▪ # Coherence of light and matter: from basic concepts to modern applications

Part II Script 1

Vorlesung im GrK 1355

WS 2013

A. Hemmerich & G. Grübel

Location: SemRm 052, Gebäude 69, Bahrenfeld

Thursdays 12.15 – 13.45

G.Grübel (GR), A.Hemmerich (HE)

Coherence of light and matter: from basic concepts to modern applications

24.10.	Introduction	(HE)
31.10.	Coherence of classical light, basic concepts and examples	(HE)
7.11.	Coherence of classical light, basic concepts and examples	(HE)
14.11.	Coherence of quantized light	(HE)
21.11.	Excursion	
28.11.	Coherence of quantized light	(HE)
5.12.	Coherence of matter waves	(HE)
12.12.	Coherence based X-ray techniques: Introduction	(GR)
19.12.	Imaging techniques (I)	(GR)
9. 1.	Imaging techniques (II)	(GR)
16.1.	X-ray Photon Correlation Spectroscopy (I)	(GR)
23.1.	X-ray Photon Correlation Spectroscopy (II)	(GR)
30.1.	Summary	(GR)

Literature

Basic concepts: The quantum theory of light
Rodney Loudon, Oxford University Press (1990)
Quantum Optics
Marlan O. Scully, M. Suhal Zubairy, Cambridge University Press (1997)
Dynamic Light Scattering with Applications
B.J. Berne and R. Pecora, John Wiley&Sons (1976)
Elements of Modern X-Ray Physics
J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)

Matter Waves: Bose-Einstein Condensation in Dilute Gases
C. J. Pethick and H. Smith, Cambridge University Press (2002)

Lecture Notes

Part I: ***http://photon.physnet.uni-hamburg.de/fileadmin/user_upload/ILP/Hemmerich/teaching.html/Coherence.pdf***

Part II: **http://photon-science.desy.de/research/studentsteaching/lectures__seminars/ws_13_14/coherence_of_light_grk1355/…..**

Coherence of light and matter: from basic concepts to modern applications

Part II: G. Grübel

Coherence based X-ray techniques

Overview, Introduction to X-ray Scattering, Sources of Coherent X-rays, Speckle pattern and their analysis

Imaging techniques

Phase Retrieval, Sampling Theory, Reconstruction of Oversampled Data, Fourier Transform Holography, Applications

X-ray Photon Correlation Spectroscopy (XPCS)

Introduction, Equilibrium Dynamics (Brownian Motion), Surface Dynamics, Non-Equilibrium Dynamics

Imaging and XPCS at FEL Sources

▪

Coherence based X-ray techniques:

