

Coherent x-rays: overview

by

Malcolm Howells

Lecture 1 of the series

COHERENT X-RAYS AND THEIR APPLICATIONS

A series of tutorial–level lectures edited by Malcolm Howells*

*ESRF Experiments Division

CONTENTS

Introduction to the series

Books

History

The idea of coherence - temporal, spatial

Young's slit experiment

Coherent experiment design

Coherent optics

The diffraction integral

Linear systems - convolution

Wave propagation and passage through a transparency

Optical propagators - examples

Future lectures:

1. Today
2. Quantitative coherence and application to x-ray beam lines (MRH)
3. Optical components for coherent x-ray beams (A. Snigirev)
4. Coherence and x-ray microscopes (MRH)
5. Phase contrast and imaging in 2D and 3D (P. Cloetens)
6. Scanning transmission x-ray microscopy: principles and applications (J. Susini)
7. Coherent x-ray diffraction imaging: history, principles, techniques and limitations (MRH)
8. X-ray photon correlation spectroscopy (A. Madsen)
9. Coherent x-ray diffraction imaging and other coherence techniques: current achievements, future projections (MRH)

COHERENT X-RAYS AND THEIR APPLICATIONS

A series of tutorial–level lectures edited by Malcolm Howells*

Mondays 5.00 pm in the Auditorium except where otherwise stated

1. **Coherent x-rays: overview (Malcolm Howells) (April 7) (5.30 pm)**
2. **Coherence theory: application to x-ray beam lines (Malcolm Howells) (April 21)**
3. **Optical components for coherent x-ray beams (Anatoli Snigirev) (April 28)**
4. **Coherence and x-ray microscopes (Malcolm Howells) (May 26) (CTRL room)**
5. **Coherence activities at the ESRF: phase-contrast x-ray imaging in two and three dimensions (Peter Cloetens) (June 2) (Room 500)**
6. **Coherence activities at the ESRF: Scanning transmission x-ray microscopy (Jean Susini) (June 9)**
7. **Coherent X-ray diffraction imaging (CXDI): principles, history, current practices and radiation damage (Malcolm Howells) (June 23)**
8. **X-ray photon correlation spectroscopy (Anders Madsen) (June 30)**
9. **Summary of present achievements and future projections in CXDI and other coherence techniques (Malcolm Howells) (July 7)**

GENERAL INTRODUCTION

- In the future the ESRF scientific program will make increasing use of the coherence properties of the x-ray beams
- I have been asked to organize a program of lectures that will provide explanations and information about coherence experiments to a wide cross section of the ESRF scientific and technical community
- The concepts of coherence theory come from physics and engineering but I and the other speakers will do our best to make them accessible to people from outside these disciplines
- The treatment I give will not involve quantum theory
- To help people who wish to dig deeper or have reference information available we will:
 - Provide a recommended reading list of well written reference books and will urge the library to keep both loan and reference copies of them
 - Make computer files of all of the talks available at <http://www.esrf.fr/events/announcements/Tutorials>
 - Make background information such as full text of proofs of some formulas, hard-to-find references, published work by the speakers etc available for download at <http://intranet.esrf.fr/events/announcements/tutorials>
 - Provide (at the same website) EndNote files of citations for the book list and other references
- Later in this session I will give some information about the other talks of the series
- This is meant to be informal so please raise questions or comments at any time

BOOK LIST (alphabetical order)

Born, M. and E. Wolf (1980). Principles of Optics. Oxford, Pergamon.

THE optics text book, Chapter 10 is the classical exposition of coherence theory

Bracewell, R. N. (1978). The Fourier Transform and its applications. New York, McGraw-Hill.

Insightful but still easy to read

Collier, R. J., C. B. Burckhardt, et al. (1971). Optical Holography, Academic Press, New York.

Outstandingly well written, still the best holography book and there are many others

Goodman, J. W. (1968). Introduction to Fourier Optics. San Francisco, McGraw Hill.

Still the best in a widening field

Goodman, J. W. (1985). Statistical Optics. New York, Wiley.

Written with thought and care - indispensable in coherence studies

Hawkes, P. W. and J. C. H. Spence, Eds. (2007). Science of Microscopy (2 vols). Berlin, Springer.

I am not unbiased but I think this is a unique and outstanding coverage of a wide field by many of the best practitioners

Mandel, L. and E. Wolf (1995). Optical Coherence and Quantum Optics. Cambridge, Cambridge University Press.

Another unique effort - it seems, and is, formidable but chapters 1- 9 (the non-quantum part of interest to us) are no more difficult to read than Born and Wolf!

Paganin, D. (2006). Coherent X-ray Optics. Oxford, Oxford University Press.

A new contribution - still evaluating but it looks good

Stark, H., Ed. (1987). Image Recovery: Theory and Application. Orlando, Academic Press.

An excellent collection of articles - no longer new but it has not been superseded by anything else

ESRF Lecture Series on Coherent X-rays and their Applications, Lecture 1, Malcolm Howells

HISTORY OF COHERENCE THEORY



Author	Year	Citation	Comment
E. Verdet	1869	Ann. Scientif. l'Ecole Supérieure, 2 , 291	Qualitative assessment of coherence volume due to an extended source
M. von Laue	1907	Ann. D. Physik, (4), 2 , 1, 795	Introduced correlations for study of the thermodynamics of light
van Cittert	1934	Physica, 1 , 201	First calculation of correlations due to an extended source
F. Zernike	1938	Phisica, 5 , 785	Used correlations to define a <i>measurable</i> "degree of coherence" thus launching modern coherence theory
P. M. Duffieux	1946	L'intégral de Fourier et ses Application à l'optique, Rennes	Application of linear system and Fourier methods to optics
H. H. Hopkins	1951	Proc. Roy. Soc. A, 208 , 263	Application coherence theory to image formation and resolution
K. Miyamoto	1961	Progress in Optics, 1 , E. Wolf (ed), 41	Application of linear system and Fourier methods to optics

WHAT ARE THE COHERENCE EXPERIMENTS ALREADY GOING ON AT SYNCHROTRONS?

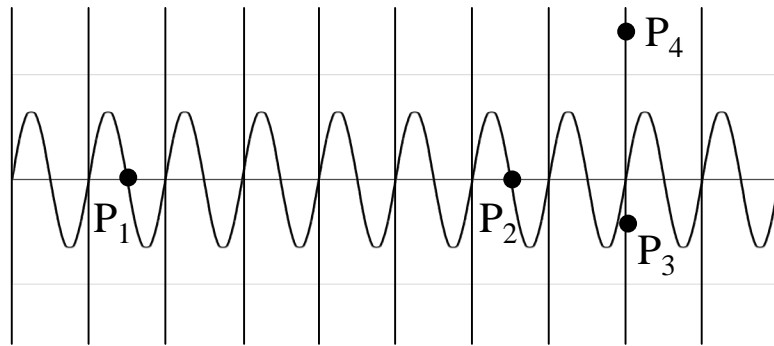


- **Scanning transmission x-ray microscopy (STXM)**
Coherent illumination required for diffraction-limited resolution but images are NOT coherent!
About 15 instruments world wide
- **X-ray holography**
Many interesting variants and demonstrations since 1972 but only the ESRF scheme has been used in scientific investigations
- **Coherent x-ray diffraction imaging**
Five synchrotron labs now including ESRF and growing
- **Phase-contrast imaging**
Phase contrast always involves some degree of coherence we will discuss how much later
- **X-ray photon correlation spectroscopy**
Two dedicated beam lines now - expected to double or triple in the next few years
- **New and specialized**
Ptychography, magnetism...

THE BASIC IDEAS OF COHERENCE

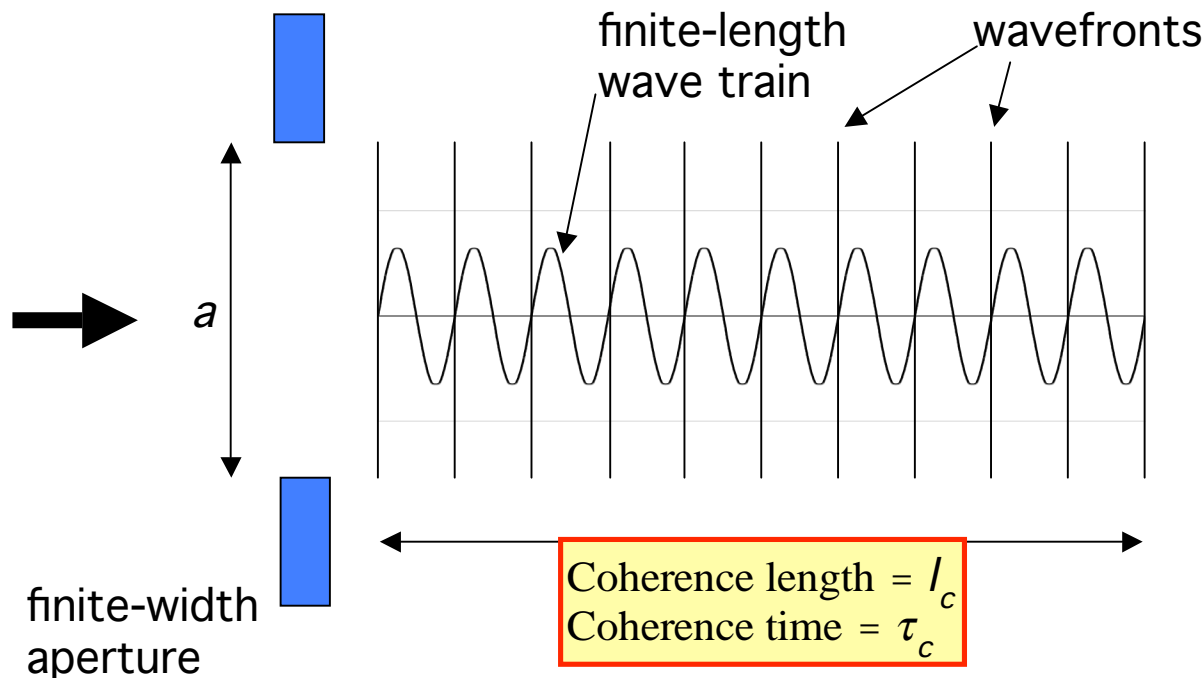
- *Optical coherence exists in a given radiating region if the phase differences between all pairs of points in that region have definite values which are constant with time*
- *The sign of good coherence is the ability to form interference fringes of good contrast*
- There are two types of coherence to specify:
 - Temporal or longitudinal coherence
Considers the phase at longitudinally separated pairs of points - $\Delta\Phi(P_1:P_2)$
 - Spatial or transverse coherence
Considers the phase at transversely separated pairs of points - $\Delta\Phi(P_3:P_4)$

