

X-Ray Crystallography

“If a picture is worth a thousand words, then a macromolecular structure is priceless to a physical biochemist.” – van Holde

Topics:

1. Protein Data Bank (PDB)

Data mining and Protein Structure Analysis Tools

2. Image Formation

Resolution / Wavelength (Amplitude, Phase) / Light Microscopy / EM / X-ray / (NMR)

3. X-Ray Crystallography (after NMR)

a) Crystal Growth – Materials / Methods

b) Crystal Lattices - Lattice Constants / Space Groups / Asymmetric Unit

c) X-ray Sources – Sealed Tube / Rotation Anode / Synchrotron

d) Theory of Diffraction – Bragg’s Law / Reciprocal Space

e) Data Collection – Methods / Detectors / Structure Factors

f) Structure Solution – Phase Problem: MIR / MR / MAD

h) Refinements and Models

i) Analysis and presentation of results

PDB Holdings List: 5-Apr-2005

		Molecule Type				Total
		Proteins, Peptides, and Viruses	Protein/Nucleic Acid Complexes	Nucleic Acids	Carbohydrates	
Exp.	X-ray Diffraction and other	23942	1147	778	11	25878
Tech.	NMR	3721	111	649	2	4483
	Total	27663	1258	1427	13	30361

Please note that theoretical models have been removed, effective July 02, 2002, as per [PDB policy](#).

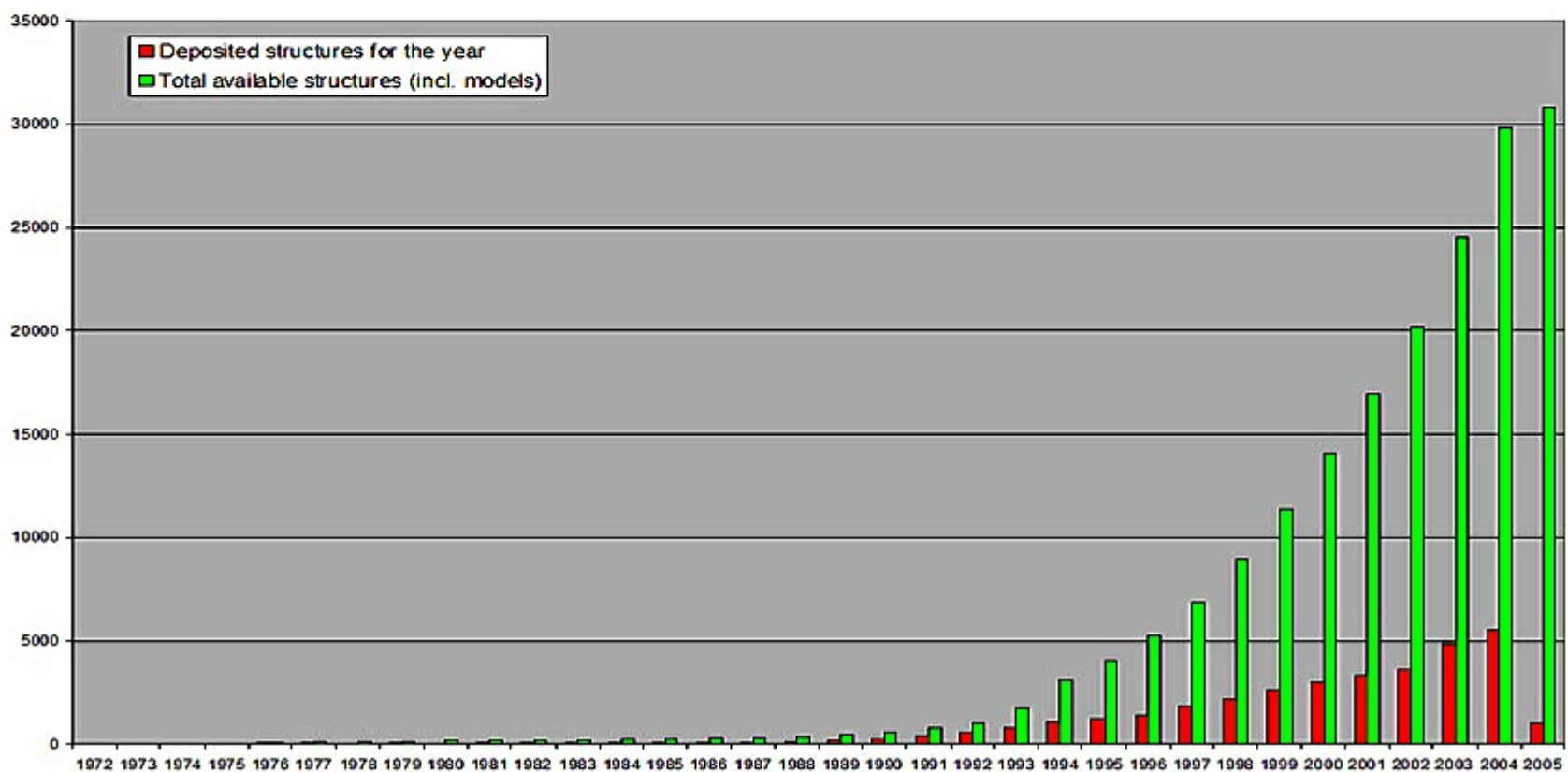
16255 Structure Factor Files

2484 NMR Restraint Files

35,917 4/6/06

42,627 4/4/07

PDB Content Growth



Protein Data Bank - 17,679 Structures - March 2002

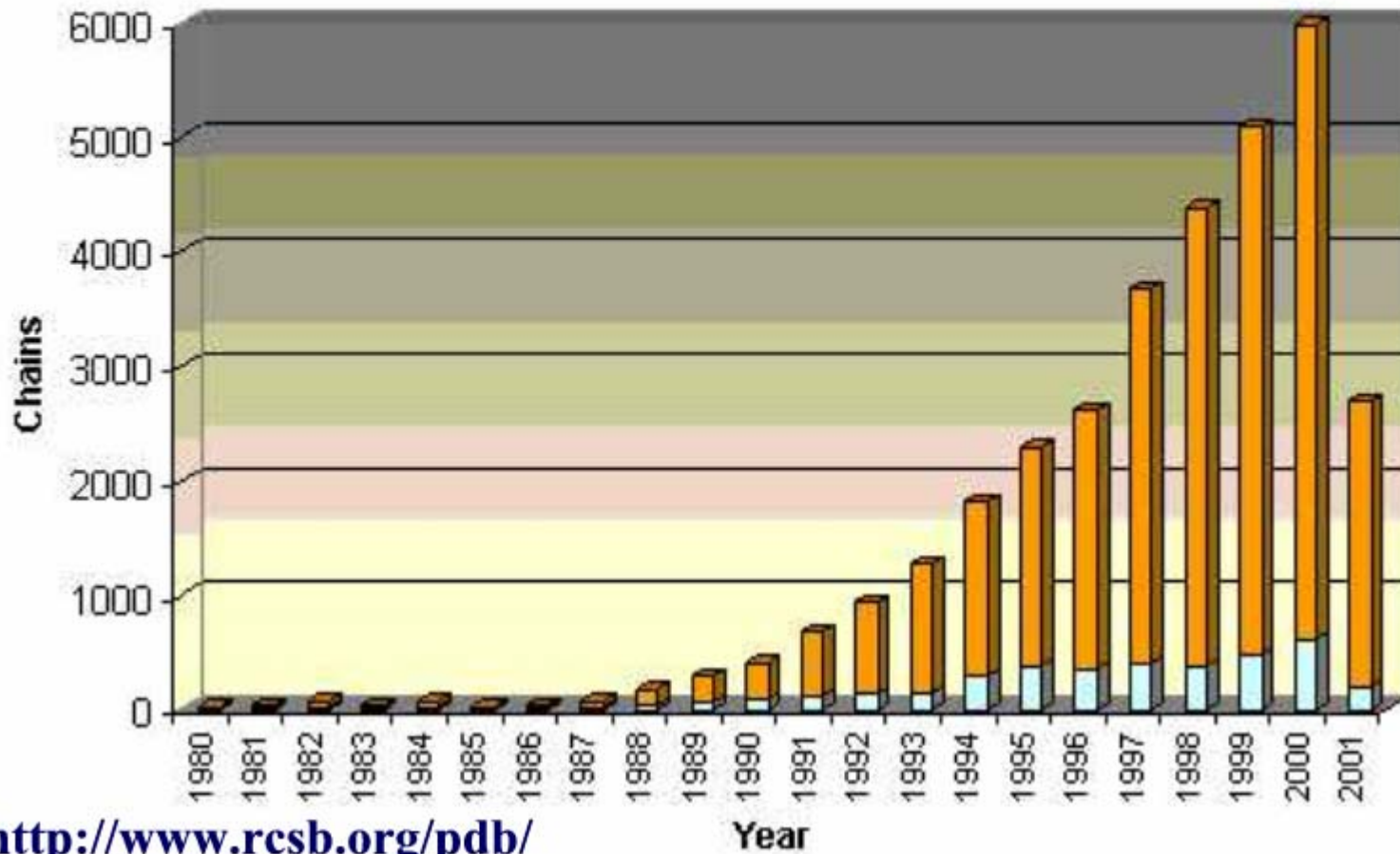
X-ray - 14595

NMR - 2706

Theory - 378

"Old" Folds

"New" Folds



<http://www.rcsb.org/pdb/>

Analyze – structure (Ramachandran Plot) and biochemistry

Publish in leading biochemical or structural biology journal

Contribute results (coordinates, etc.) to PDB

Data Mining

Visualization programs (Cn3D / RasMol / SwissPDBV / etc)

SCOP – Structural Classification of Proteins

CATH – Classification / Arch / Topology

SCOP































Structural Classification of Proteins

Structural Classification of Proteins



Root: scop

Classes:

1. [All alpha proteins](#) (151)   
2. [All beta proteins](#) (111)   
3. [Alpha and beta proteins \(a/b\)](#) (117)   
Mainly parallel beta sheets (beta-alpha-beta units)
4. [Alpha and beta proteins \(a+b\)](#) (212)   
Mainly antiparallel beta sheets (segregated alpha and beta regions)
5. [Multi-domain proteins \(alpha and beta\)](#) (39)   
Folds consisting of two or more domains belonging to different classes
6. [Membrane and cell surface proteins and peptides](#) (12)   
Does not include proteins in the immune system
7. [Small proteins](#) (59)   
Usually dominated by metal ligand, heme, and/or disulfide bridges
8. [Coiled coil proteins](#) (5)   
Not a true class
9. [Low resolution protein structures](#) (17)  
Not a true class
10. [Peptides](#) (95)   
Peptides and fragments. Not a true class
11. [Designed proteins](#) (36)   
Experimental structures of proteins with essentially non-natural sequences. Not a true class

