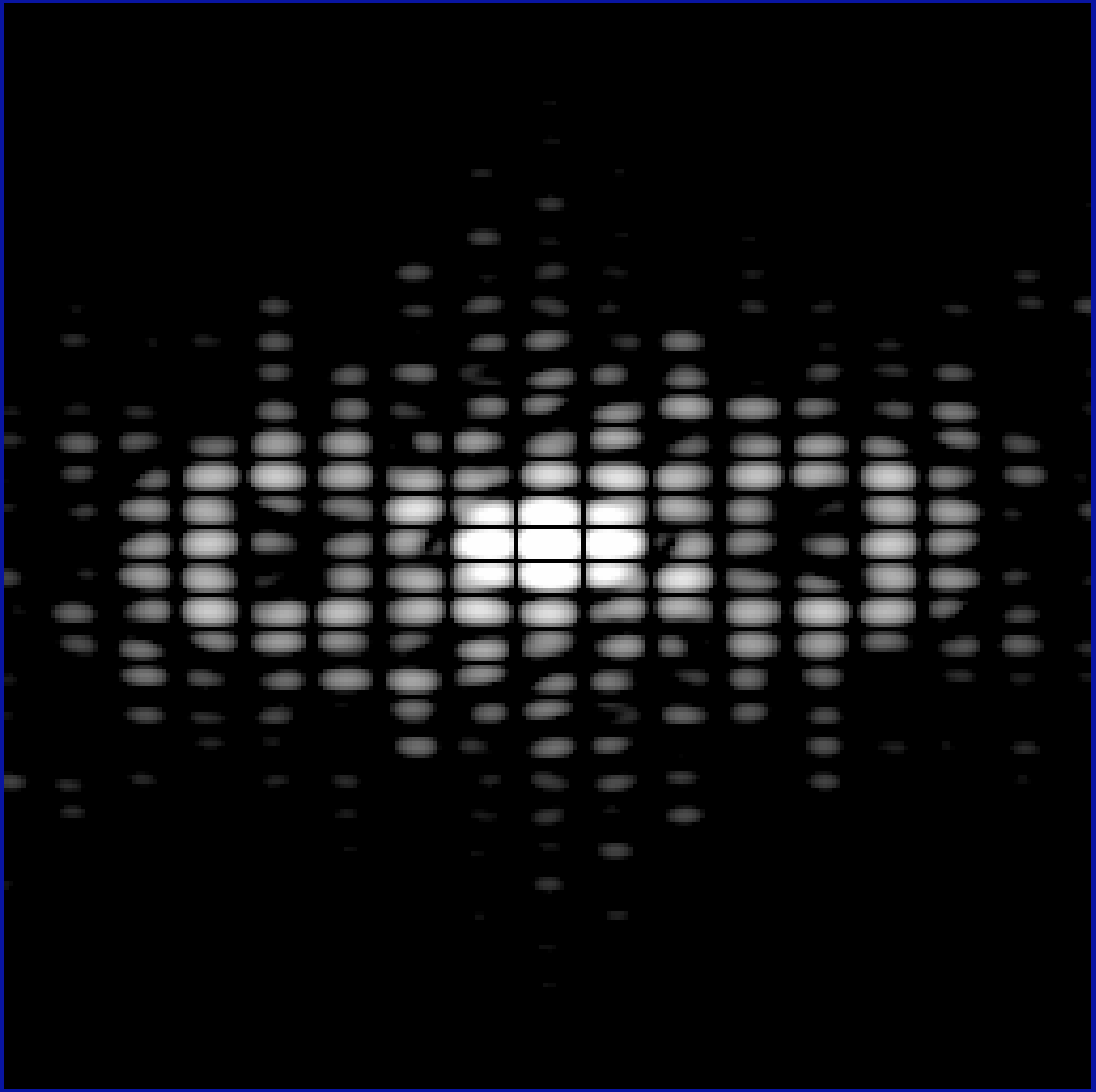
Effect of 2-D Crystal Lattice on Transform
(Transform Sampling)

2 x 1 crystal



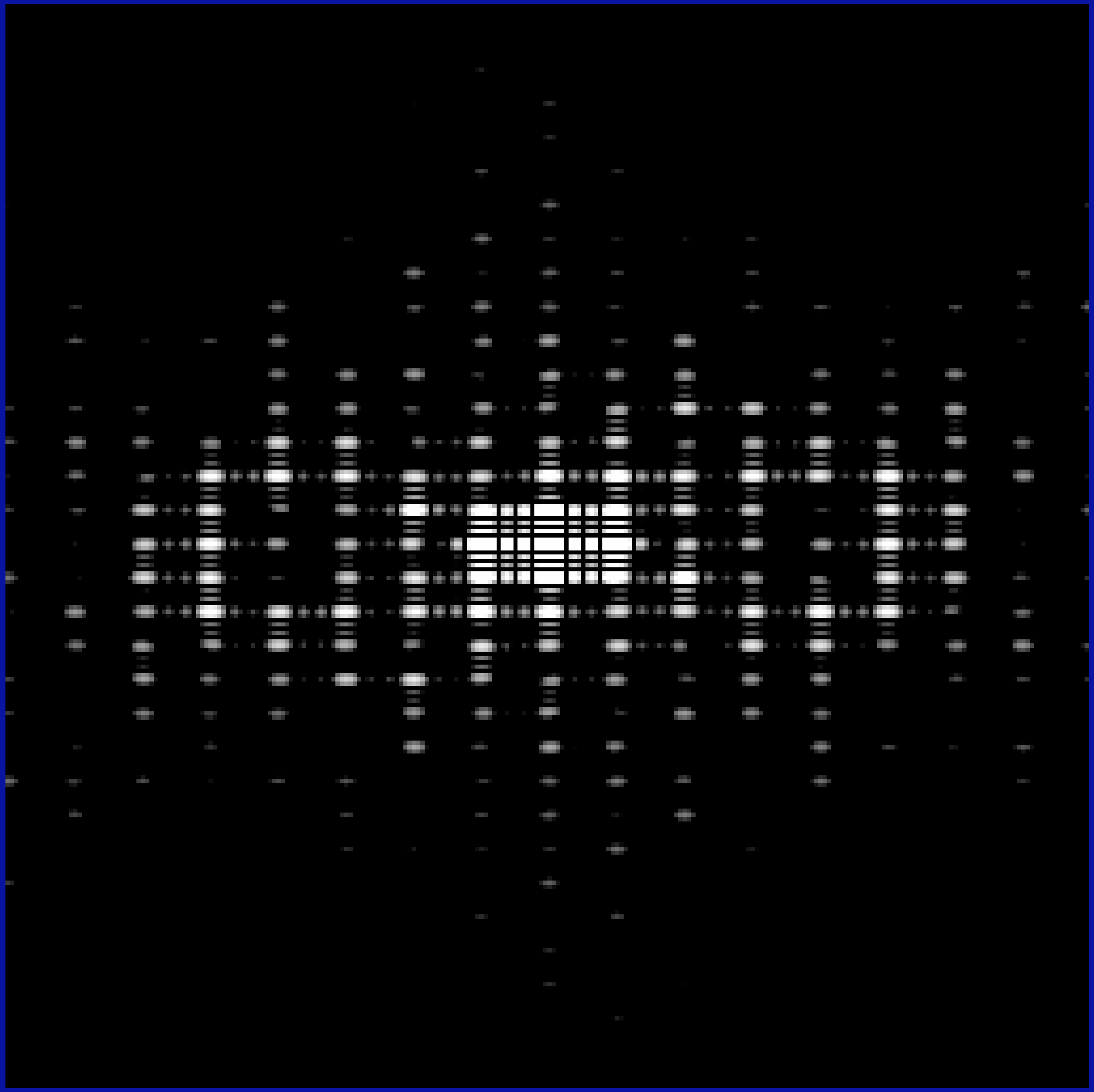
Effect of 2-D Crystal Lattice on Transform
(Transform Sampling)

2 x 2 crystal



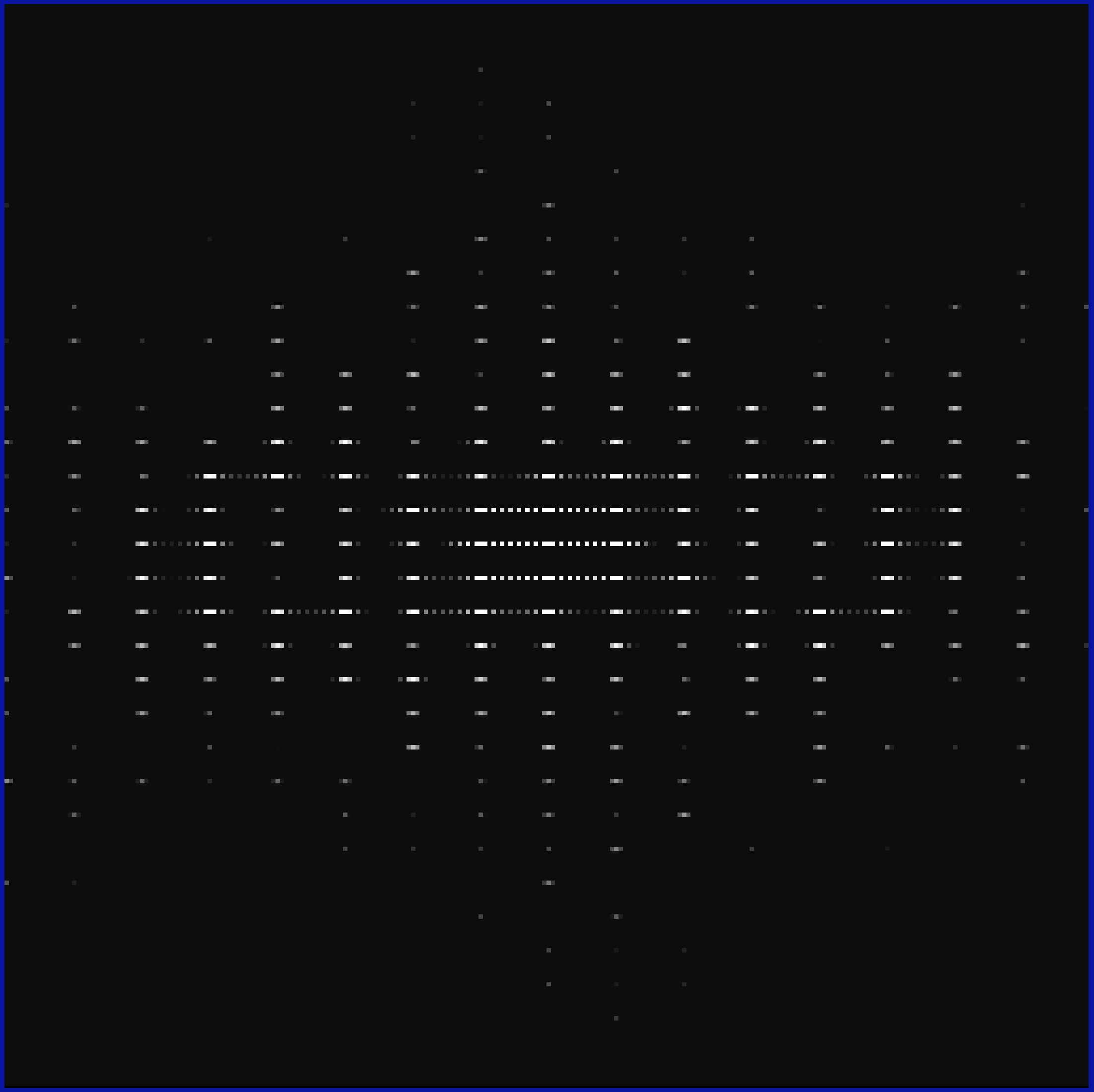
Effect of 2-D Crystal Lattice on Transform (Transform Sampling)

4 x 4 crystal



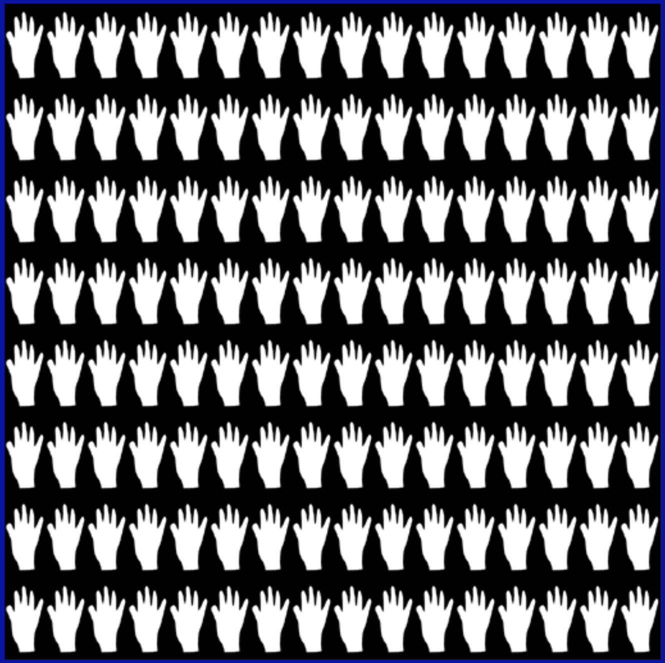
Effect of 2-D Crystal Lattice on Transform (Transform Sampling)

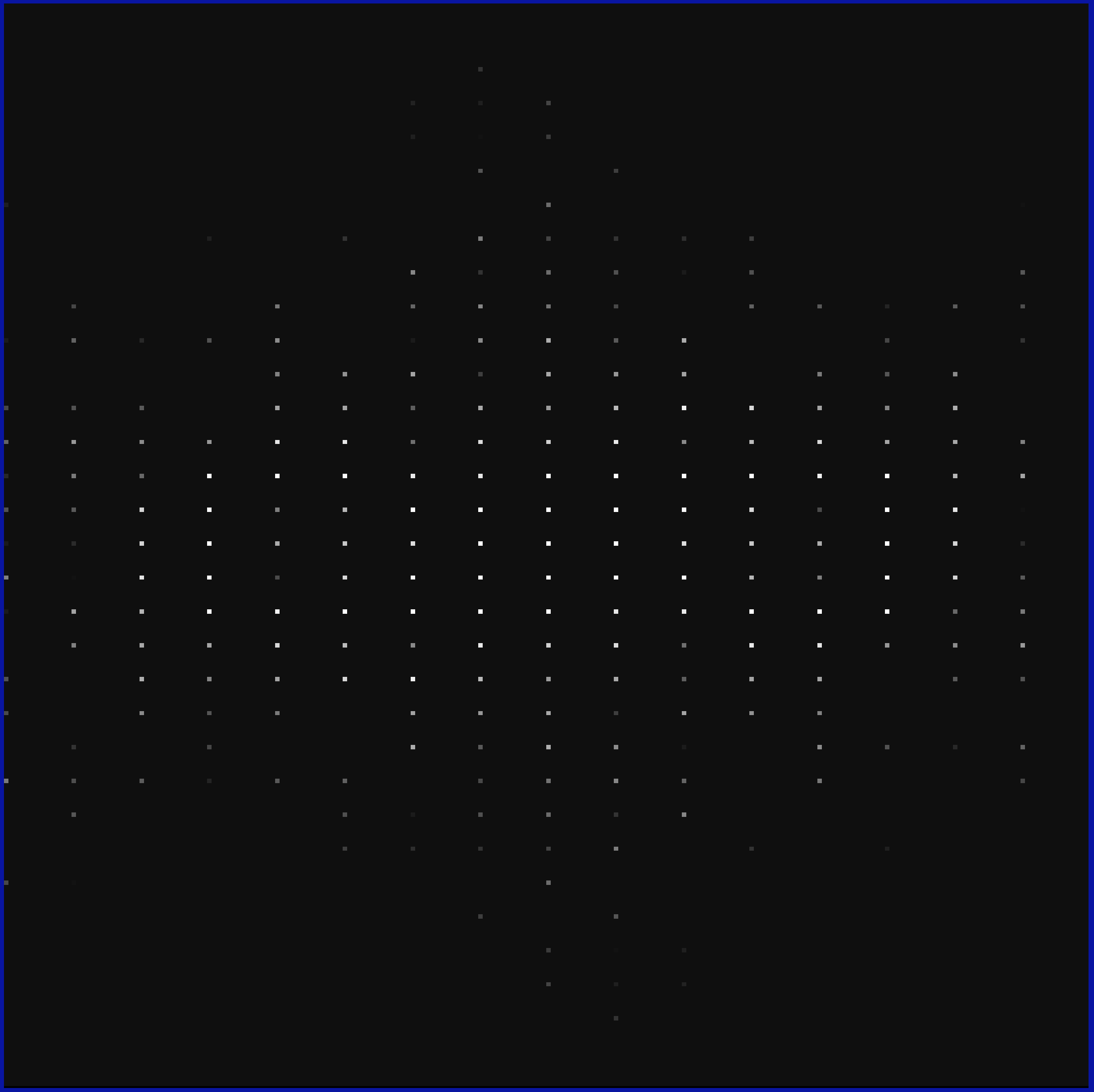
8 x 8 crystal



Effect of 2-D Crystal Lattice on Transform
(Transform Sampling)

16 x 8 crystal





III.C.6.g Convolution and Multiplication

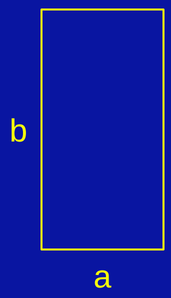
1-D lattices give rise to transforms sampled in only one direction

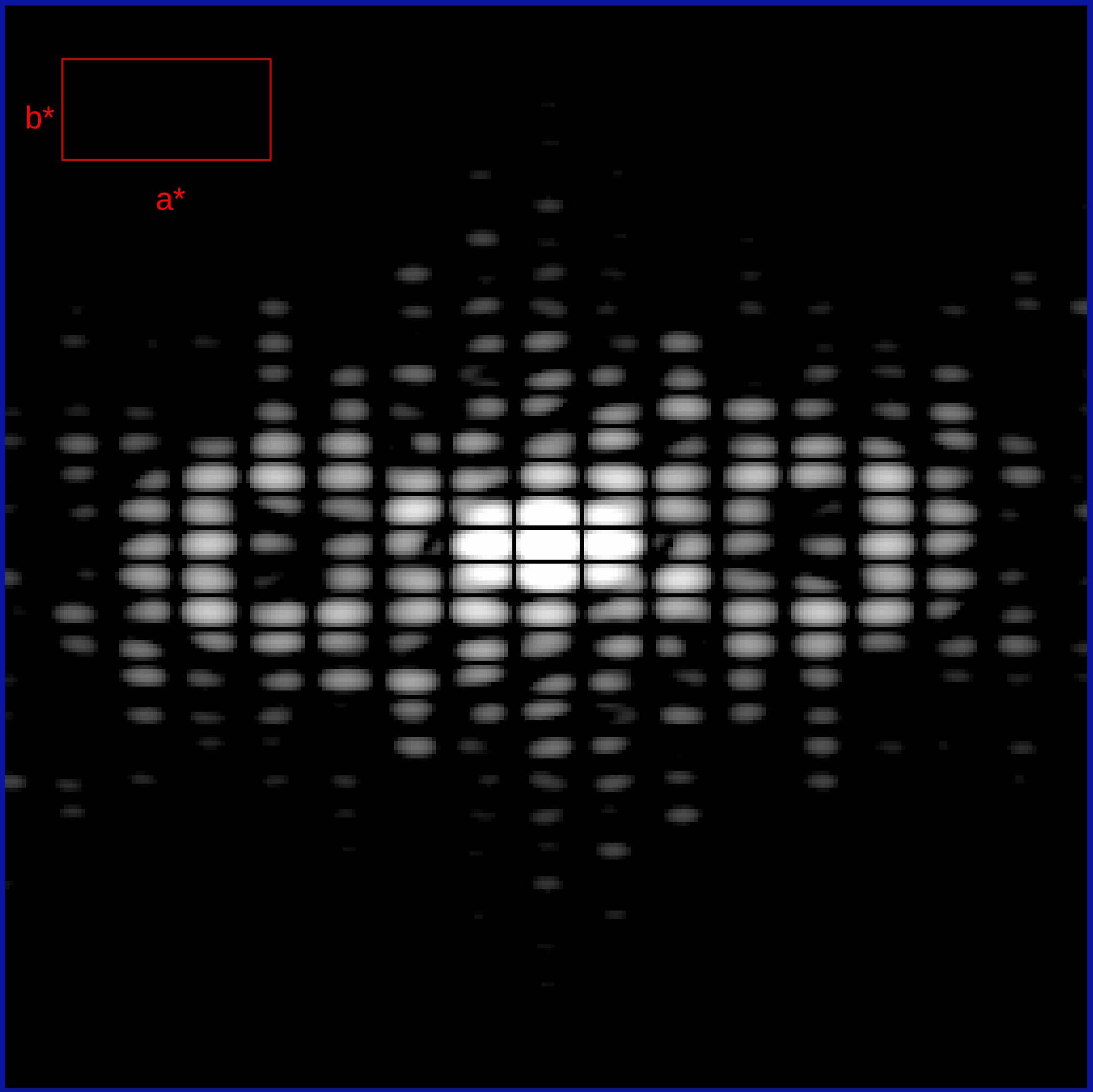
2-D lattices produce sampling on a 2-D grid or reciprocal lattice

Example 2: Non-orthogonal 2-D lattice

Effect of 2-D Crystal Lattice on Transform
(Transform Sampling)

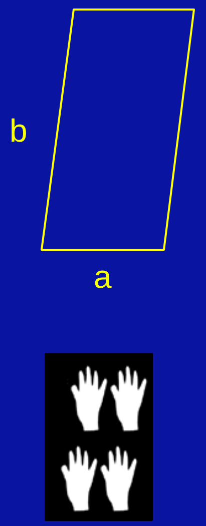
2 x 2 crystal

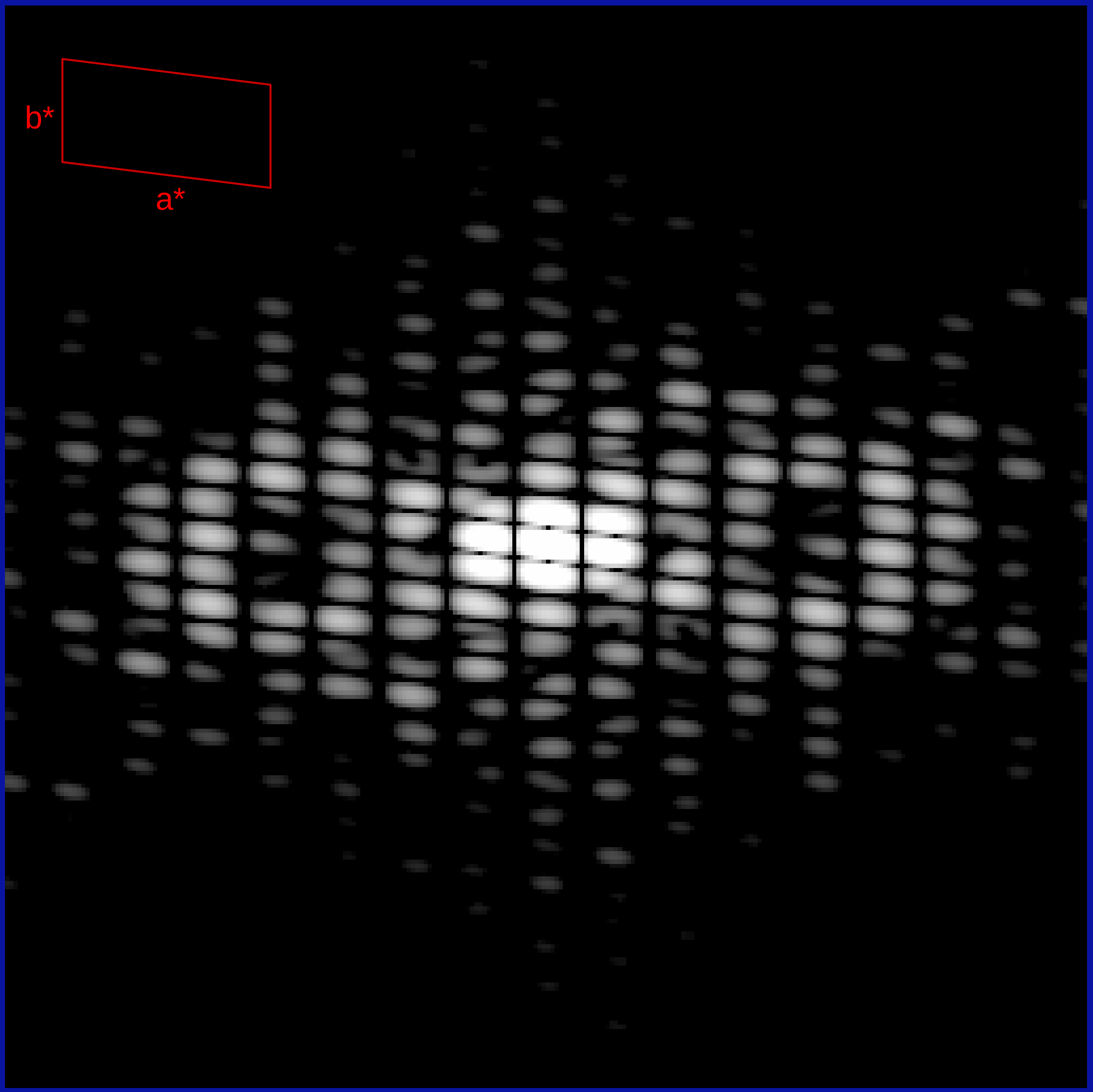




Effect of 2-D Crystal Lattice on Transform
(Transform Sampling)

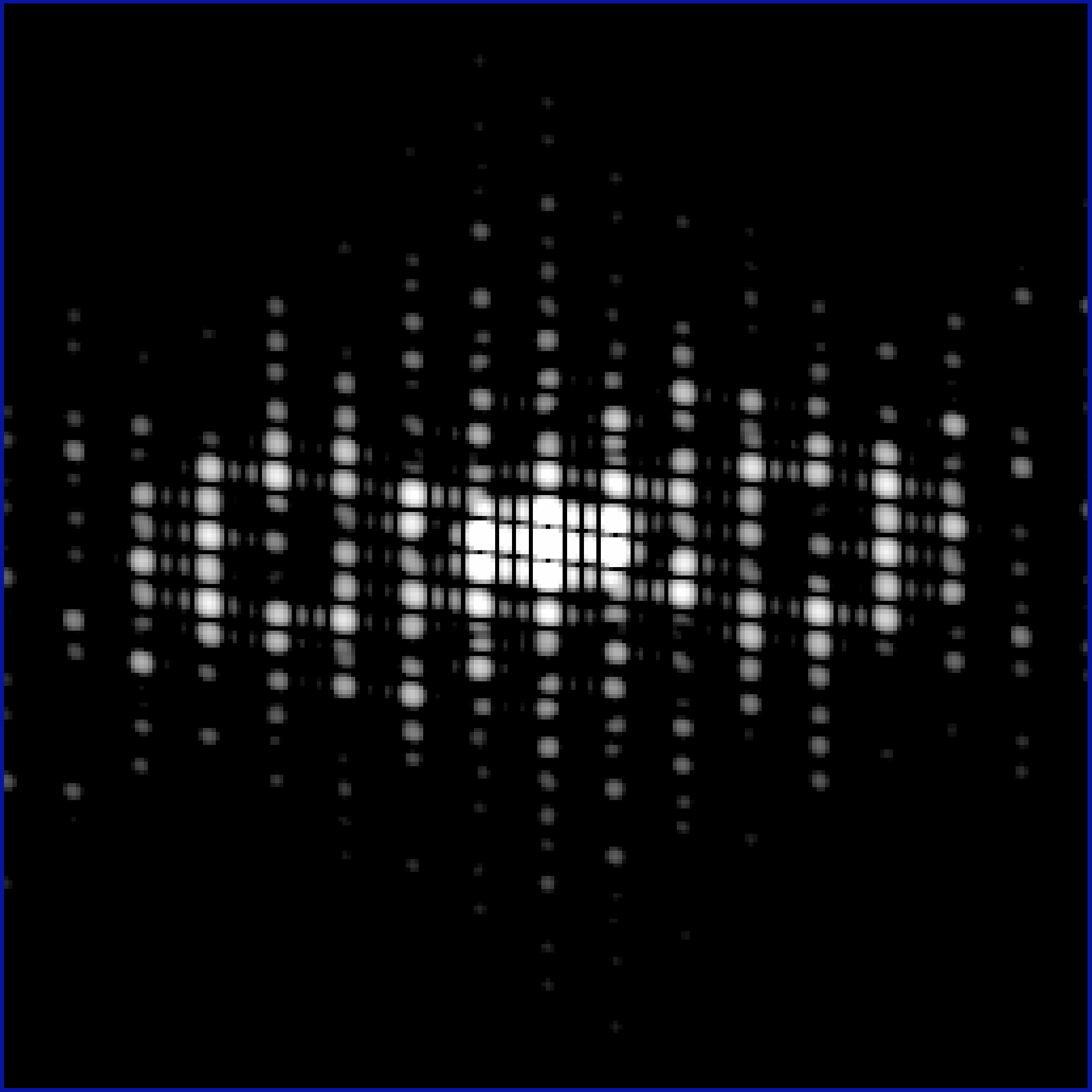
2 x 2 crystal





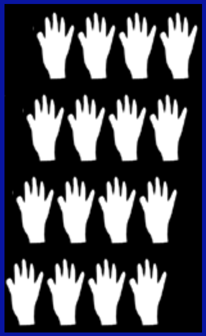
Effect of 2-D Crystal Lattice on Transform
(Transform Sampling)

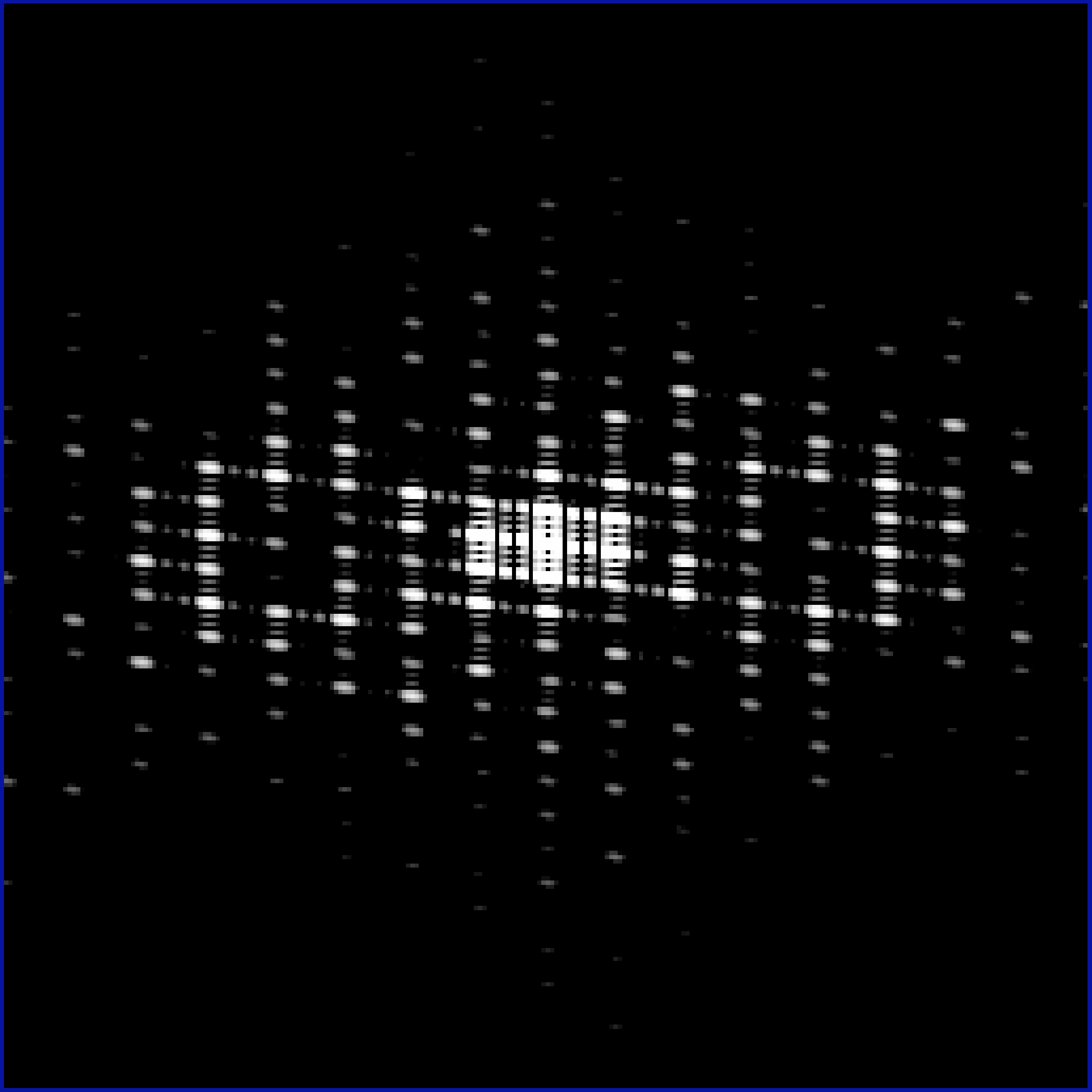
4 x 2 crystal



Effect of 2-D Crystal Lattice on Transform (Transform Sampling)