- Temporal coherence is determined by monochromaticity
- Spatial coherence is determined by collimation



Note that the wave train duration at any point is usually much less than the illumination time (even if the latter is only one ESRF pulse)

TEMPORAL COHERENCE COMES FROM THE LENGTH OF THE WAVE TRAIN WHICH COMES FROM MONOCHROMATICITY



Wave train properties:

$$c = v\lambda$$

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta v}{v} = \frac{\Delta E}{E} \approx \frac{1}{N}$$

$$l_c = N\lambda = \frac{\lambda^2}{\Delta\lambda}$$

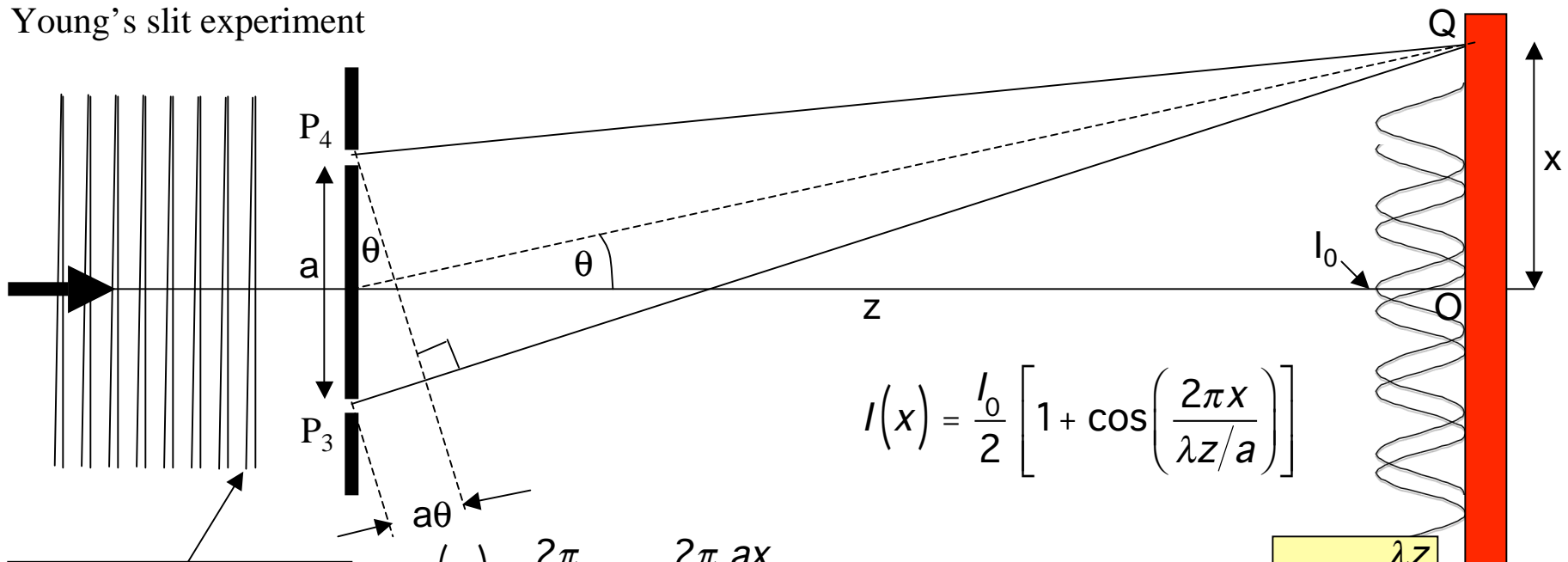
Using distance=velocity \times time

$$\tau_c = \frac{l_c}{c} = \frac{\lambda^2}{v \Delta\lambda} = \frac{1}{\Delta v}$$

- If a and $l_c \rightarrow \infty$ we have an ideal monochromatic plane wave - always perfectly coherent
- Our wave train has a limited length ($N=10$ periods) - as produced by a 10-period undulator for example - thus it has length $l_c = \lambda^2/\Delta\lambda$ and time duration $\tau_c = 1/\Delta v$ as shown above
- So we have defined the coherence length and coherence time l_c and τ_c of the wave packet
- Now suppose that $\Delta\lambda/\lambda = 10^{-4}$, $\lambda = 1 \text{ \AA}$ - then $l_c \approx 1 \mu\text{m}$, $\tau_c \approx 3 \text{ fs}$
- Compare this to $l_{\text{ESRF pulse}} \approx 15 \text{ mm (FWHM)}$, $\tau_{\text{ESRF pulse}} \approx 50 \text{ ps (FWHM)}$

A FINITE COHERENCE WIDTH IS A CONSEQUENCE OF IMPERFECT COLLIMATION

Young's slit experiment



$$I(x) = \frac{I_0}{2} \left[1 + \cos\left(\frac{2\pi x}{\lambda z/a}\right) \right]$$

$$\Delta\phi(Q) = \frac{2\pi}{\lambda} a\theta = \frac{2\pi}{\lambda} \frac{ax}{z} \quad \text{set } \Delta\phi = 2\pi \Rightarrow \text{fringe period } \Delta x = \frac{\lambda z}{a}$$

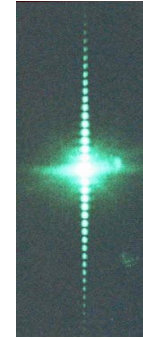
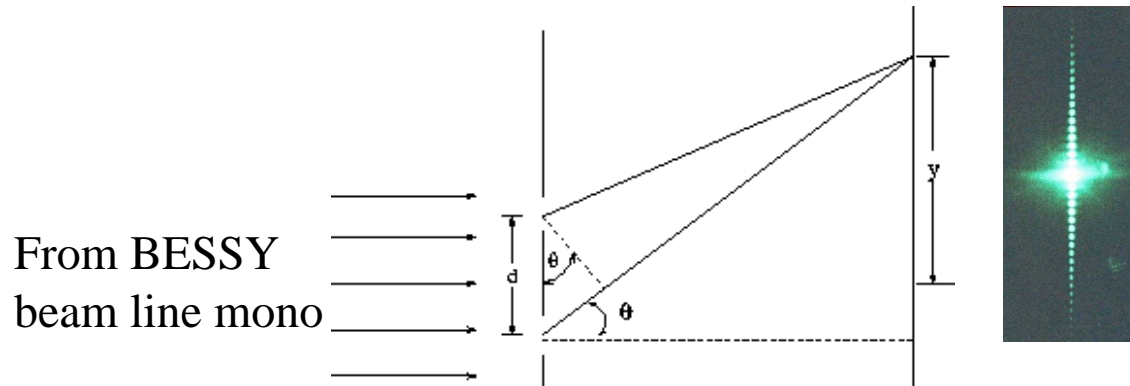
Second wave tilted by $\epsilon = \lambda/(4a)$ giving an additional path lag of $\lambda/4$ of the signal from P_3 relative to that from P_4

Conclusions:

- Tilted wave shows the effect of imperfect collimation - the $\lambda/4$ path lag reduces the contrast of the fringes somewhat but does not destroy them - so this gives a rough guide to the collimation needed for coherence experiments - we give a more exact one later
- Beam angular spread is often given by the angular subtense of the effective source
- The coherence width is thus the maximum transverse spacing of a pair of points from which the light signals can interfere to give fringes of "reasonable" contrast

- If the beam spread FULL angle is A then the coherence width is given by $aA \cong \lambda/2$

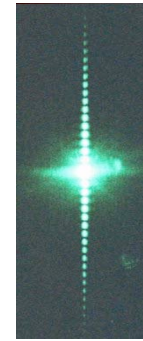
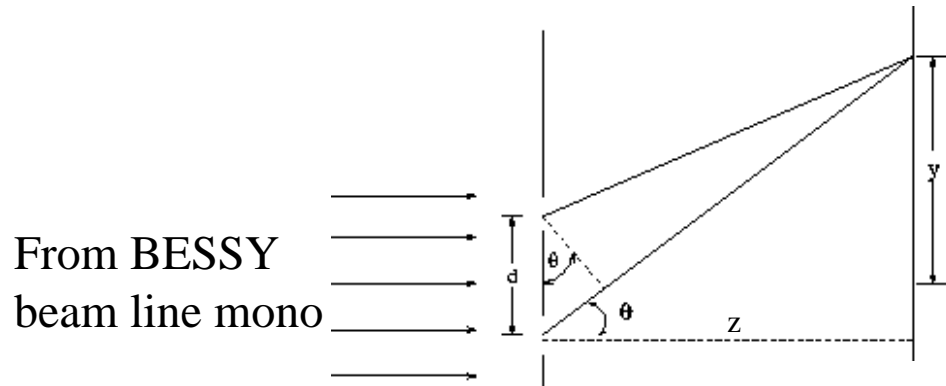
Young's double slit experiment with synchrotron x-rays