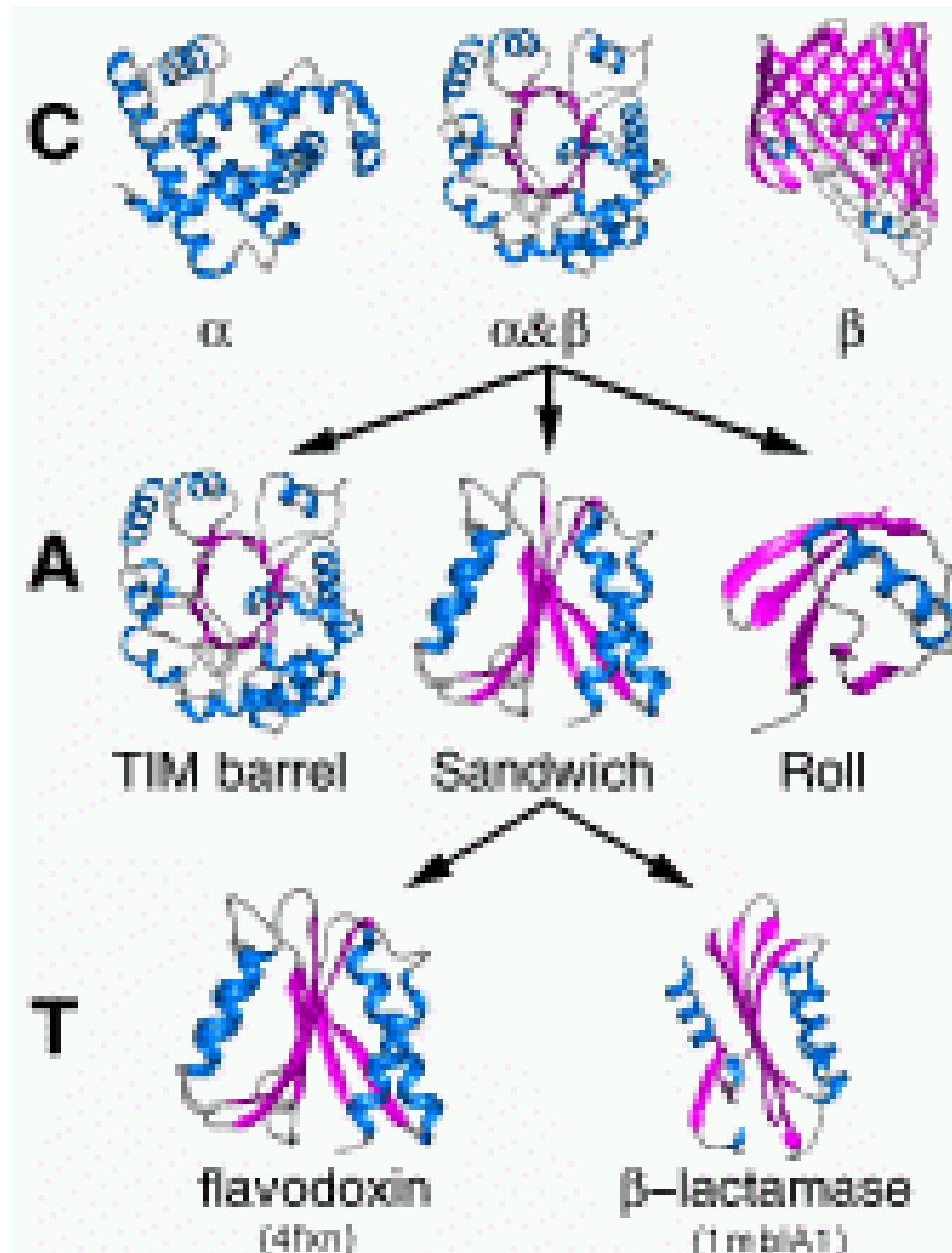
CATH - Protein Structure Classification

CATH is a novel hierarchical classification of protein domain structures, which clusters proteins at four major levels: **Class (C)**, **Architecture (A)**, **Topology (T)**, and **Homologous (H) Superfamily**

Class, derived from **secondary structure** content, is assigned for more than 90% of protein structures automatically.

Architecture, which describes the **gross orientation of secondary structures**, independent of connectivities, is currently assigned manually. The **topology** level clusters structures according to their **topological connections and numbers of secondary structures**. The **homologous superfamilies** cluster proteins with **highly similar structures and functions**. The assignments of structures to topology families and homologous superfamilies are made by sequence and structure comparisons.

CATH



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Object



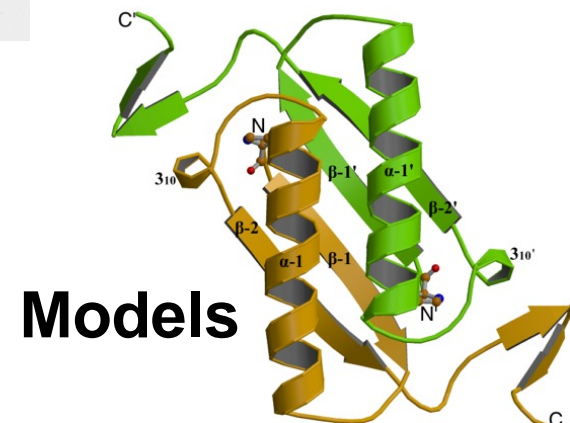
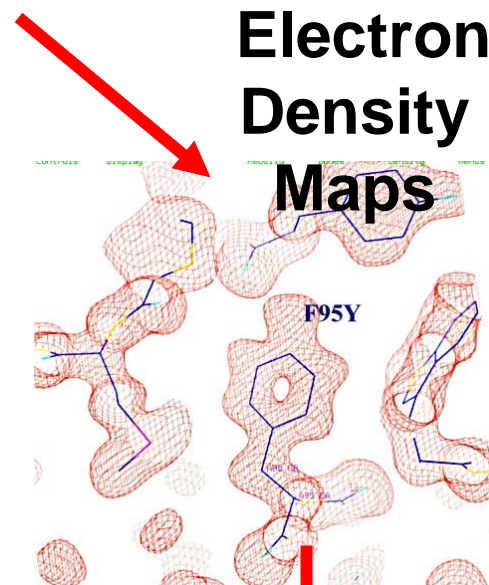
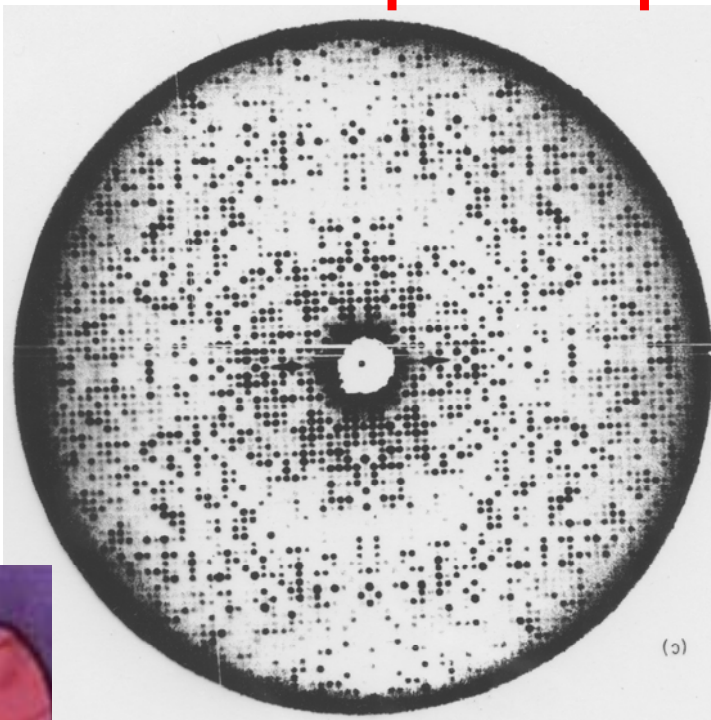
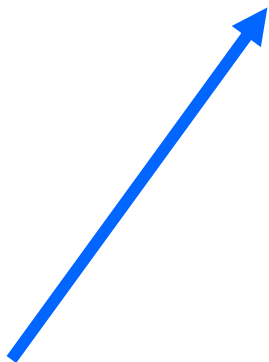
Transform



Image

Transform / Reciprocal Space

Object / Real Space



“If a picture is worth a thousand words, then a macromolecular structure is priceless to a physical biochemist.” – van Holde



- Light Photography

$\lambda \sim 400 - 700 \text{ nm}$

- Electron Microscopy

$\lambda \sim 0.001 - 0.1 \text{ nm}$

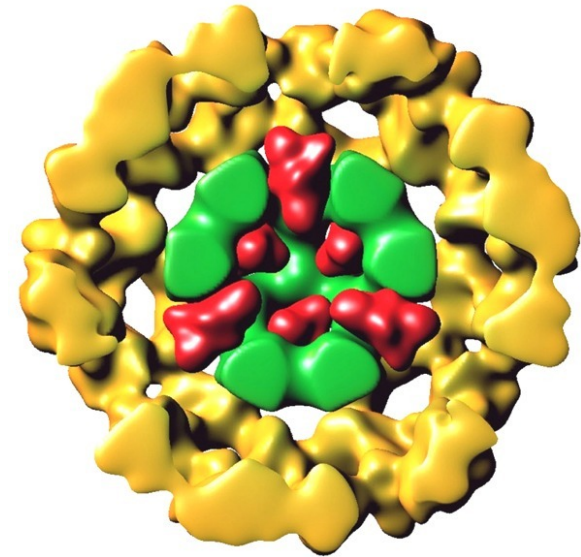


Image Formation

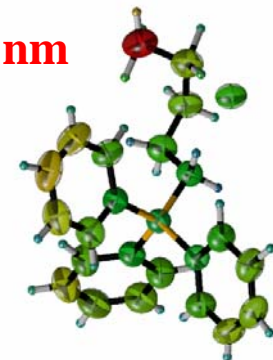
Abbe (~1873):