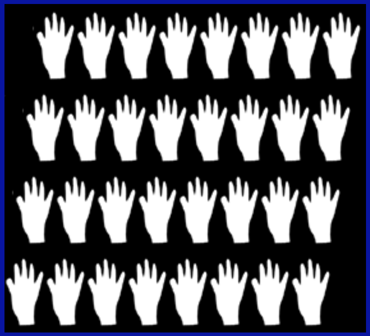
4 x 4 crystal

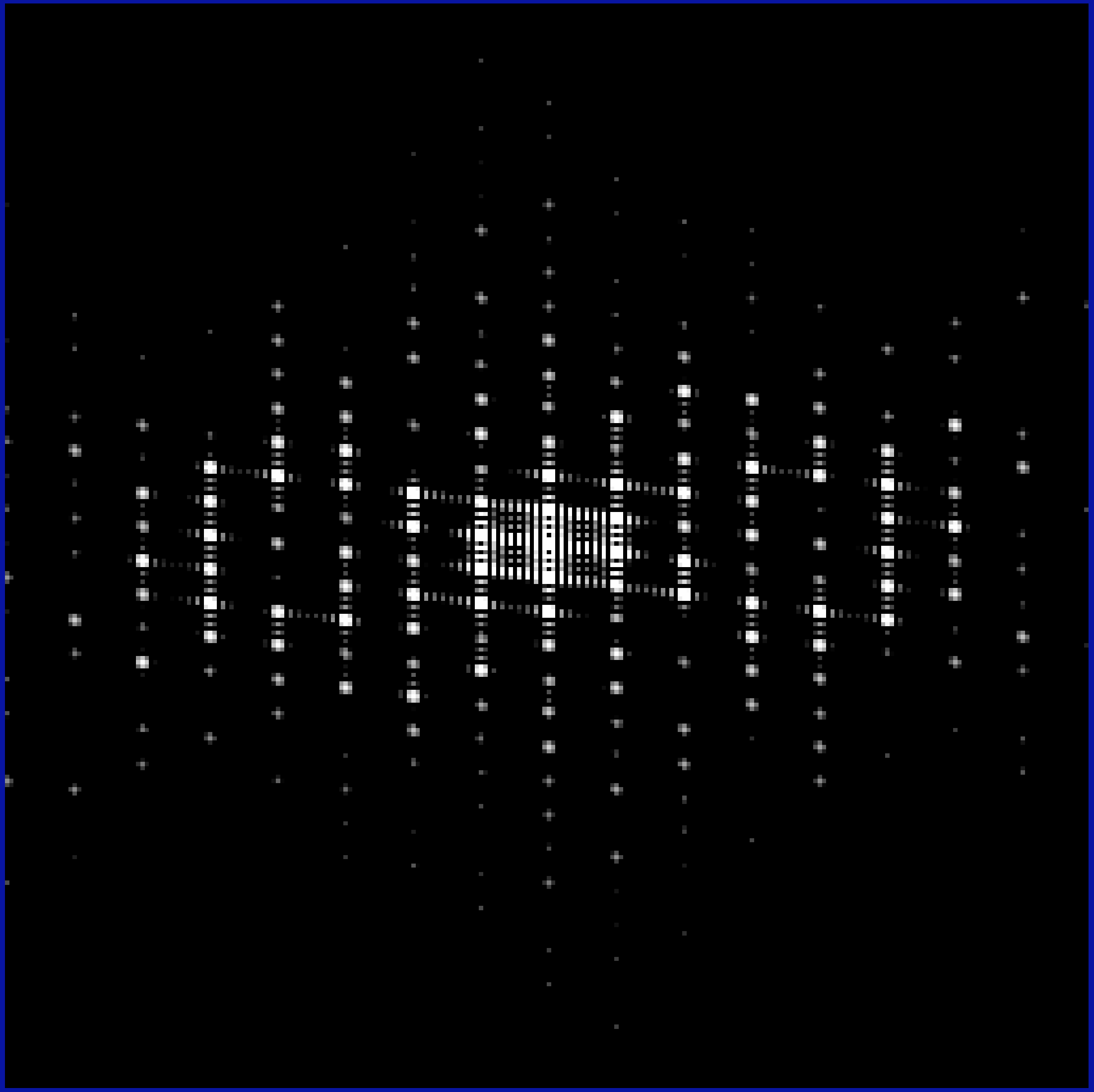




Effect of 2-D Crystal Lattice on Transform (Transform Sampling)

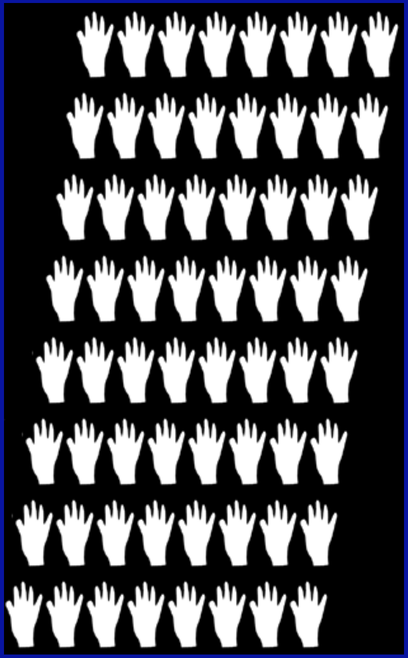
8 x 4 crystal

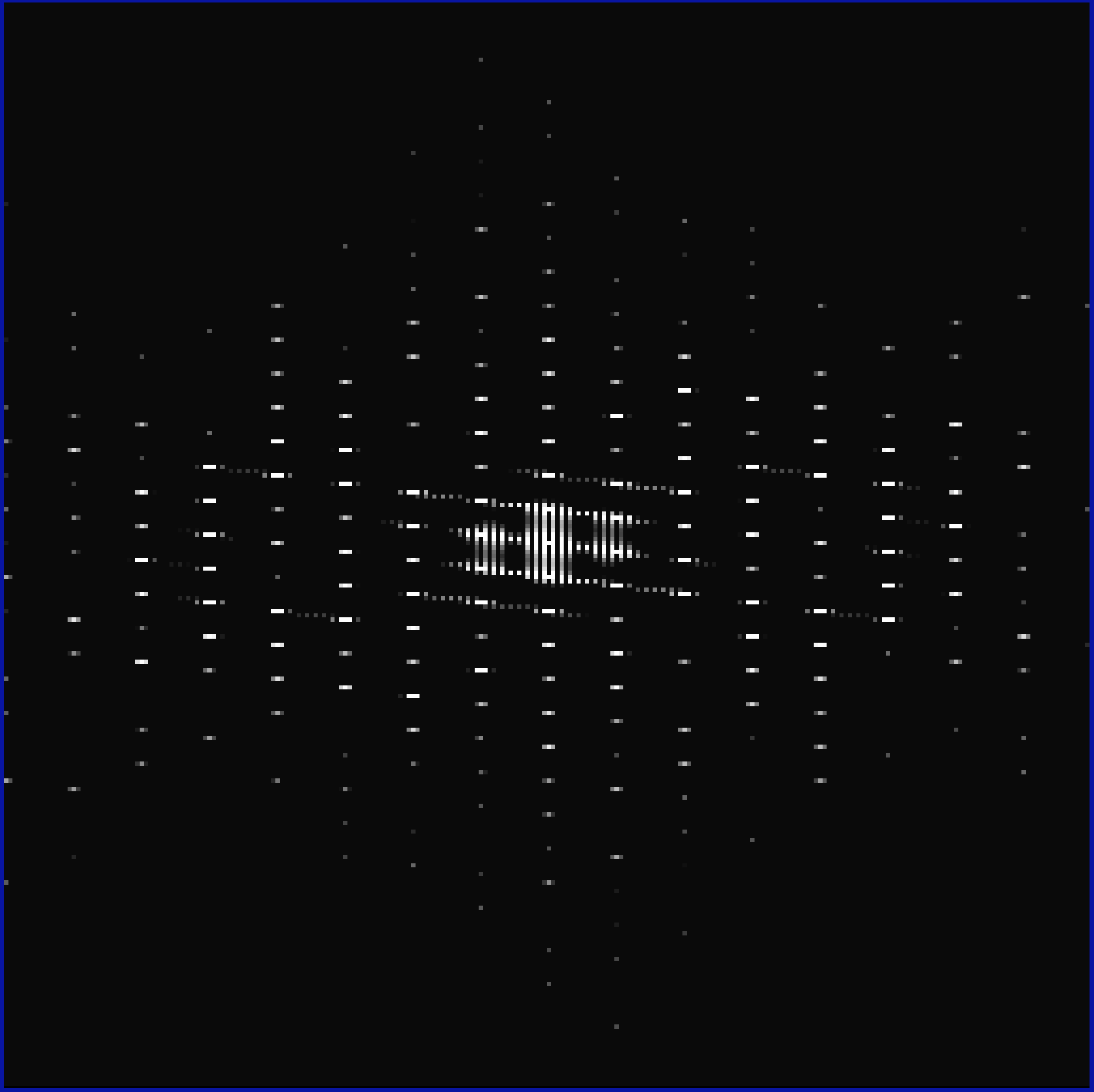




Effect of 2-D Crystal Lattice on Transform (Transform Sampling)

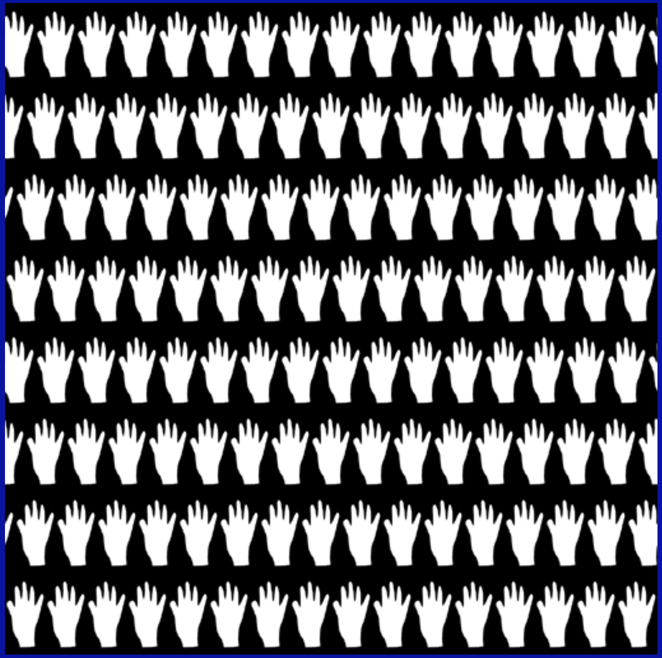
8 x 8 crystal

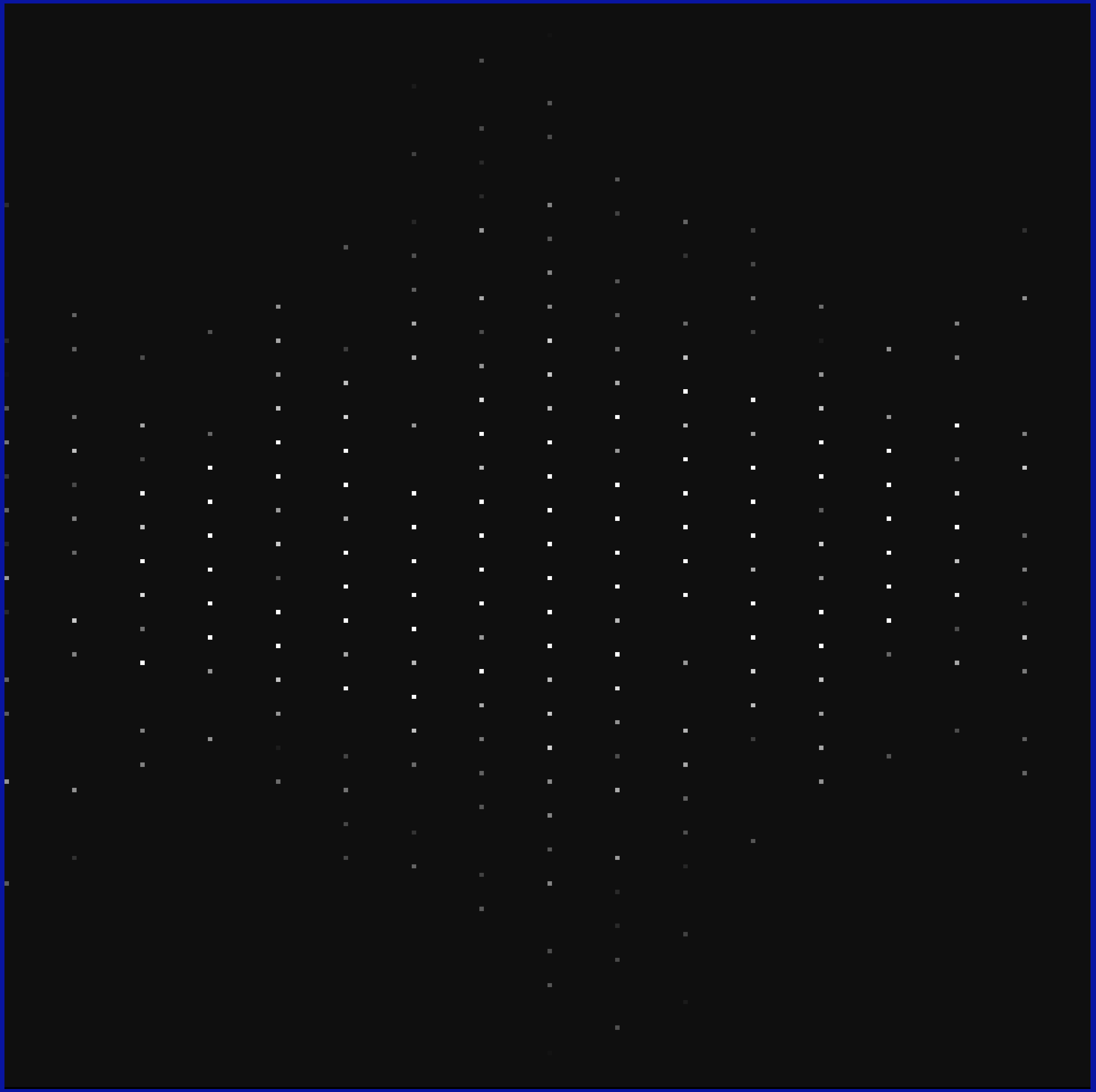




Effect of 2-D Crystal Lattice on Transform (Transform Sampling)

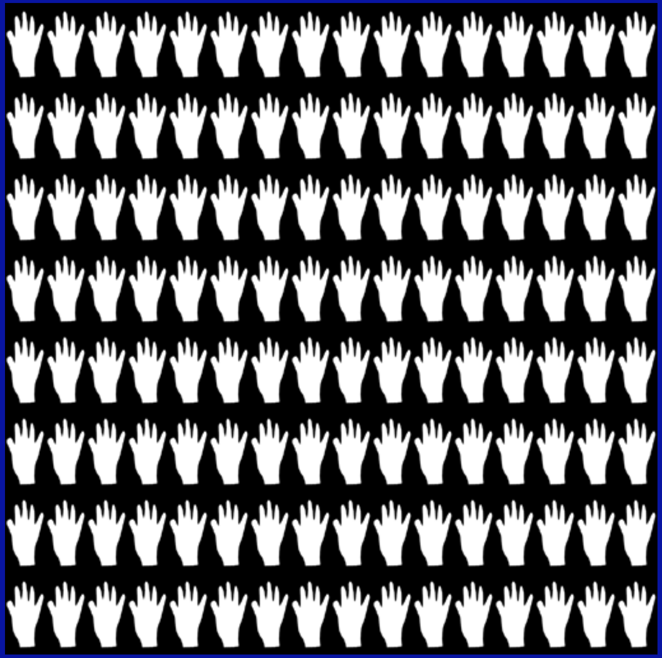
16 x 8 crystal

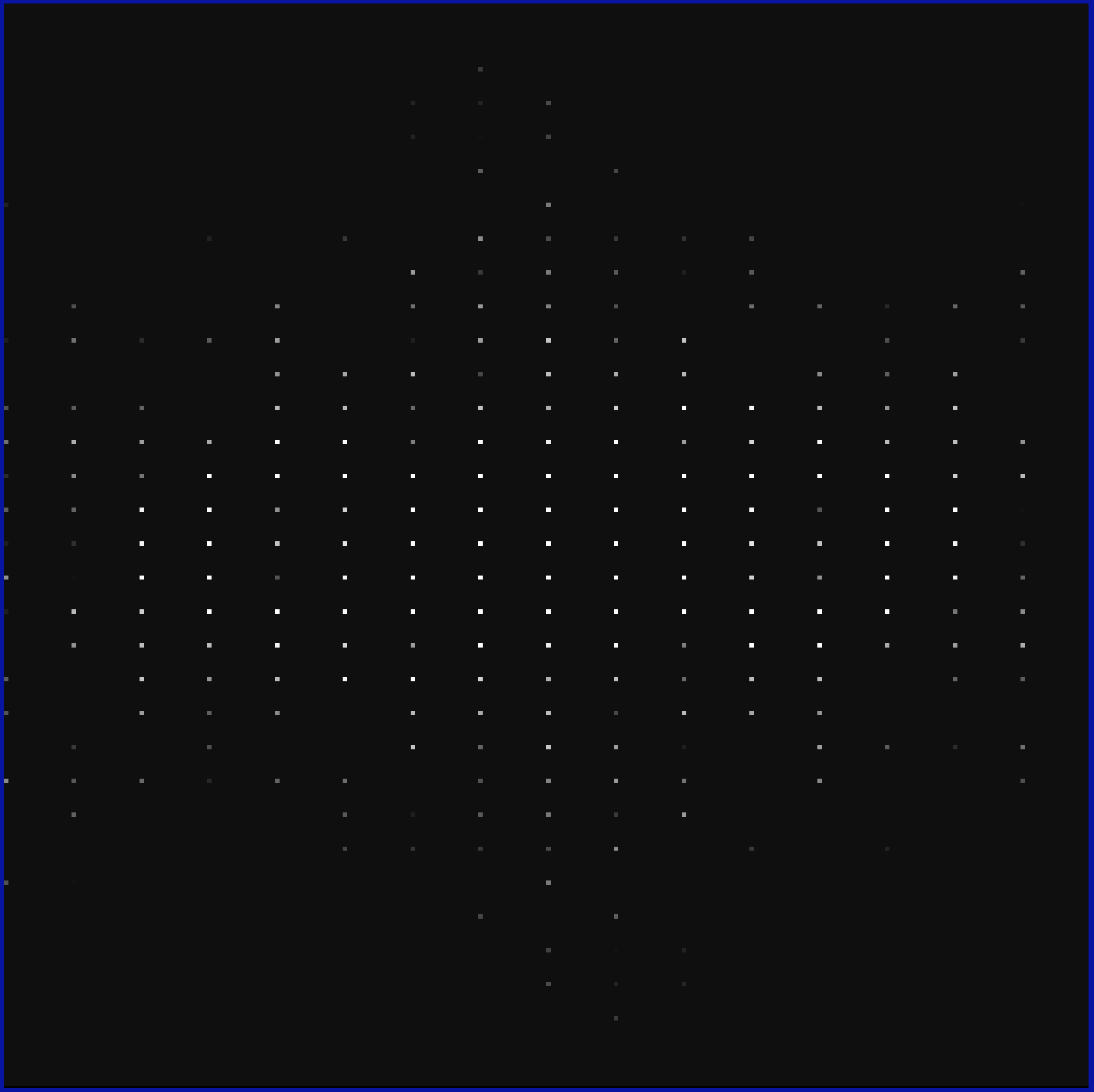




Effect of 2-D Crystal Lattice on Transform (Transform Sampling)

16 x 8 crystal





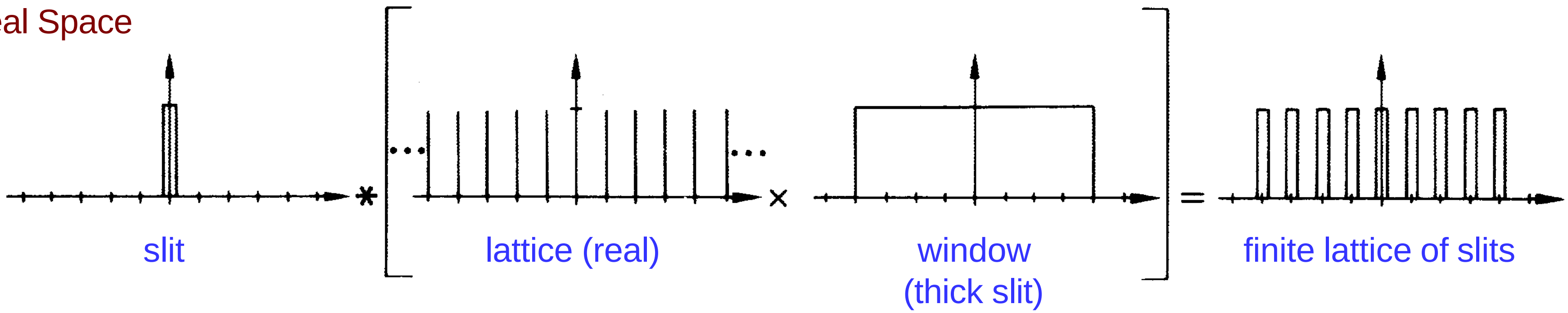
III.C.6.g Convolution and Multiplication

If the phase and amplitude (structure factor) at each point *hk* in the 2-D reciprocal lattice can be obtained, the **crystal and motif structures** can be solved by **mathematical** Fourier synthesis (inverse Fourier transformation)

Diffraction Pattern of N Wide Slits

(Fourier Transform and Convolution Relationships)

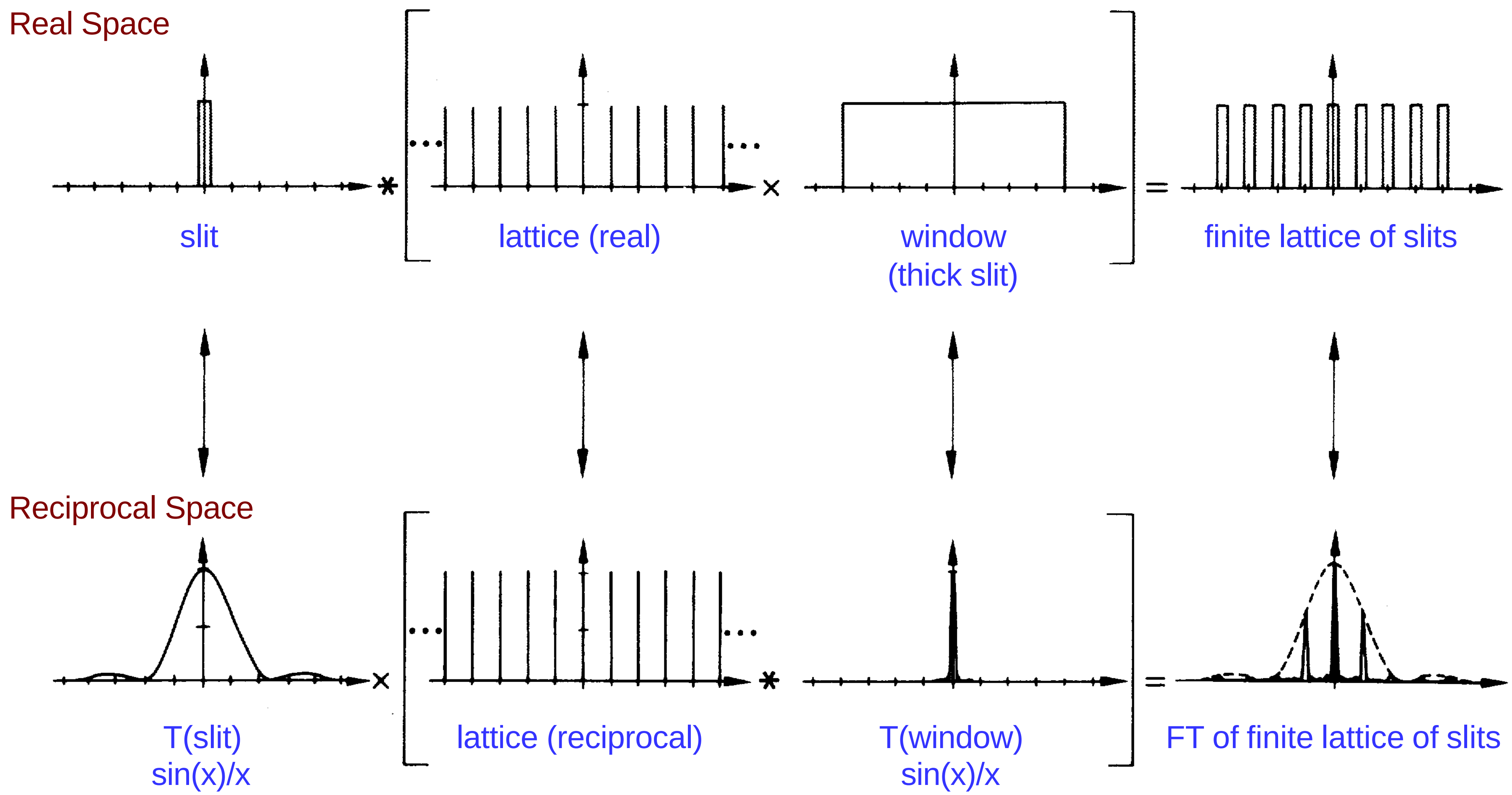
Real Space



From Sherwood, Fig. 7.21, p.255

Diffraction Pattern of N Wide Slits

(Fourier Transform and Convolution Relationships)



From Sherwood, Fig. 7.21, p.255

III.C CRYSTALS, SYMMETRY AND DIFFRACTION

III.C.6 Diffraction

KEY CONCEPTS:

- Fourier transform
- Fourier Synthesis and Analysis
- Image formation is a double diffraction process
- Bragg's Law
- Structure factor and Argand diagram
- Convolution and multiplication

III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

1) Analogy between OD and "Mathematical" FTs

2) Asymmetric / Symmetric Objects / Transforms

3) Reciprocity

4) Resolution

5) Sharpness of Diffraction Spots

6) Geometry, Intensity and Symmetry

7) Projection Theorem

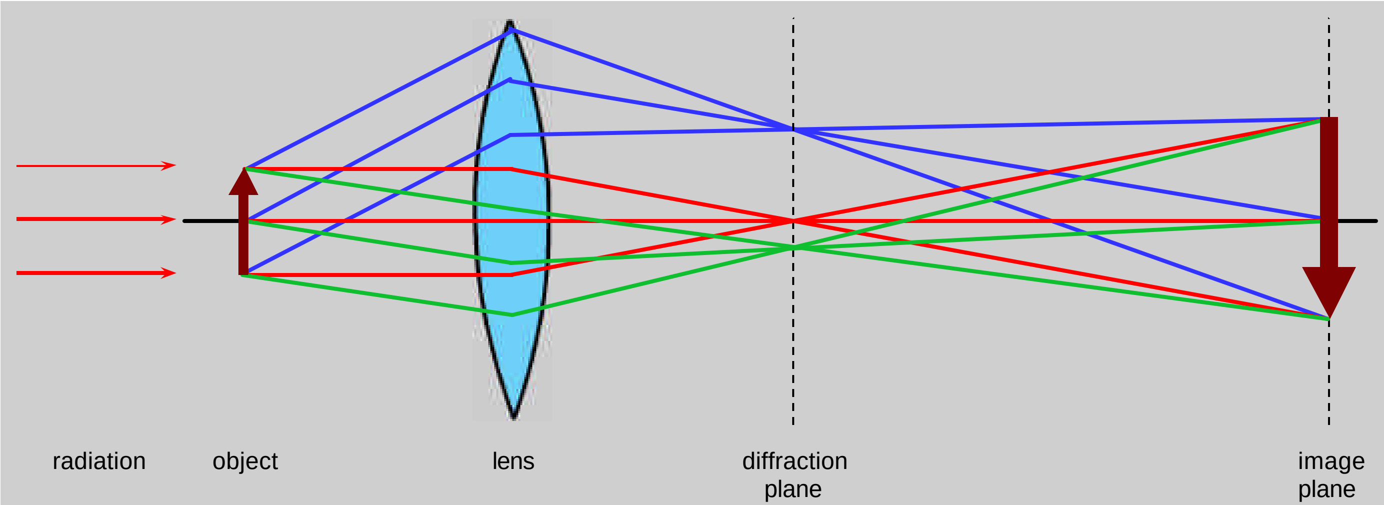
8) Friedel's Law

III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Analogy between OD and "Mathematical" FTs

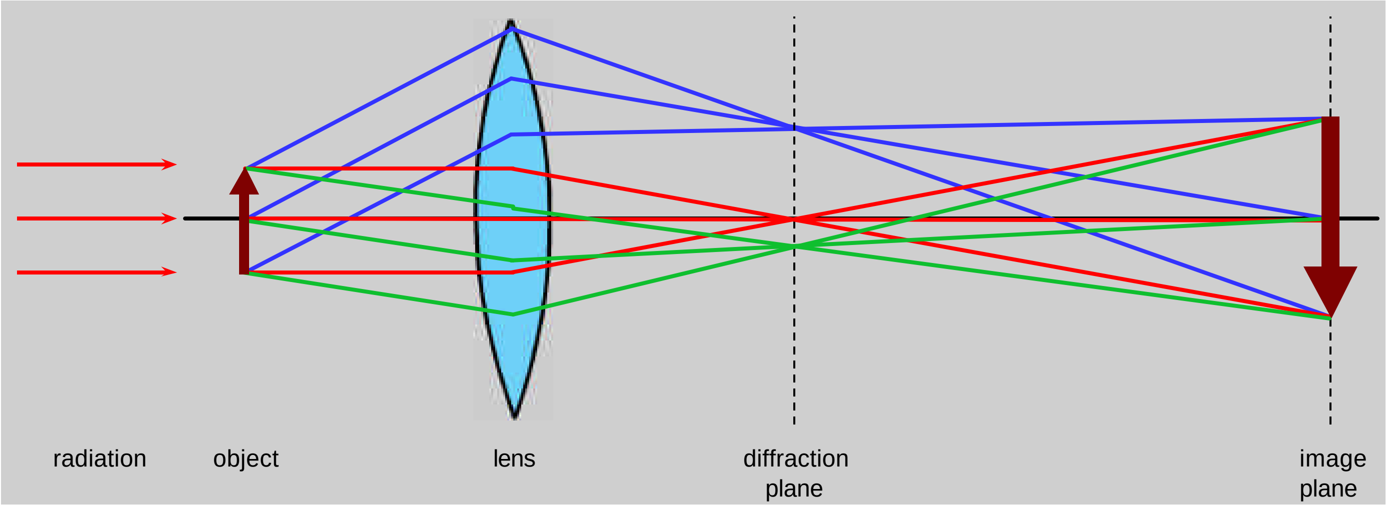
Optical bench is an excellent device for demonstrating properties of Fourier transforms and diffraction patterns