W. Leitenberger *et al.*
Physica B 336, 36 (2003)

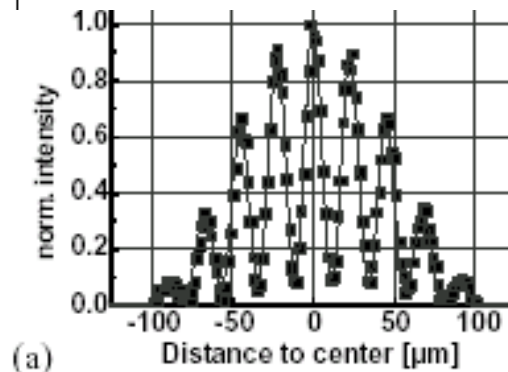
- With coherent illumination we expect to see interference fringes
- What are the requirements to see fringes?
 - The diffraction patterns of the slits must overlap - consequence for failing; get fringes only in the overlap region
 - The coherence width must be greater than d so that the two slits are coherently illuminated - consequence for failing; reduced fringe contrast
 - The coherence length must be greater than the path difference between the interfering rays - consequence for failing; number of fringes limited to the monochromaticity $\lambda/(\Delta\lambda)$
- Synchrotron beams from a monochromator usually do not limit the number of fringes but in using a pink beam, for example to make a hologram, this could happen

Young's double slit experiment with synchrotron x-rays

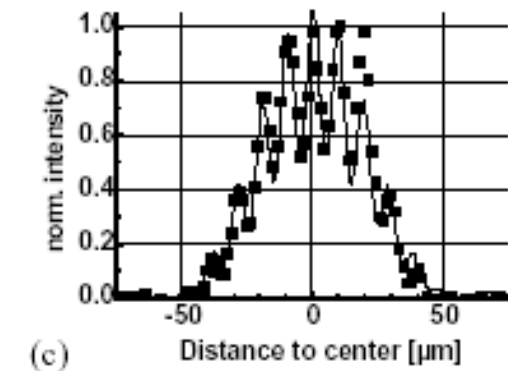
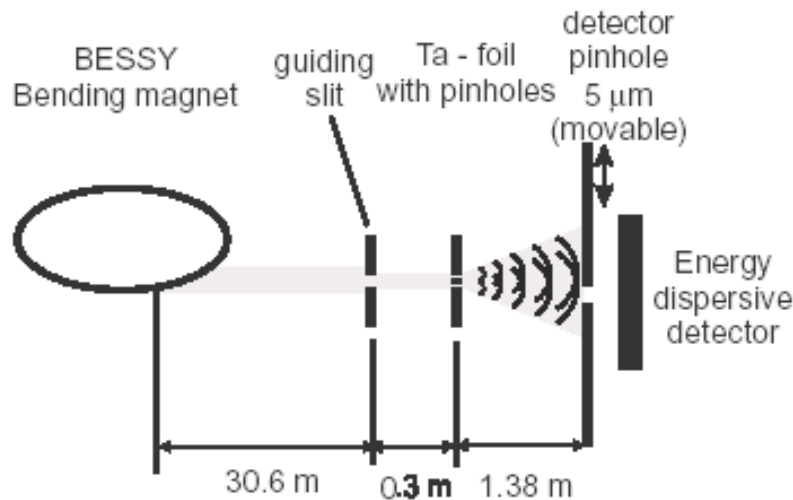


W. Leitenberger *et al.*
Physica B 336, 36 (2003)

Coherence width = $\lambda/(2\Delta)$



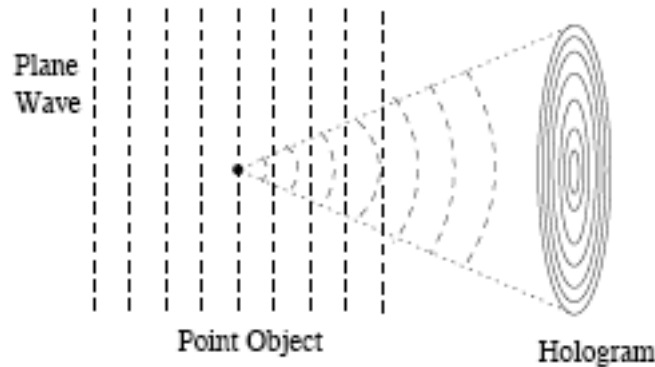
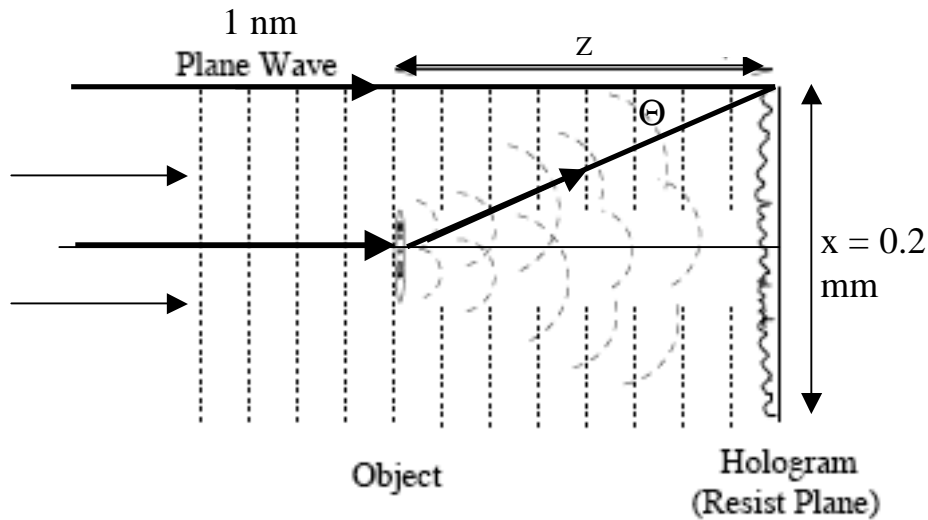
$\lambda=2.1\text{\AA}$, $d=11\mu\text{m}$
Visibility ~ 80%



$\lambda=0.9\text{\AA}$, $d=11\mu\text{m}$
Visibility ~ 30%
Coherence width
less in ratio to λ_s

Slides courtesy
of Anders Madsen

DESIGN STUDY FOR AN X-RAY GABOR HOLOGRAM



1. Suppose we want a resolution of 20 nm with a sample of size 20 μm
2. Fringe period (twice the zone plate outer zone width) must be 40 nm so $40 \text{ nm} = \lambda/\Theta$ or $\Theta = 25 \text{ mrad}$
3. From the diagram this gives $z = 20 \text{ mm}$
4. The maximum path difference between the interfering rays is

$$\left[\left(\frac{x}{2} \right)^2 + z^2 \right]^{1/2} - z \approx 1.2 \mu\text{m}$$
5. So a coherence length $> 1.2 \mu\text{m}$ is needed
6. Thus a monochromaticity $\lambda/\Delta\lambda$ of greater than $1.2 \mu\text{m}/1 \text{ nm} = 1200$ is required - OK
7. By looking at the object plane we conclude that a coherence width of 0.1 mm is required
8. This means collimation better than $5 \mu\text{r}$ is required - OK but we will need to lose some flux

$$\text{Fringe period} = \lambda/\Theta, \quad l_c = \lambda^2/(\Delta\lambda), \quad aA = \lambda/2$$

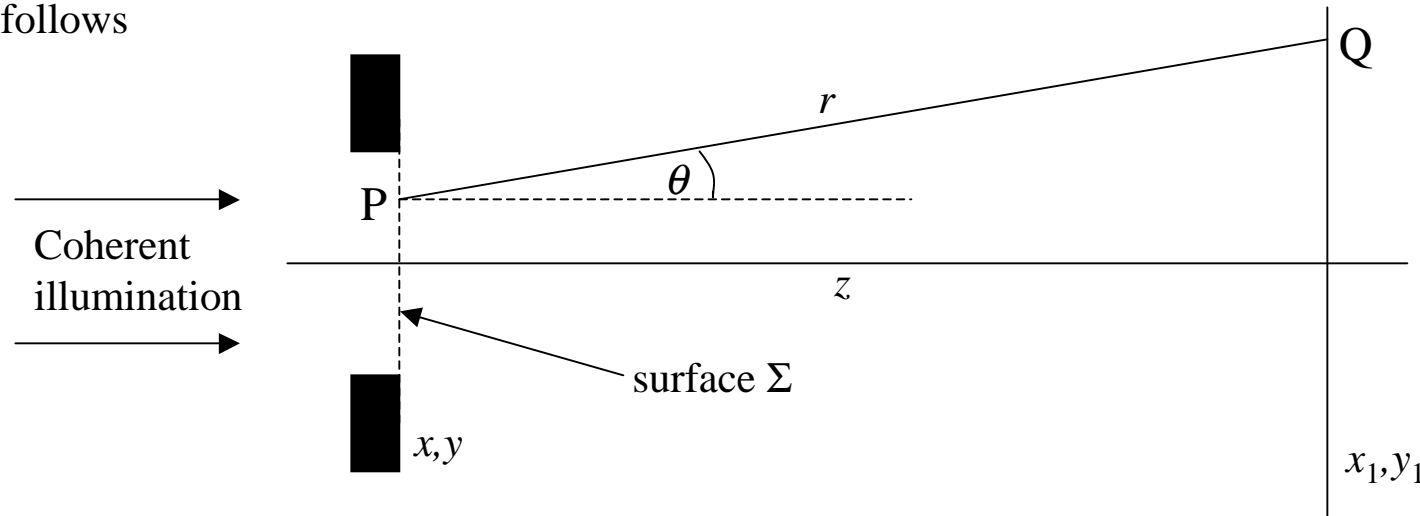
WHAT IS COHERENT OPTICS?