Limit Res. $\sim \lambda/2$



- X-Ray or NMR

$\lambda \sim 0.1 \text{ nm}$

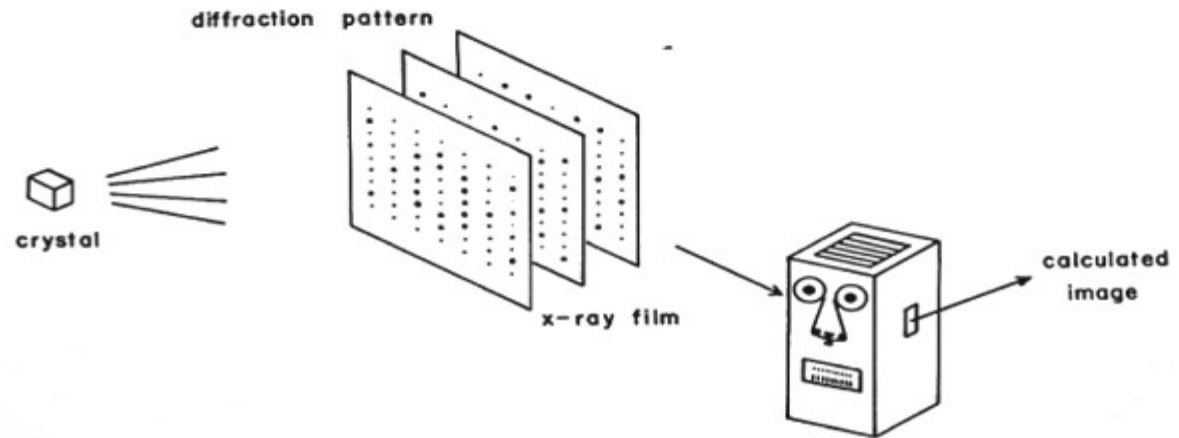
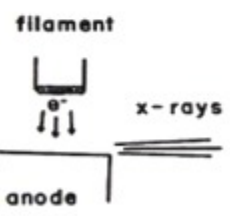
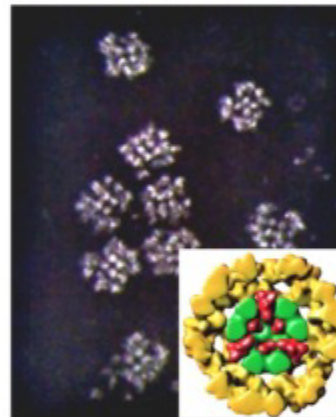
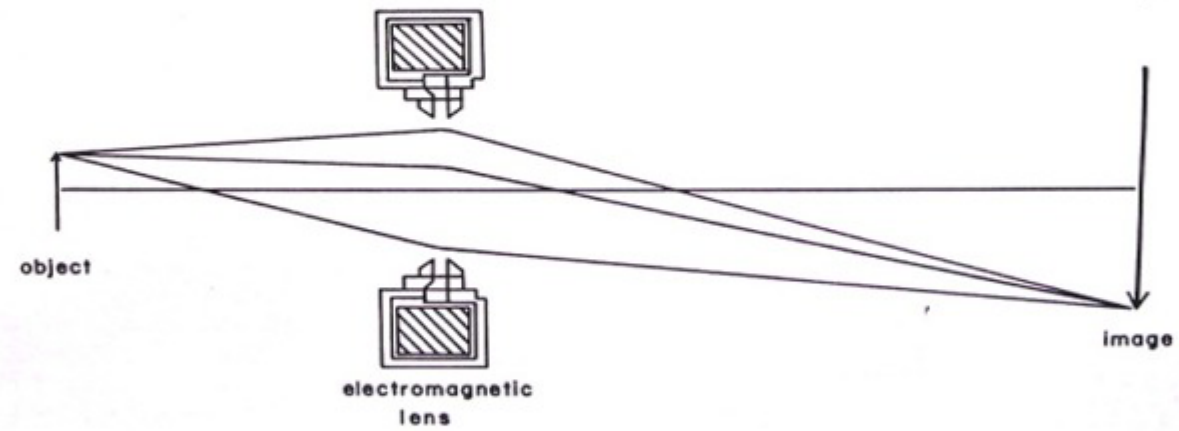
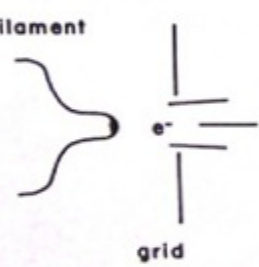
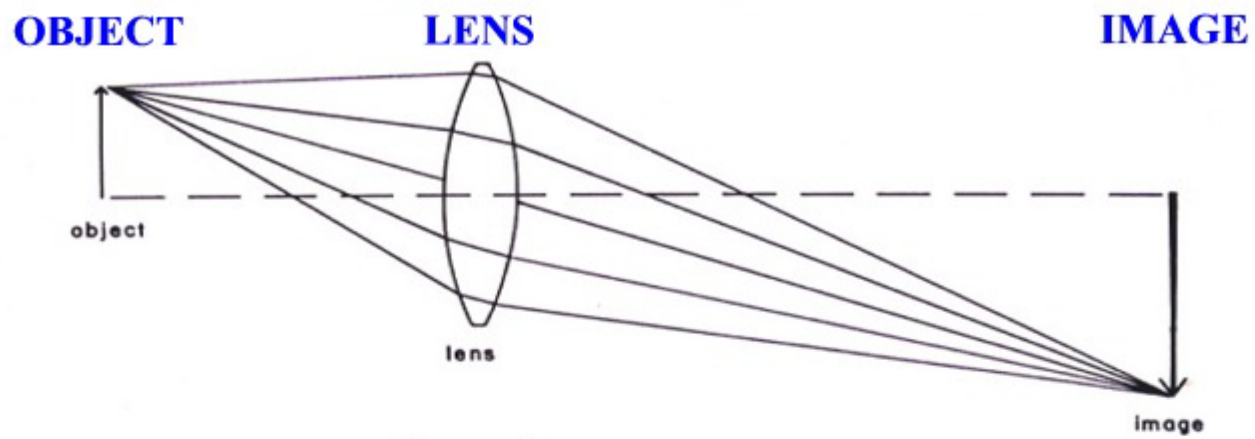


SOURCE

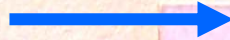
SCATTERING

RECOMBINATION

EXAMPLE



Object



Transform

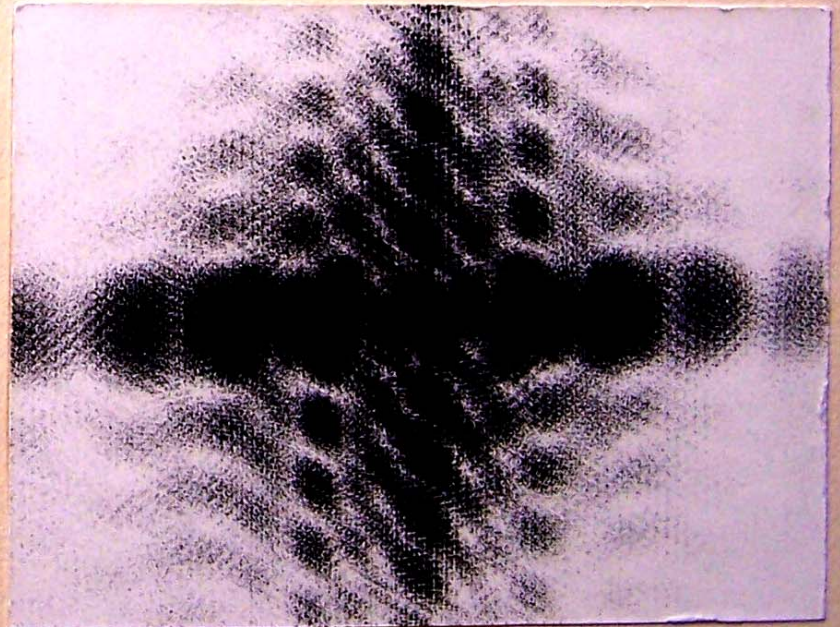
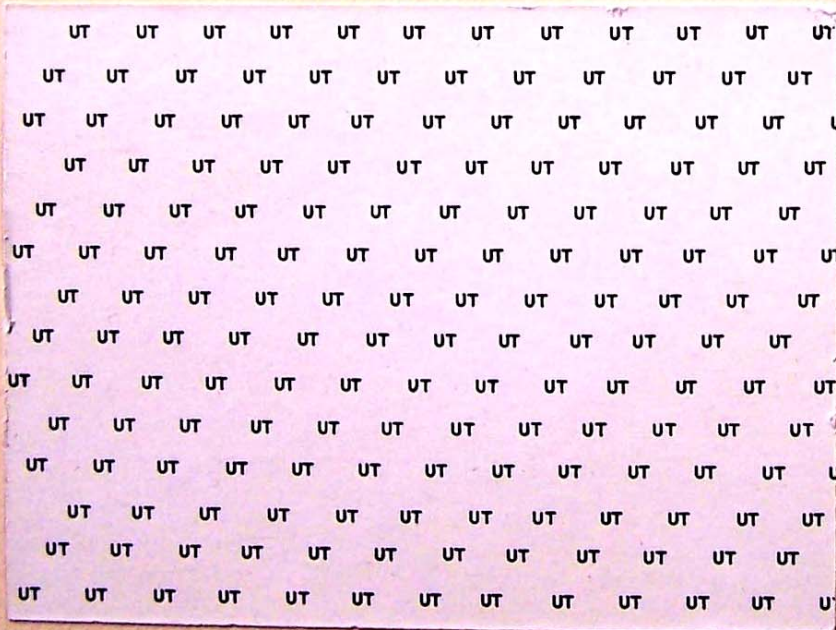
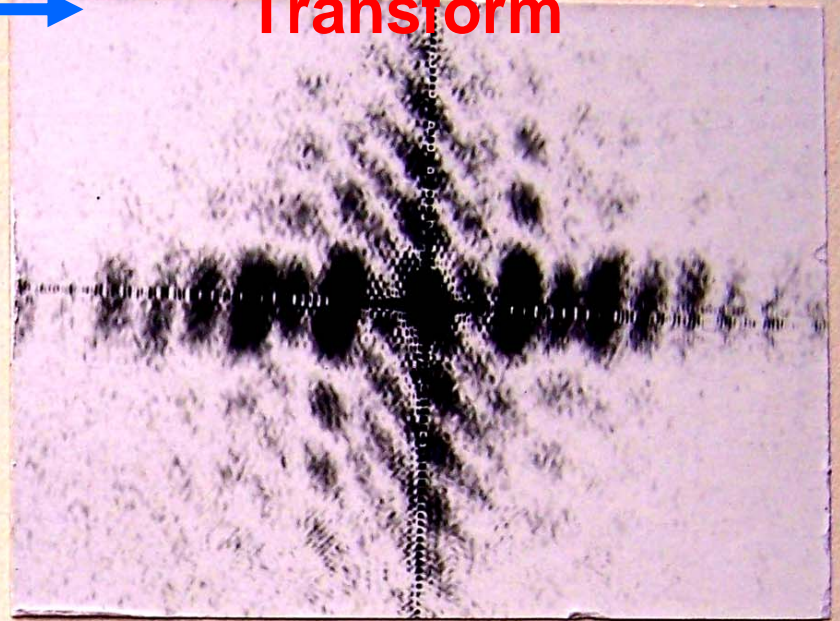


Image (high resolution)