III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Analogy between OD and "Mathematical" FTs



Optical Diffraction:

- Incident radiation is laser beam

- Diffraction grating (object) is transparency (*e.g.* EM micrograph) or mask

III.C.6.h Other Properties of FTs and Diffraction Patterns

Asymmetric vs. Symmetric Objects and Their Transforms

Simple, symmetric structures $\Rightarrow$ simple, symmetric transforms

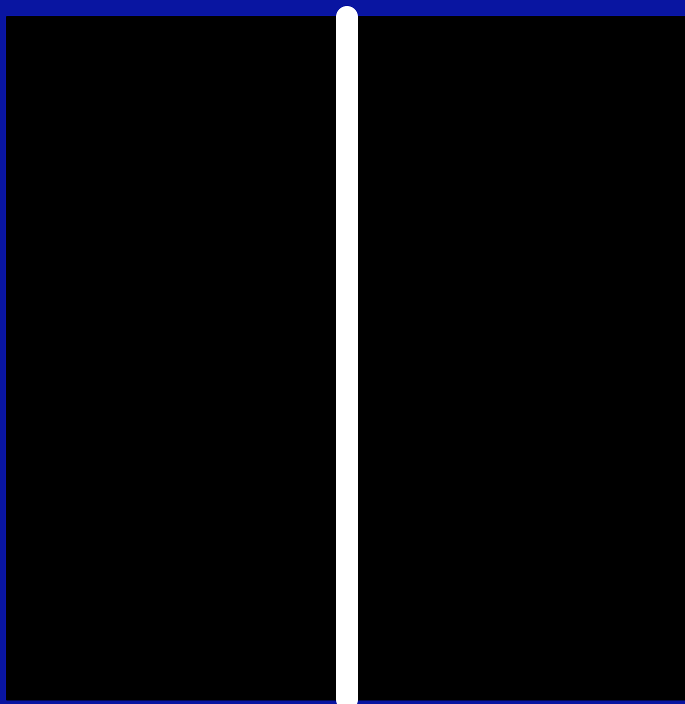
Asymmetric structures $\Rightarrow$ complex transforms

Transforms are like **fingerprints**:

- Specific object features often give rise to **characteristic features** in the transform

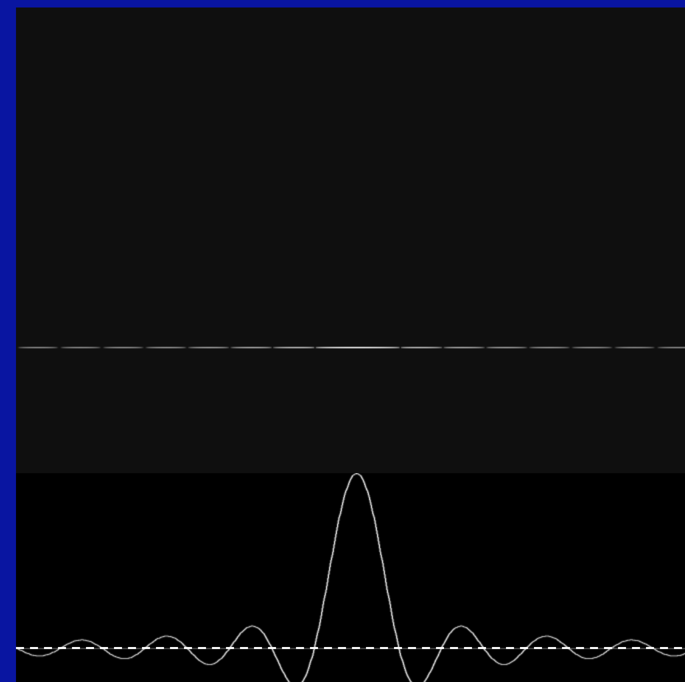
Simple Objects and Their Transforms

Single Slit



FT

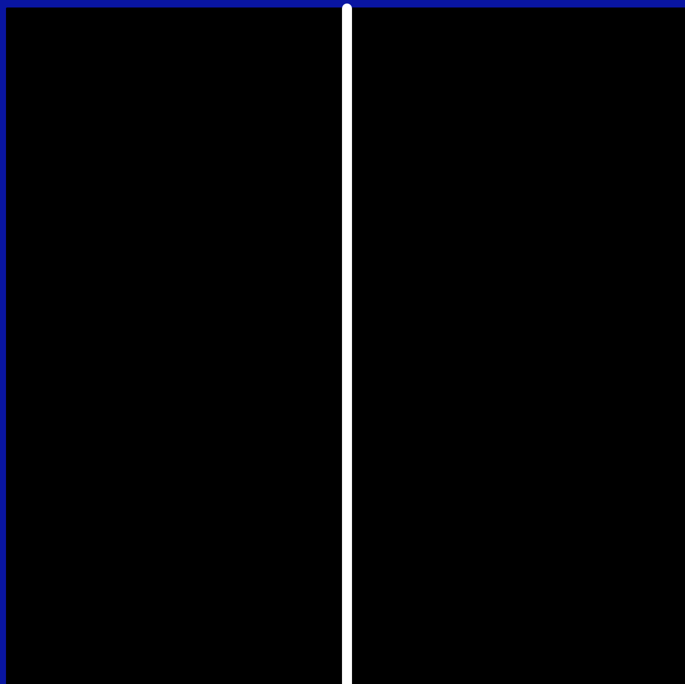
Slit Transform



$$\frac{\sin(x)}{x}$$

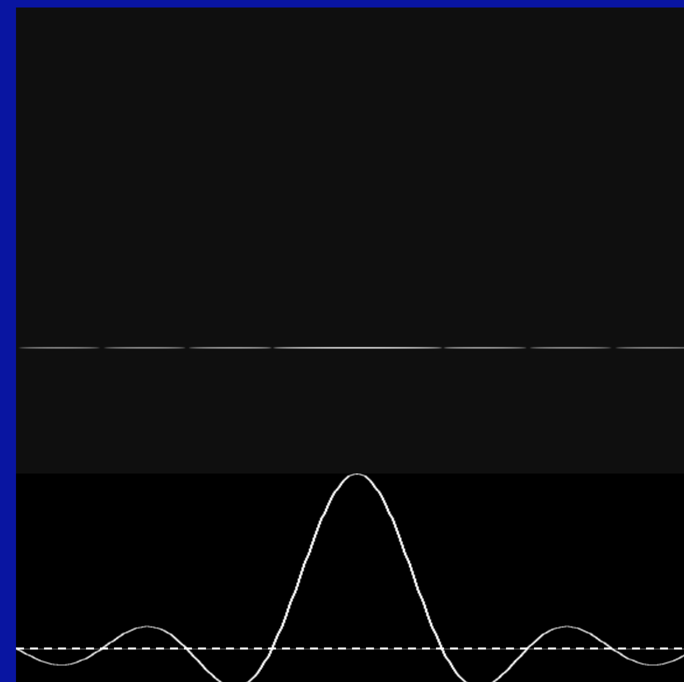
Simple Objects and Their Transforms

Single Slit



FT

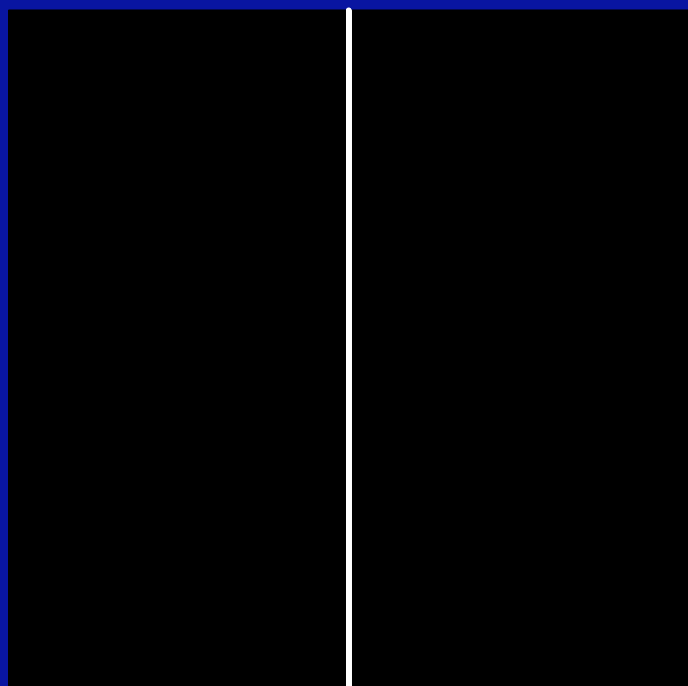
Slit Transform



$$\frac{\sin(x)}{x}$$

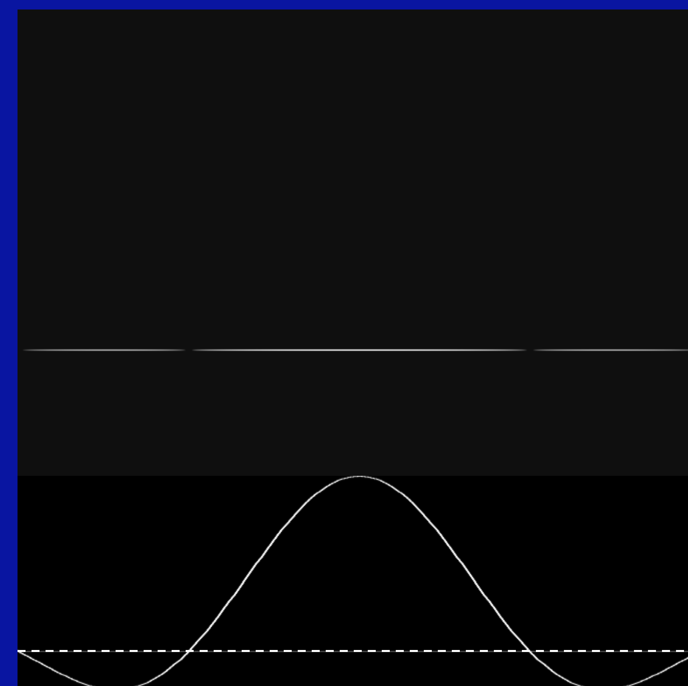
Simple Objects and Their Transforms

Single Slit



FT

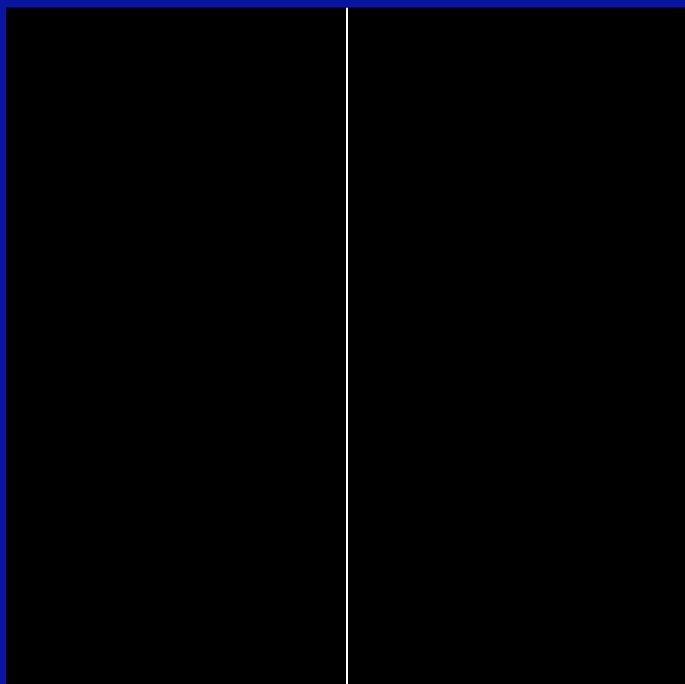
Slit Transform



$$\frac{\sin(x)}{x}$$

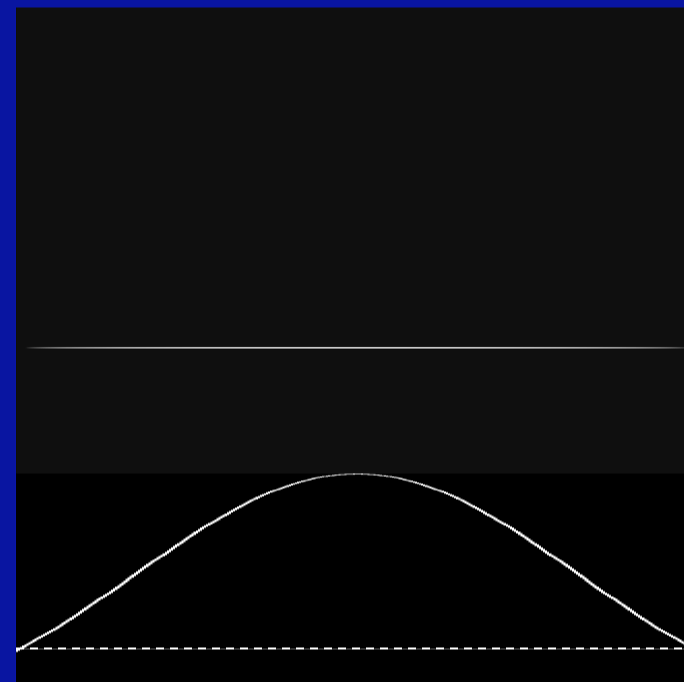
Simple Objects and Their Transforms

Single Slit



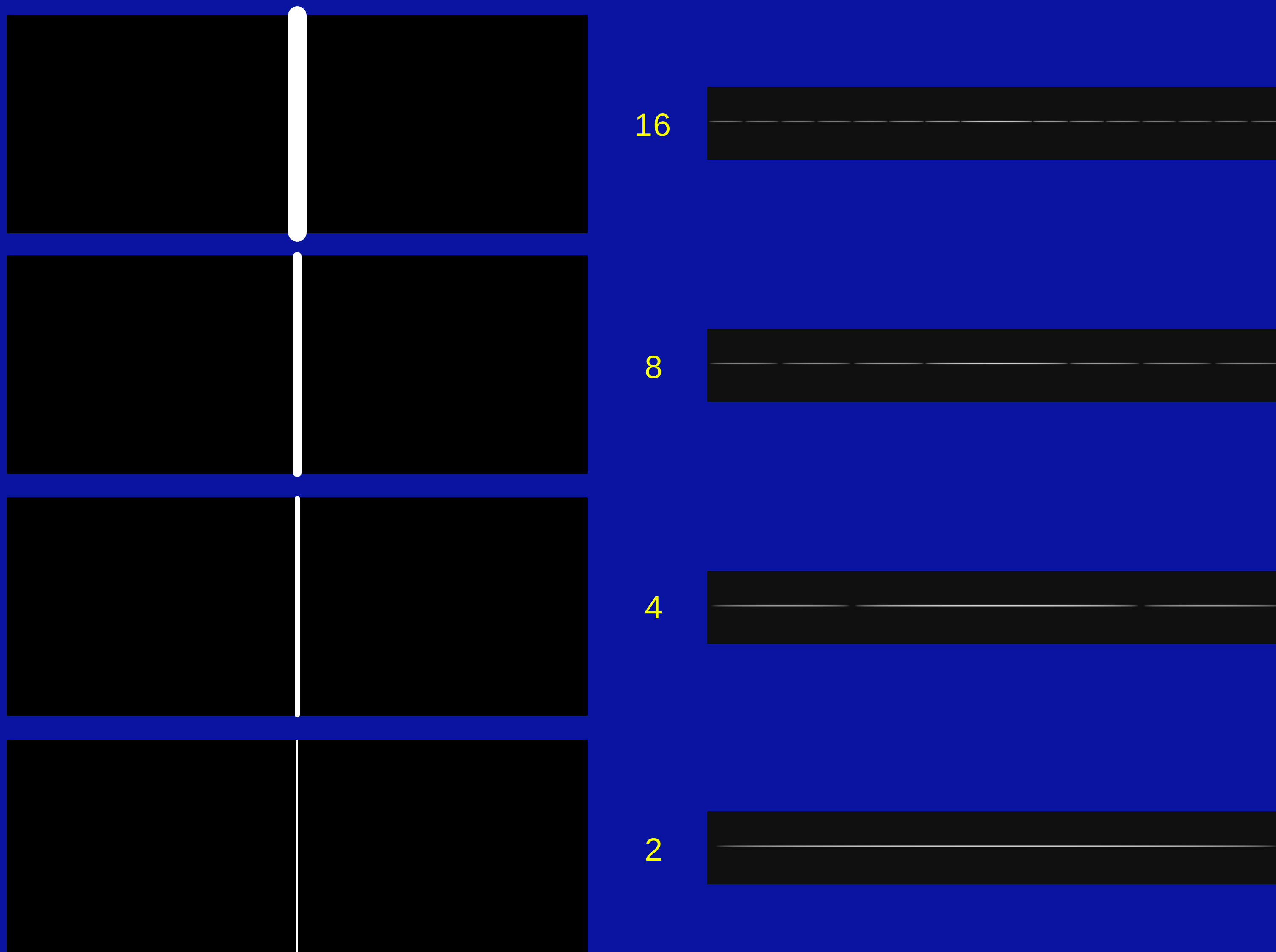
FT

Slit Transform



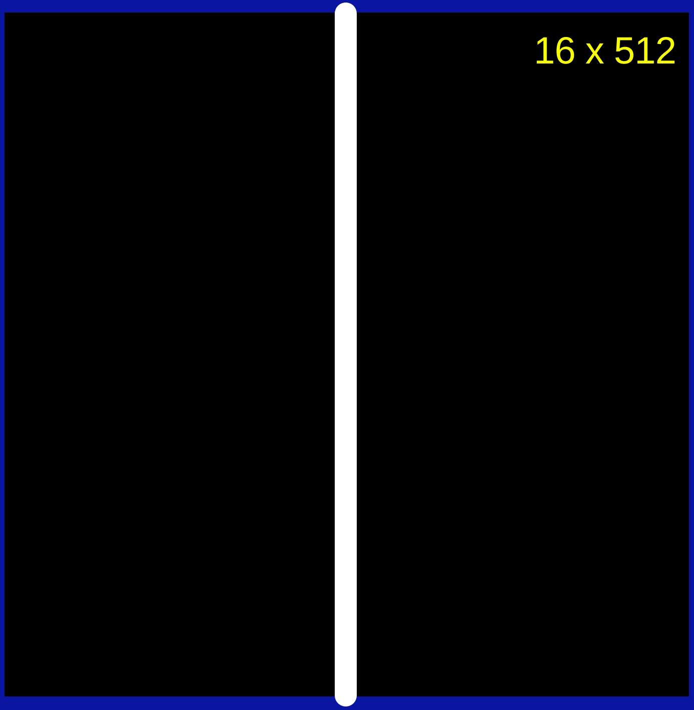
$$\frac{\sin(x)}{x}$$

Simple Objects and Their Transforms



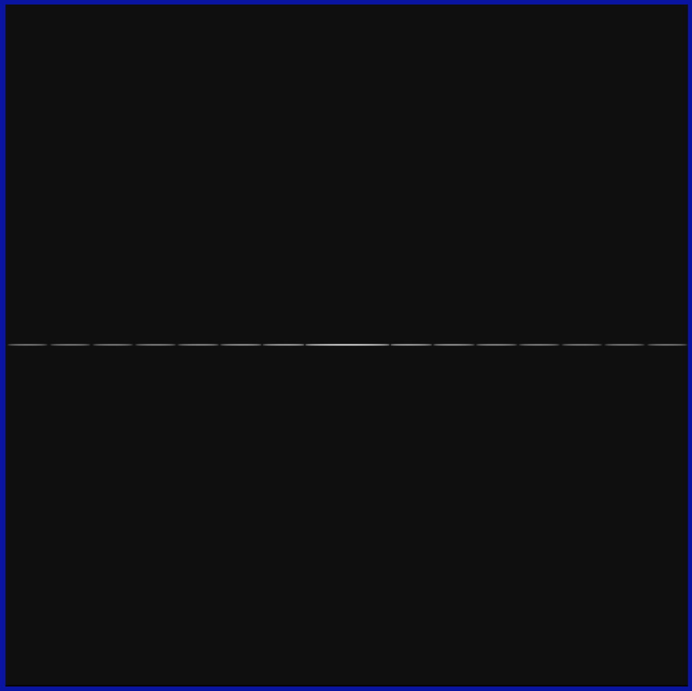
Simple Objects and Their Transforms

Rectangle



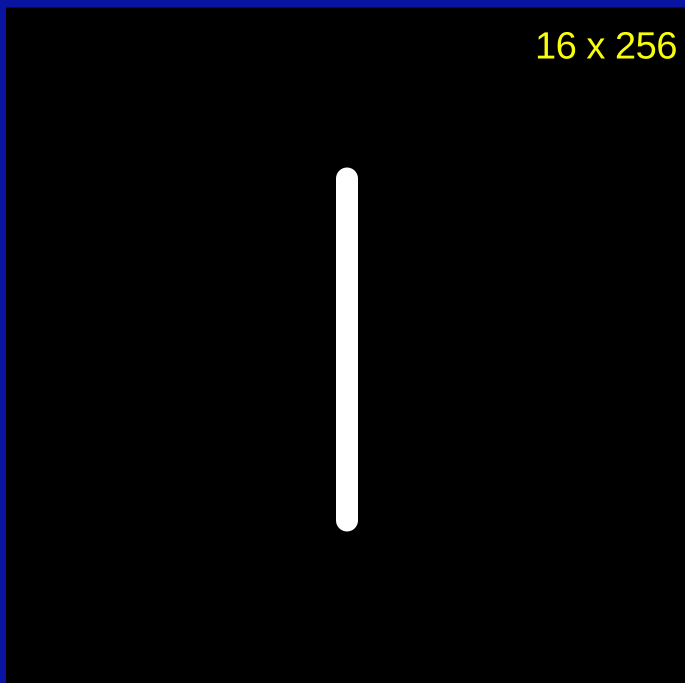
FT

Rectangle Transform



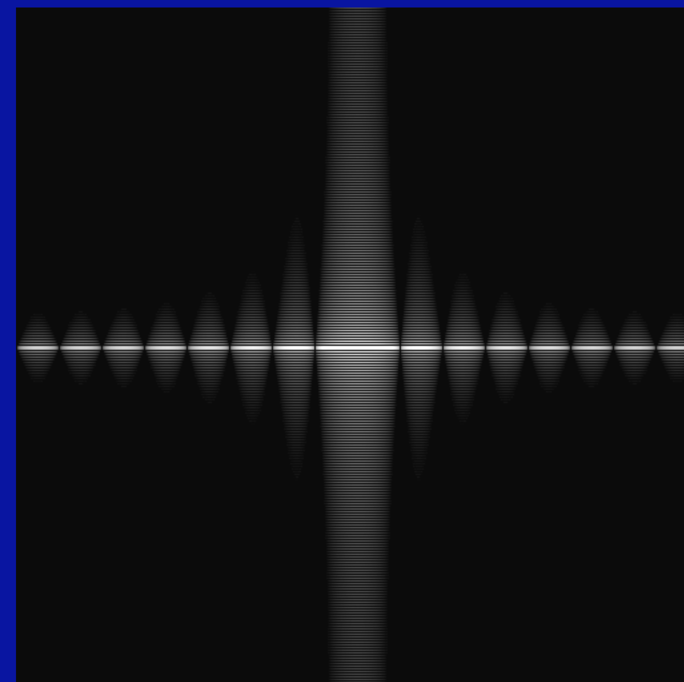
Simple Objects and Their Transforms

Rectangle



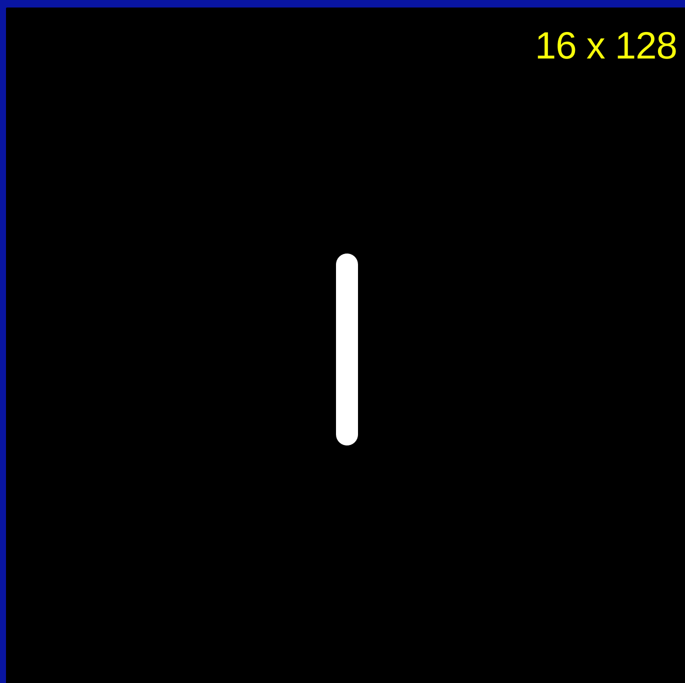
FT

Rectangle Transform



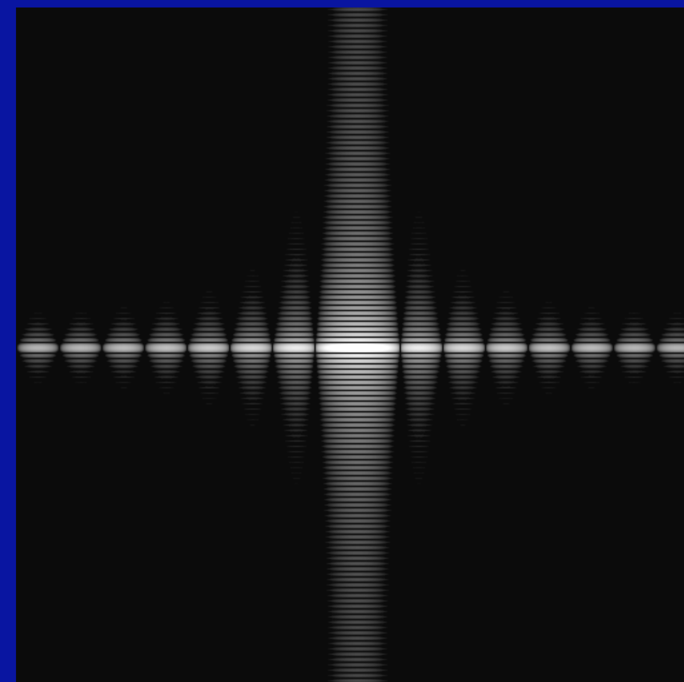
Simple Objects and Their Transforms

Rectangle



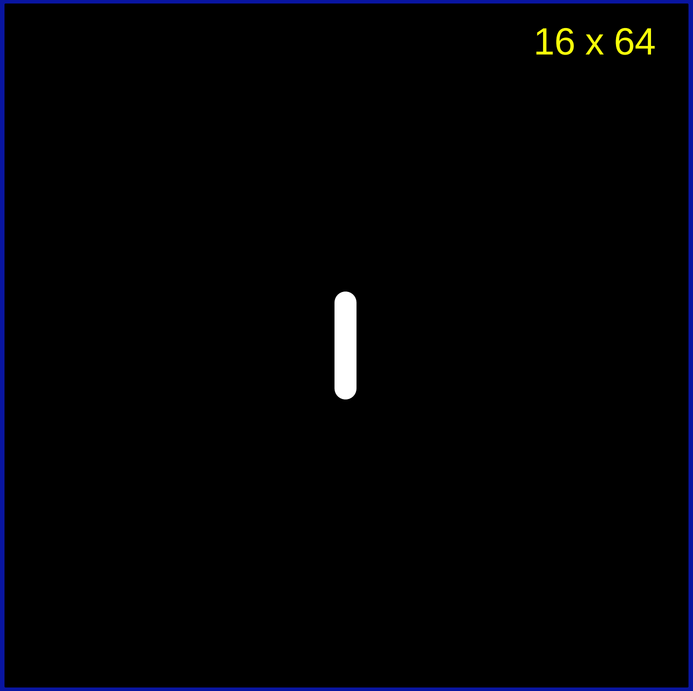
FT

Rectangle Transform



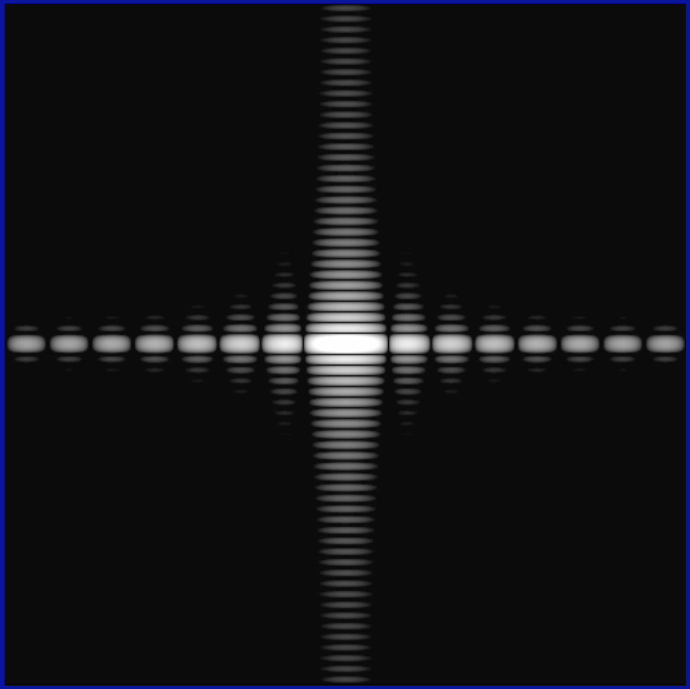
Simple Objects and Their Transforms

Rectangle



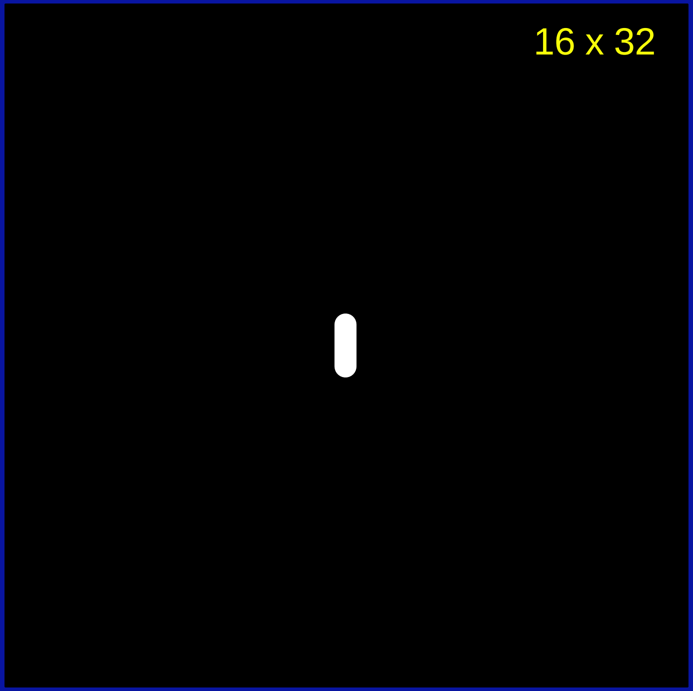
FT

Rectangle Transform



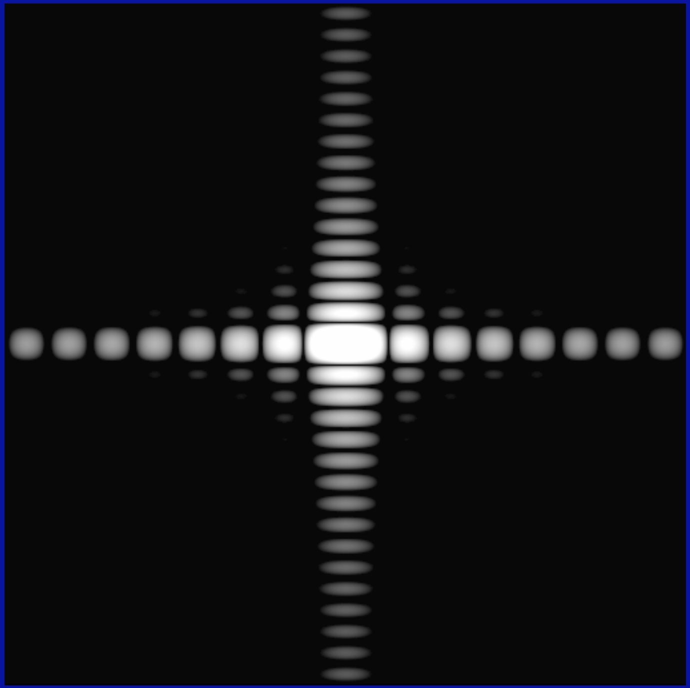
Simple Objects and Their Transforms

Rectangle



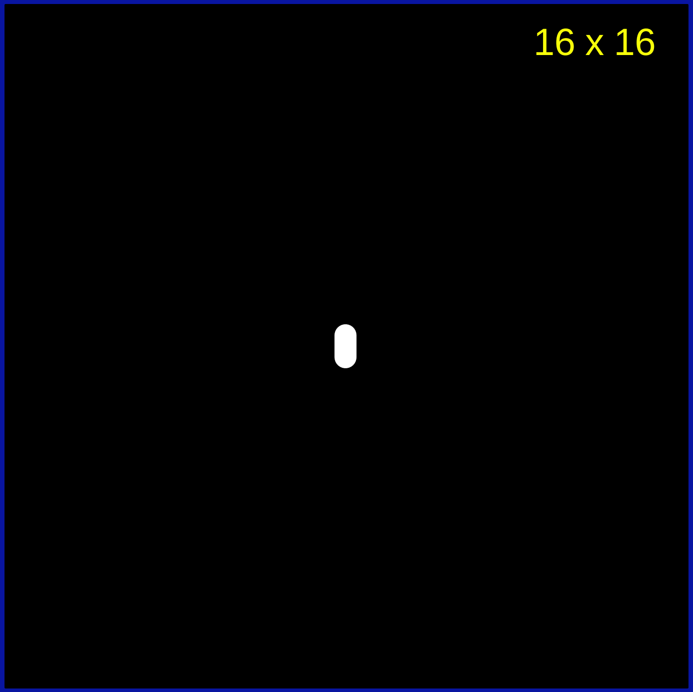
FT

Rectangle Transform



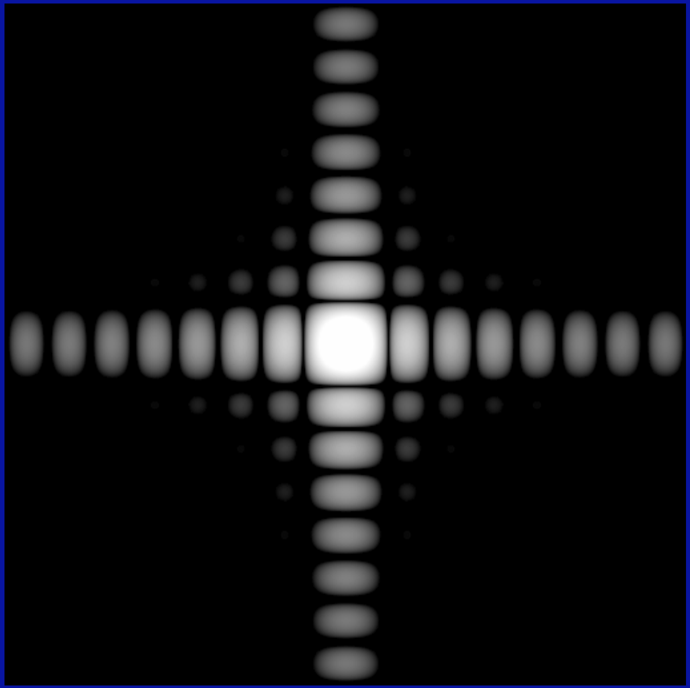
Simple Objects and Their Transforms

"Rectangle"