EARLIER WE SAID:

- *Optical coherence exists in a given radiating region if the phase difference between all pairs of points in that region has a definite value which is constant with time*
- *The sign of good coherence is the ability to form interference fringes of good contrast*
- Now suppose that a set of points P_i in some region radiates signals coherently in the above sense. This implies that the detected x-ray intensity at some given point Q can be found by adding together the (appropriately delayed) complex amplitudes of the signals radiated from the points P_i
- Thus the intensity at Q is given by the COHERENT SUM $I_Q = \left| \sum_i u_i \right|^2$ *where u_i are the arriving complex amplitudes*
- Note that the complex amplitudes of the signals are summed first. After that the square modulus is taken. This is the essence of coherent optics
- If the points P_i radiated signals with a random phase relationship then the intensity would be given by the INCOHERENT SUM $I_Q = \sum_i |u_i|^2$
- When wave *amplitudes* are added in a coherent sum it is possible for them to either reinforce or cancel. Thus it is possible for a coherent sum to lead to interference fringes.
- On the other hand the wave *intensities* that are added in an incoherent sum are always positive and can never cancel. Thus an incoherent sum can never lead to fringes
- Coherent optics has become extremely important since the invention of the laser

THE DIFFRACTION INTEGRAL

We are especially interested in diffraction by a transparency distribution in a plane screen. In this case the discrete source points P_i can be replaced by small elements of the surface area and the intensity can be calculated by an integral known as the RAYLEIGH-SOMMERFELD DIFFRACTION INTEGRAL as follows



So what is the coherence condition?

$$I_Q(x_1, y_1) = |u_Q|^2 = \left| \frac{1}{i\lambda} \int_{\Sigma} u_P(x, y) \frac{e^{ikr} \cos \theta}{r} ds \right|^2$$

See Goodman 1968, equation 3-26 for an excellent treatment

ds is an area element of the surface in the open aperture Σ in the otherwise opaque screen. u_P and u_Q are the complex amplitudes at the typical points P and Q and $k_0 = 2\pi/\lambda$.

RECASTING THE DIFFRACTION INTEGRAL FOR OUR APPLICATIONS



$$I_Q(x_1, y_1) = |u_Q|^2 = \left| \frac{1}{i\lambda} \int_{\Sigma} u_P(x, y) \frac{e^{ikr} \cos \theta}{r} ds \right|^2$$

Approximations:

1. We assume that the diffracting object can be represented by a planar complex-transparency function $t(x, y)$ [Goodman 1985, para 7.1.1] - for hard x-ray experiments with a monochromator this is often valid - thus for illumination of the object by a wave $u_P(x, y)$ the exit wave is $u_P(x, y)t(x, y)$
2. θ is small so $\cos(\theta) \approx 1$
3. r in the denominator can be replaced by the constant z and taken outside the integral
4. r in the exponent can be replaced by the following binomial approximation

$$r = \sqrt{z^2 + (x_1 - x)^2 + (y_1 - y)^2} \approx z \left\{ 1 + \frac{1}{2} \left(\frac{x_1 - x}{z} \right)^2 + \frac{1}{2} \left(\frac{y_1 - y}{z} \right)^2 + \dots \right\}$$

This is known as the Fresnel approximation. The diffraction integral thus becomes

$$I_Q(x_1, y_1) = |u_Q|^2 = \left| \frac{1}{i\lambda z} \int_{-\infty}^{+\infty} u_P(x, y) t(x, y) e^{\frac{i\pi}{\lambda z} [(x_1 - x)^2 + (y_1 - y)^2]} dx dy \right|^2 \quad [\text{Goodman 1968 equation 4-10}]$$

Comments:

1. The Fresnel approximation apparently includes focusing but not aberrations ("high-school optics") - however its validity is much wider than that suggests
2. Our latest form of the diffraction integral is a *convolution* integral which we will explore shortly

THE FRAUNHOFER APPROXIMATION

(the diffraction pattern of the object is its Fourier transform)

$$I_Q(x_1, y_1) = |u_Q|^2 = \left| \frac{1}{i\lambda z} \int_{-\infty}^{+\infty} u_P(x, y) t(x, y) e^{\frac{i\pi}{\lambda z} [(x_1-x)^2 + (y_1-y)^2]} dx dy \right|^2$$

Let's expand the squares in the exponent

$$I_Q(x_1, y_1) = \left| \frac{1}{i\lambda z} \underbrace{e^{\frac{i\pi}{\lambda z} [x_1^2 + y_1^2]}}_{\substack{\text{Disappears on} \\ \text{taking the square} \\ \text{modulus}}} \int_{-\infty}^{+\infty} \underbrace{u_P(x, y)}_{\substack{\text{Disappears if we} \\ \text{assume plane wave} \\ \text{illumination}}} t(x, y) \underbrace{e^{\frac{i\pi}{\lambda z} [x^2 + y^2]}}_{\substack{\text{Disappears under a} \\ \text{certain condition}}} e^{-\frac{2\pi i}{\lambda z} [x_1 x + y_1 y]} dx dy \right|^2$$

Disappears on
taking the square
modulus

Disappears if we
assume plane wave
illumination

Disappears under a
certain condition

$$I_Q(x_1, y_1) = \left| \frac{1}{i\lambda z} \int_{-\infty}^{+\infty} t(x, y) e^{-\frac{2\pi i}{\lambda z} [x_1 x + y_1 y]} dx dy \right|^2$$

Goodman 1968 equation 4-13

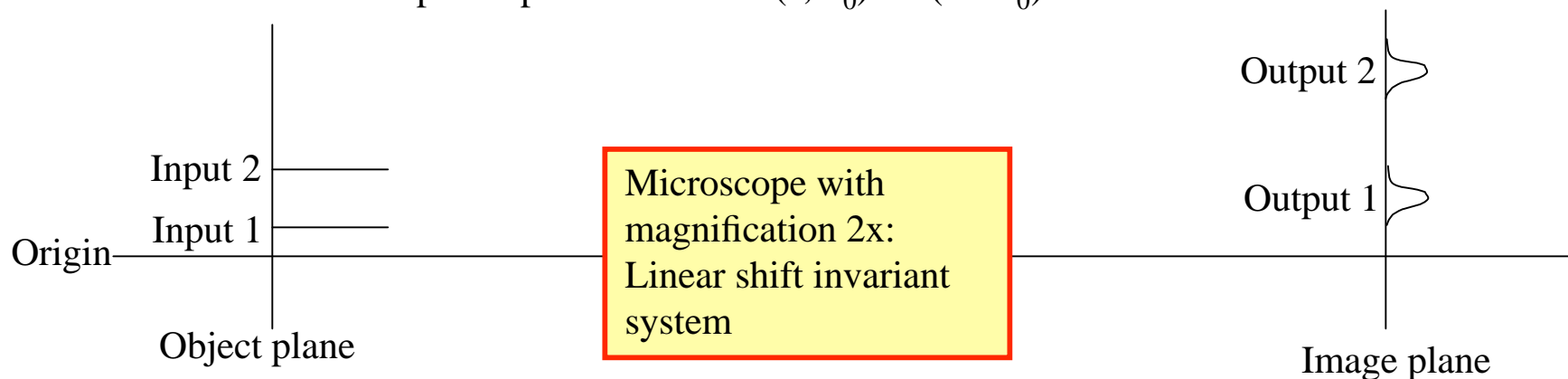
- The condition is called the *far-field* condition
- It is $\frac{\pi(x^2 + y^2)_{\max}}{\lambda z} \ll 1$
- If z is large enough to satisfy it, the detector provides a linear mapping of the diffraction angles with position
- When the condition is not satisfied then we have the *Fresnel* Transform