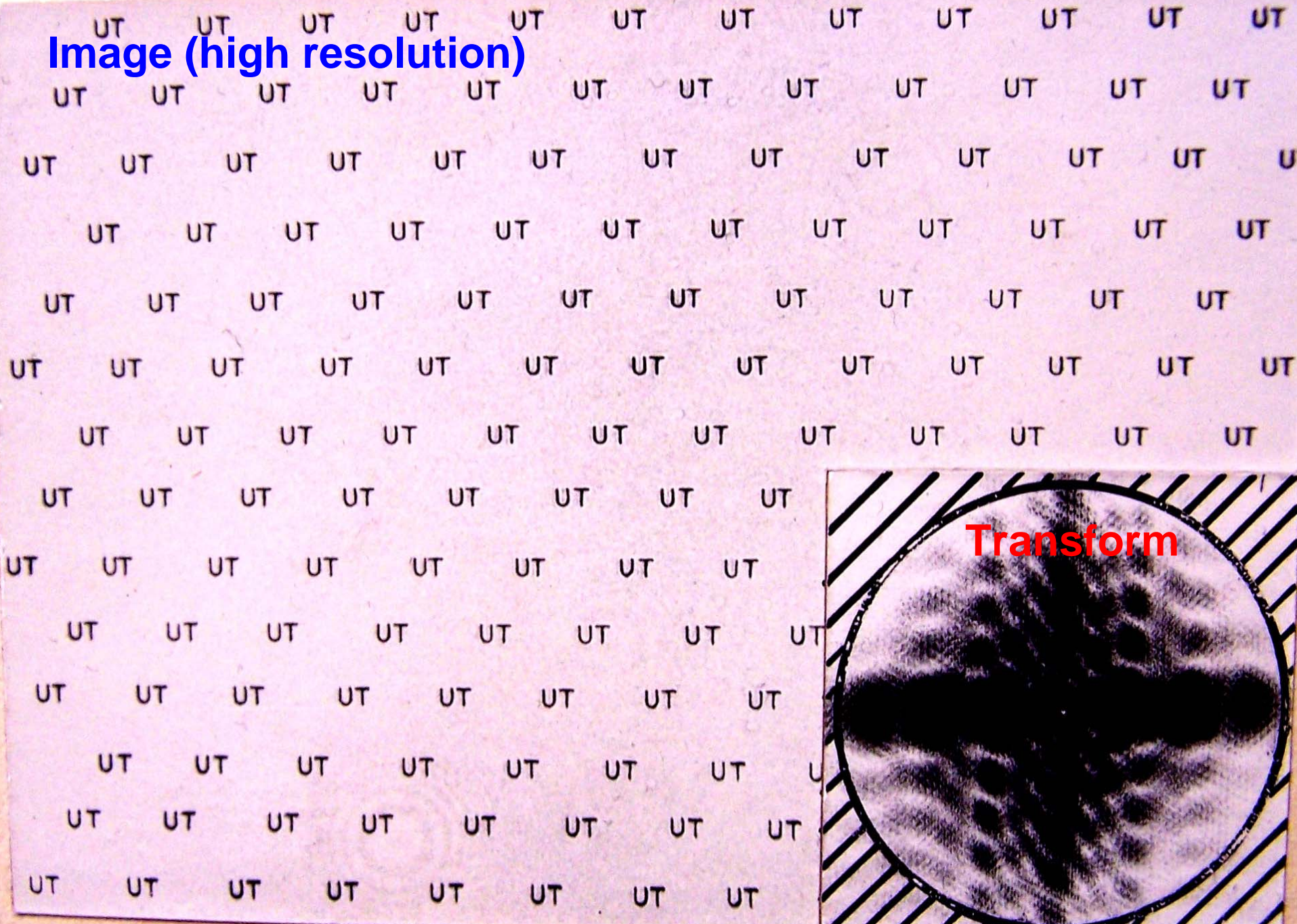
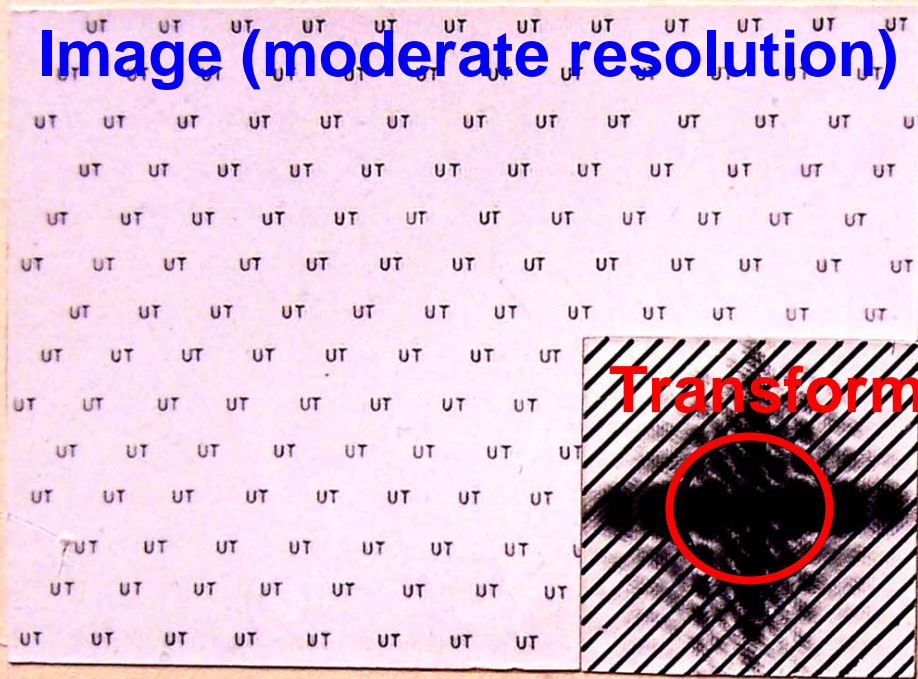
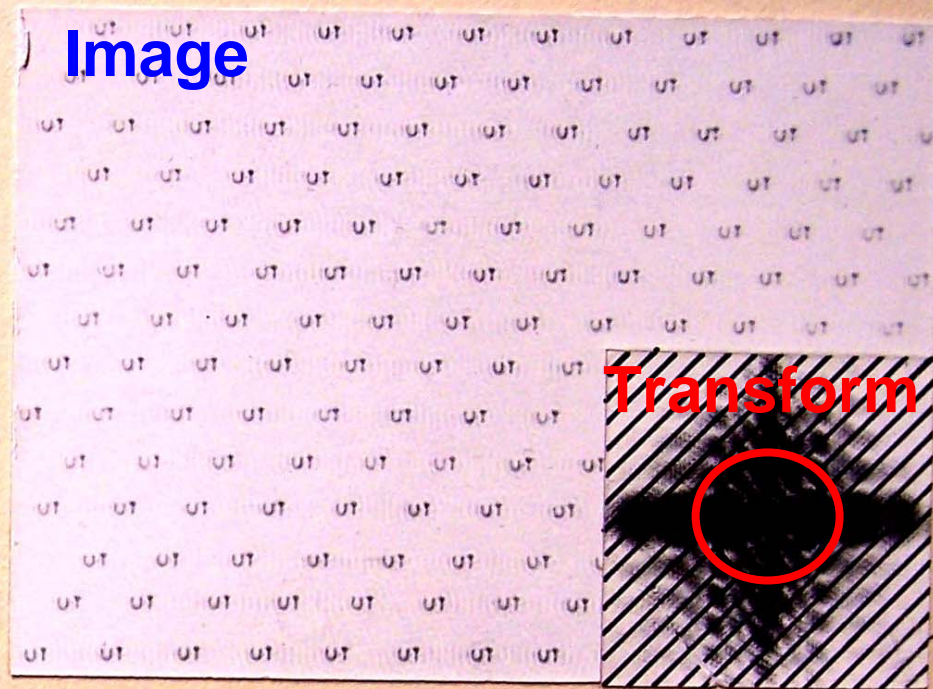


Image (moderate resolution)



Image



Image

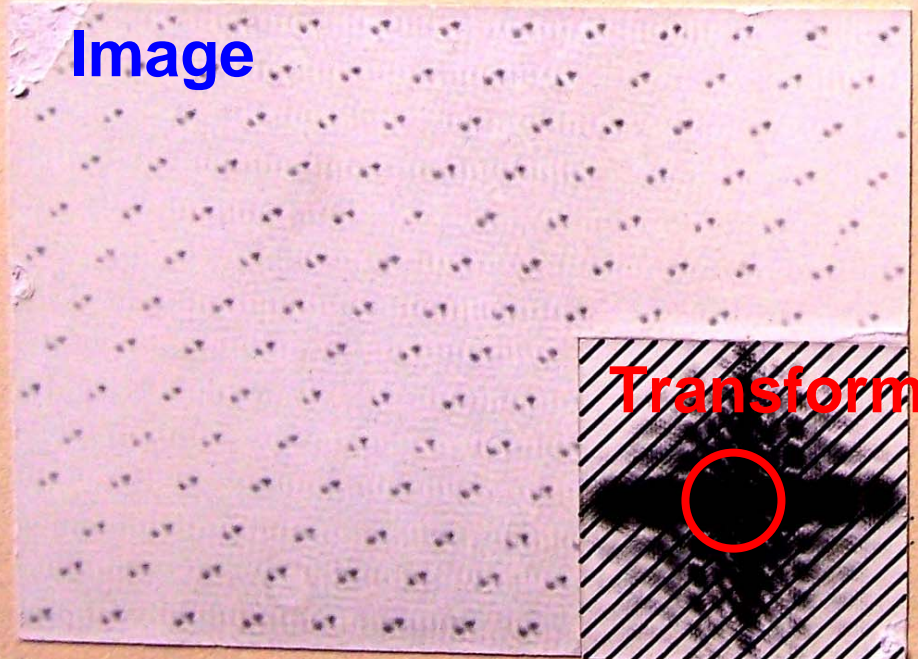
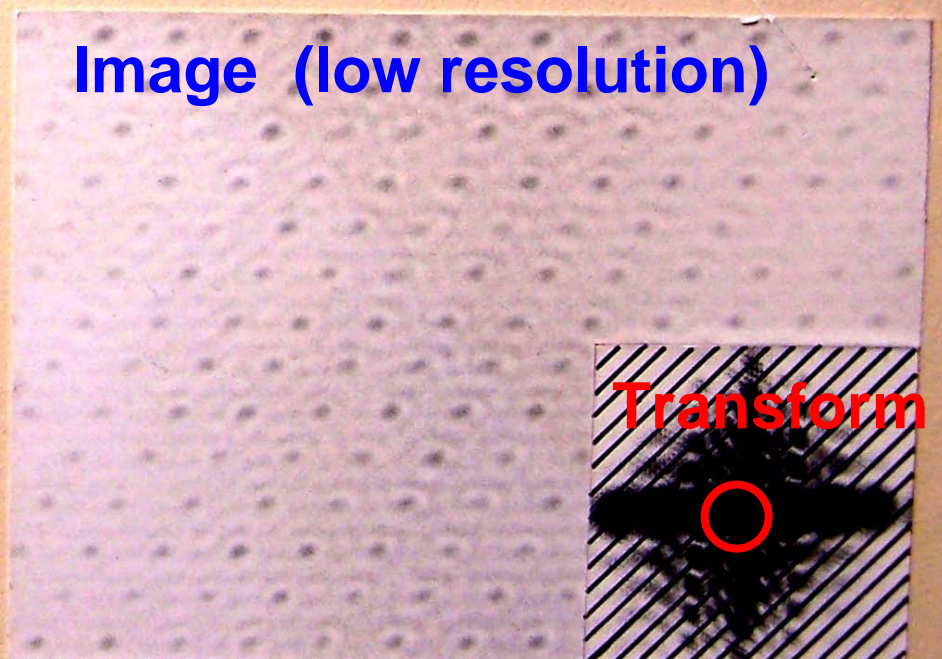
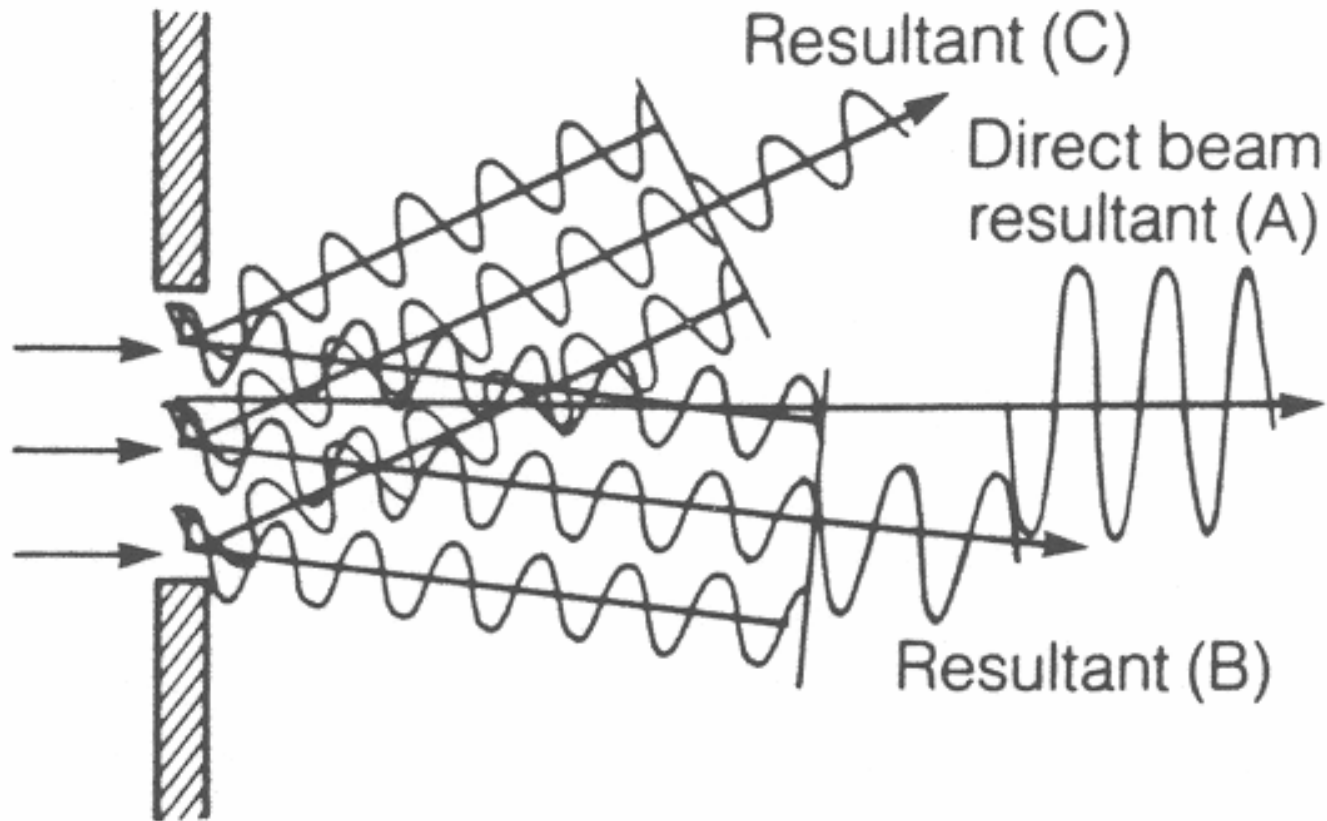