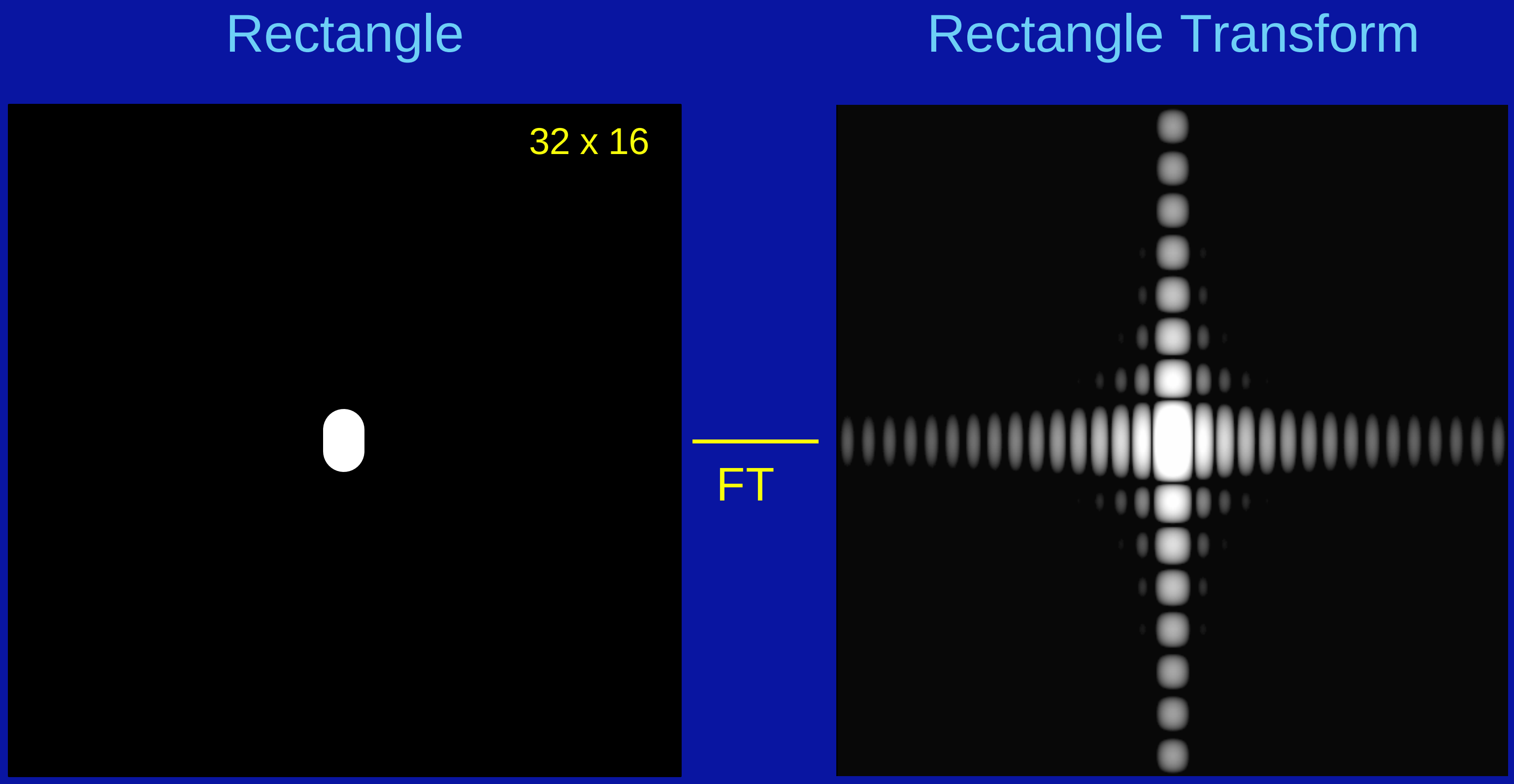


FT

"Rectangle" Transform

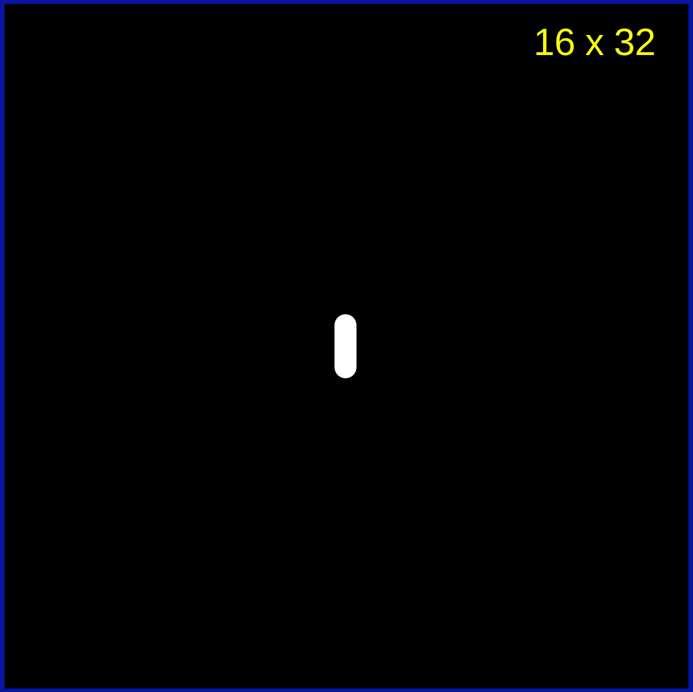


Simple Objects and Their Transforms



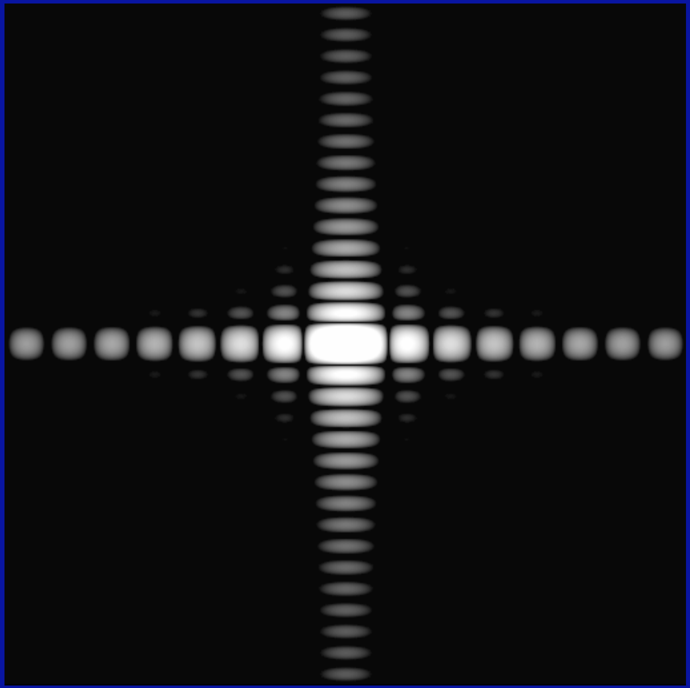
Simple Objects and Their Transforms

Rectangle



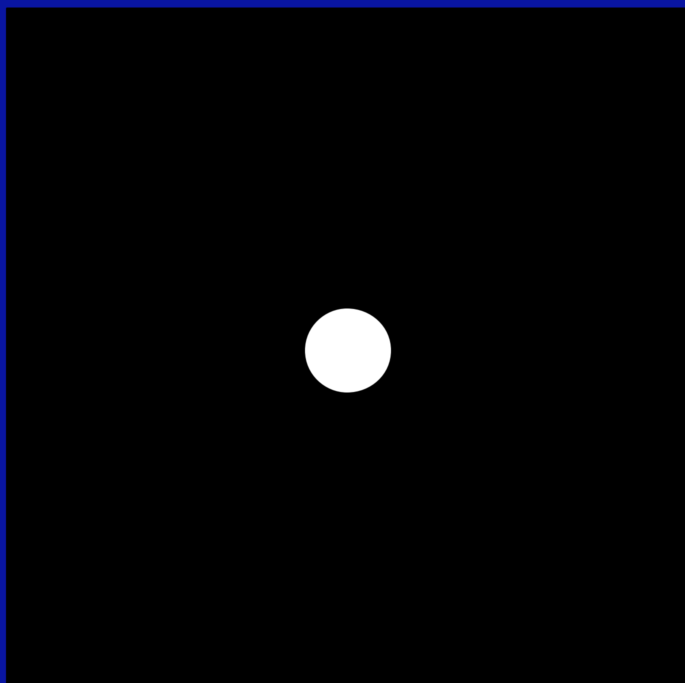
FT

Rectangle Transform



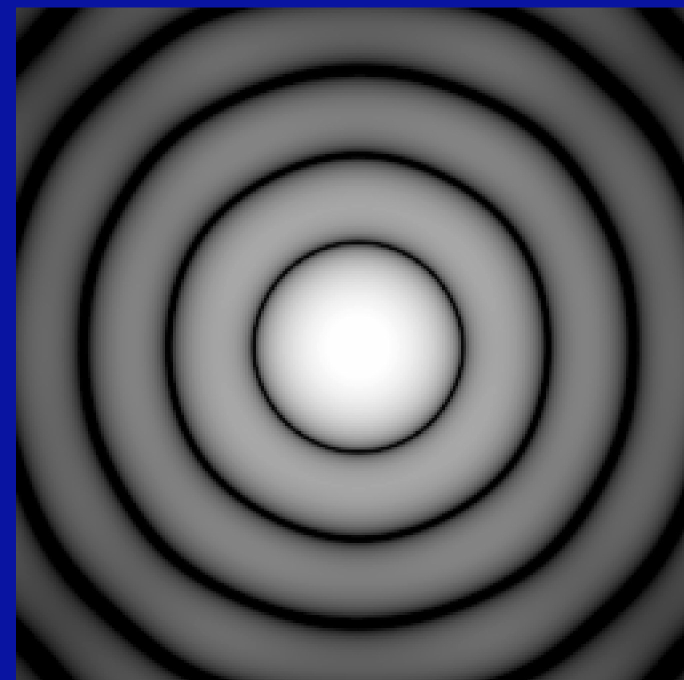
Simple Objects and Their Transforms

Circle



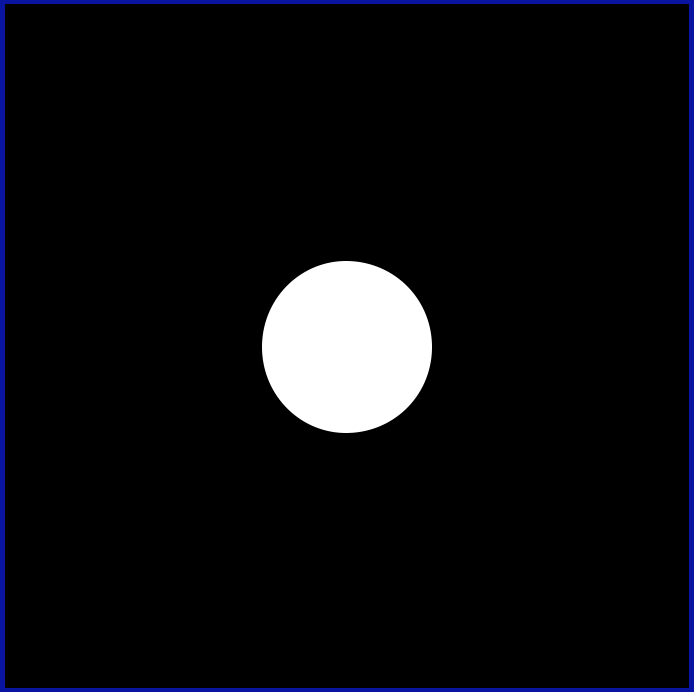
FT

Circle Transform



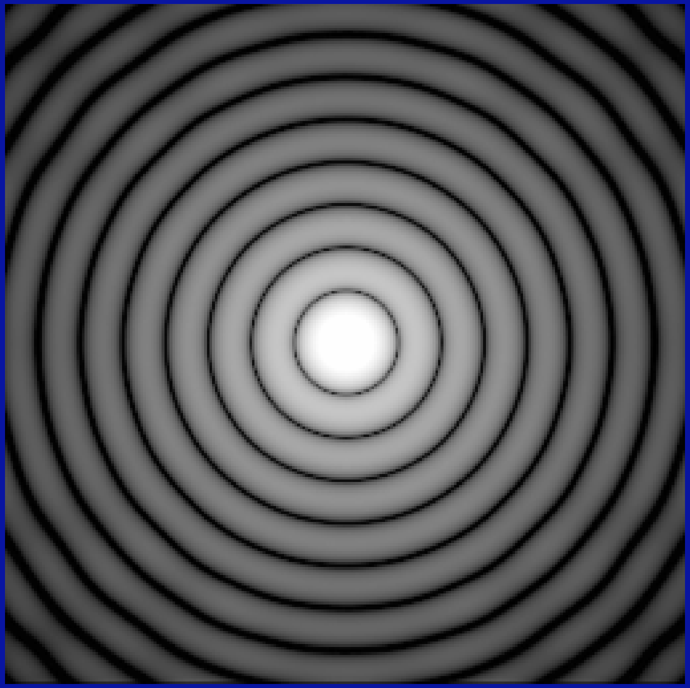
Simple Objects and Their Transforms

Circle



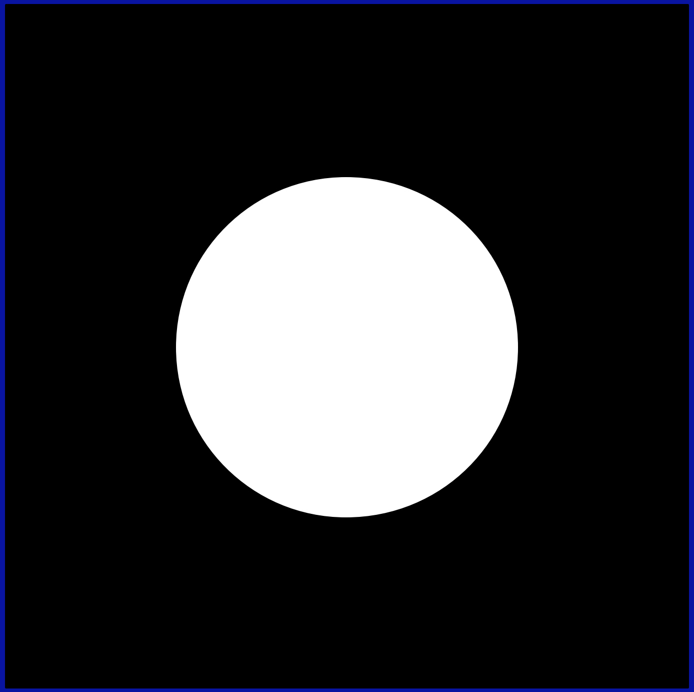
FT

Circle Transform



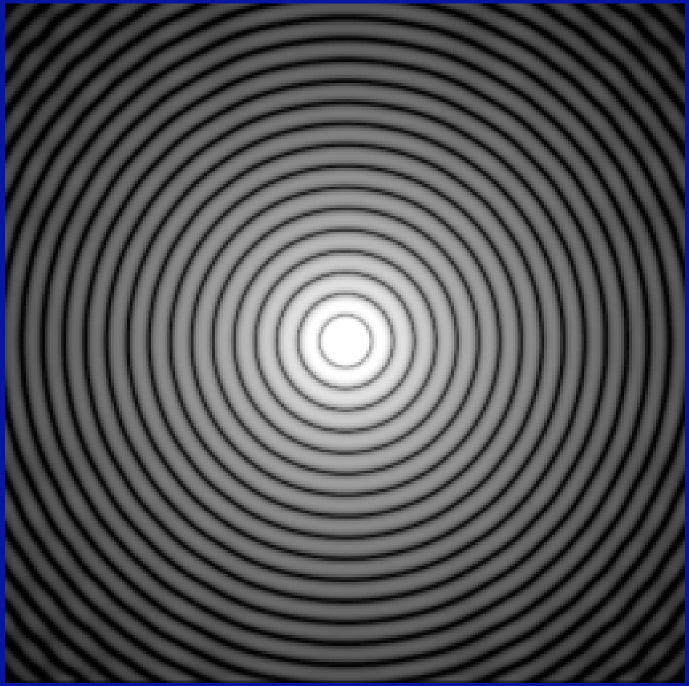
Simple Objects and Their Transforms

Circle



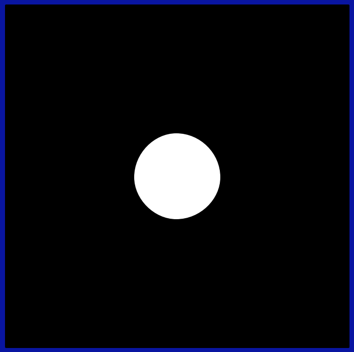
FT

Circle Transform



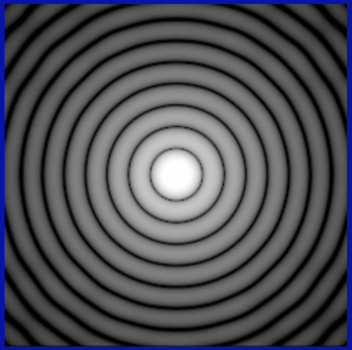
Simple Objects and Their Transforms

Circle

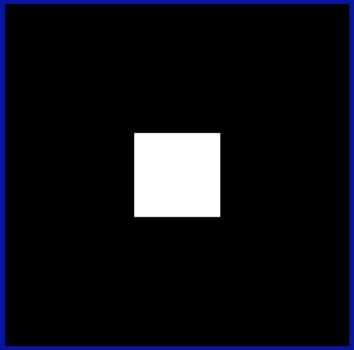


FT

Circle Transform

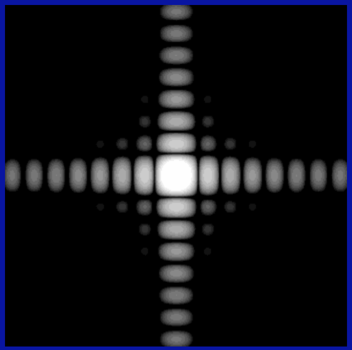


Square



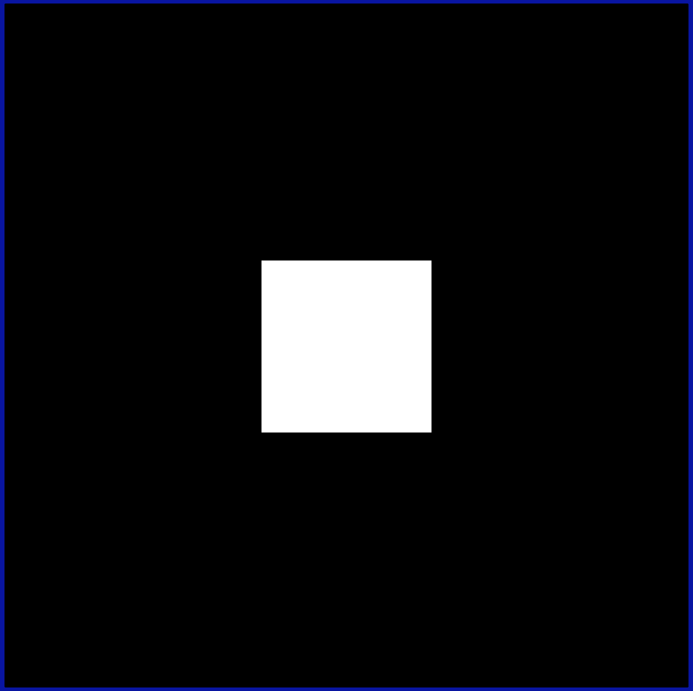
FT

Square Transform



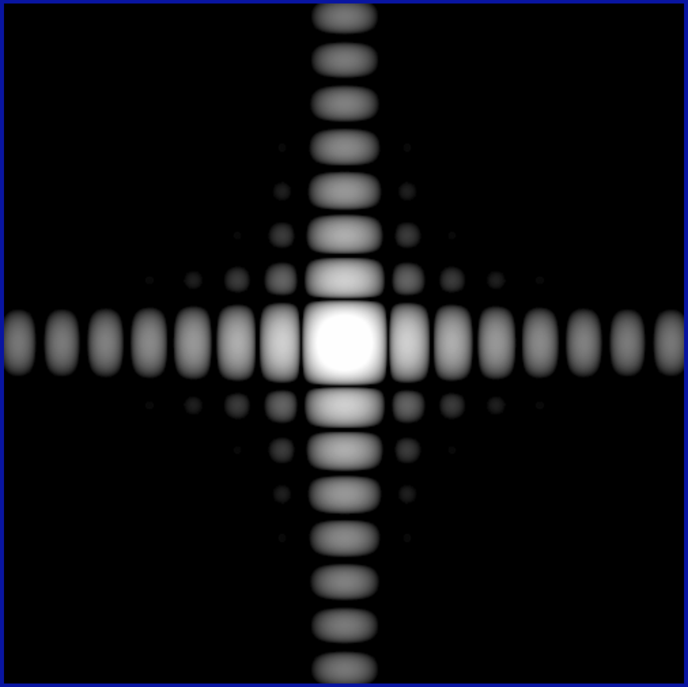
Simple Objects and Their Transforms

Square



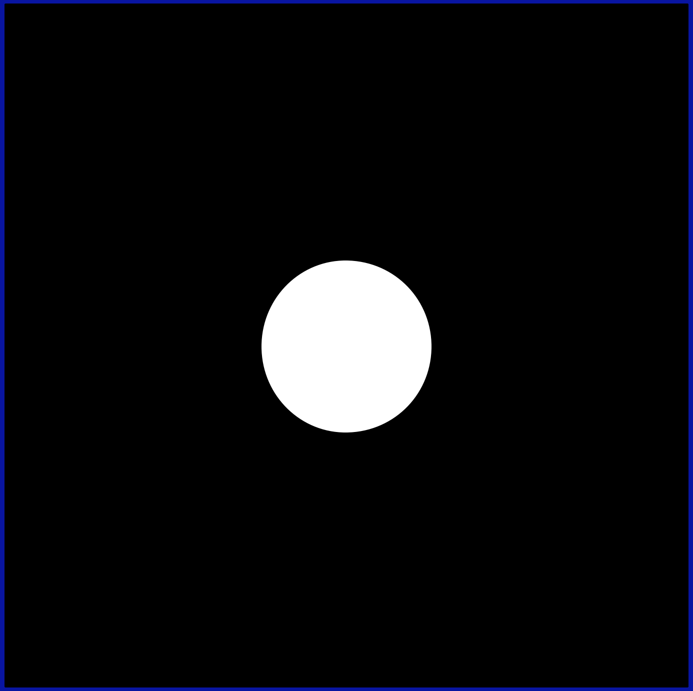
FT

Square Transform



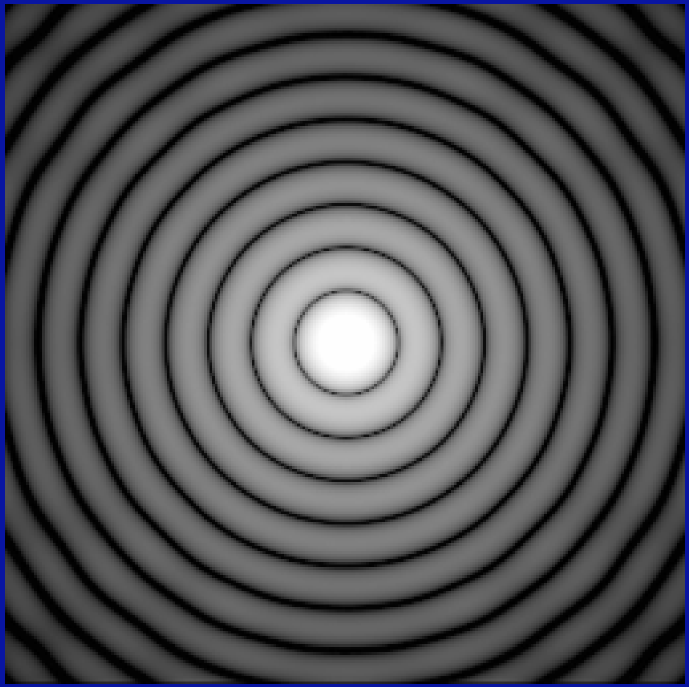
Simple Objects and Their Transforms

Circle



FT

Circle Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

Asymmetric vs. Symmetric Objects and Their Transforms

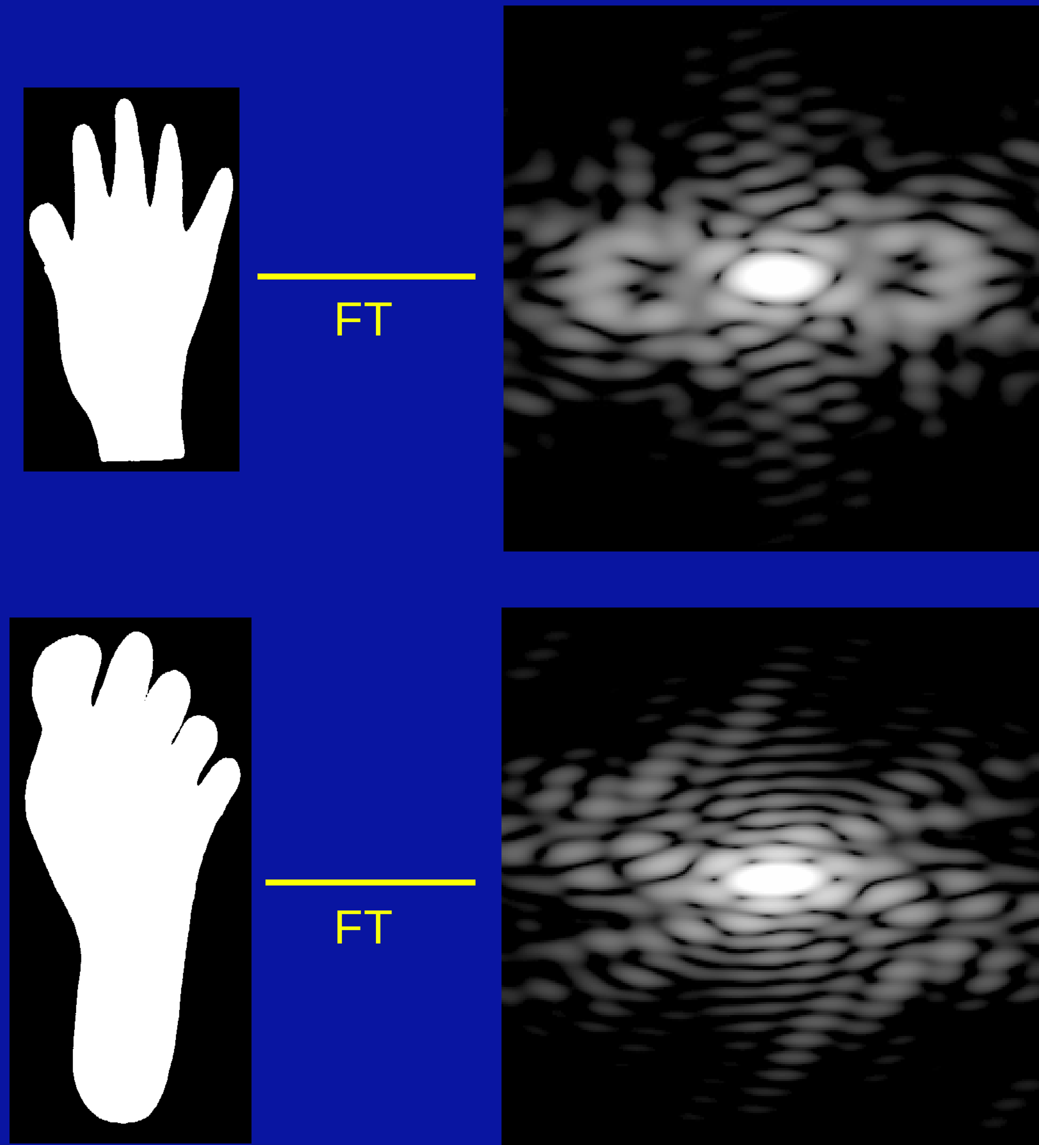
Simple, symmetric structures $\Rightarrow$ simple, symmetric transforms