DIGRESSION ON LINEAR SYSTEMS

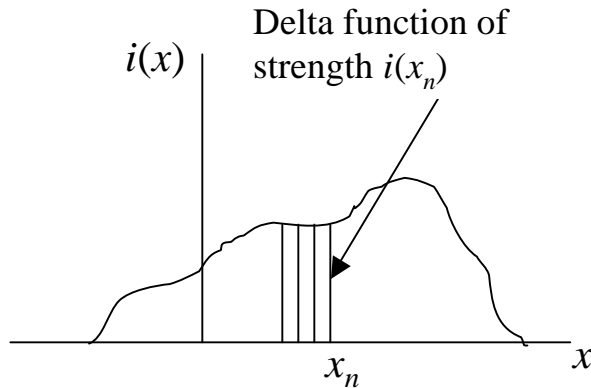
- Suppose an input signal $i(x)$ is acted on by an operator L producing an output signal $o(x)$

$$i(x) \rightarrow \boxed{L} \rightarrow o(x)$$

- If L changes $i_1 \rightarrow o_1$ and $i_2 \rightarrow o_2$, AND $ai_1 + bi_2 \rightarrow ao_1 + bo_2$ for all a and b , then L is *linear*
- Important special case: $i(x) = \delta(x - x_0) \rightarrow \boxed{L} \rightarrow o(x) = h(x, x_0)$
- $h(x; x_0)$ is the output $h(x)$ for a delta-function input at x_0 - it is variously known as Green's function, the impulse response or (in optics) the **point spread function** - for example it could be the response in the image plane of a microscope to a delta function input in the object plane at $x = x_0$
- Now suppose that when the delta function in the object plane shifts, the impulse response makes a corresponding shift but does *does not change shape*. We then say that the linear system represented by L is **shift invariant** and its point spread function $h(x; x_0) = h(x - x_0)$



CONVOLUTION



We can represent the input signal as a sum of many delta functions

$$i(x) \equiv \sum_n i(x_n) \delta(x - x_n) \rightarrow \boxed{\text{L}} \rightarrow \sum_n i(x_n) h(x - x_n)$$

We can represent the output signal as an integral

$$o(x) = \int_{-\infty}^{+\infty} i(x_0) h(x - x_0) dx_0 \quad \text{or}$$

$$o(x) \equiv i(x) * h(x)$$

The integral is known as a **convolution** and allows us to calculate the output signal of a linear shift-invariant system due to a given input signal when the point-spread function of the system is known. Using Capital letters to indicate a Fourier transform (FT), the **Convolution Theorem** states that if the last equation is true then

$$O(\xi) = I(\xi) H(\xi)$$

O, I - FT's of o and i
 ξ is the spatial frequency variable conjugate to x

H the **contrast transfer function** - the system response to a delta function in frequency i. e. to a sine wave input - H is the FT of h - Note the sine wave here is a *spatial* sine wave which might be a special test sample in the object plane of a microscope.

WHY ARE SINE WAVES SO IMPORTANT

Suppose that the input to a shift-invariant linear system is a sine wave of spatial frequency ξ_0 - then

$$i(x) = e^{2\pi i \xi_0 x}$$

$$o(x) = e^{2\pi i \xi_0 x} * h(x) \quad (\text{from the last slide})$$

$$O(v) = \delta(\xi - \xi_0) H(\xi) \quad (\text{by the Convolution theorem (last slide) plus FT}[\delta(\xi)] = 1, \text{ shift theorem}^*)$$

$$o(x) = FT^{-1}[\delta(\xi - \xi_0) H(\xi)] \quad (\text{by taking the inverse FT of both sides})$$

$$= \int_{-\infty}^{+\infty} \delta(\xi - \xi_0) H(\xi) e^{2\pi i \xi x} d\xi$$

$$= e^{2\pi i v_0 x} H(\xi_0) \quad (\text{by the sifting property of the delta function})$$

$$= i(x) H(\xi_0)$$

Thus we could write this in normal operator notation as

$$L i(x) = i(x) H(\xi_0)$$

In other words the action of a linear operator on a sine wave is to produce another sine wave of the *same* frequency multiplied by a constant ($H(\xi_0)$). Therefore the sine waves are eigenfunctions of *any* linear operator and have eigenvalue equal to the $H(\xi_0)$ value corresponding to that operator

*The shift theorem of the Fourier transform: see [Goodman 1968] p277, [Bracewell 1978] p121 for the forward transform. For the inverse transform (used here) the theorem is the same except the sign of the exponent in the exponential is reversed

RULES OF COHERENT FOURIER OPTICS IN THE SPATIAL DOMAIN



$$I_Q(x_1, y_1) = |u_Q|^2 = \left| \frac{1}{i\lambda z} \int_{-\infty}^{+\infty} u_P(x, y) t(x, y) e^{\frac{i\pi}{\lambda z} [(x_1-x)^2 + (y_1-y)^2]} dx dy \right|^2$$

Returning to the diffraction integral in the Fresnel approximation we see that it can be written as a convolution of the input wave field with the **point spread function** (x, y are now dummy variables)

$$I_Q(x_1, y_1) = \left| u_P(x, y) t(x, y) * \frac{1}{i\lambda z} e^{\frac{i\pi}{\lambda z} [x^2 + y^2]} \right|_{x_1, y_1}^2$$

We see that the general rules of Coherent Fourier optics in the spatial domain are as follows:

$u_Q(x_1, y_1) = u_P(x, y) t(x, y) * \frac{1}{i\lambda z} e^{\frac{i\pi}{\lambda z} [x^2 + y^2]} \Big _{x_1, y_1}$	PROPAGATION IN FREE SPACE
$u_{\text{EXIT}}(x, y) = u_P(x, y) t(x, y)$	PASSAGE THROUGH A TRANSPARENCY

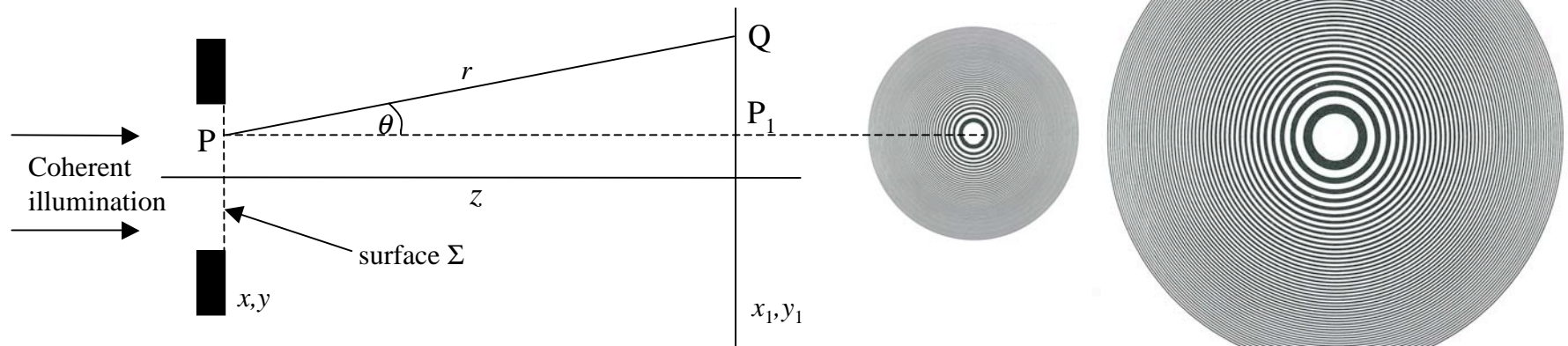
- Note that for propagation $u_P(x, y) t(x, y)$ is the input, $u_Q(x, y)$ is the output and the point spread function is

$$\frac{1}{i\lambda z} e^{\frac{i\pi}{\lambda z} [x_1^2 + y_1^2]}$$

- We can see this from the above by imagining that the input is a delta function at the origin

WHAT HAPPENS PHYSICALLY WHEN A COHERENT DIFFRACTION PATTERN IS FORMED?

Signal at points Q due to the area element at P = $u(x_P, y_P) t(x_P, y_P) \frac{1}{i\lambda z} e^{\frac{i\pi}{\lambda z} [(x_P - x_Q)^2 + (y_P - y_Q)^2]}$



- The complex amplitude of the signal at Q due to the area element at P is the value of the point spread function centered on P₁.
- It's phase relative to the phase at P is constant with time
- In the diagram one should count the black zones to be + and white ones to be – (they are Fresnel's half-period zones)
- Most of the energy from P is delivered near to P₁ which is the point of minimum phase for signals from P
- The resultant signal at Q is formed by adding vectorially the signals from all the area elements in Σ - it is then squared to give the intensity which is detected

$r_n^2 = n\lambda z$
zone-plate pattern
magnified

RULES OF COHERENT FOURIER OPTICS IN THE SPATIAL FREQUENCY DOMAIN

By applying the Convolution theorem to "the rules of coherent Fourier optics in the spatial domain" we obtain the corresponding rules in the spatial frequency domain

$$U_{z=z}(\xi, \eta) = U_{z=0}(\xi, \eta) e^{-i\pi\lambda z[\xi^2 + \eta^2]}$$

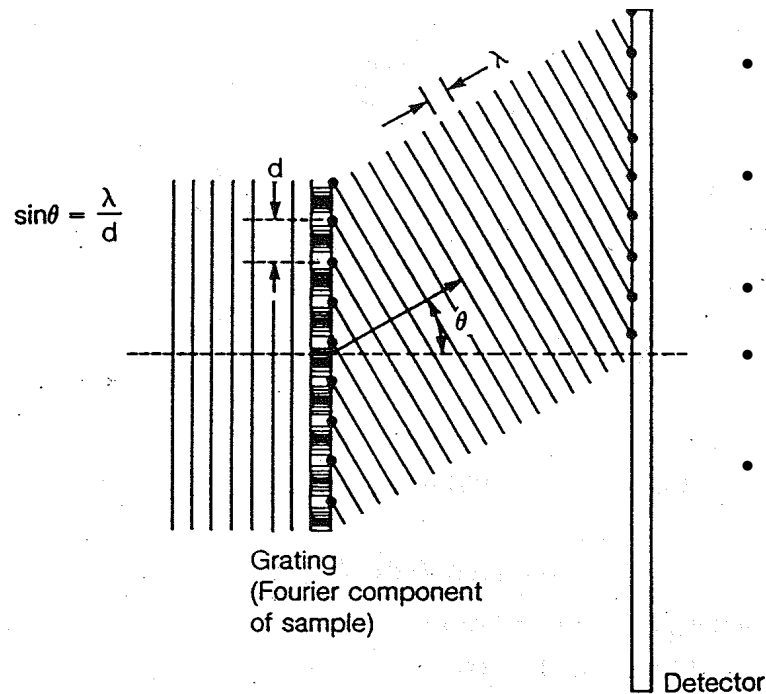
PROPAGATION IN FREE SPACE

(note that the transfer function is a pure phase factor)

$$U_{\text{OUT}}(\xi, \eta) = U_{\text{IN}}(\xi, \eta) * T(\xi, \eta)$$

PASSAGE THROUGH A TRANSPARENCY

ξ is the spatial frequency corresponding to x - it is expressed in cycles per distance unit where the distance unit is the same as for x