Image (low resolution)



Transforms / Reciprocal Space

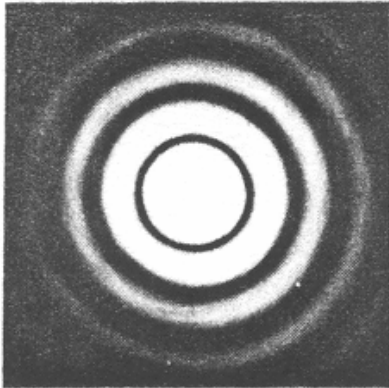


(b)

Transforms / Reciprocal Space

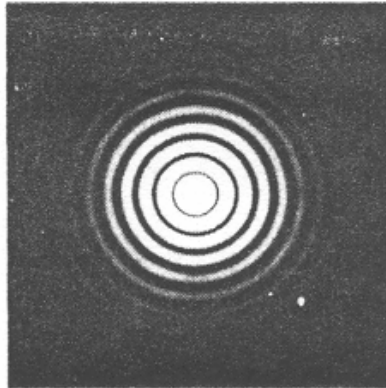
Different size holes

(a) ●



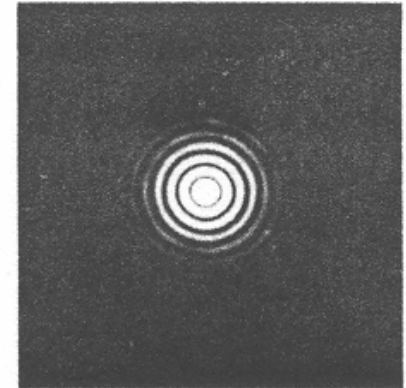
(a)

(b) ●



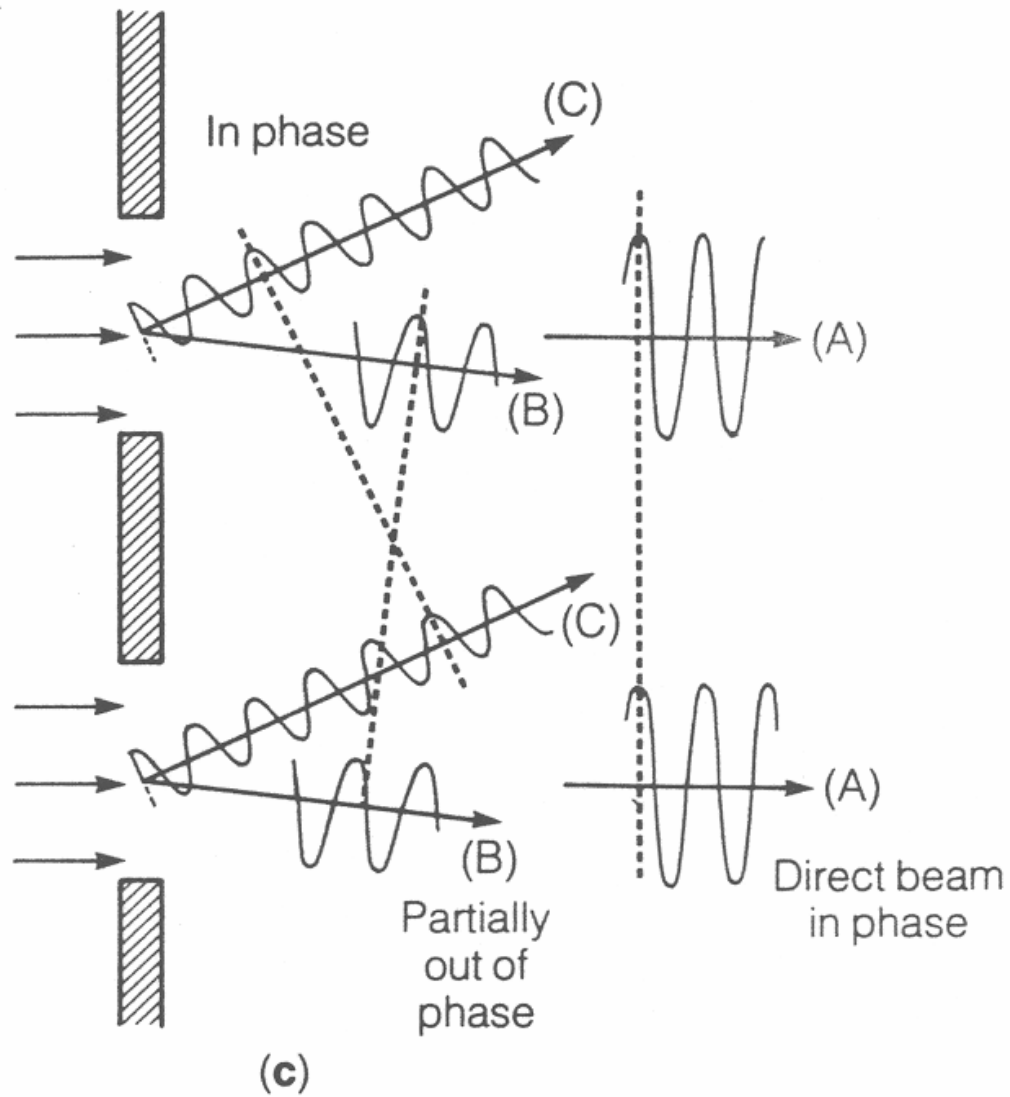
(b)

(c) ●

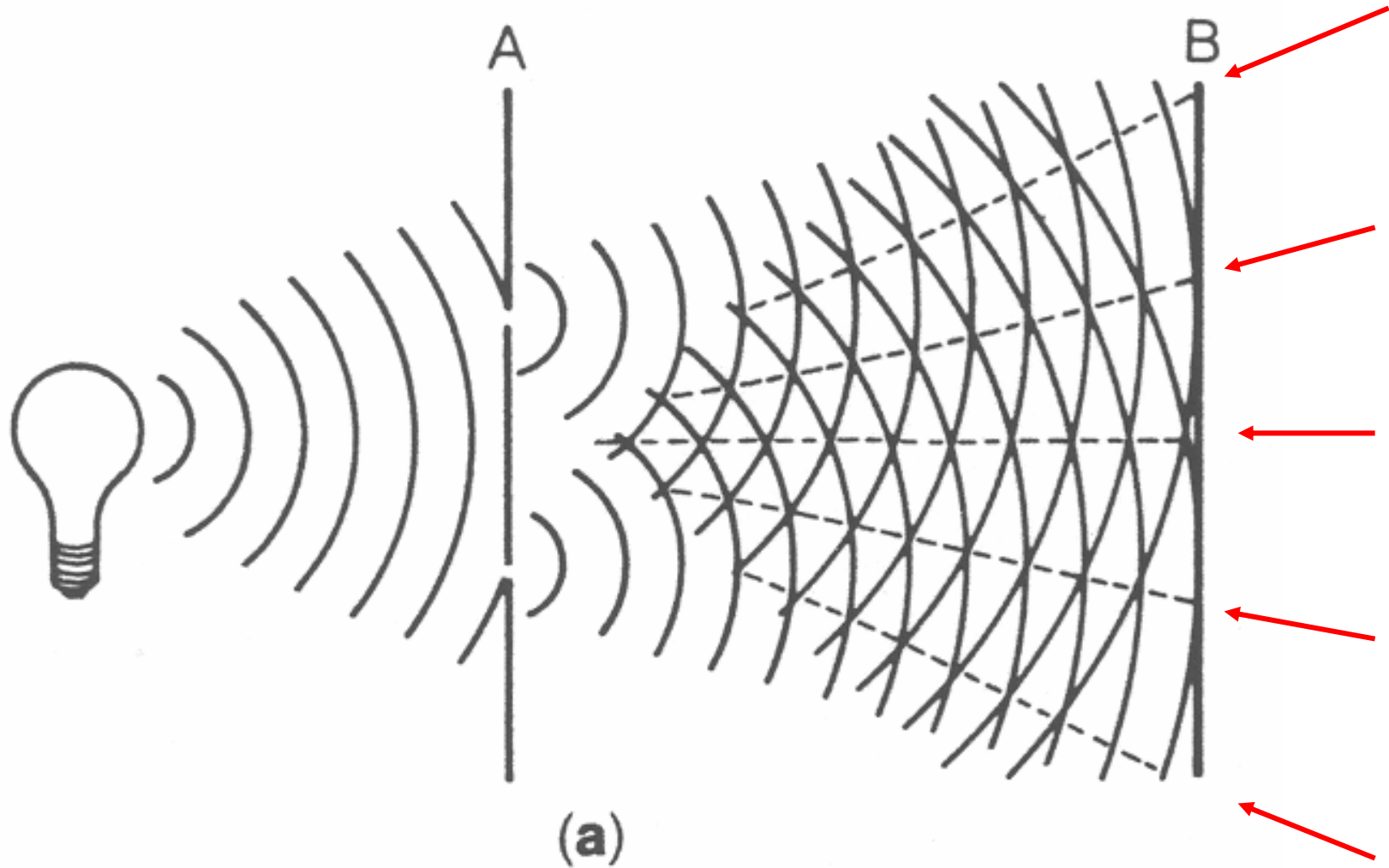


(c)