Asymmetric structures $\Rightarrow$ complex transforms

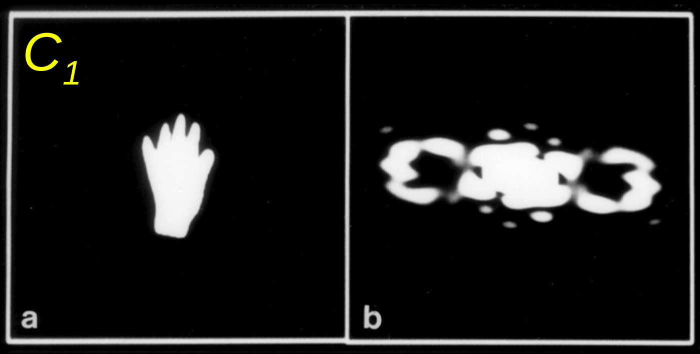
Transforms are like **fingerprints:**

- Specific object features often give rise to **characteristic features** in the transform

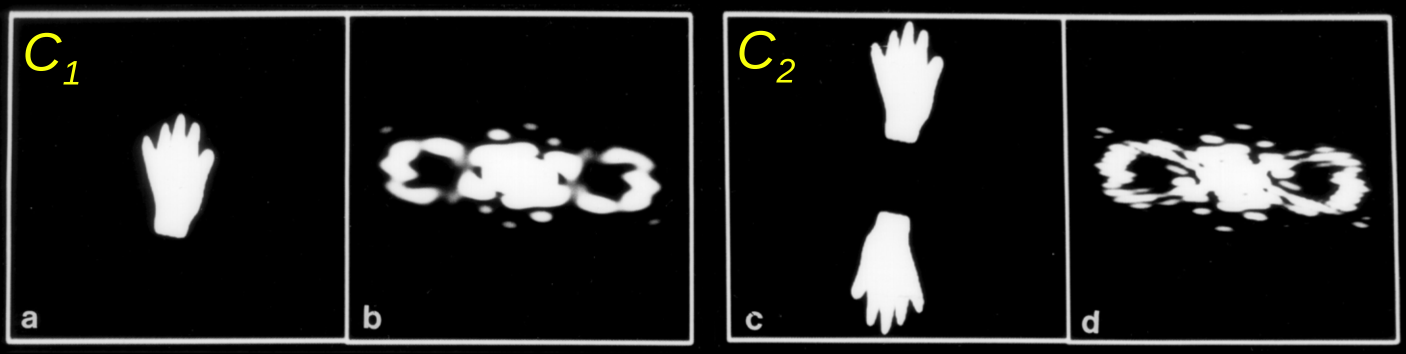
Asymmetric Objects and Their Transforms



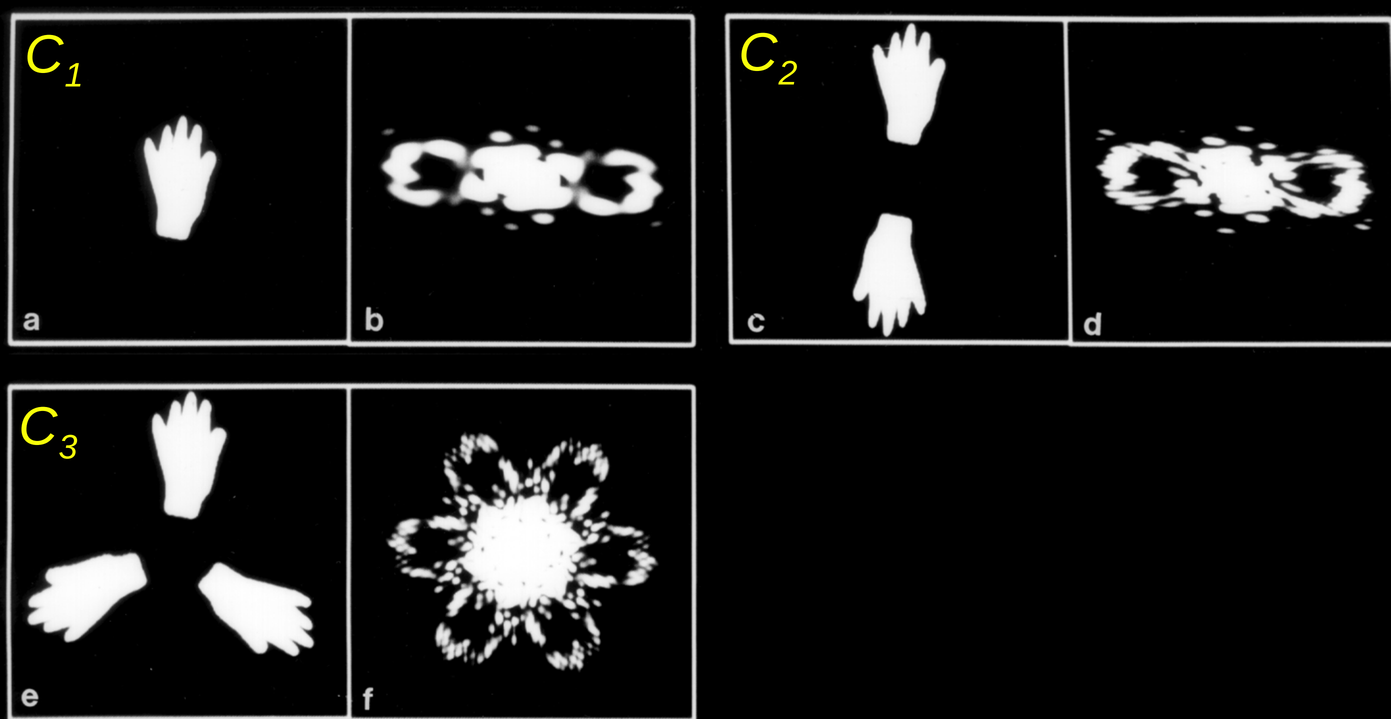
Objects with Cyclic Symmetry and Their Transforms



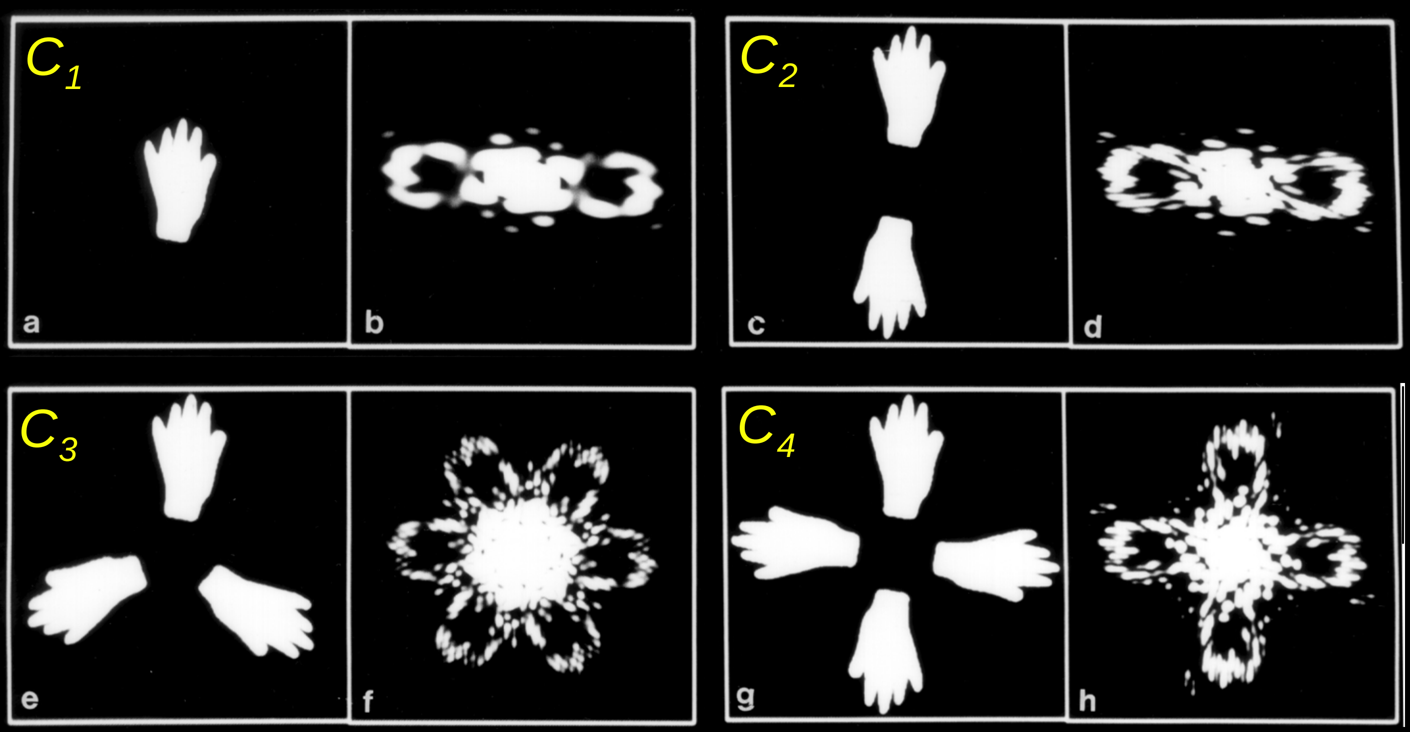
Objects with Cyclic Symmetry and Their Transforms



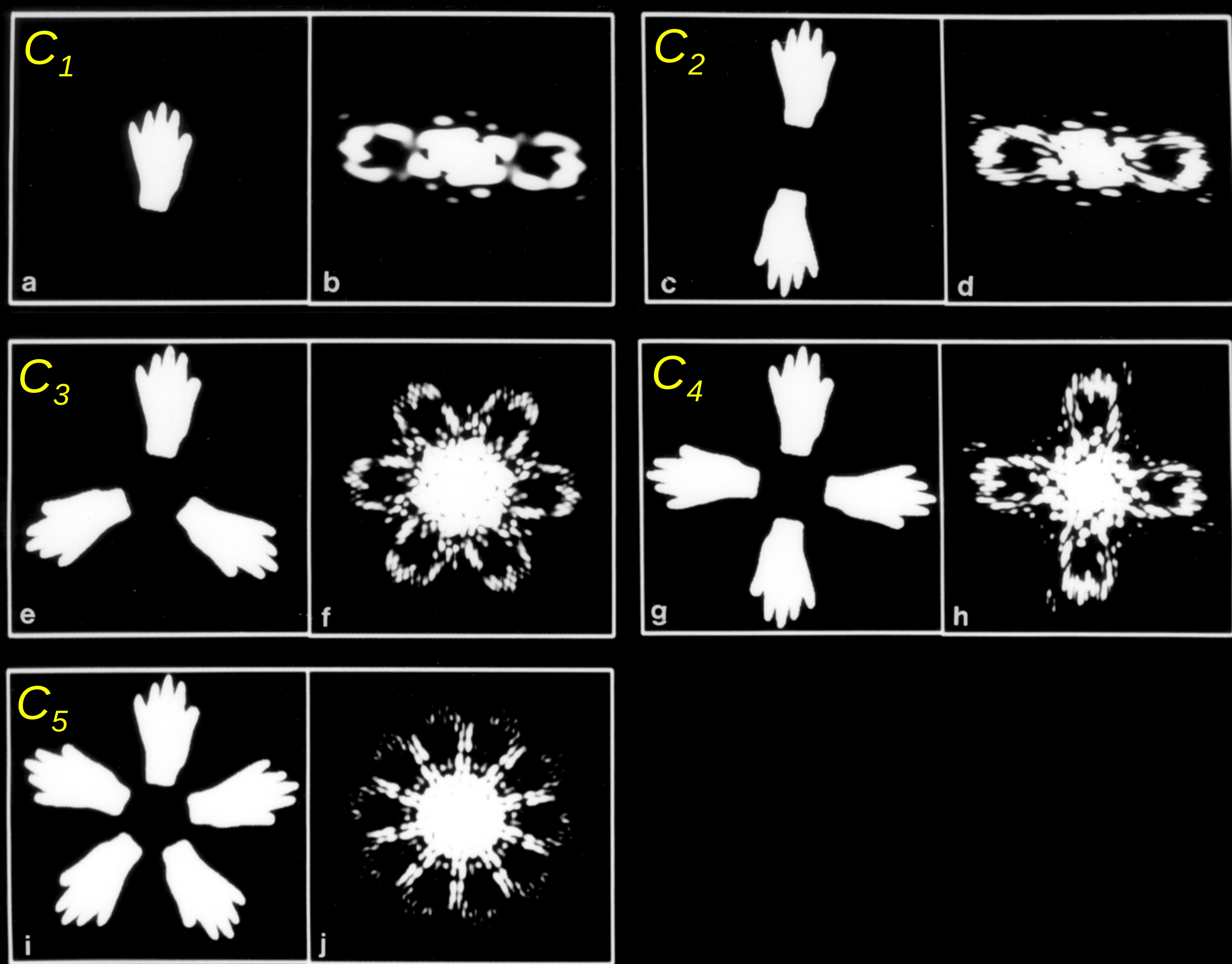
Objects with Cyclic Symmetry and Their Transforms



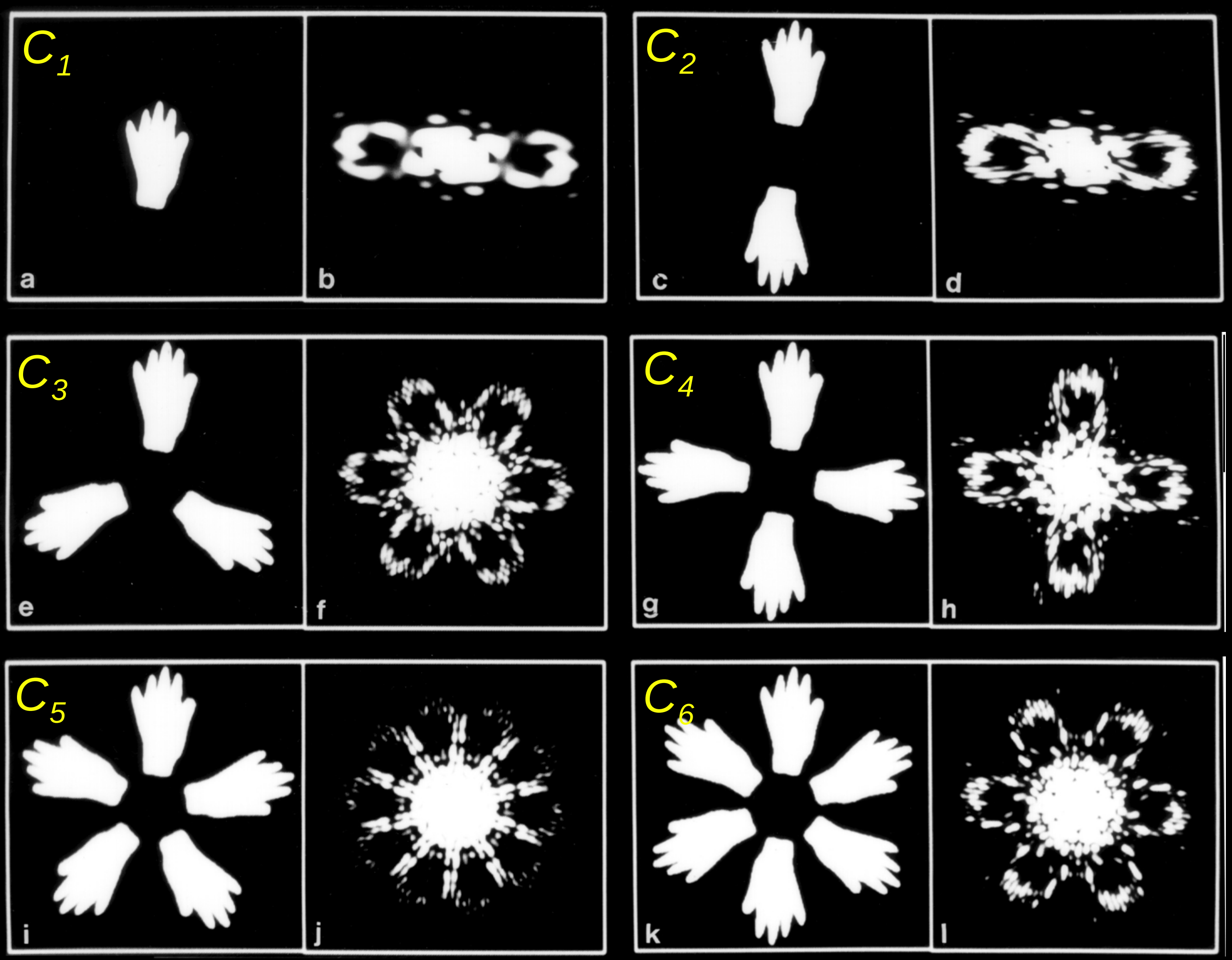
Objects with Cyclic Symmetry and Their Transforms



Objects with Cyclic Symmetry and Their Transforms



Objects with Cyclic Symmetry and Their Transforms



III.C.6.h Other Properties of FTs and Diffraction Patterns

Asymmetric vs. Symmetric Objects and Their Transforms

Structure can be regenerated by back transformation **ONLY** if the **amplitudes and phases** at **ALL** points of the FT are available

May be accomplished for:

Visible light (optical reconstruction)

Electrons (electron microscopy)

Can only be achieved by **mathematical** computation for:

X-rays and neutrons (phases indirectly measured)

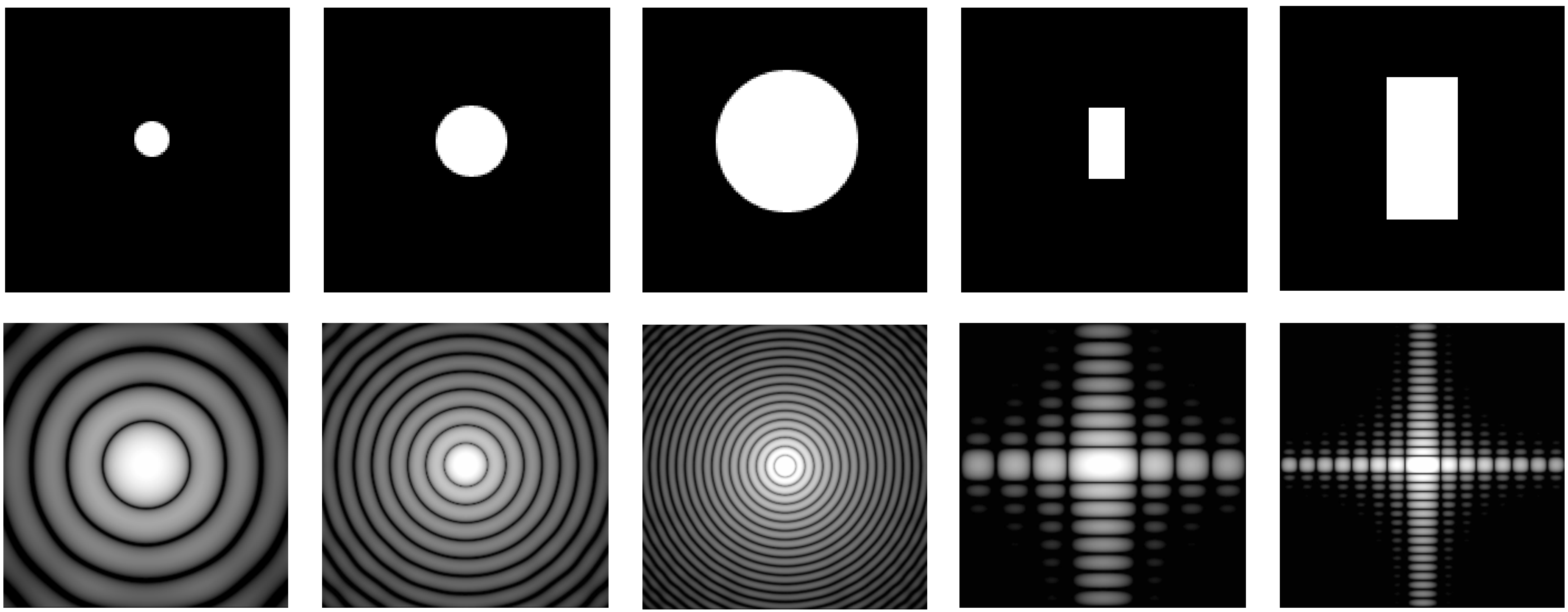
Simple inspection of most transforms does **NOT** directly lead to a unique determination of structure

III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Reciprocity

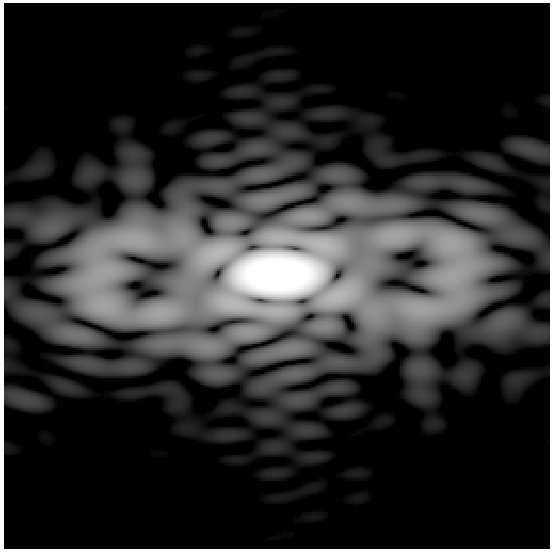
Dimensions in object (**real space**) are **inversely** related to dimensions in the transform (**reciprocal space**)



III.C.6.h Other Properties of FTs and Diffraction Patterns

Reciprocity

Small spacings in object - represented by features spaced **far apart** in reciprocal space

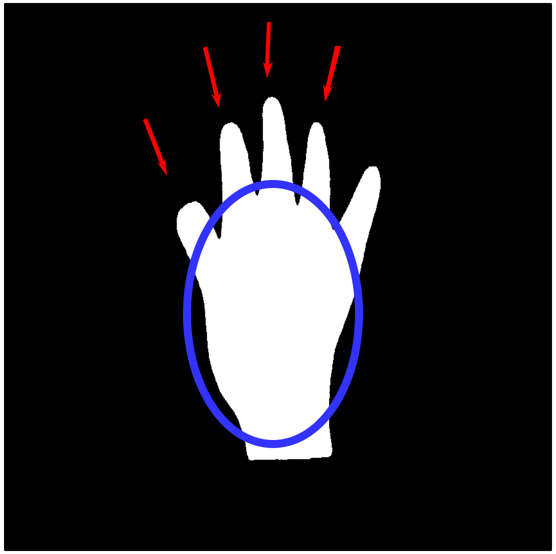


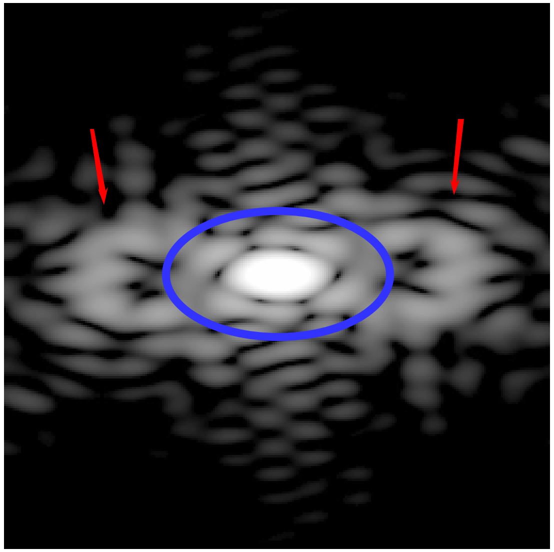
III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Resolution

Outer regions of FT arise from fine (**high resolution**) details in the object





Coarse (**low resolution**) object features contribute near the **central region** of the FT

III.C.6.h Other Properties of FTs and Diffraction Patterns

Resolution

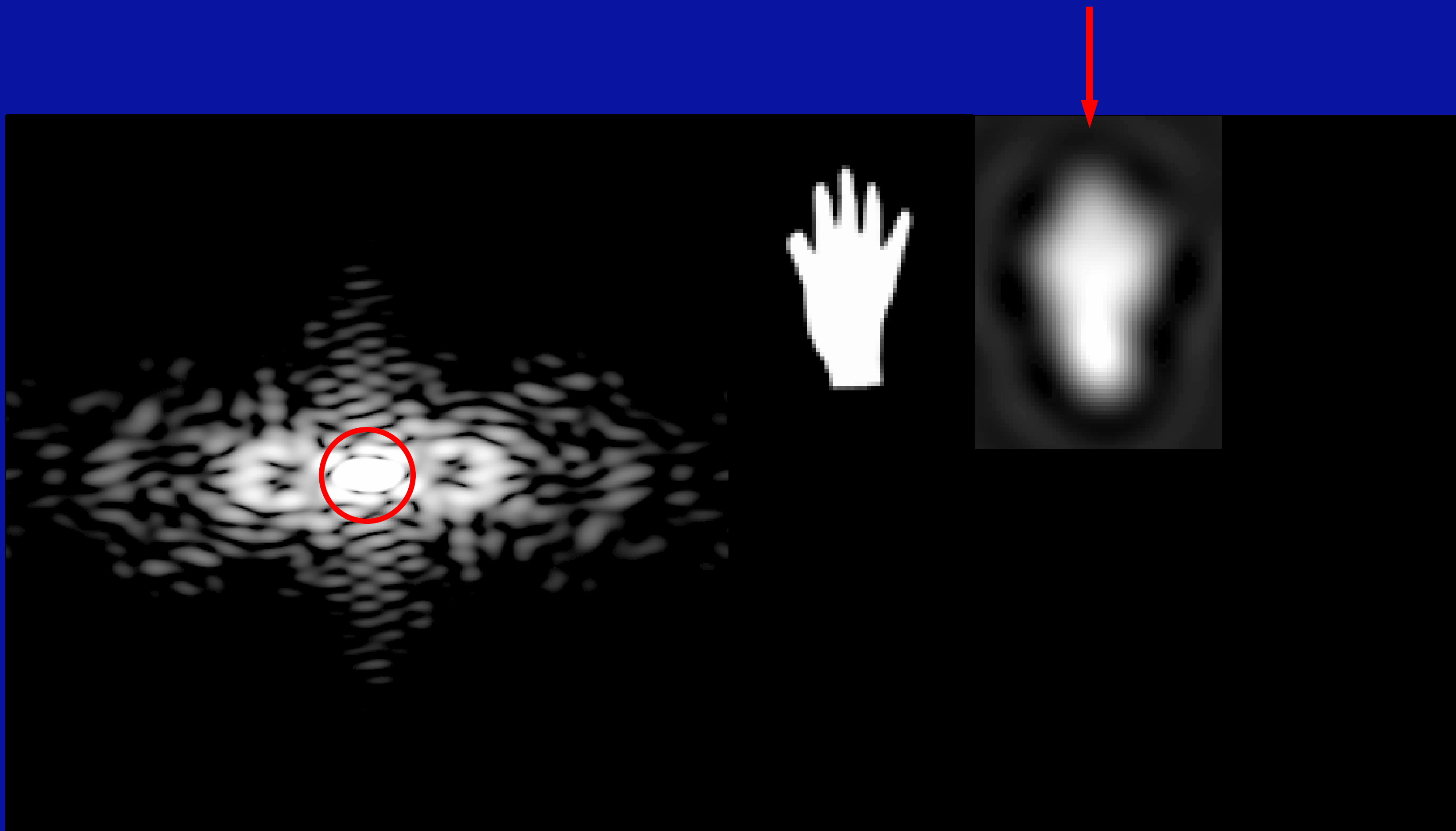
Low-pass/High-pass filtering

Low-pass: low-resolution features (near center of transform) are allowed to "pass" through filter and interfere (resynthesize) at image plane while high resolution features are removed

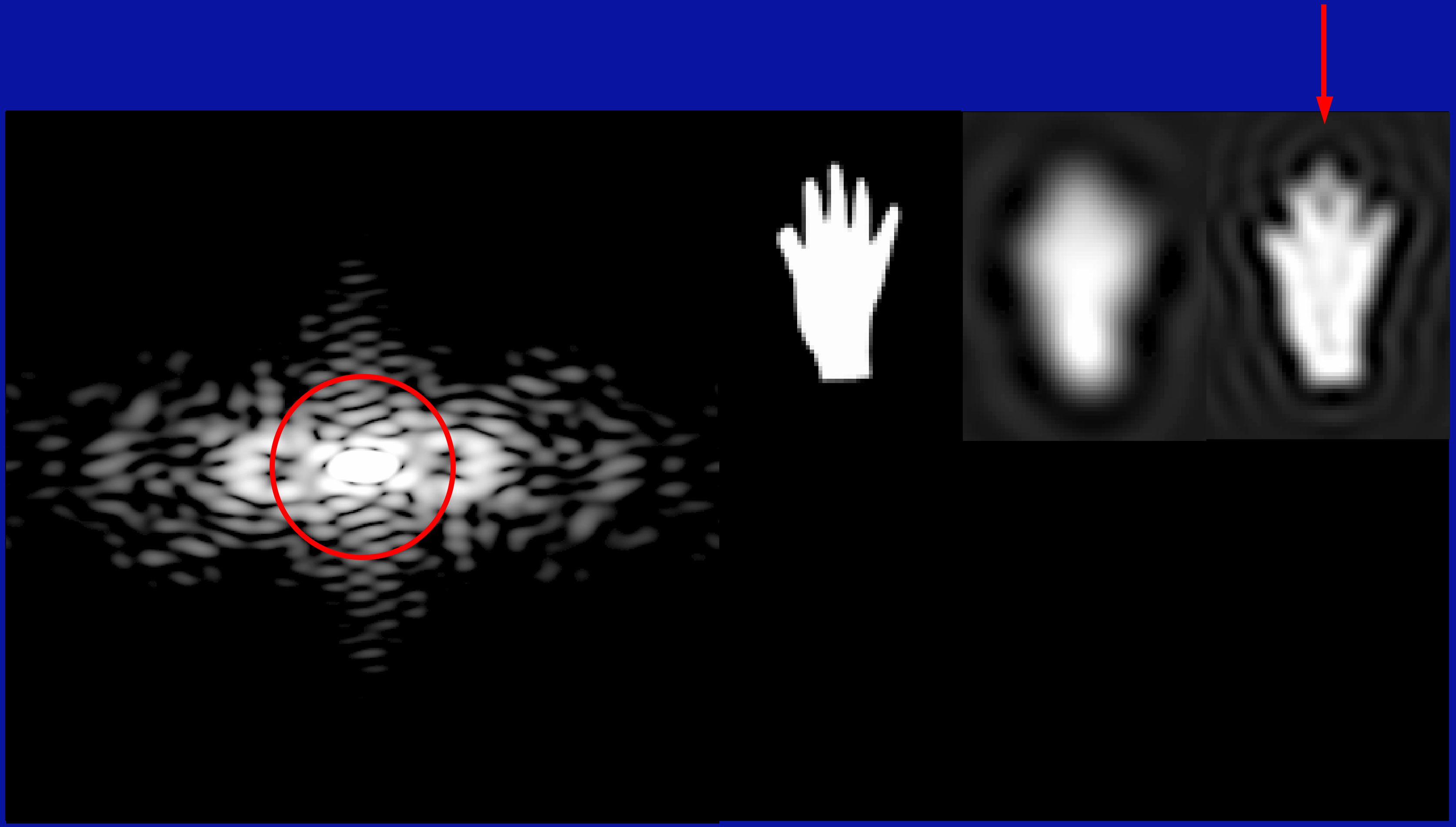
High-pass: low resolution Fourier components are **removed** (*i.e.* blocked by filter) while high resolution Fourier components are allowed to "pass" through filter and form an image (leads to accentuation of high resolution features such as edges)