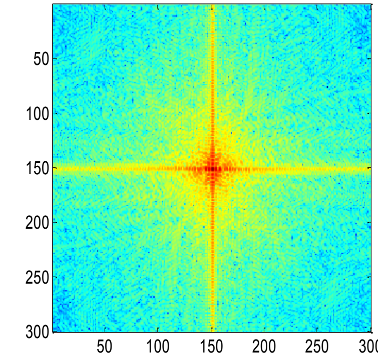
Introduction

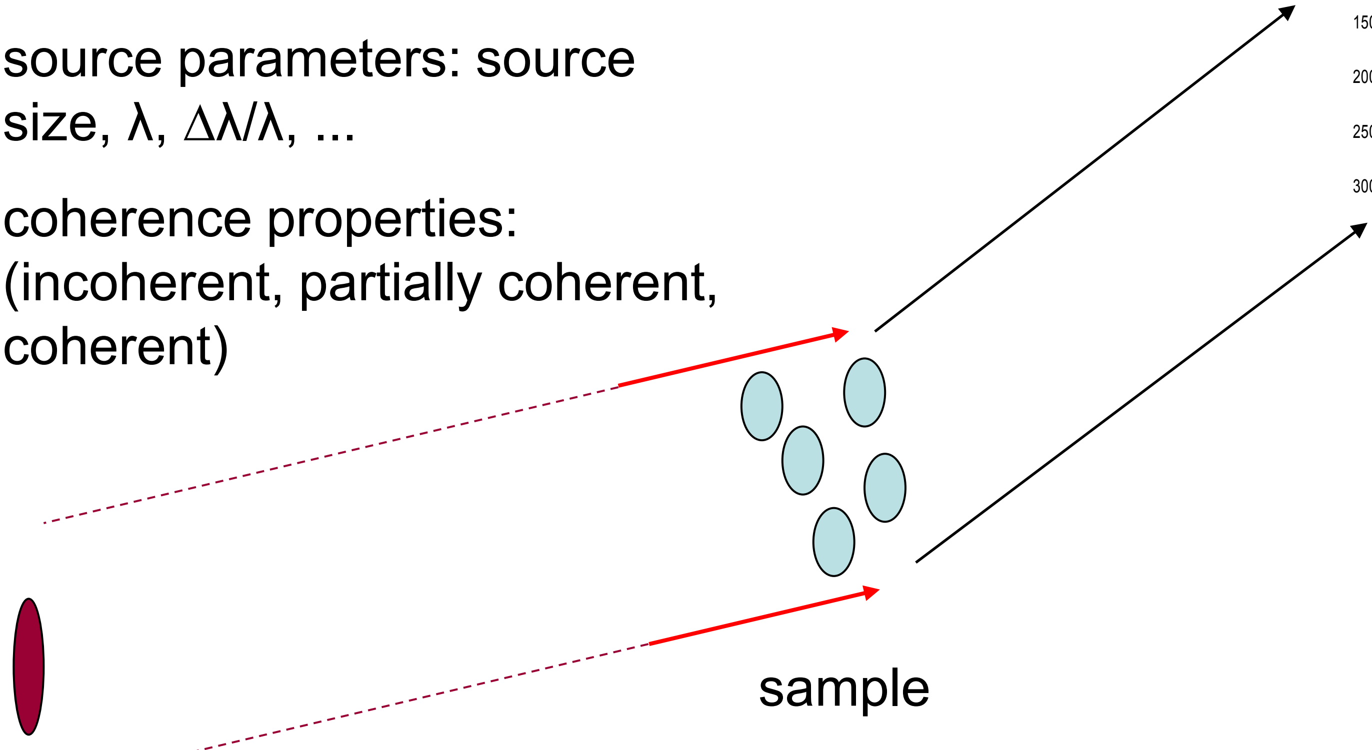
Introduction: Experimental Set-Up

source (visible light, x-rays,..)

source parameters: source size, λ, Δλ/λ, ...

coherence properties: (incoherent, partially coherent, coherent)





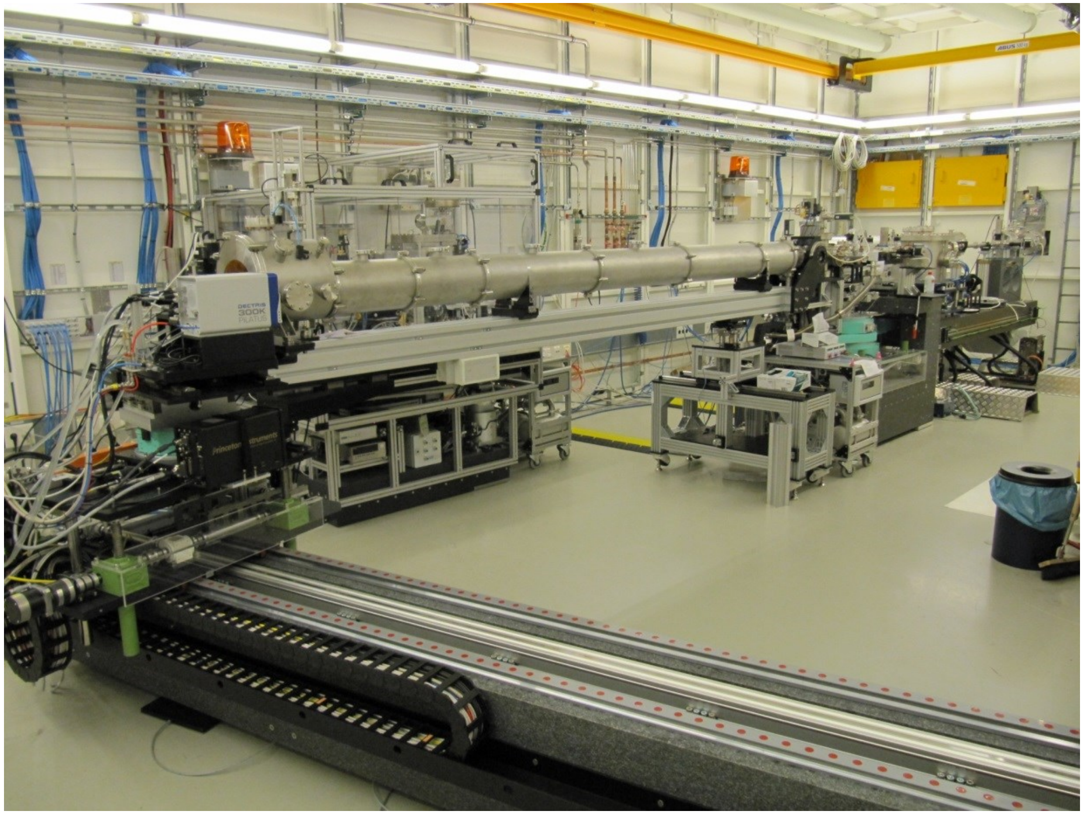
detector

sample

interacts with radiation (e.g. x-rays)