Transforms / Reciprocal Space



Transforms / Reciprocal Space



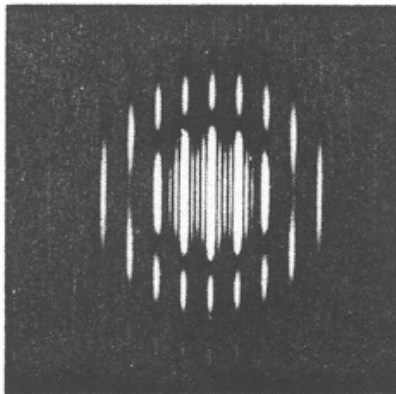
Transforms / Reciprocal Space

Five horizontal holes
with various spacings

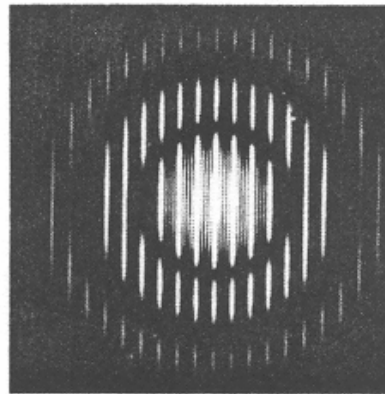
(j) ● ● ● ● ●

(k) ● ● ● ● ●

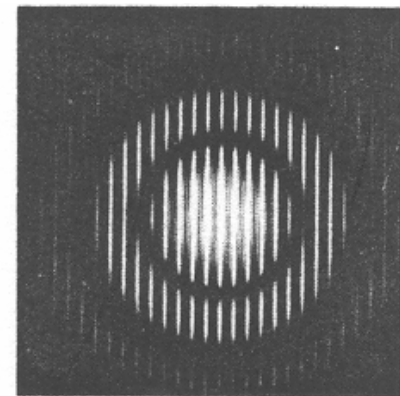
(l) ● ● ● ● ●



(j)



(k)

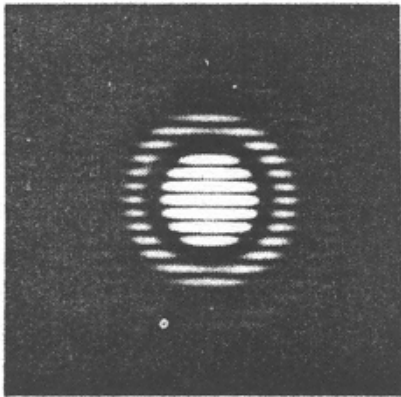


(l)

Transforms / Reciprocal Space

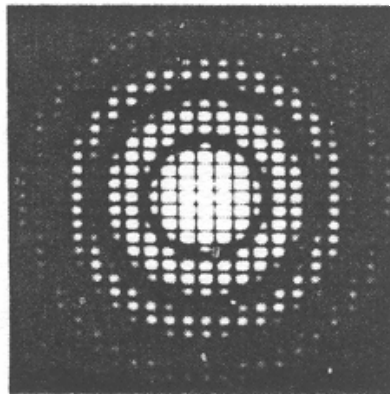
Vertical holes and nets of holes

(g)



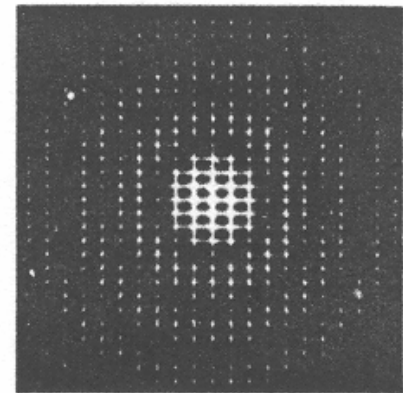
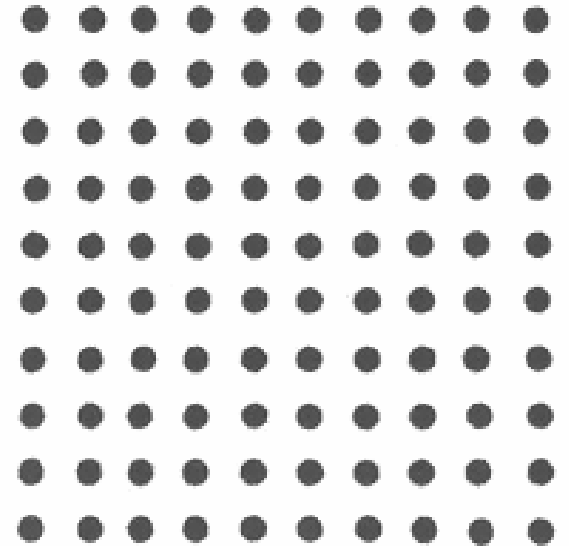
(g)

(h)



(h)

(i)



(i)



Back



Forward



Reload



Home



Search



Netscape



Print



Security



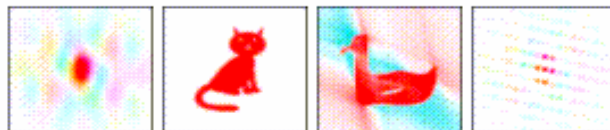
Shop



Stop



Kevin Cowtan's Book of Fourier



This is a book of pictorial 2-d Fourier Transforms. These are particularly relevant to my own field of *X-ray crystallography*, but should be of interest to anyone involved in signal processing or frequency domain calculations.

Contents:

<http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html>

- [Introduction](#)
- [Book of Crystallography](#)
- [Duck Tales](#) and missing data.
- [A little Animal Magic](#) and cross phasing.
- [A Tail of Two Cats](#) and image restoration.
- [Animal Liberation](#) and free-sets.

- [The Gallery](#). Other interesting pictures.

Other topics:

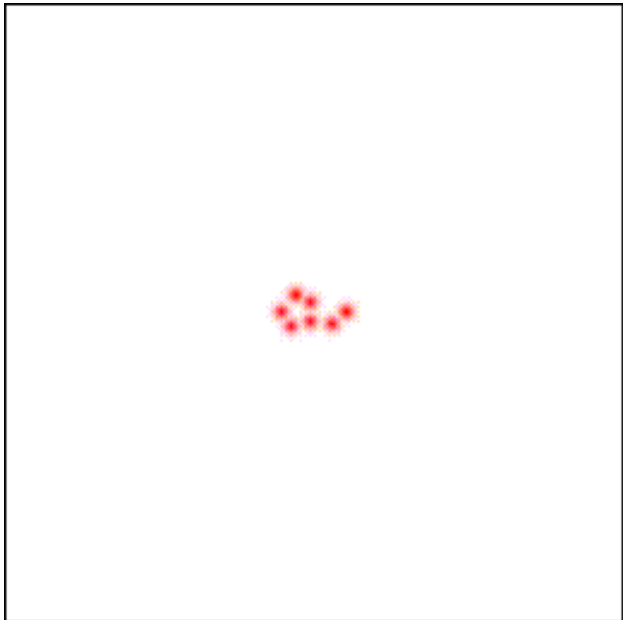
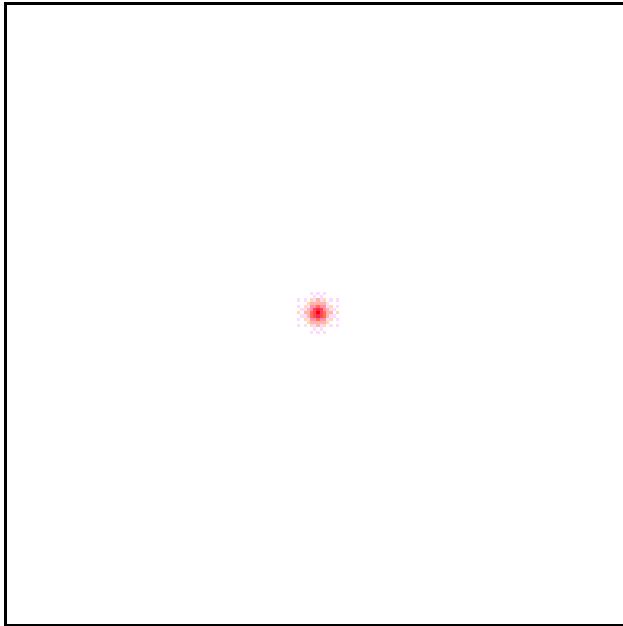
[The Interactive Structure Factor Tutorial](#): Learn about structure factors and maps.

An introduction to crystallographic [Fourier transforms](#). The mathematical link between [Scattering theory](#) and Fourier theory. An explanation of the [convolution theorem](#).

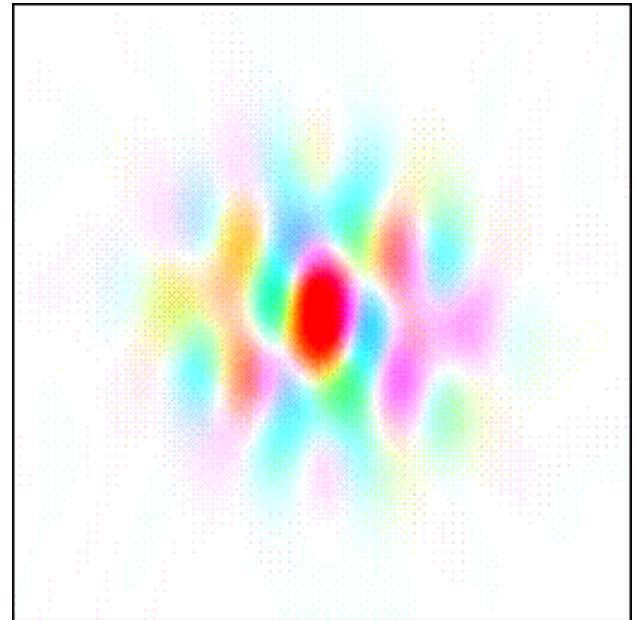
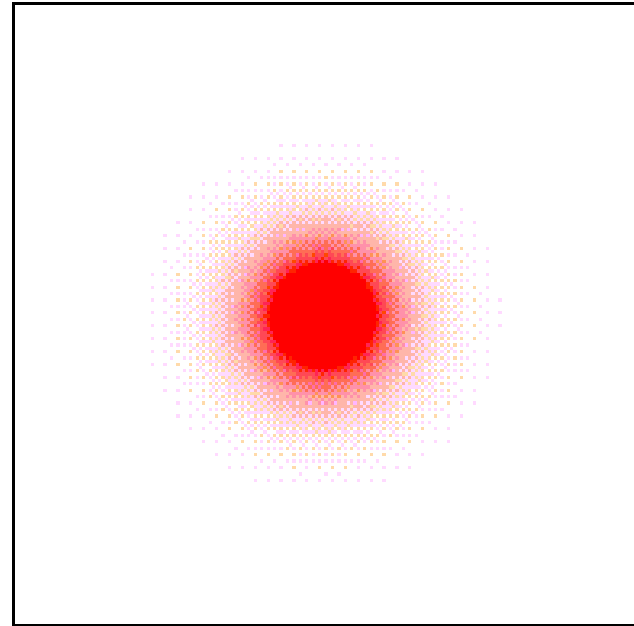
Teaching materials elsewhere