Fourier Transform Filtering

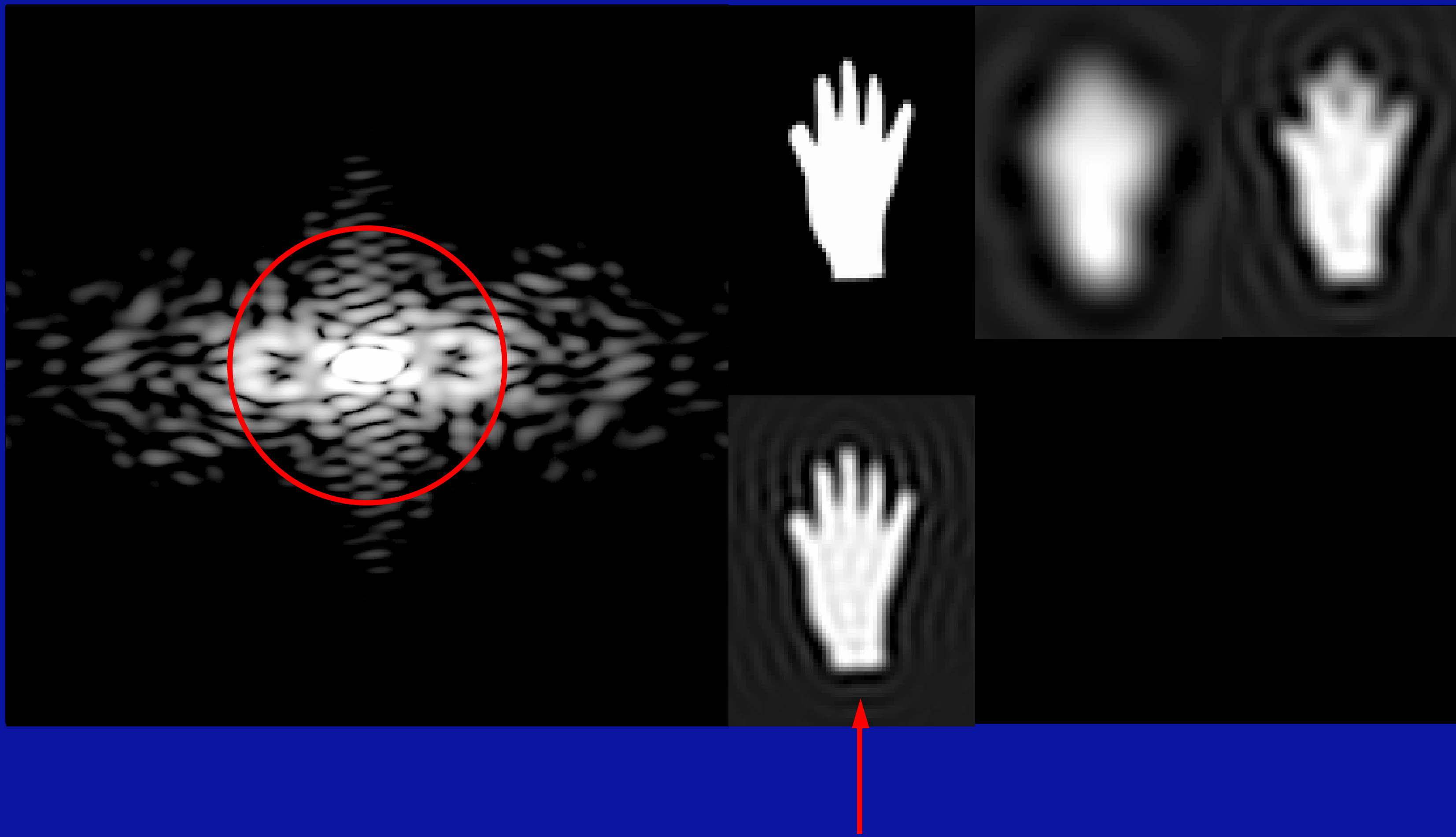
Fourier Transform Filtering



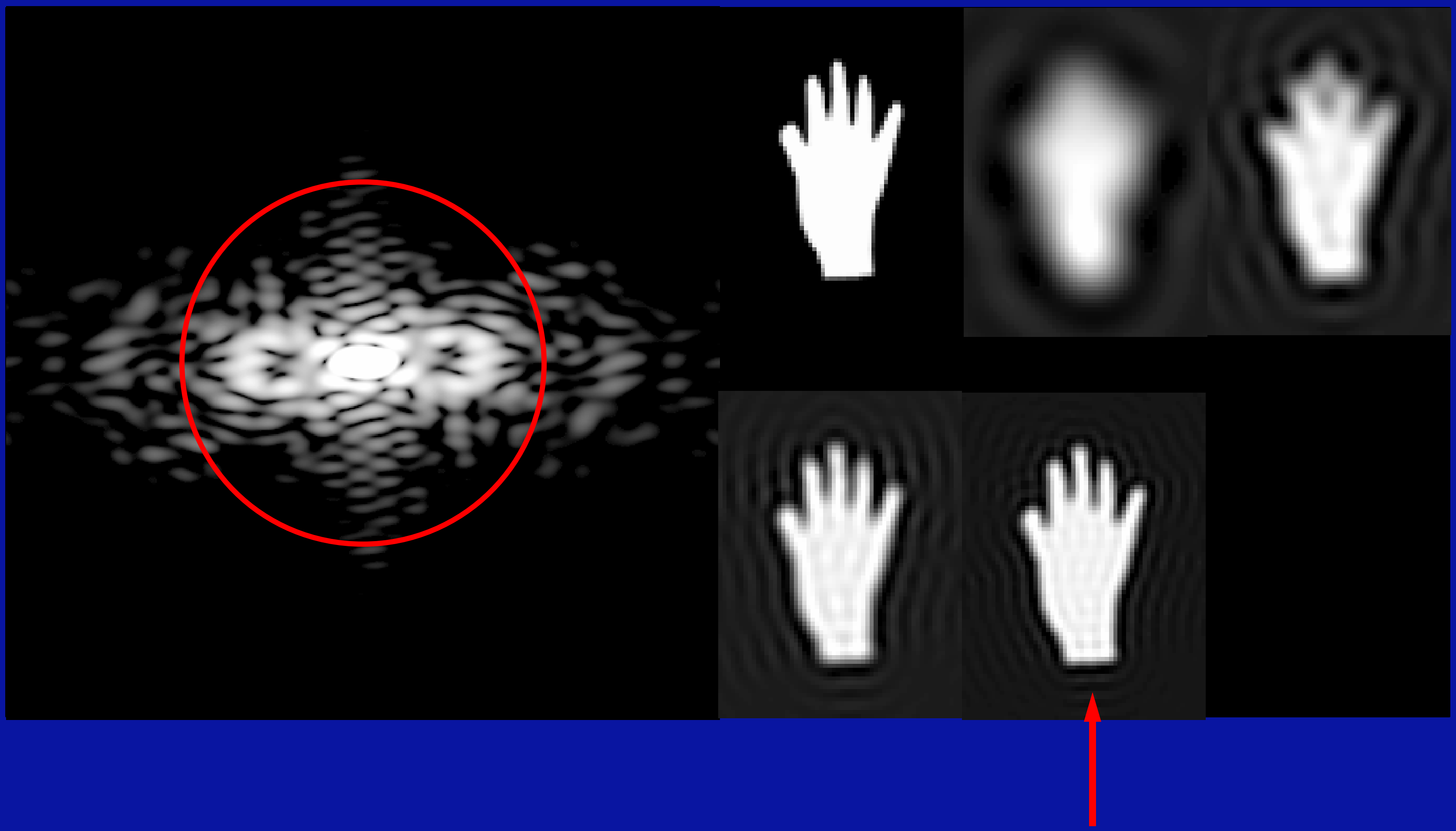
Fourier Transform Filtering



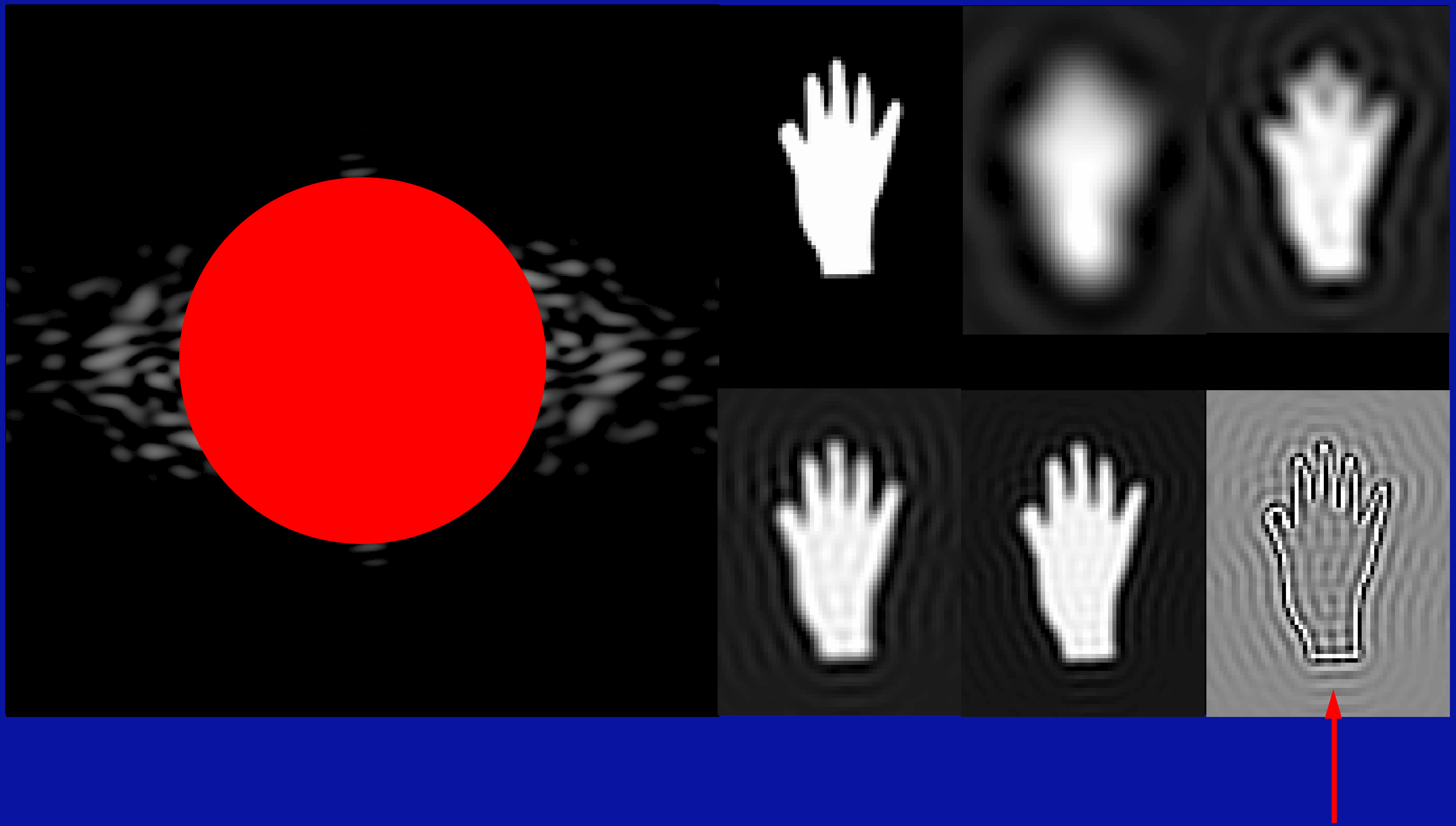
Fourier Transform Filtering



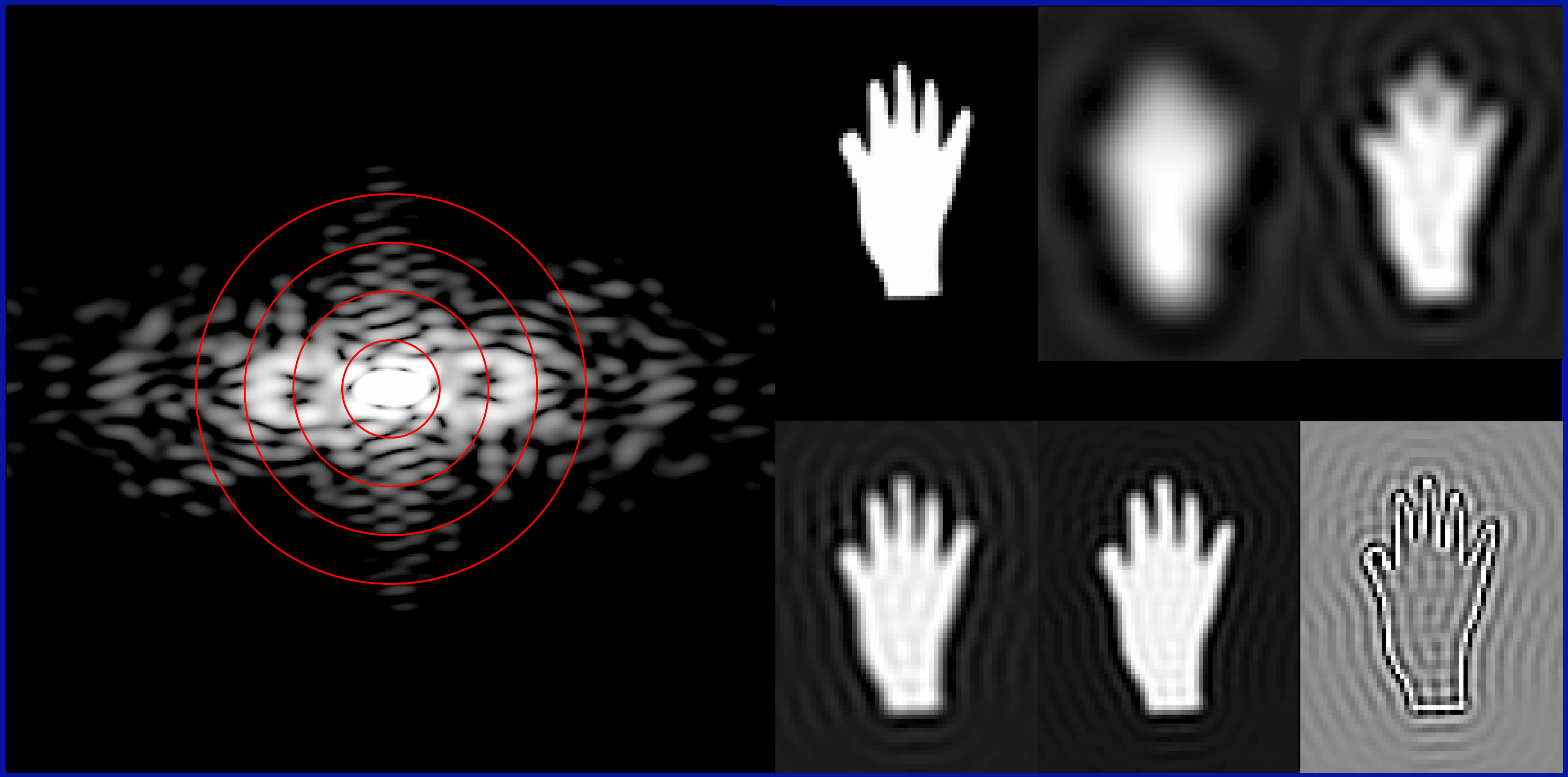
Fourier Transform Filtering

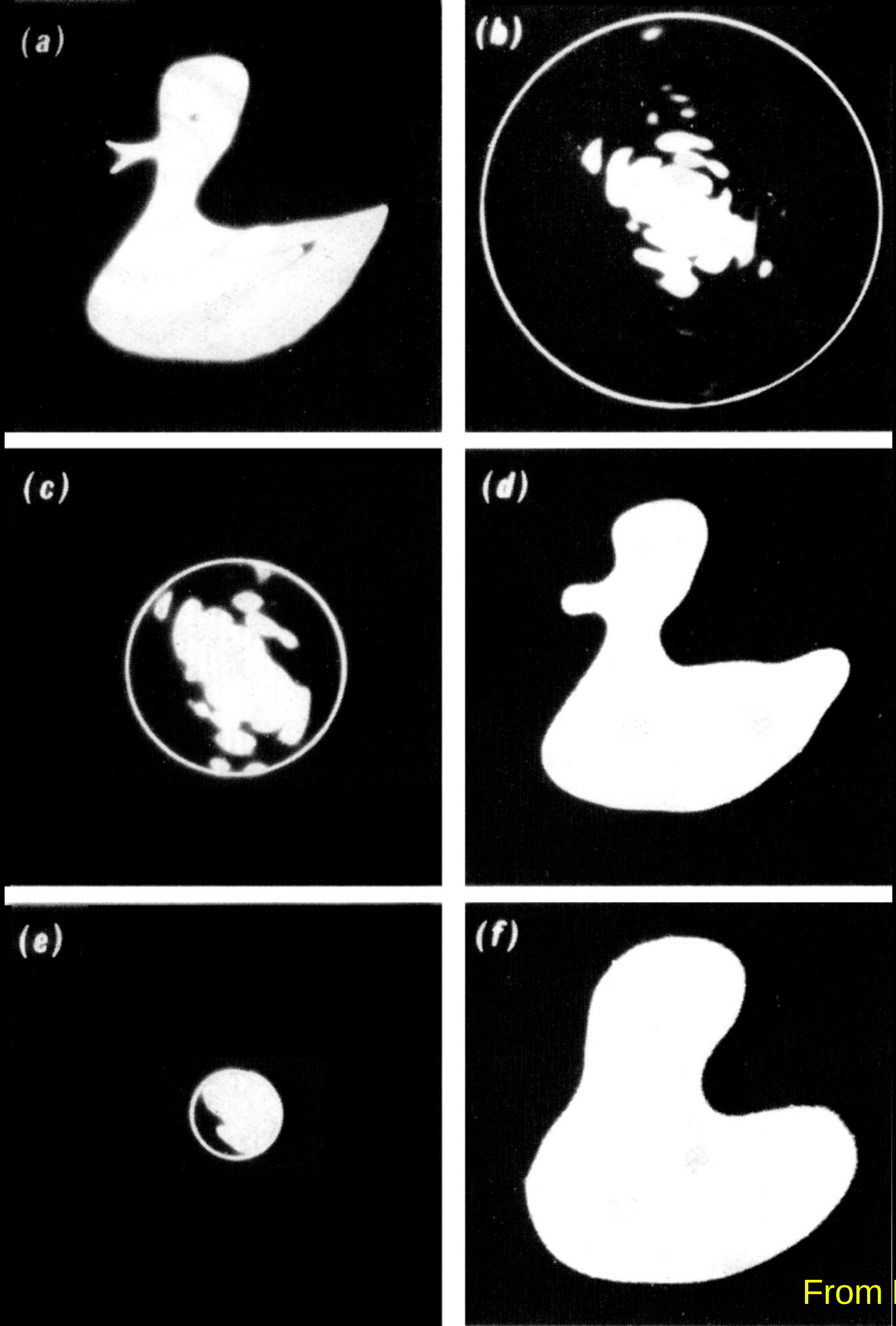


Fourier Transform Filtering



Fourier Transform Filtering





From Holmes and Blow, Fig. 3, p.120

III.C.6.h Other Properties of FTs and Diffraction Patterns

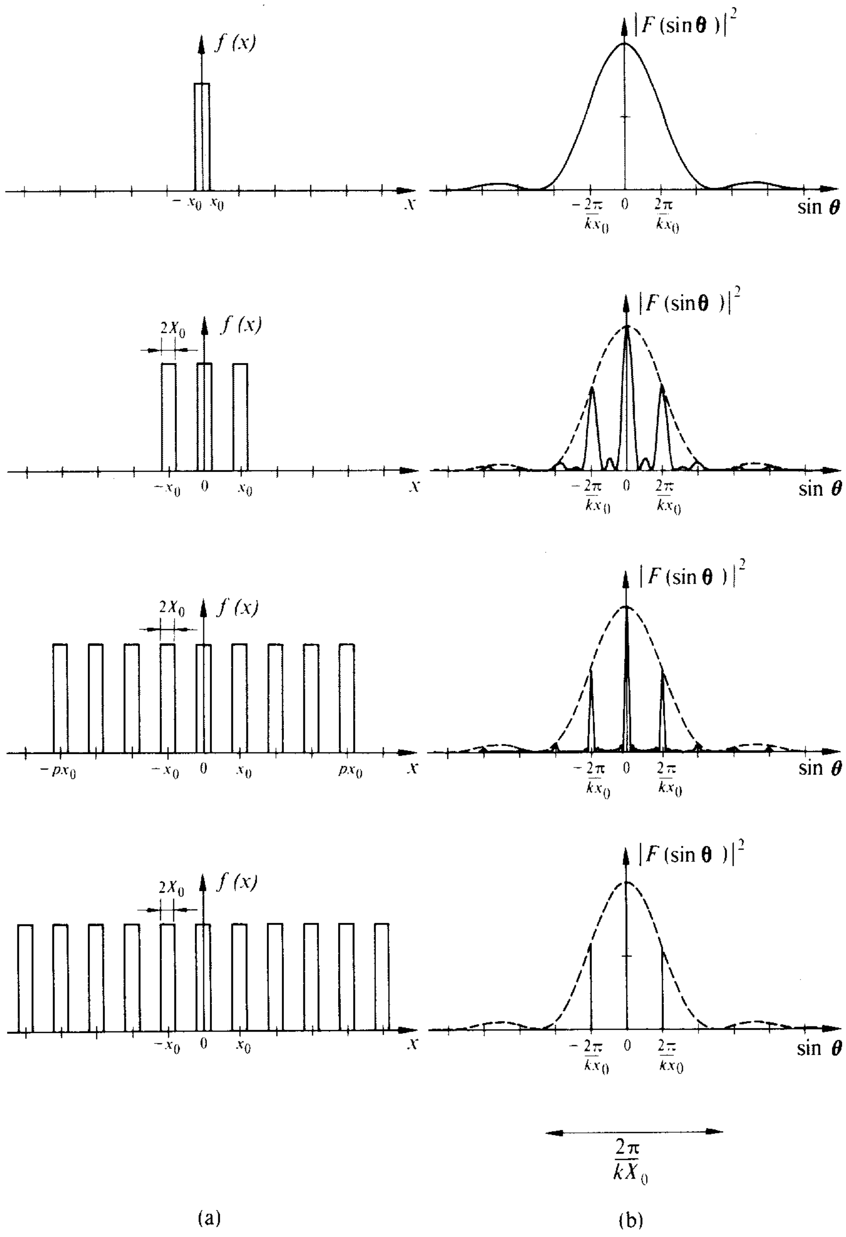
Sharpness of Diffraction Spots

Features in the diffraction pattern become **sharper** as the **number** of diffracting **objects** or the **distance between them increases**

Sharpening reflects a situation of more complete, destructive interference away from the reciprocal lattice positions