- The spatial frequency of a wave in Fourier optics is closely related to its angle of propagation
- The frequency of the grating is in the diagram $1/d$ and the frequency of the wave diffracted by it is evidently the same
- By the grating equation - $1/d = \sin \theta / \lambda$
- Thus for small angles the spatial frequency of the wave is proportional to the angle
- The beam diffracted by a sample and measured at a known angle (frequency) thus provides information on the strength of that frequency in the Fourier decomposition of the sample - this why diffraction experiments are so useful

OPTICAL PROPAGATORS

The point spread function $\frac{1}{i\lambda z} e^{\frac{i\pi}{\lambda z}[x^2+y^2]}$ is the quadratic approximation to the distribution of wave amplitude on a receiving plane due to a diverging spherical wave. Analogously its complex conjugate approximates the amplitudes describing a *converging* spherical wave (action of a *lens*). The quadratic phase factor above is known as an optical propagator or Vander Lugt function and is clearly very useful in analyzing optical systems.

$u_Q(x_1, y_1) = u_P(x, y) t(x, y) \left. \frac{1}{i\lambda z} e^{\frac{i\pi}{\lambda z}[x^2+y^2]} \right _{x_1, y_1}$	PROPAGATION A DISTANCE z IN FREE SPACE
$u_{\text{EXIT}}(x, y) = u_P(x, y) e^{-\frac{i\pi}{\lambda f}[x^2+y^2]}$	PASSAGE THROUGH A LENS OF FOCAL LENGTH f

Example 1: Fourier transforming properties of a lens

Going back to the expanded diffraction integral in the Fresnel approximation

$$I_Q(x_1, y_1) = \left| \frac{1}{i\lambda z} e^{\frac{i\pi}{\lambda z}[x_1^2+y_1^2]} \int_{-\infty}^{+\infty} u_P(x, y) t(x, y) e^{\frac{i\pi}{\lambda z}[x^2+y^2]} e^{-\frac{2\pi i}{\lambda z}[x_1 x + y_1 y]} dx dy \right|^2$$

Inserting the lens propagator in place of $t(x, y)$ (which is in contact with u_P) the output wavefield is

$$u_Q(x_1, y_1) = \int_{\text{aperture}} u_P(x, y) e^{-\frac{i\pi}{\lambda f}[x^2+y^2]} e^{\frac{i\pi}{\lambda z}[x^2+y^2]} e^{-\frac{2\pi i}{\lambda z}[x_1 x + y_1 y]} dx dy$$

Thus when $z = f$ the quadratic phase factors cancel and the output wave field is the FT of the input wave field - this is a well known property of a simple lens - [Goodman 1968] equation 5-14

PROPAGATOR ALGEBRA

We use the notation $\mathbf{x} = \mathbf{i}x + \mathbf{j}y$ in the spatial domain and $\mathbf{u} = \mathbf{i}\xi + \mathbf{j}\eta$ in the spatial frequency domain in the following list of properties - these are thus *two-dimensional* formulas

$$\psi(\mathbf{x}; d) = e^{\frac{i\pi|\mathbf{x}|^2}{\lambda d}}$$

Carlson and Francis 1977

Goodman 1995

Handbook of holography 1992

$$\psi^*(\mathbf{x}; d) = \psi(\mathbf{x}; -d), \quad (\text{A2})$$

$$\psi(-\mathbf{x}; d) = \psi(\mathbf{x}; d), \quad (\text{A3})$$

$$\psi(c\mathbf{x}; d) = \psi(\mathbf{x}; d/c^2), \quad (\text{A4})$$

$$\psi(\mathbf{x}; d_1)\psi(\mathbf{x}; d_2) = \psi[\mathbf{x}; d_1d_2/(d_1 + d_2)], \quad (\text{A5})$$

$$\psi(\mathbf{x}_1 - \mathbf{x}_2; d) = \psi(\mathbf{x}_1; d)\psi(\mathbf{x}_2; d) \exp\{-(2\pi i/\lambda d)\mathbf{x}_1 \cdot \mathbf{x}_2\}, \quad (\text{A6})$$

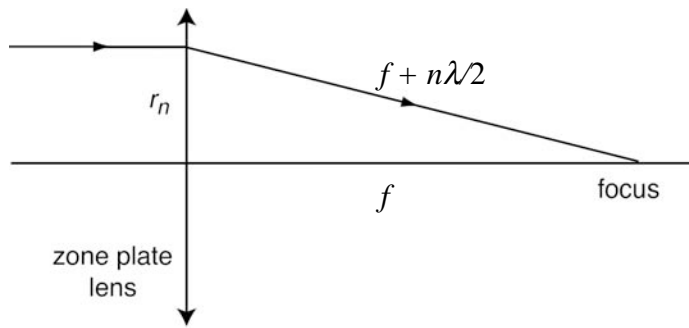
$$\psi(\mathbf{x}; \infty) = 1, \quad (\text{A7})$$

$$\text{FT}\{\psi(\mathbf{x}; d)\} = i\lambda d\psi^*(\lambda d\mathbf{u}; d), \quad (\text{A8})$$

$$\psi(\mathbf{x}; d_1) * \psi(\mathbf{x}; d_2) = i\lambda[d_1d_2/(d_1 + d_2)]\psi(\mathbf{x}; d_1 + d_2), \quad (\text{A9})$$

$$\lim_{d \rightarrow 0} (1/i\lambda d)\psi(\mathbf{x}; d) = \delta(\mathbf{x}). \quad (\text{A10})$$

EXAMPLE 2: FRESNEL ZONE PLATES

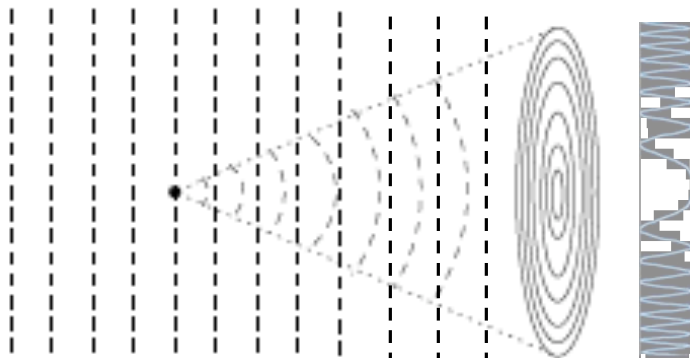


$$\sqrt{r_n^2 + f^2} = f + \frac{n\lambda}{2}$$

$$f \left[1 + \frac{1}{2} \frac{r_n^2}{f^2} + \dots \right] = f + \frac{n\lambda}{2}$$

$$r_n^2 = n\lambda f$$

- The zones are called Fresnel's half-period zones
- The ray from each zone is delayed half a wave more than the previous one by the lengthening distance to the focus
- The zones are rectangular in shape and alternate zones are opaque
- A Fresnel zone plate is similar to a [Gabor zone plate](#) which is the hologram of a point and has the same zone positions



Formation of a hologram of a point

$$I_H = (1 + u_Q)(1 + u_Q^*) \equiv \text{transparency}$$

$$= [1 + \psi(\mathbf{x}; f)] [1 + \psi^*(\mathbf{x}; f)]$$

$$= 2 \left(1 + \cos \left(\frac{i\pi r^2}{\lambda f} \right) \right)$$

$$\cos \left(\frac{\pi r^2}{\lambda f} \right) = \pm 1 \text{ when } \frac{\pi r^2}{\lambda f} = n\pi \text{ whence } r_n^2 = n\lambda f$$