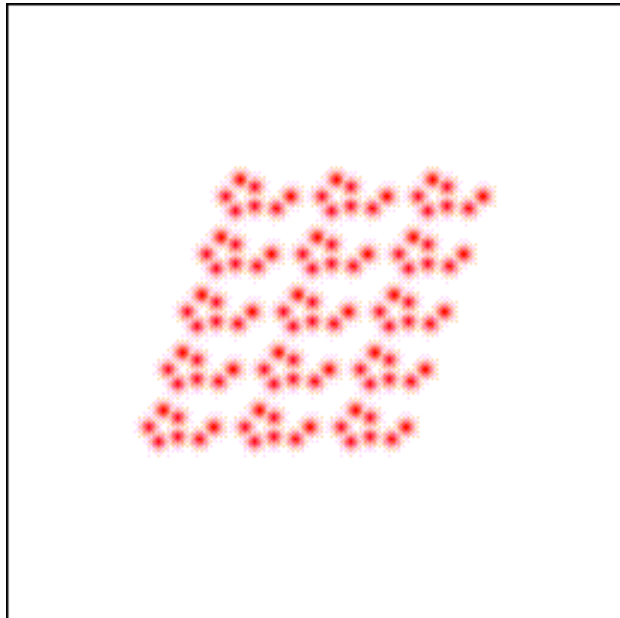
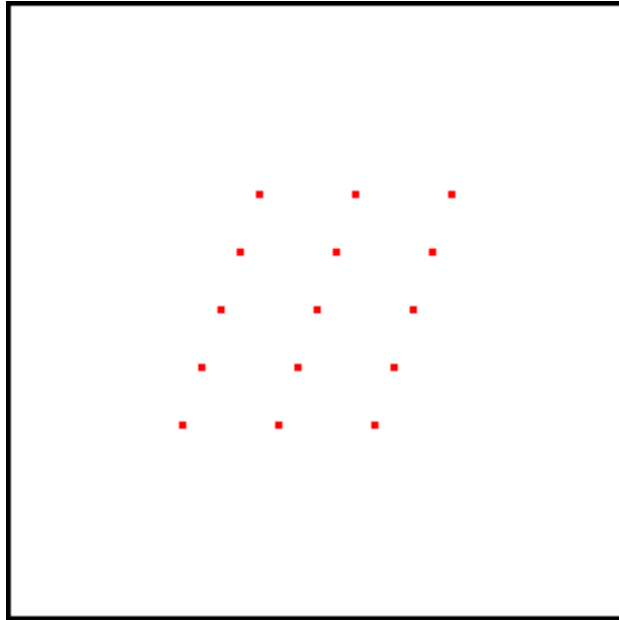
Object / Real Space



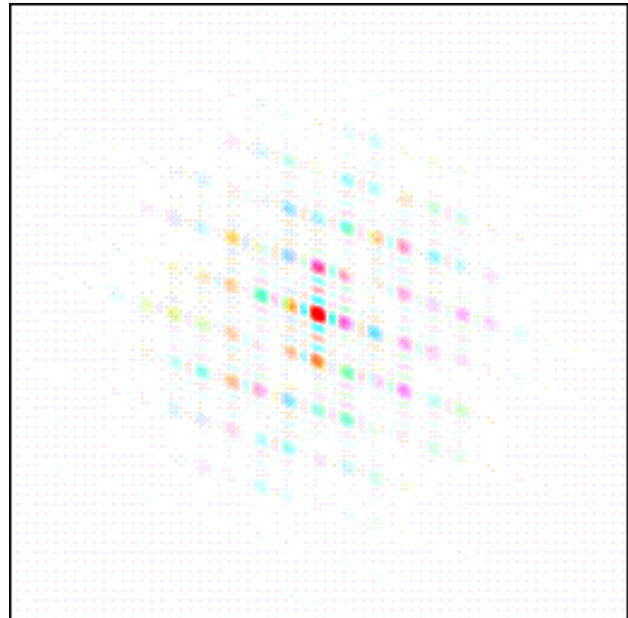
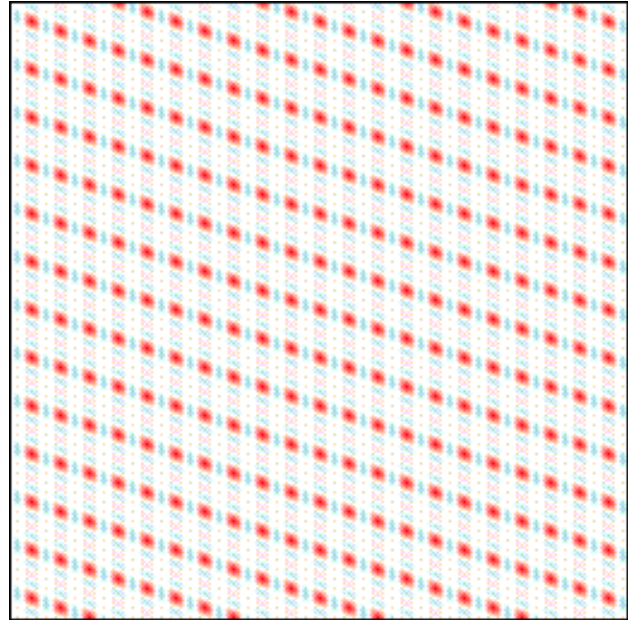
Transform / Reciprocal Space



Object / Real Space



Transform / Reciprocal Space

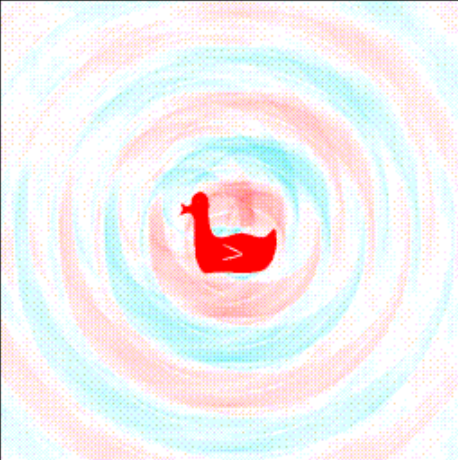
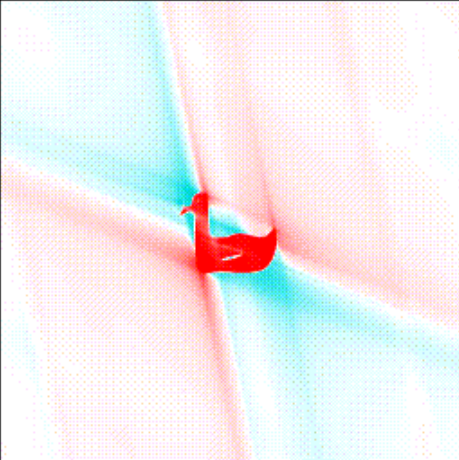
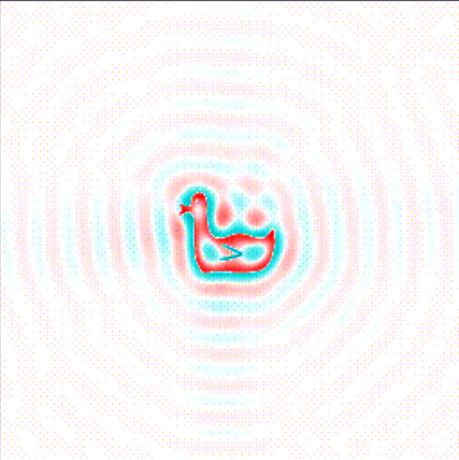
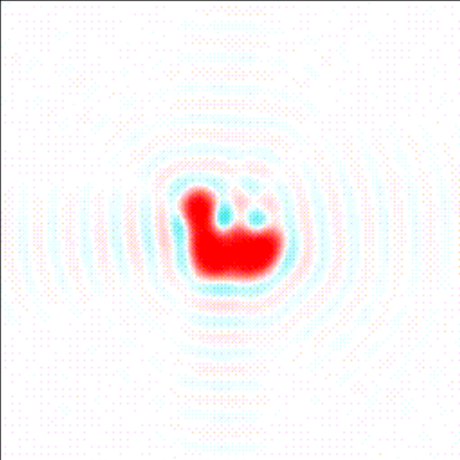
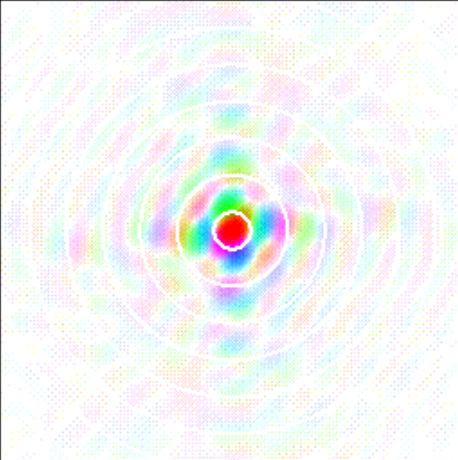
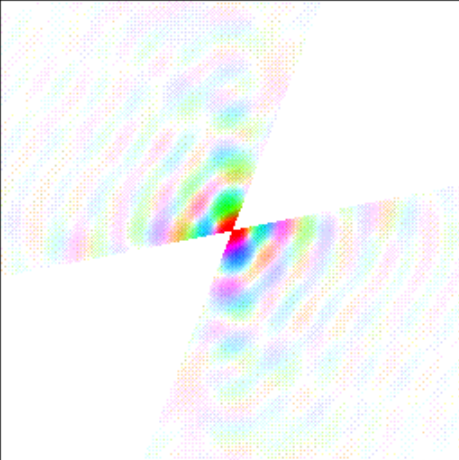
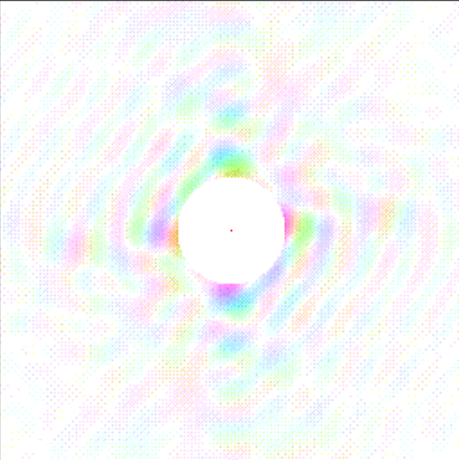
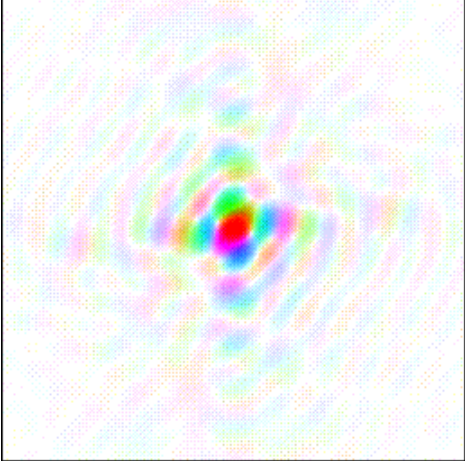