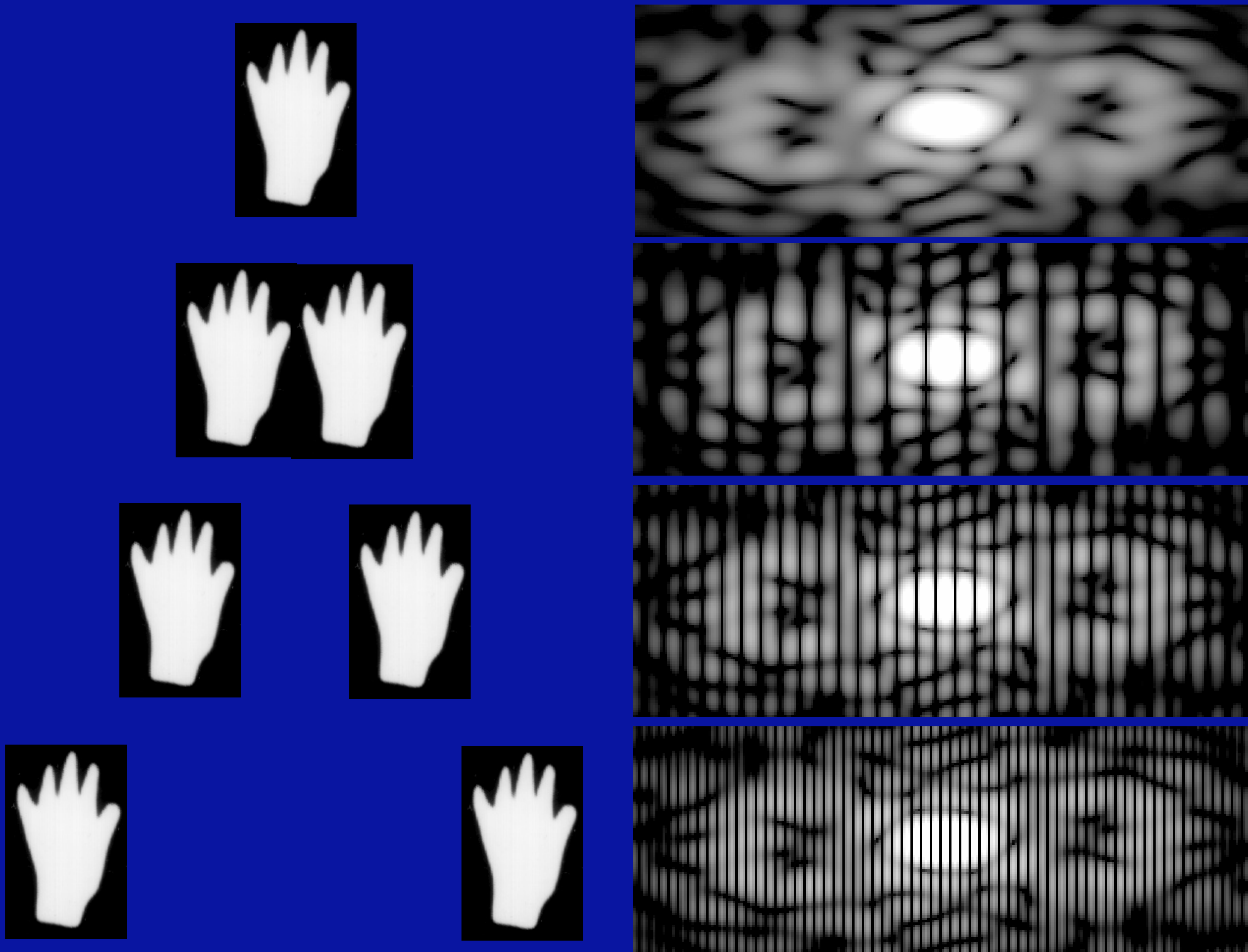
Transform Sampling

Diffraction patterns of one, three, nine and 8 number of slits

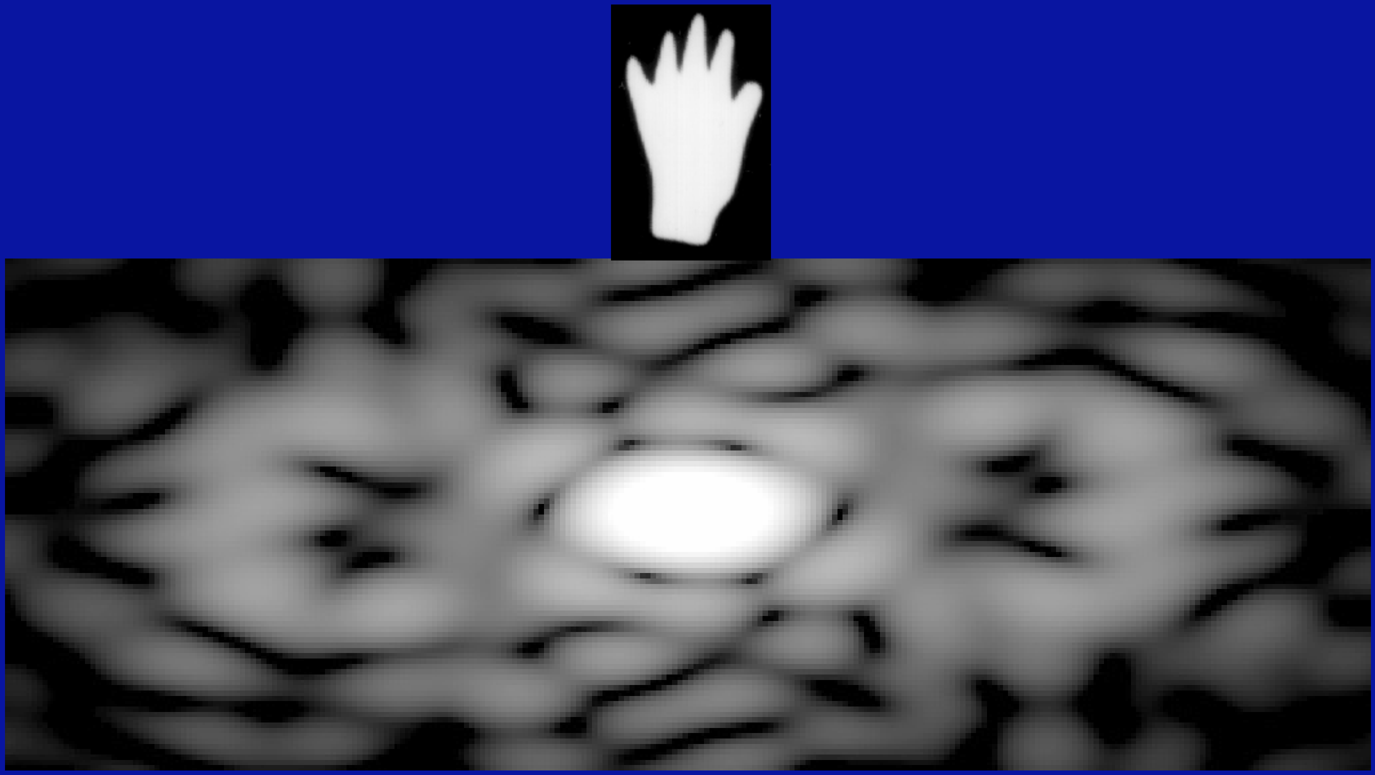


From Sherwood, Fig. 7.16, p.249

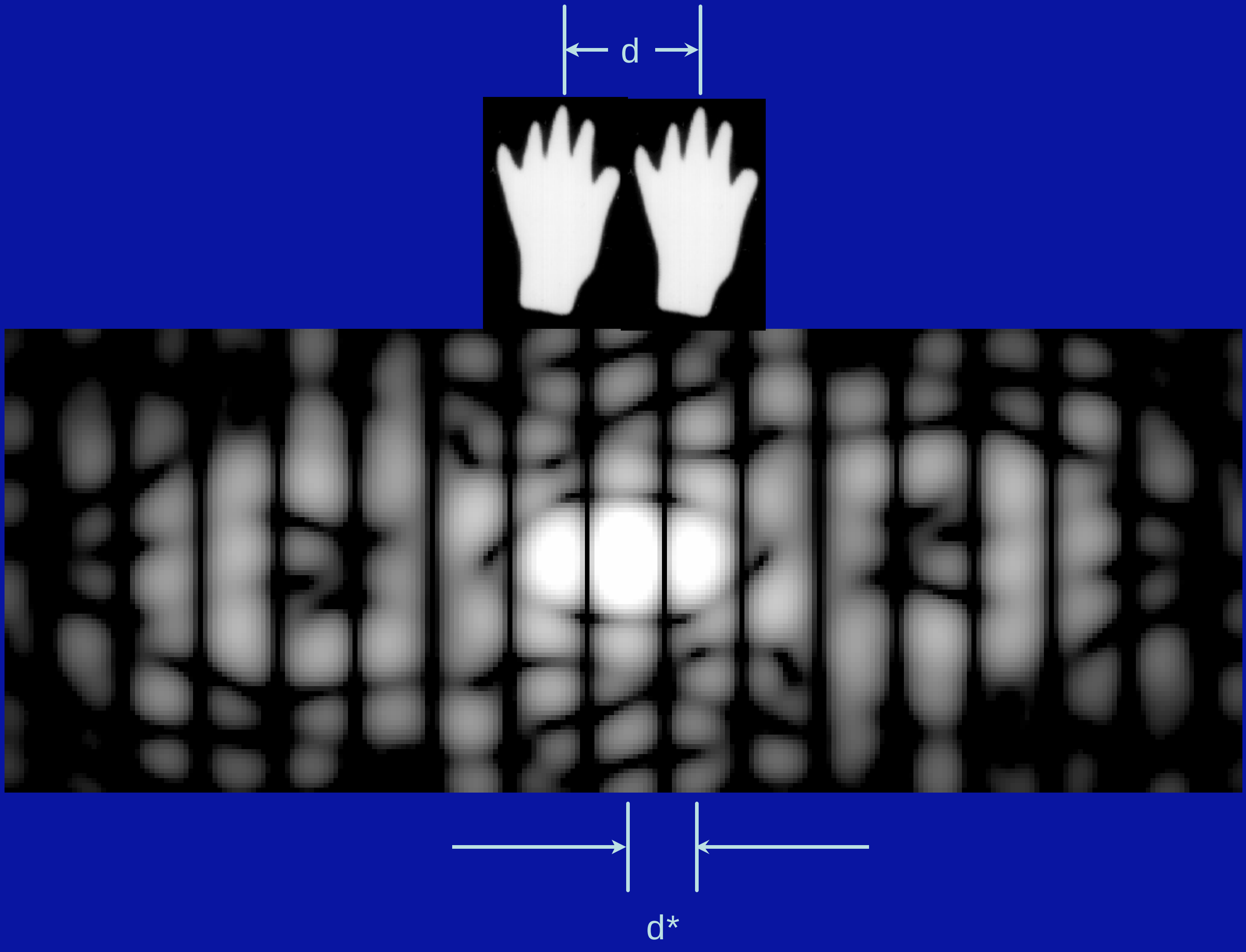
Sharpening of Diffraction Features



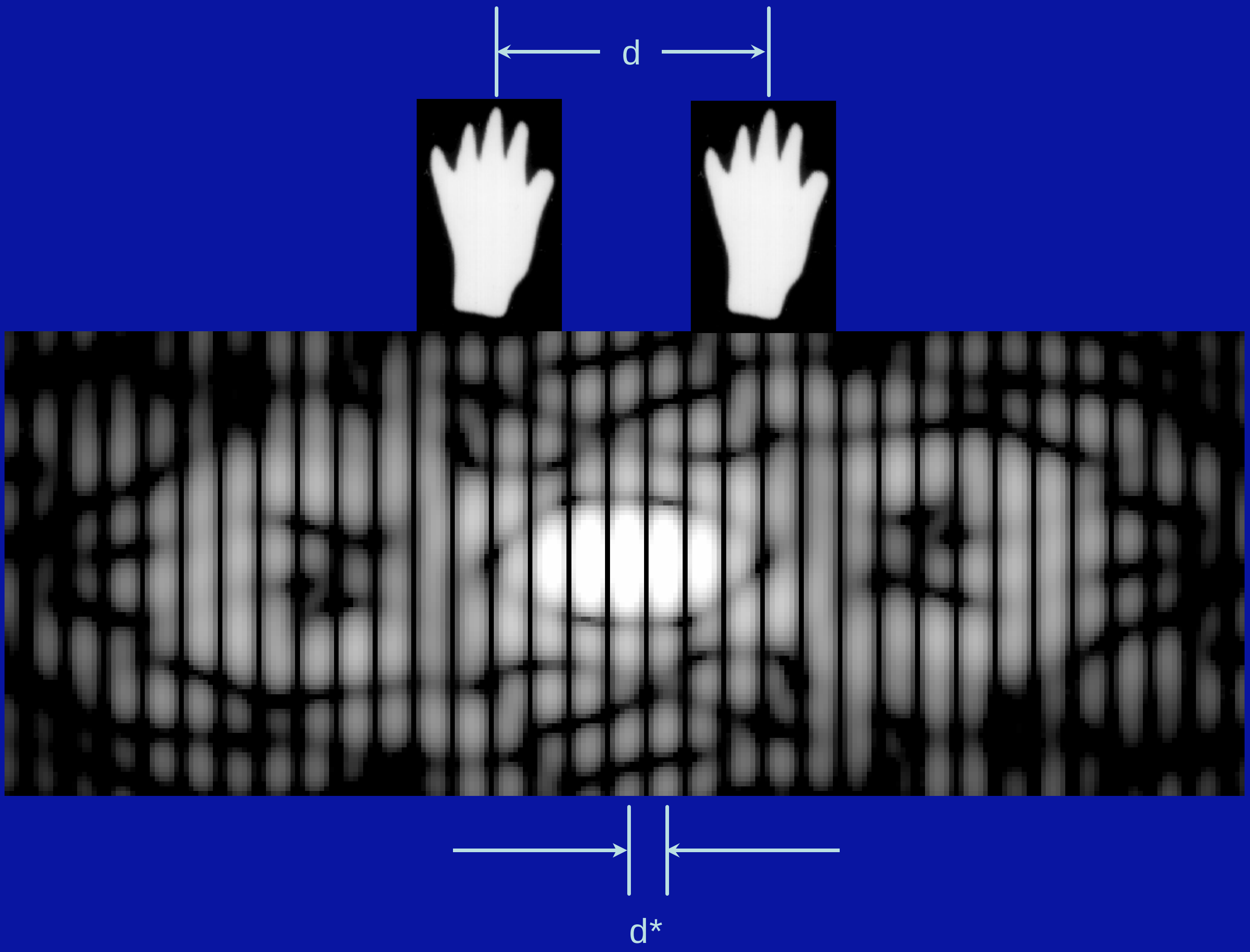
Sharpening of Diffraction Features



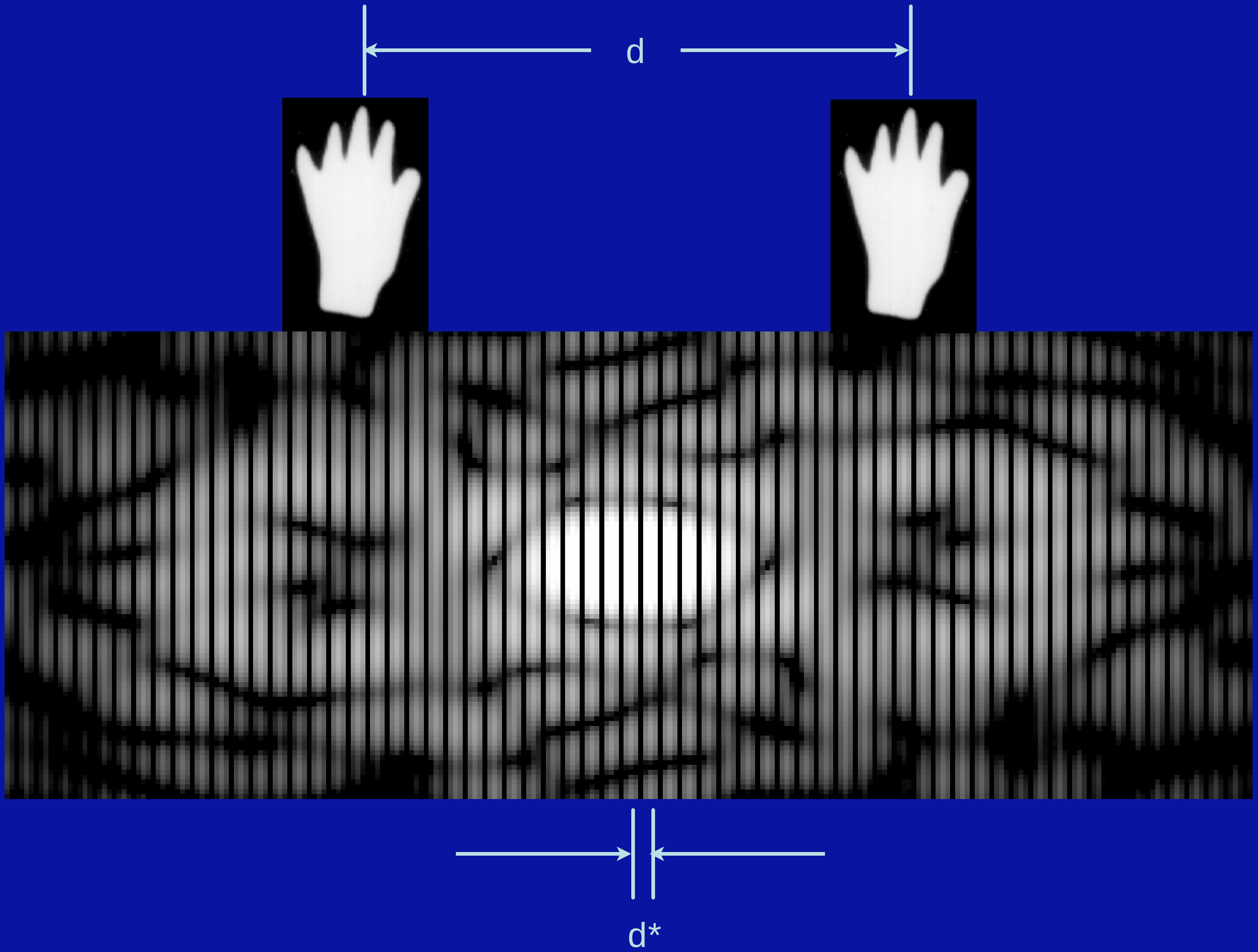
Sharpening of Diffraction Features



Sharpening of Diffraction Features



Sharpening of Diffraction Features



4-01-04

III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

1) Analogy between OD and "Mathematical" FTs

2) Asymmetric / Symmetric Objects / Transforms

3) Reciprocity

4) Resolution

5) Sharpness of Diffraction Spots

6) Geometry, Intensity and Symmetry

7) Projection Theorem

8) Friedel's Law

III.C.6.h Other Properties of FTs and Diffraction Patterns

Transforms are like **fingerprints**

Asymmetric structures $\Rightarrow$ complex transforms

Simple, symmetric structures $\Rightarrow$ simple, symmetric transforms

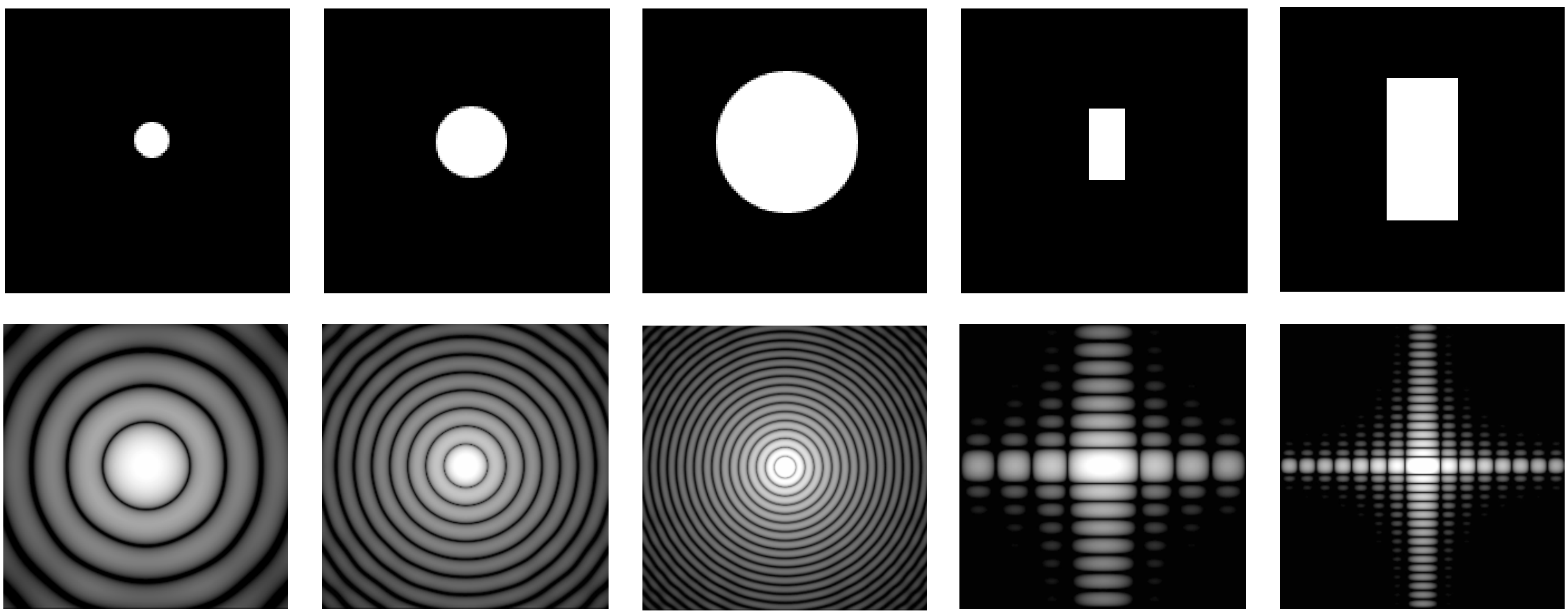
Simple inspection of most transforms does **NOT** directly lead to a unique determination of structure

III.C.6 Diffraction

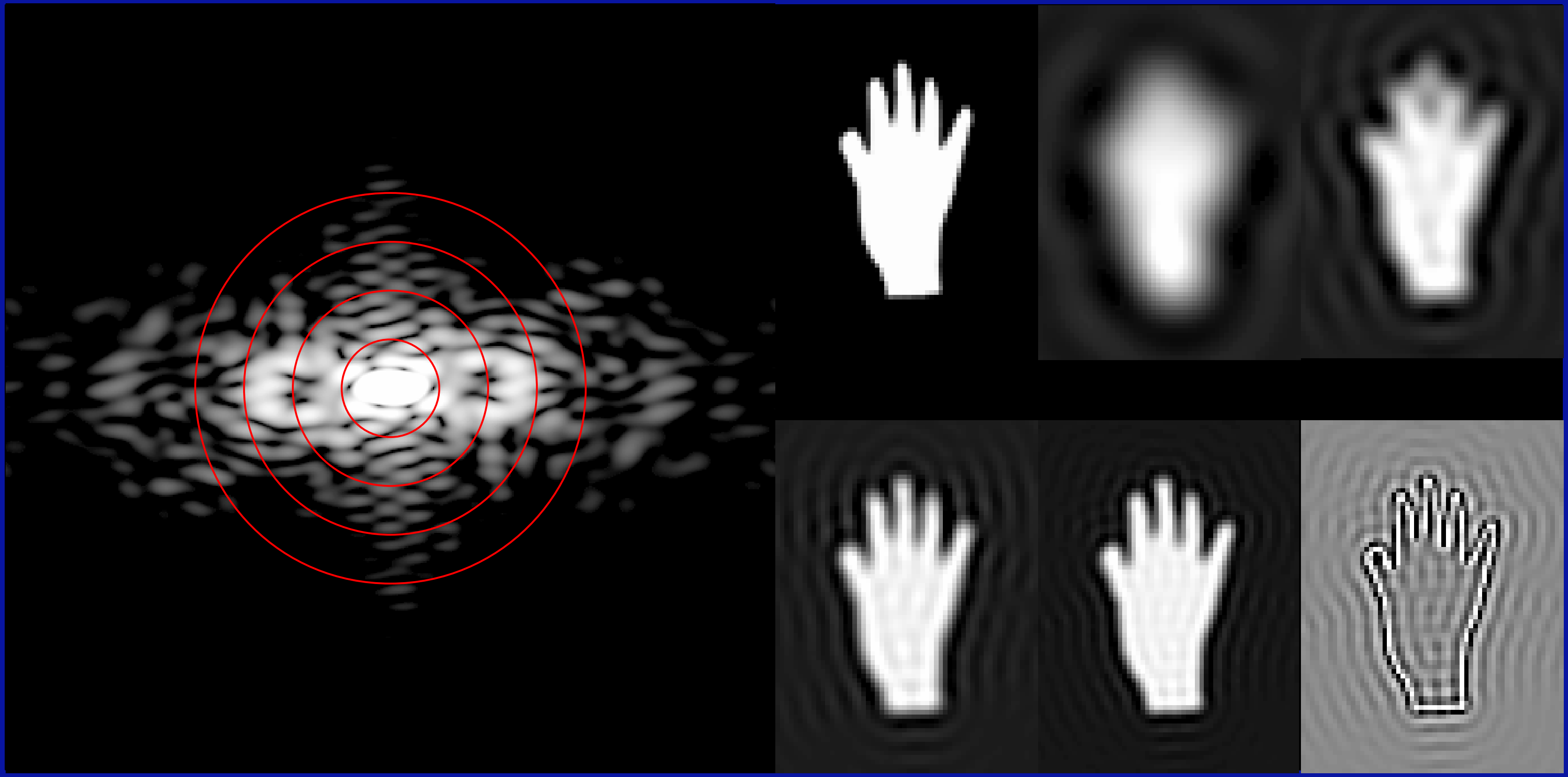
III.C.6.h Other Properties of FTs and Diffraction Patterns

Reciprocity

Dimensions in object (**real space**) are **inversely** related to dimensions in the transform (**reciprocal space**)



Fourier Transform Filtering



III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Sharpness of Diffraction Spots

Features in the diffraction pattern become **sharper** as the **number** of diffracting **objects** **or** the **distance between them increases**

Sharpening reflects a situation of more complete, destructive interference away from the reciprocal lattice positions

III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Geometry, Intensity and Symmetry

Geometry and spacings of the crystal and reciprocal lattices obey a reciprocal relationship

$$d^* = \frac{K}{d \sin g^*}$$

$$\text{and} \quad g^* = 180 - g$$

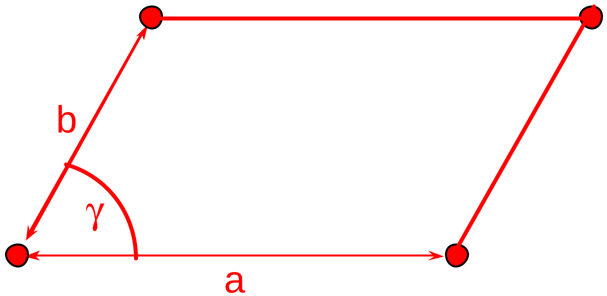
- d = unit cell spacing (a or b)
- d^* = reciprocal lattice spacing (a^* or b^*)
- g = angle between unit cell axes
- g^* = angle between reciprocal lattice axes
- K = constant of diffraction (= λL)
- λ = wavelength of monochromatic radiation
- L = camera length (distance from specimen to diffraction plane)

III.C.6.h Other Properties of FTs and Diffraction Patterns

Geometry, Intensity and Symmetry

$$d^* = \frac{K}{d \sin g^*}$$

$$g^* = 180 - g$$



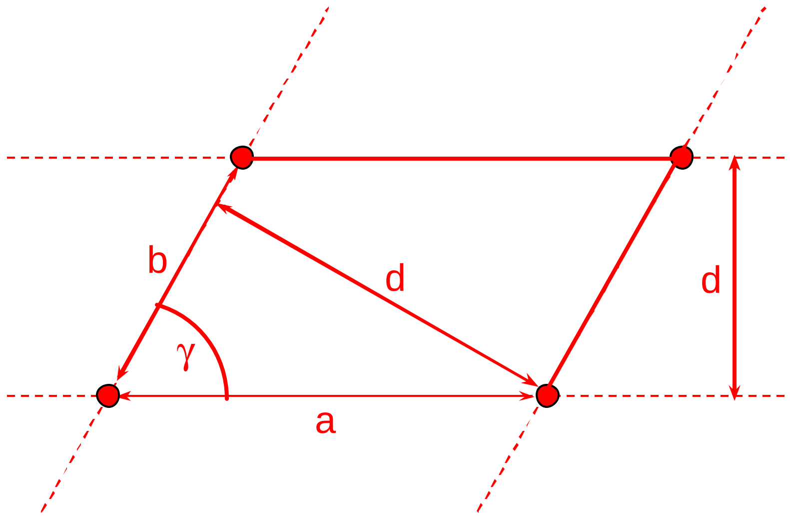
Real Lattice

III.C.6.h Other Properties of FTs and Diffraction Patterns

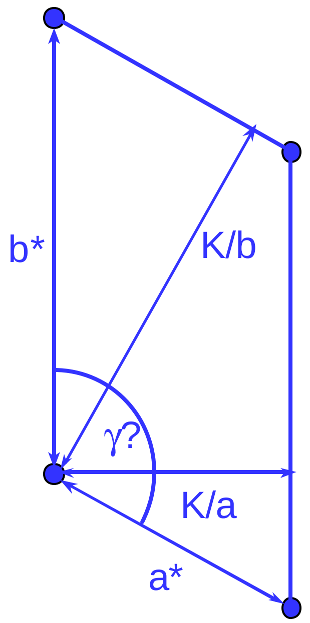
Geometry, Intensity and Symmetry

$$d^* = \frac{K}{d \sin g^*}$$

$$g^* = 180 - g$$



Real Lattice

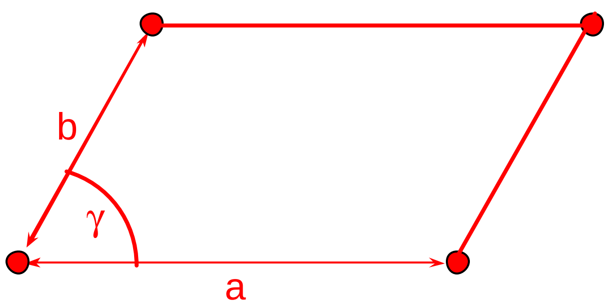


Reciprocal Lattice

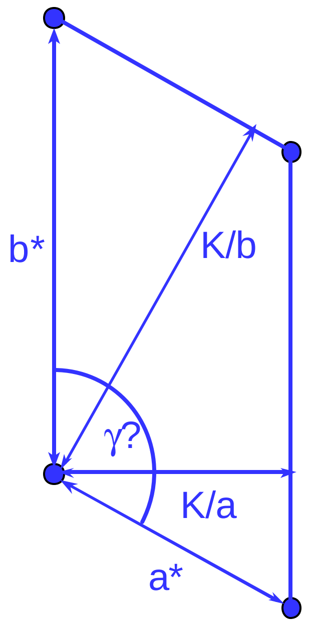
III.C.6.h Other Properties of FTs and Diffraction Patterns

Geometry, Intensity and Symmetry

The reciprocal lattice edges, of dimensions *a** and *b**, are respectively perpendicular to the cell edges *b* and *a*



Real Lattice



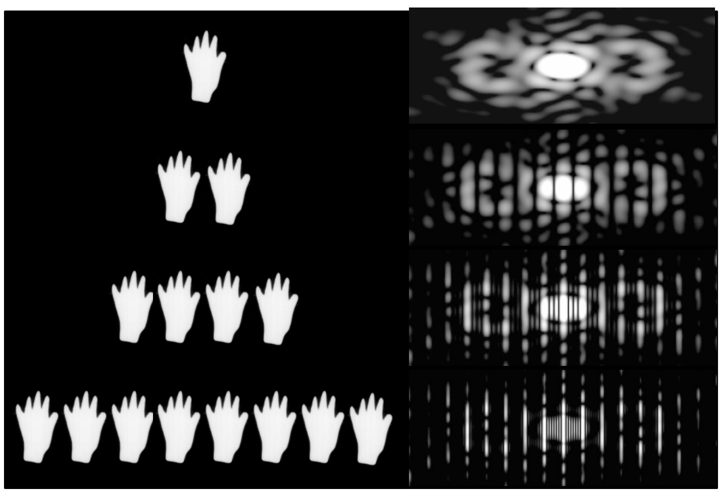
Reciprocal Lattice

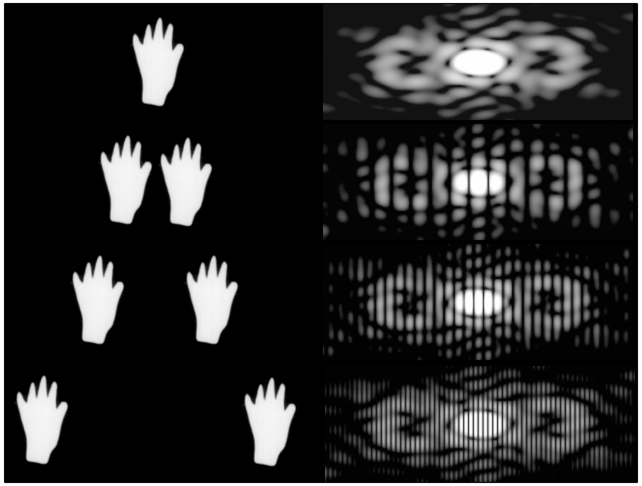
III.C.6.h Other Properties of FTs and Diffraction Patterns

Geometry, Intensity and Symmetry

Each spot is indexed according to its position in the reciprocal lattice, and is considered to arise by diffraction from a set of density (Bragg) planes/lines in the 3-D/2-D crystal

Motif structure, **NOT** spacings or geometry of crystal lattice, determine the **intensity distribution** in transform





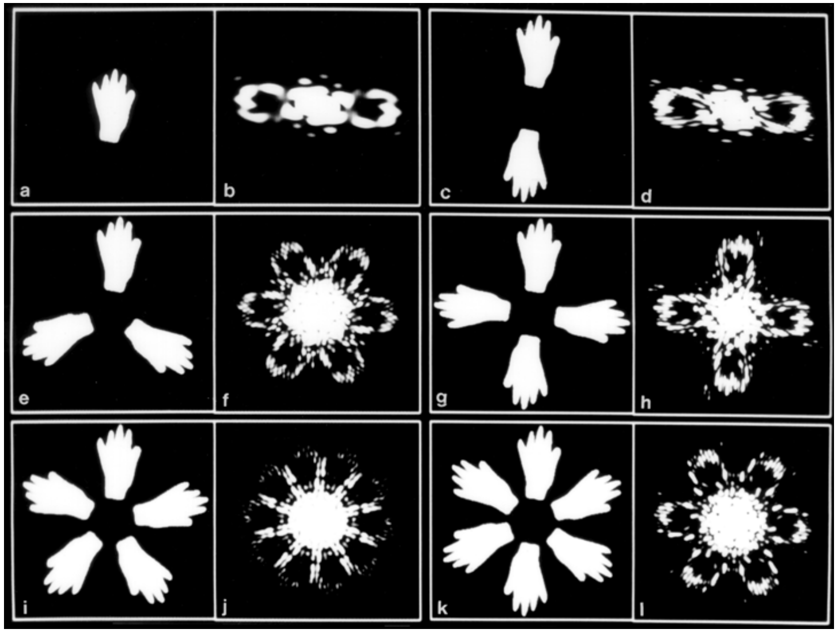
Spacings and geometry of crystal lattice only determine **where** the motif transform is **sampled**

III.C.6.h Other Properties of FTs and Diffraction Patterns

Geometry, Intensity and Symmetry

Structural symmetry produces symmetrical intensity distributions in the transform (aside from Friedel symmetry)

Object rotational symmetry	Transform rotational symmetry
***n* even**	***n***
***n* odd**	**2*n***



One of major reasons why OD is powerful method for diagnosing presence of symmetry in biological specimens

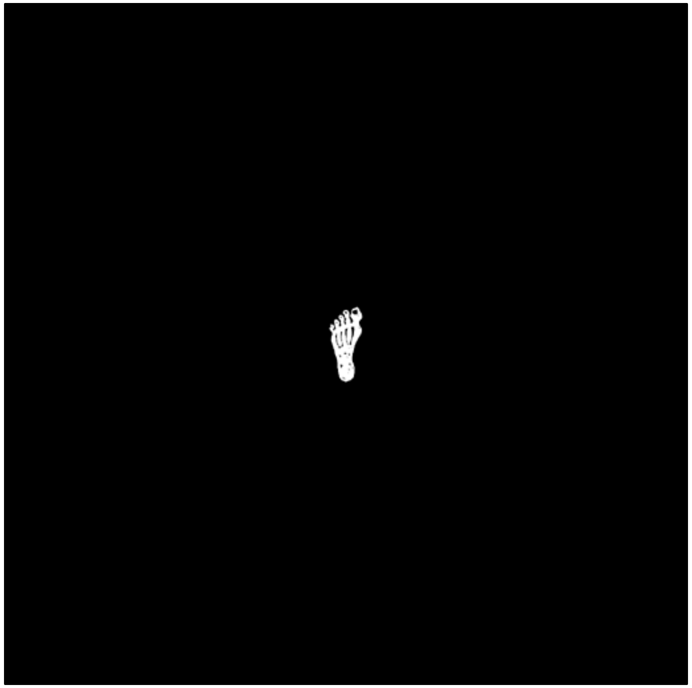
Geometry, Intensity and Symmetry

Screw-axis symmetry in a crystal produces **systematic absences** in the transforms

III.C.6.h Other Properties of FTs and Diffraction Patterns

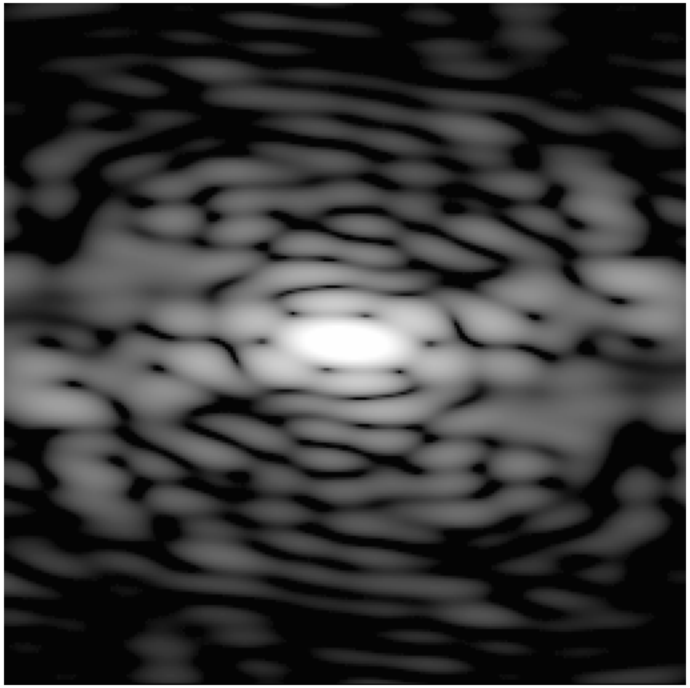
Geometry, Intensity and Symmetry

Foot



FT

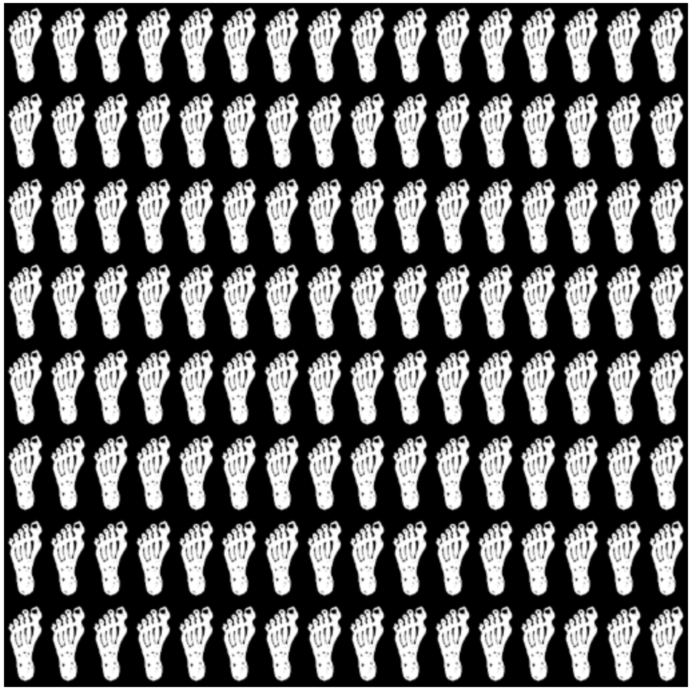
Foot Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