thus the zone positions are the same

ZONE PLATES IN FOURIER OPTICS LANGUAGE

Consider a plane-wave illuminated Gabor zone plate

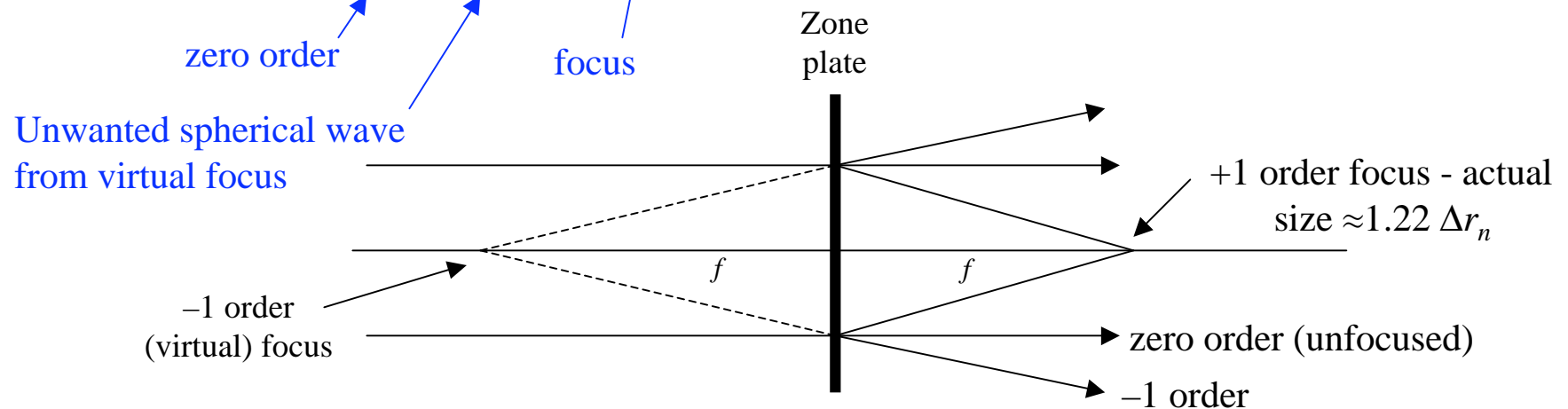
$$t(\mathbf{x}) = \frac{1}{2} + \frac{1}{2} \cos\left(\frac{\pi \mathbf{x}^2}{\lambda f}\right) = \frac{1}{2} + \frac{1}{2} \frac{[\psi(\mathbf{x}; f) + \psi^*(\mathbf{x}; f)]}{2} \text{ so at distance } z$$

$$u_P(\mathbf{x}) = \frac{1}{i\lambda z} \left\{ \frac{1}{2} + \frac{1}{2} \frac{[\psi(\mathbf{x}; f) + \psi^*(\mathbf{x}; f)]}{2} \right\} * \psi^*(\mathbf{x}; z)$$

Now consider what happens near the focus when $z \rightarrow f$ and $z - f = \Delta$ (small)

$$u_{\text{FOCAL PLANE}}(\mathbf{x}) = \frac{1}{2} + \frac{\psi(\mathbf{x}; 2f)}{8} - \frac{i\lambda f}{4} \left\{ \lim_{\Delta \rightarrow 0} \frac{1}{i\lambda \Delta} \psi(\mathbf{x}; \Delta) \right\} \text{ using A9 twice}$$

$$u_{\text{FOCAL PLANE}}(\mathbf{x}) = \frac{1}{2} + \frac{\psi(\mathbf{x}; 2f)}{8} - \frac{i\lambda f}{4} \delta(\mathbf{x}) \text{ using A10}$$



COHERENCE THEORY APPLIED TO X-RAY BEAM LINES

By Malcolm Howells, ESRF Experiments Division, April 21



- Development of coherence ideas with visible light, mathematical description, experimental meaning
- Spatial coherence by propagation
- Undulators, the one-electron pattern
- Definition of a mode, phase space
- The degeneracy parameter
- Statistics and modeling of a synchrotron light source
- Depth of field effects
- Partially coherent diffraction, why do nearly all synchrotron beams have horizontal stripes?

OPTICAL COMPONENTS FOR COHERENT X-RAY BEAMS

By Anatoli Snigirev, ESRF Experiments Division, April 28)



Practical aspects of temporal and spatial coherence for hard X-rays,
how can we measure spatial coherence?

Definition of the coherence requirements on mirrors, crystals and windows,
how close are we to meeting them?

Consequences of failing to meet requirements, strategies for improvement,
what remains to be done?

What new challenges do the “purple-book” experiments pose for optics?

Coherence matching for nanofocusing optics,
single-bounce single-capillary reflectors versus compound refractive lenses
and Fresnel zone plates

COHERENCE AND X-RAY MICROSCOPES

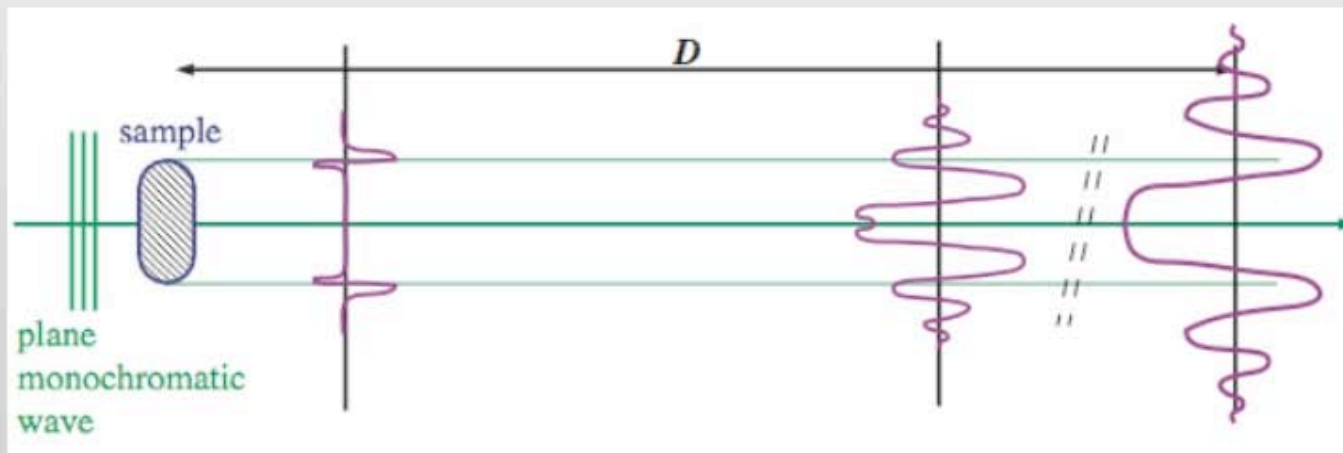
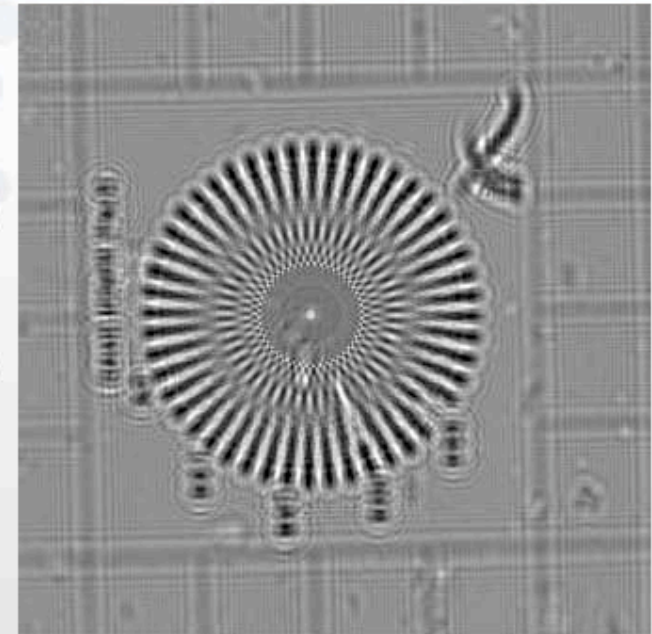
By Malcolm Howells, ESRF Experiments Division, May 26, (CTRL room)



- Introduction to x-ray microscopes at synchrotrons
- Zone plates
- Transmission x-ray microscopes (TXMs) and scanning transmission x-ray microscopes (STXMs)
- Sample illumination (condenser) systems, should the illumination be coherent, is the image coherent?
- Role of beam angle in determining resolution, Fourier optics treatment
- Contrast transfer, reciprocity, influence of coherence on resolution
- Coherence and Zernike phase contrast, Wigner phase contrast
- Are microscopes flux or a brightness experiments?
- Some example results.

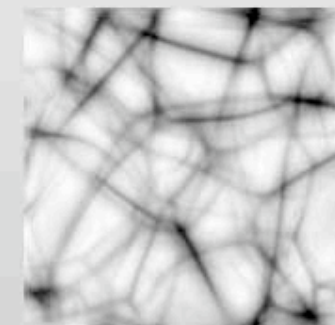
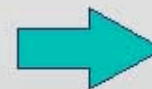
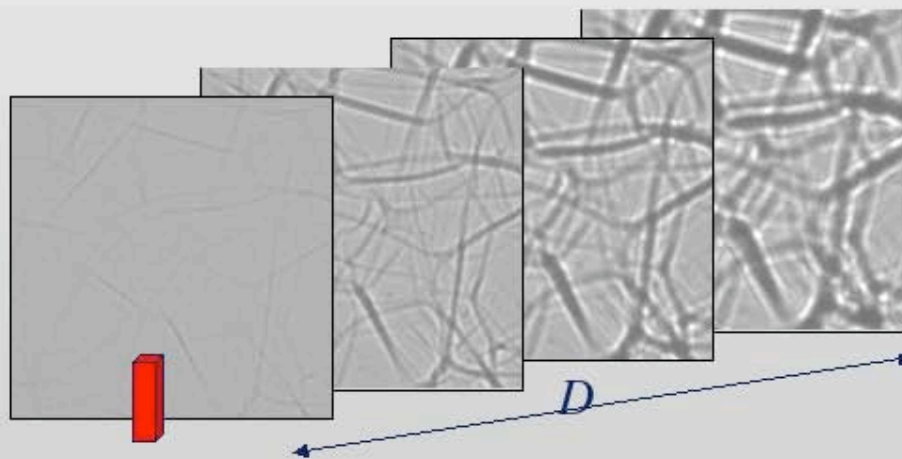
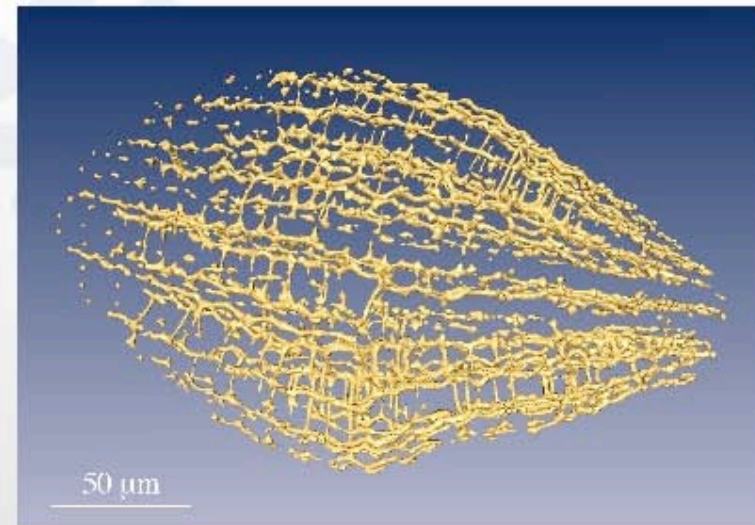
Peter Cloetens, June 2, room 500