Objects – Transforms and Image Formation

A Duck



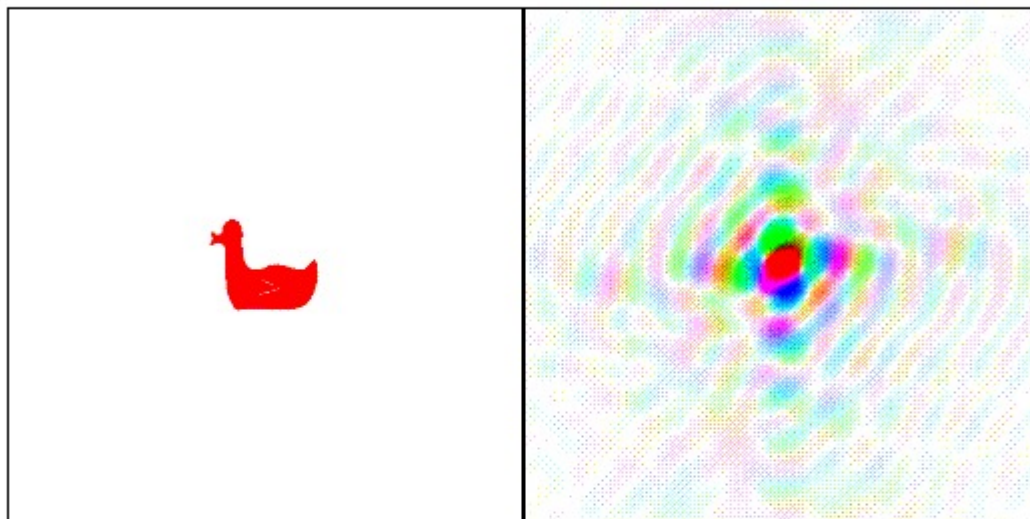
Transform
of a Duck



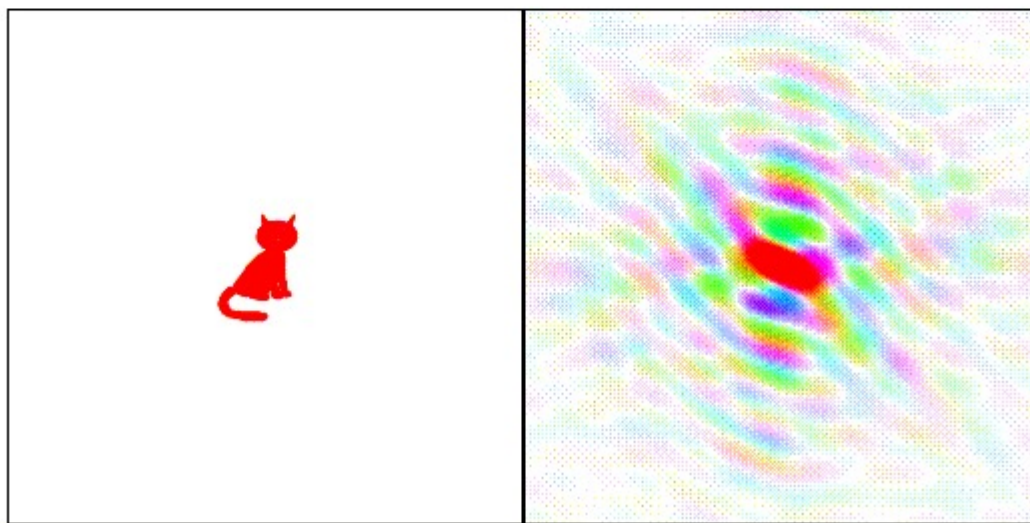
Kevin Cowtan's Book of Fourier

<http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html>

Here is our old friend; the Fourier Duck, and his Fourier transform:



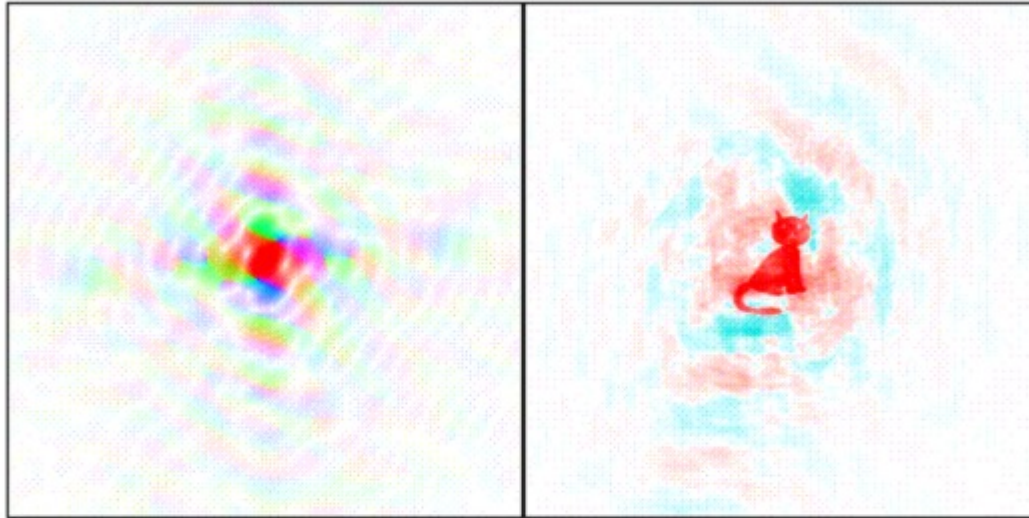
And here is a new friend; the Fourier Cat and *his* Fourier transform:



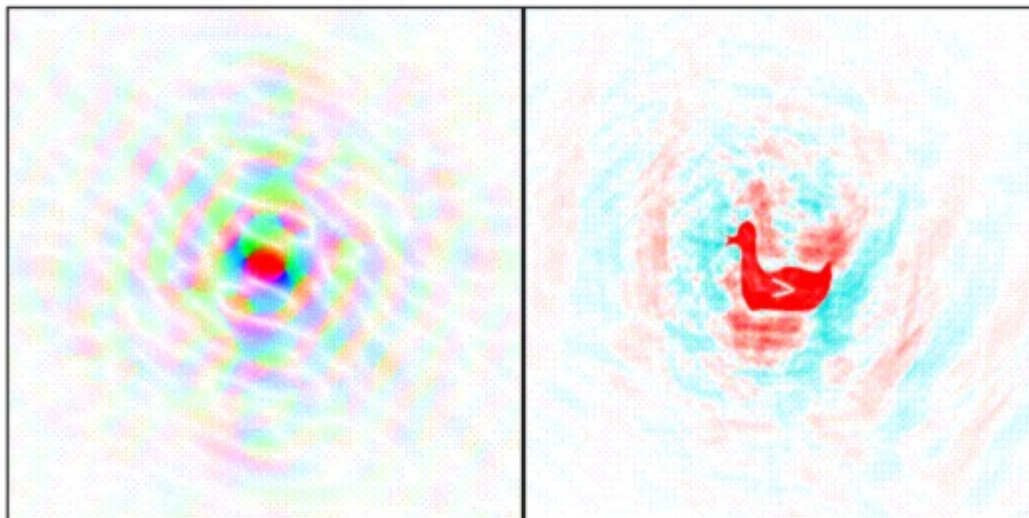
Kevin Cowtan's Book of Fourier

<http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html>

Duck Transform Amplitudes + Cat Phases

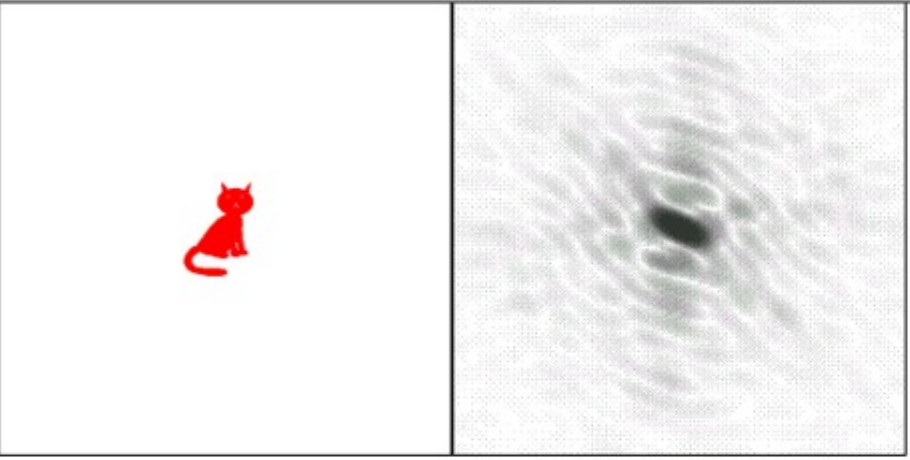


Cat Transform Amplitudes + Duck Phases

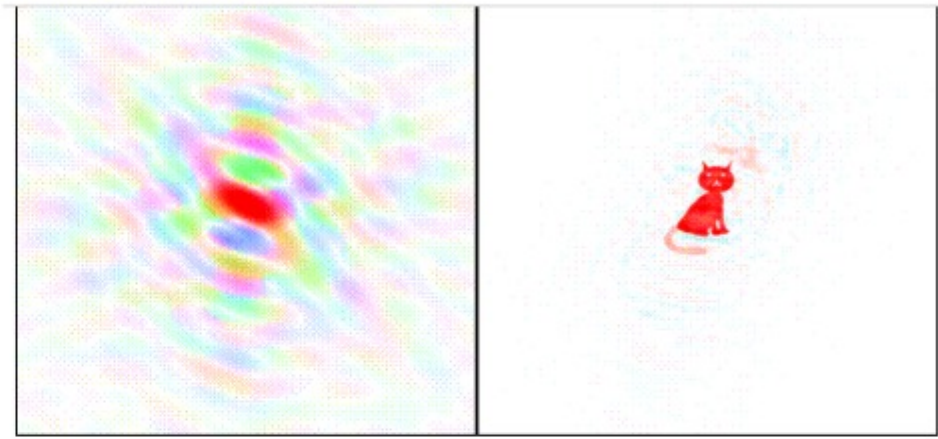


Kevin Cowtan's Book of Fourier

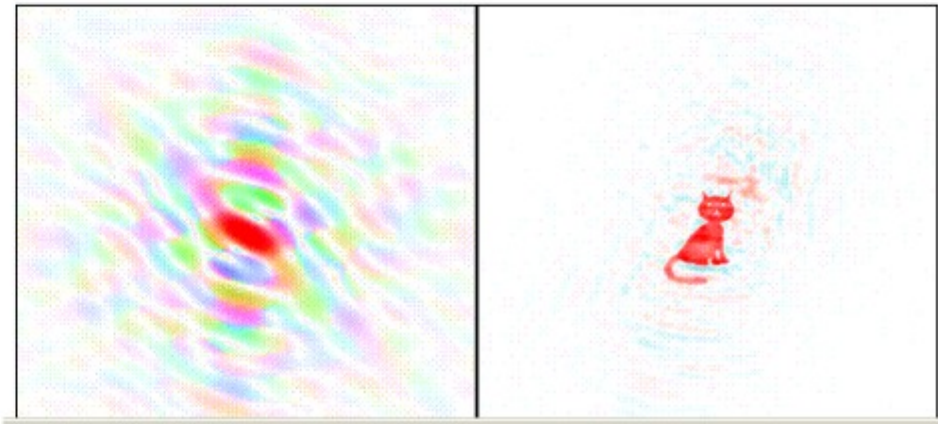
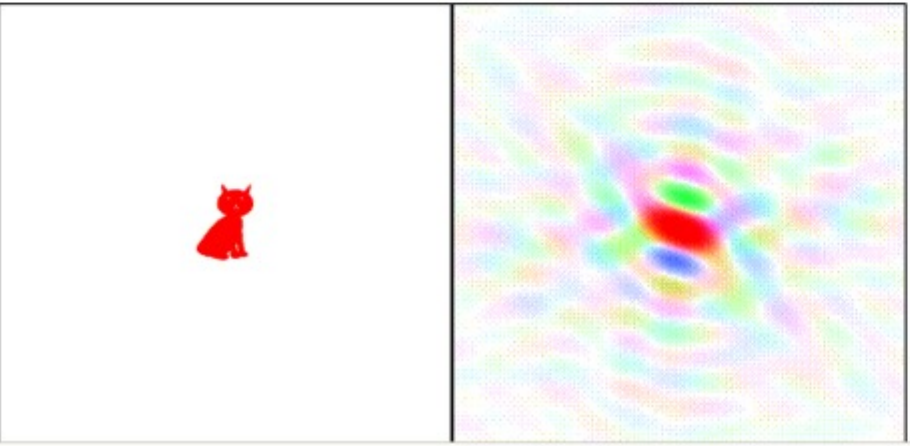
<http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html>



a) Cat - Cat Transform (Amplitudes only)
b) Manx (tailless) Cat - Manx Transform



c) Cat Amplitudes + Manx Phases
d) $[2x(\text{Cat Amplitudes}) - \text{Manx Amplitudes}] + \text{Manx Phases}$



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