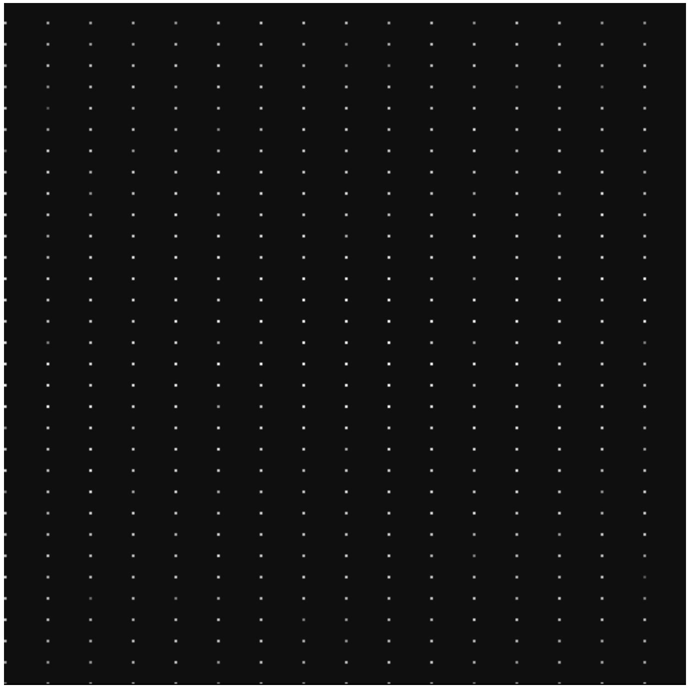
Geometry, Intensity and Symmetry

Foot p1 Crystal



FT

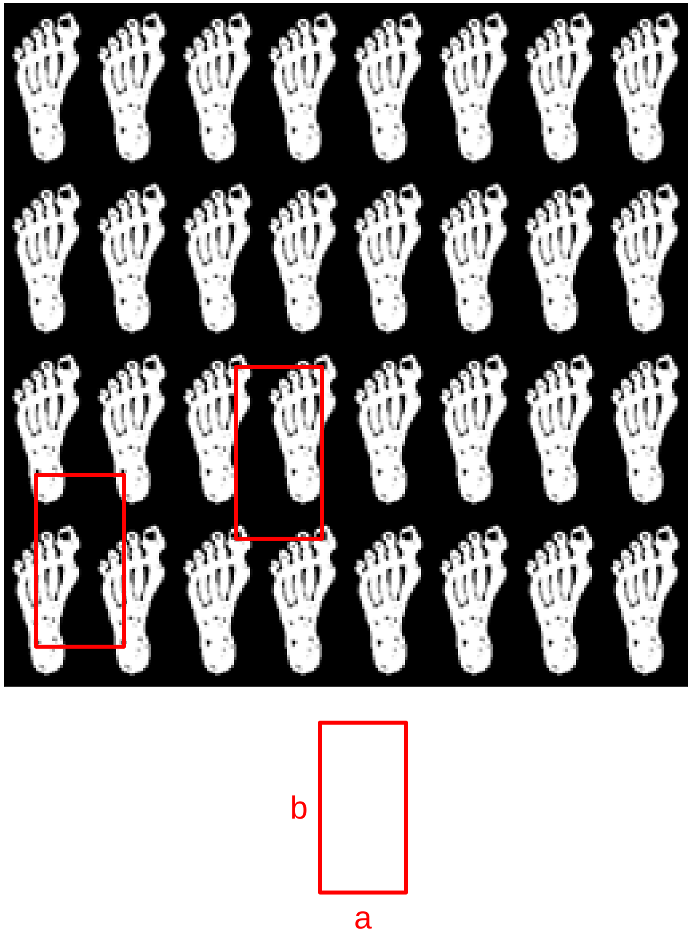
Foot p1 Crystal Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

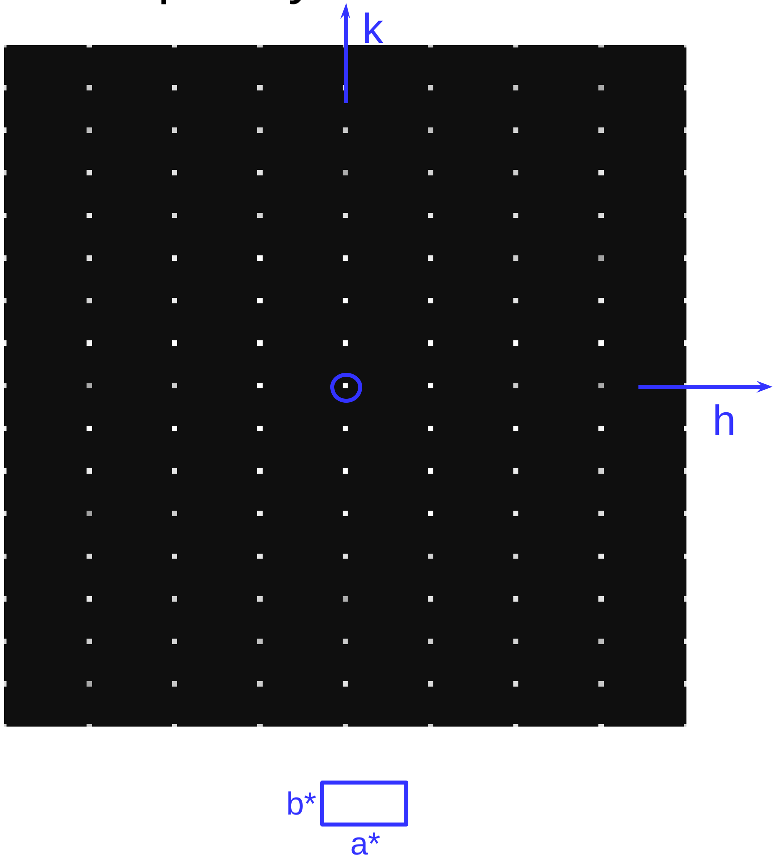
Geometry, Intensity and Symmetry

Foot p1 Crystal



FT

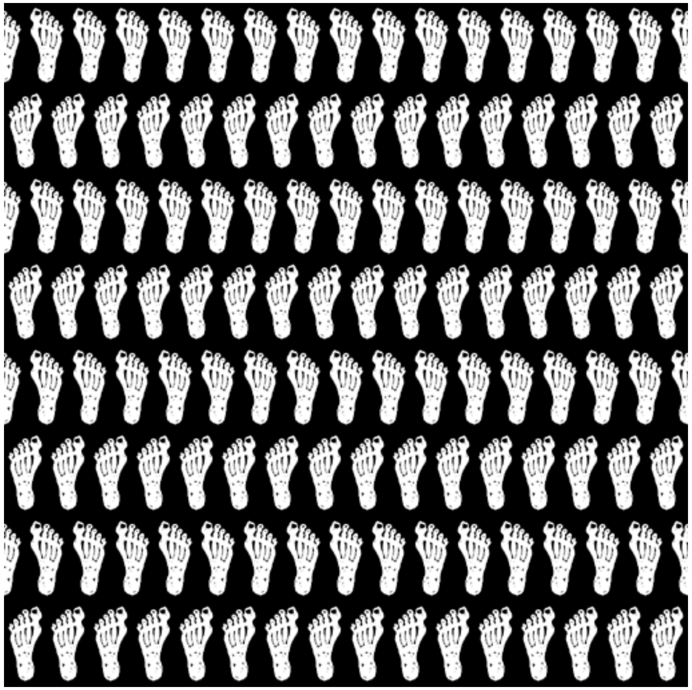
Foot p1 Crystal Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

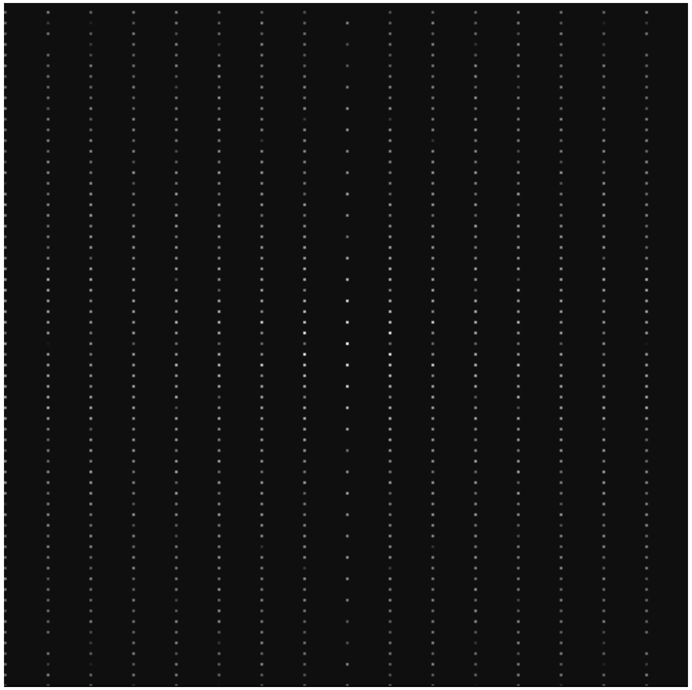
Geometry, Intensity and Symmetry

Foot pg Crystal



FT

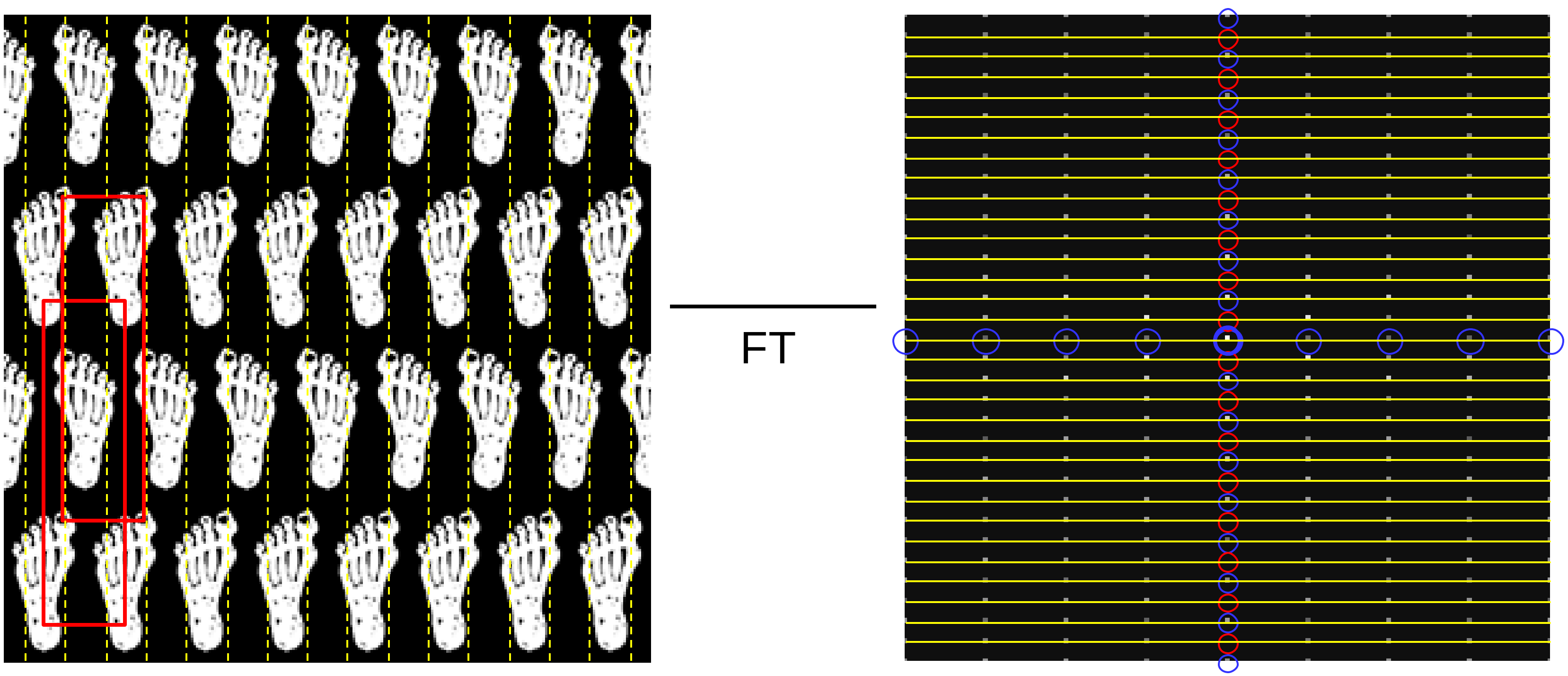
Foot pg Crystal Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

Geometry, Intensity and Symmetry

Foot pg Crystal   Foot pg Crystal Transform



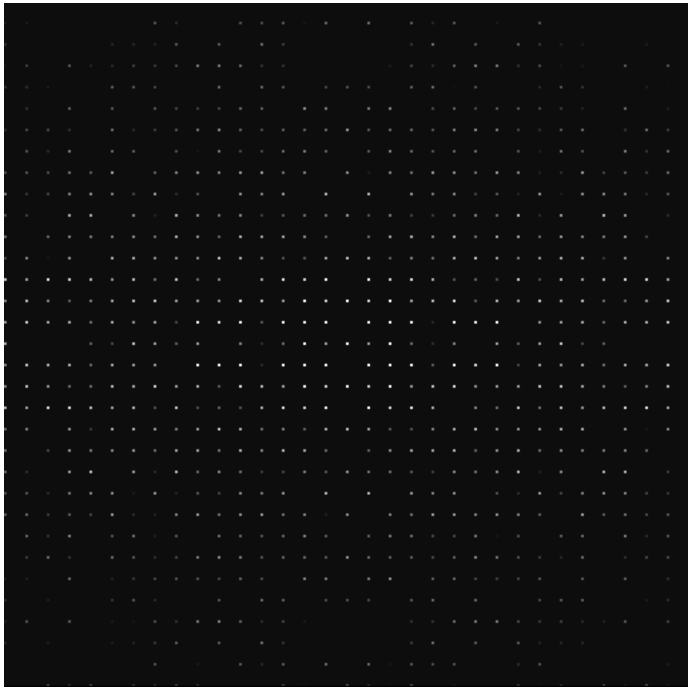
III.C.6.h Other Properties of FTs and Diffraction Patterns

Geometry, Intensity and Symmetry

Foot pg Crystal

FT

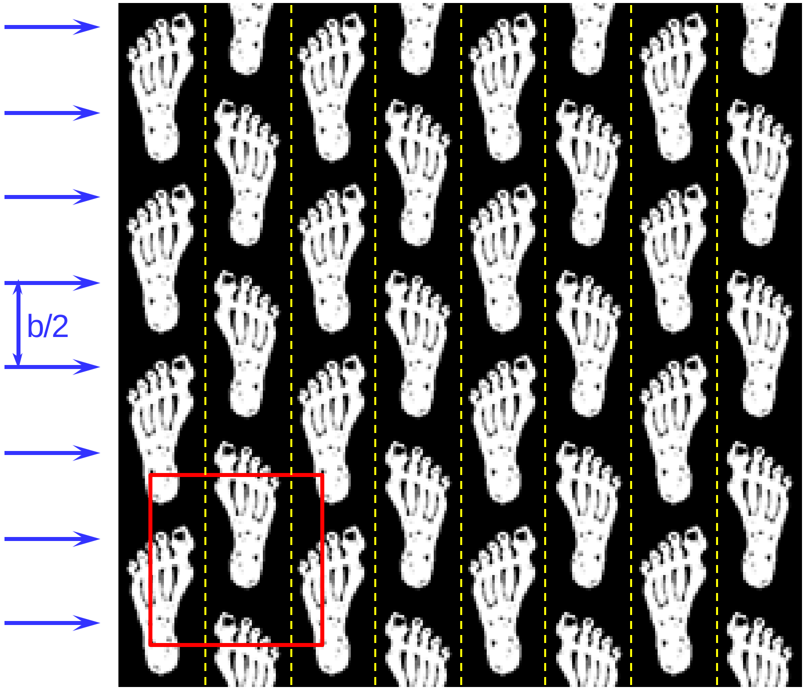
Foot pg Crystal Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

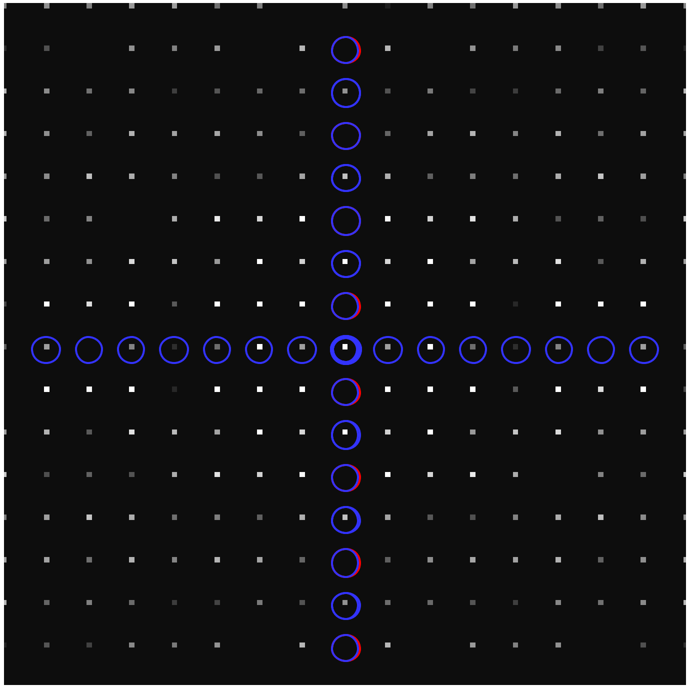
Geometry, Intensity and Symmetry

Foot pg Crystal



FT

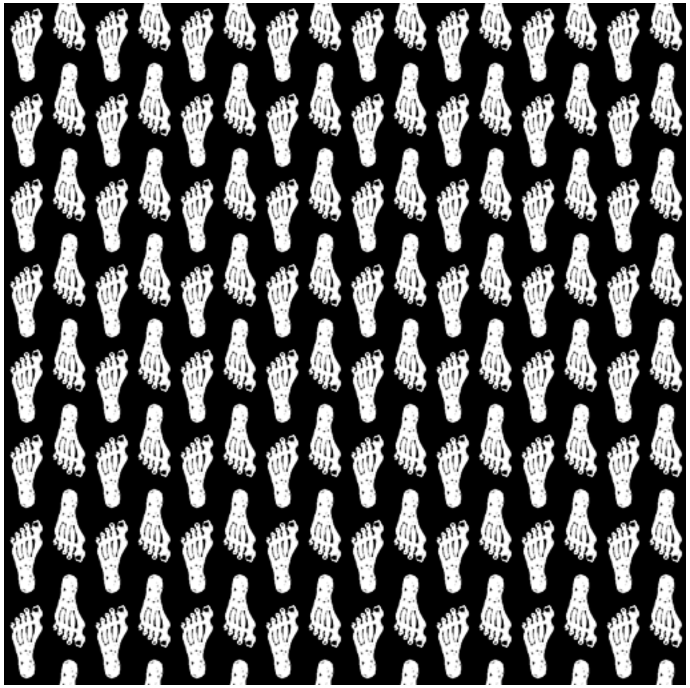
Foot pg Crystal Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

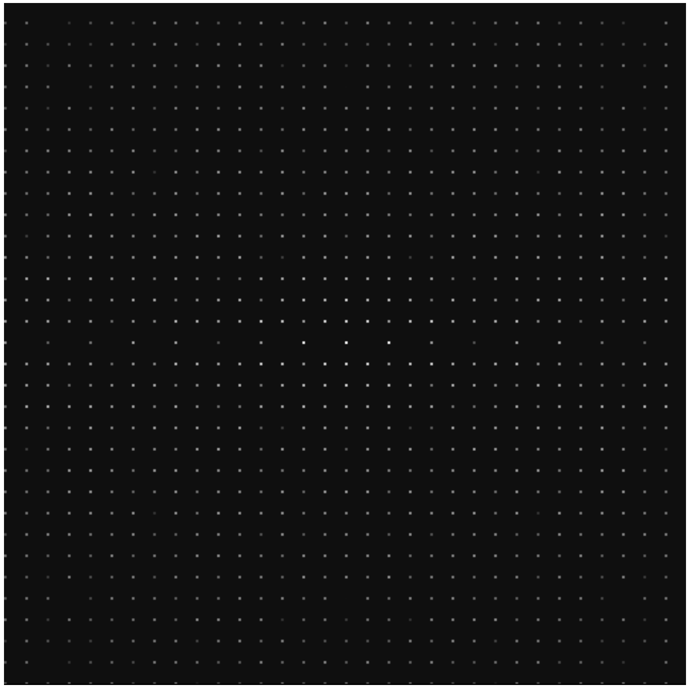
Geometry, Intensity and Symmetry

Foot pg Crystal



FT

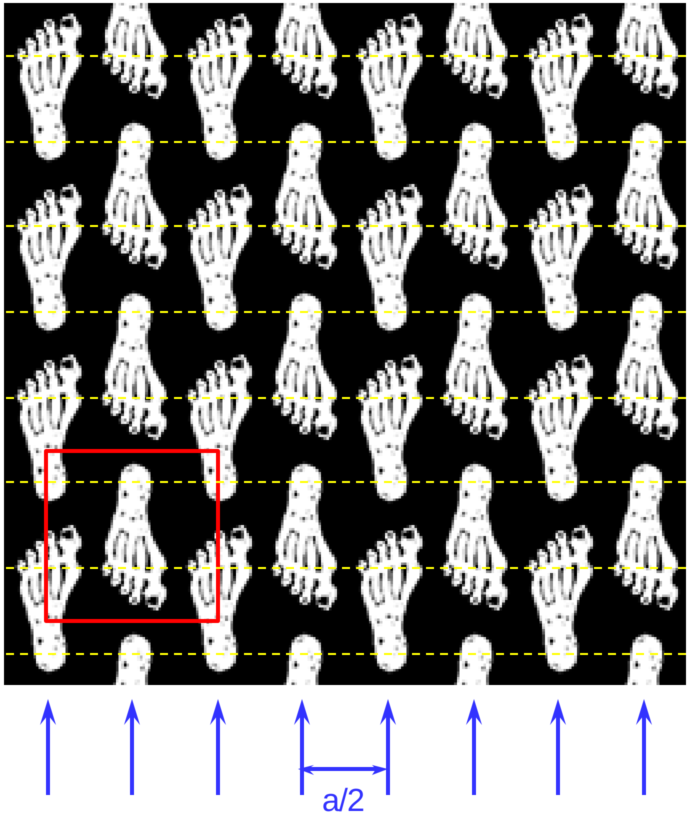
Foot pg Crystal Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

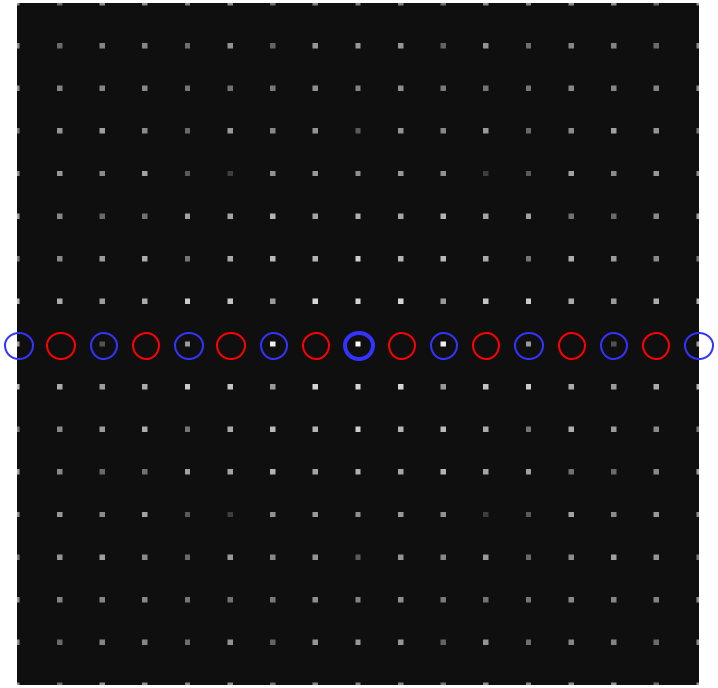
Geometry, Intensity and Symmetry

Foot pg Crystal



FT

Foot pg Crystal Transform



III.C.6.h Other Properties of FTs and Diffraction Patterns

Projection Theorem

FT of the **projected** structure of a **3-D** object is equivalent to a **2-D central section** of the 3-D FT of the object

Central section **intersects the origin** of the 3-D transform and is perpendicular to the direction of projection

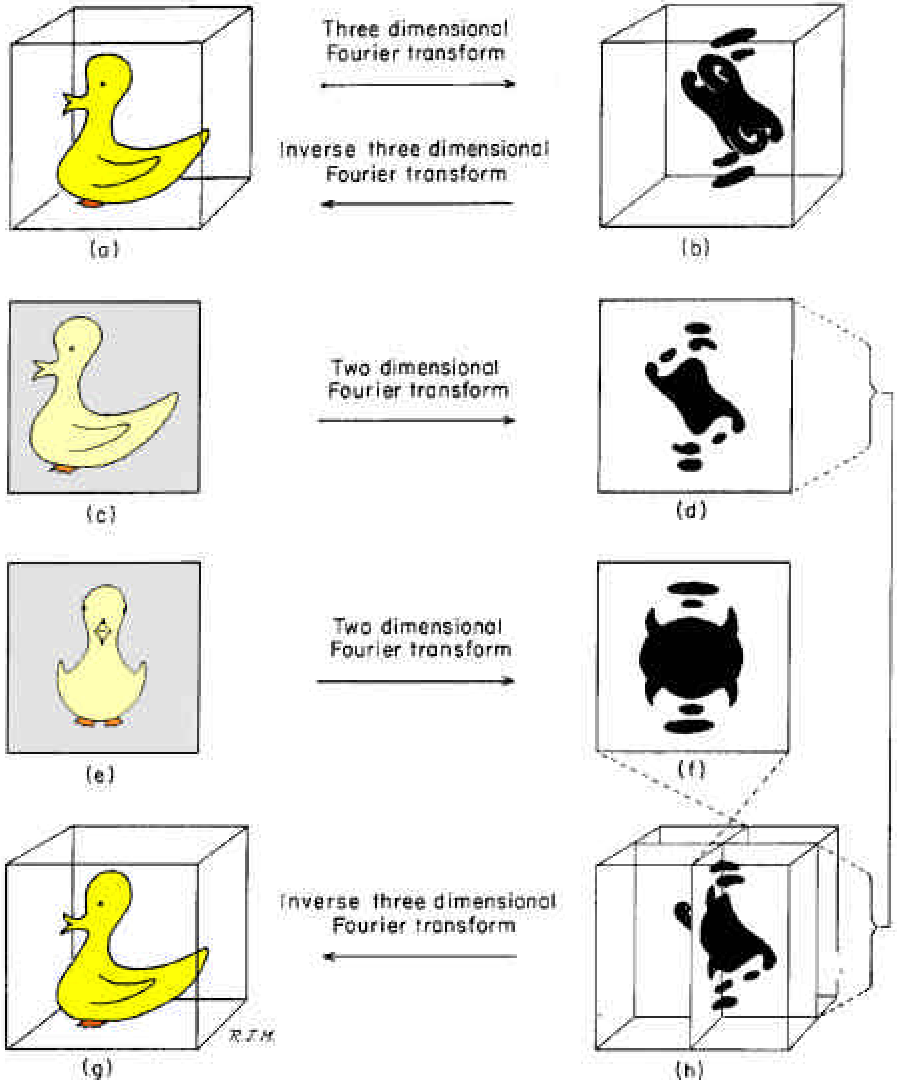
Basis of 3D reconstruction by Fourier methods:

- Several **independent views** of the projected structure are recorded and their 2-D transforms calculated to **build up a complete 3-D transform**

- 3-D structure is **reconstructed** from 2-D views by inverse Fourier transformation of 3-D FT

III.C.6.h Other Properties of FTs and Diffraction Patterns

Projection Theorem



From Lake (Lipson), Fig. 14, p.174

III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Friedel's Law

Diffraction pattern from the projected structure of a real object has an **inversion center** in the **intensity** distribution

Amplitude at any point in the pattern is identical at a point equidistant and opposite in direction from the transform origin: $|F_{hkl}| = |F_{-h,-k,-l}|$

Phases at these two points are opposite: $\alpha_{hkl} = -\alpha_{-h,-k,-l}$

For periodic specimens with periodic patterns consisting of discrete spots (reflections), Friedel related spots are called **Friedel pairs**

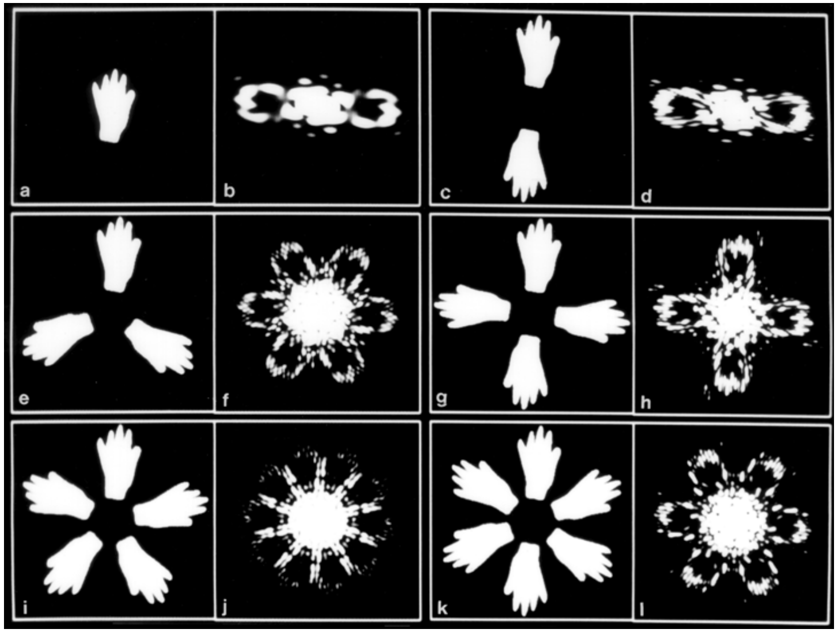
III.C.6 Diffraction

III.C.6.h Other Properties of FTs and Diffraction Patterns

Friedel's Law

Friedel symmetry causes the transform of **any real** object to display **2-fold** symmetry in the **intensity** distribution

Object rotational symmetry	Transform rotational symmetry
***n* even**	***n***
***n* odd**	**2*n***



III.C.6.h Other Properties of FTs and Diffraction Patterns

Friedel's Law

Optical diffraction:

Friedel's law generally fails (pattern does **not** exhibit perfect inversion symmetry in intensity distribution) because the object is a photographic transparency which causes **irregular phase shifts** of the incident radiation (laser light) as it passes through the emulsion and backing of the film

Mathematically computed diffraction patterns:

Should have **PERFECT** Friedel symmetry (if software is bug-free of course!)

End of Sec.III.C.6