- Propagation-based phase-contrast imaging
 - coherence conditions
 - the forward problem; Fresnel diffraction
 - in-line holography



Peter Cloetens, June 2, room 500

- The inverse problem
 - phase retrieval methods
- Three-dimensional imaging
 - holo-tomography
- Projection microscopy
 - KB-based imaging



Phase map

Coherence activities at the ESRF: Scanning transmission x-ray microscopy

By Jean Susini, ESRF Experiments Division

- ❖ **Basic principles**
- ❖ **Optical design**
 - **Zone plates vs to Kirkpatrick-Baez systems?**
 - **High-beta vs low-beta sources?**
 - **Source demagnification vs use of secondary sources?**
- ❖ **Spectromicroscopy and energy tuning**
 - **Use of multi-keV x-rays**
 - **Chemical mapping and X-ray fluorescence**
 - **Radiation damage**
- ❖ **Some applications**

Synchrotron based microprobe techniques

X-Ray Fluorescence

- Composition
- Quantification
- Trace element mapping

X-ray Diffraction & scattering

- Long range structure
- Crystal orientation mapping
- Stress/strain/texture mapping

Phase contrast X-ray imaging

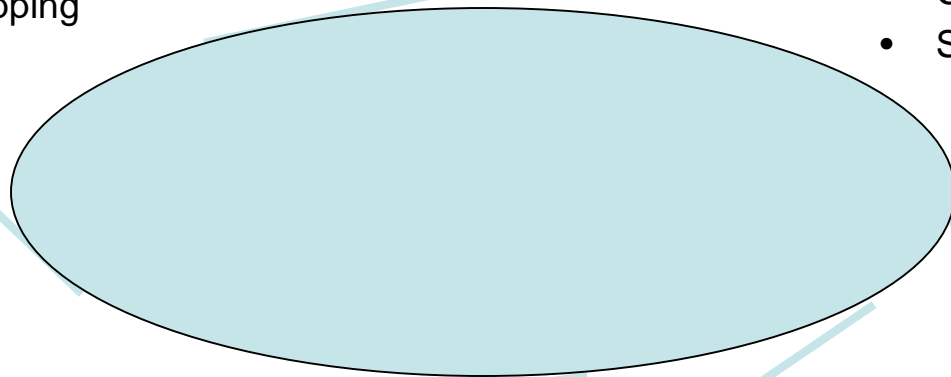
- 2D/3D Morphology
- High resolution
- Density mapping

Infrared FTIR-spectroscopy

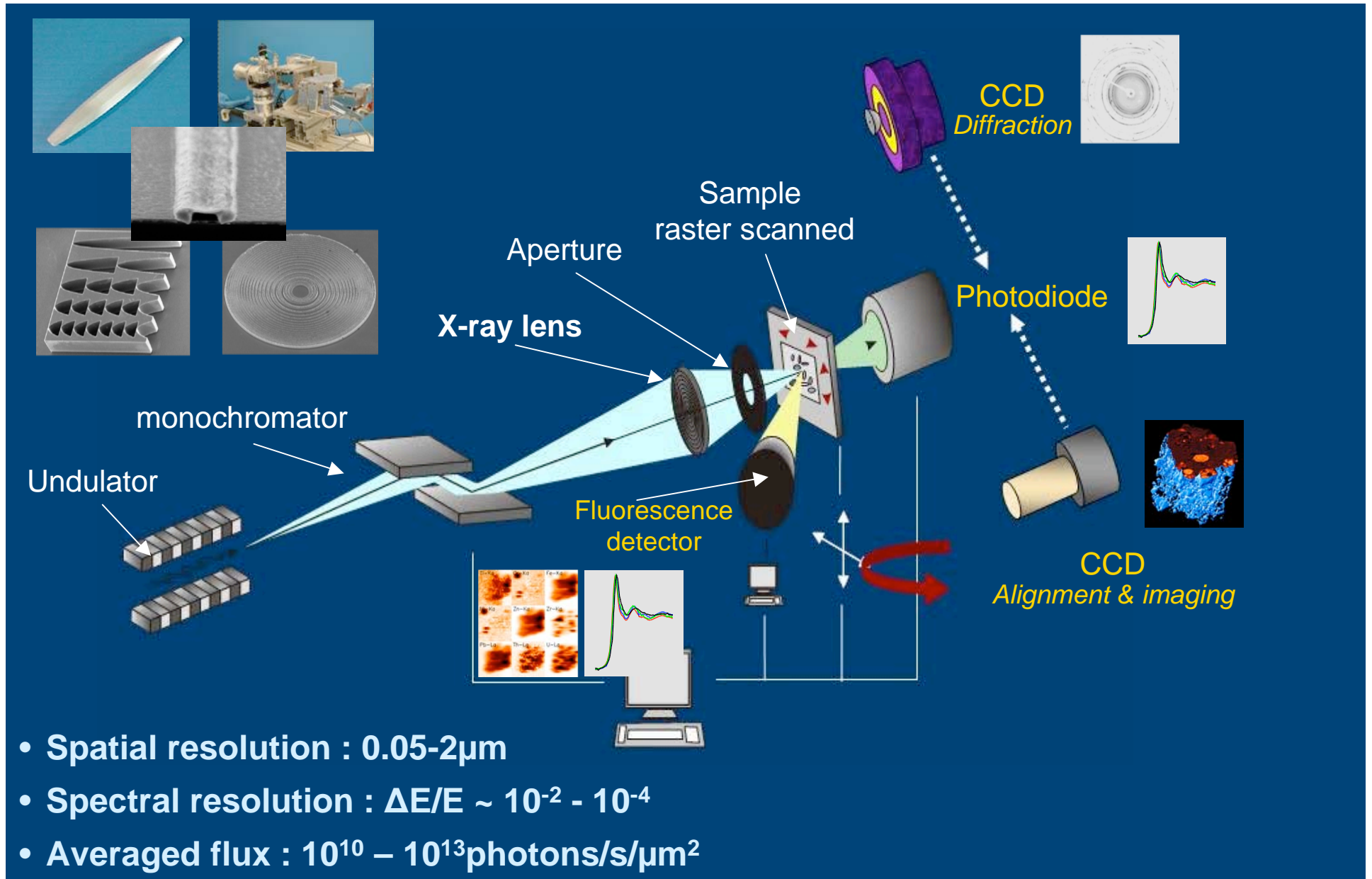
- Molecular groups & structure
- High S/N for spectroscopy
- Functional group mapping

X-ray spectroscopy

- Short range structure
- Electronic structure
- Oxidation/speciation mapping



Synchrotron based hard X-ray microprobe



COHERENT X-RAY DIFFRACTION IMAGING: I

Malcolm Howells, ESRF, Experiments Division, June 23



- The basic idea: measure the intensities, compute the phases
- Why the need for coherence?
- Schematic experiments and algorithms
- Oversampling: is it necessary?
- History, active groups and their achievements
- Experimental realities and limitations, computational challenges
- Radiation damage limitations
- Resolution-flux scaling, ways around the damage limit?
- Alternative schemes – ptychography

X-ray Photon Correlation Spectroscopy

Anders Madsen, June 30

- **XPCS overview**
- **Speckle**
- **Correlation functions**
- **Setup and detectors for XPCS**
- **Scientific highlights**
- **Complementary methods**
- **XPCS at 4th generation sources**

COHERENT X-RAY DIFFRACTION IMAGING: II

Malcolm Howells, ESRF Experiments Division, July 7



- Summary of present achievements and future projections in CXDI and other coherence techniques
- Details of ALS results and their implications
- How do we know the resolution?
- Detectors, multiple exposures
- Choice of wavelength
- Resolution-exposure-time tradeoffs with a purpose-built beam line
- Beam-line design, the Berkeley COSMIC project
- What are reasonable performance expectations for the future?
- Benefits of the ESRF upgrade, Comparison with other techniques
- New opportunities for time-resolved and damage-avoiding experiments with x-ray free-electron lasers
- Conclusion

Anatoly Snigirev (April 28)

Optical components for coherent x-ray beams

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