L

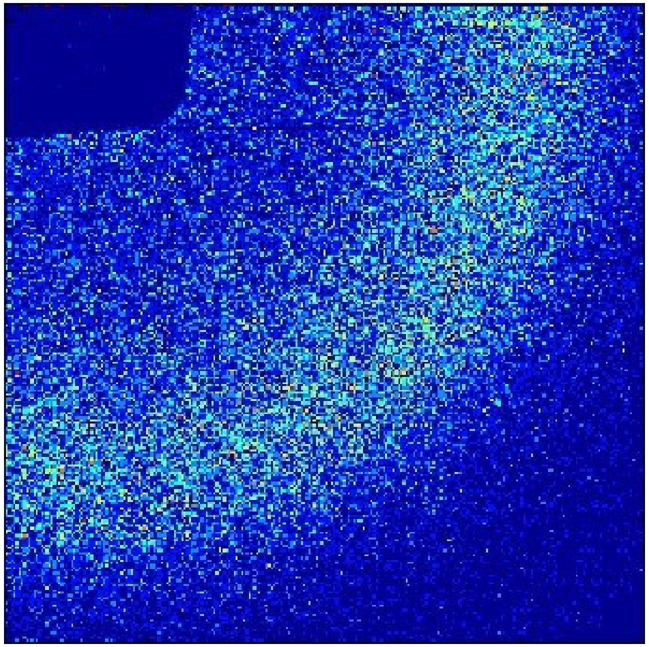
Experimental Set-up



Introduction: Scattering with coherent X-rays

If coherent light is scattered from a disordered system it gives rise to a random (grainy) diffraction pattern, known as "speckle". A speckle pattern is an interference pattern and related to the exact spatial arrangement of the scatterers in the disordered system.

$$I(Q,t) \sim S_c(Q,t) \sim \left| \sum e^{iQRj(t)} \right|^2$$



j in coherence volume $c = \xi_t^2 \xi_l$

Incoherent Light:

$S(Q,t) = \langle S_c(Q,t) \rangle_{V>>c}$

ensemble average

Introduction: Speckle Pattern

A speckle pattern contains information on both, the source and sample that produced it.

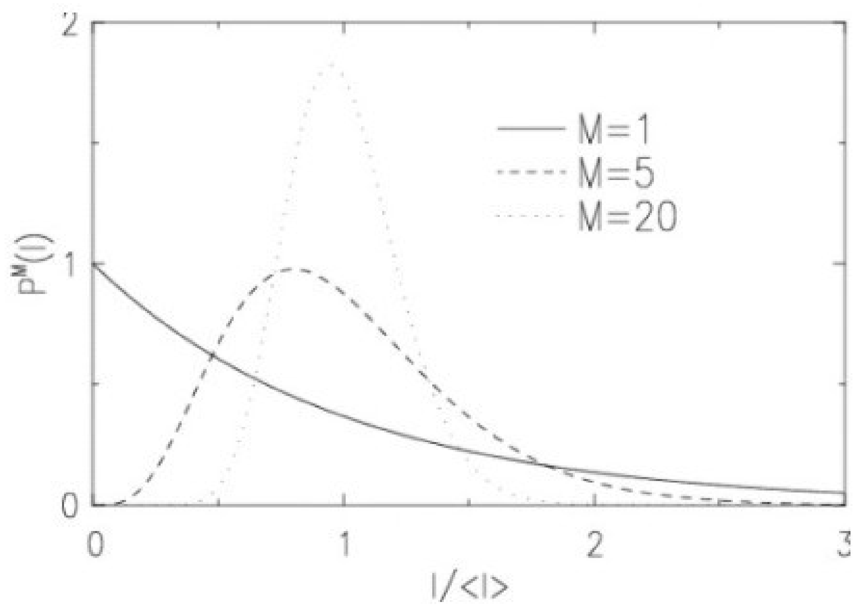
If the source is fully coherent and the scattering amplitudes and phases of the scattering are statistically independent and distributed over 2π one finds for the probability amplitude of the intensities:

$$P(I) = (1/\langle I\rangle) \exp(- I/\langle I\rangle)$$

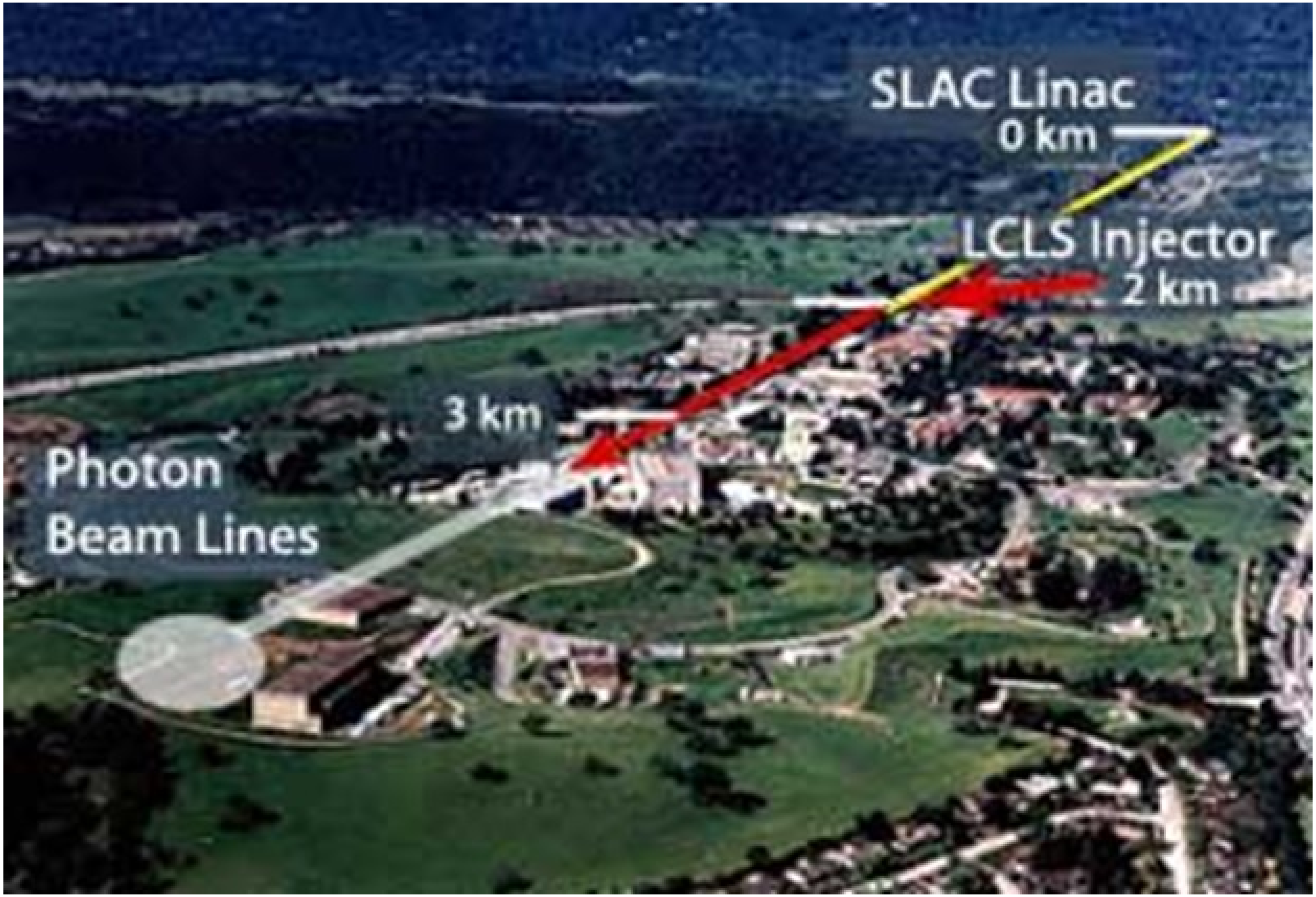
Mean: $\langle I\rangle$

Std.Dev. σ: $\text{sqrt}(\langle I^2\rangle - \langle I\rangle^2) = \langle I\rangle$

Contrast: $ß = \sigma^2/\langle I\rangle^2 = 1$



The Linac Coherent Light Source (LCLS)



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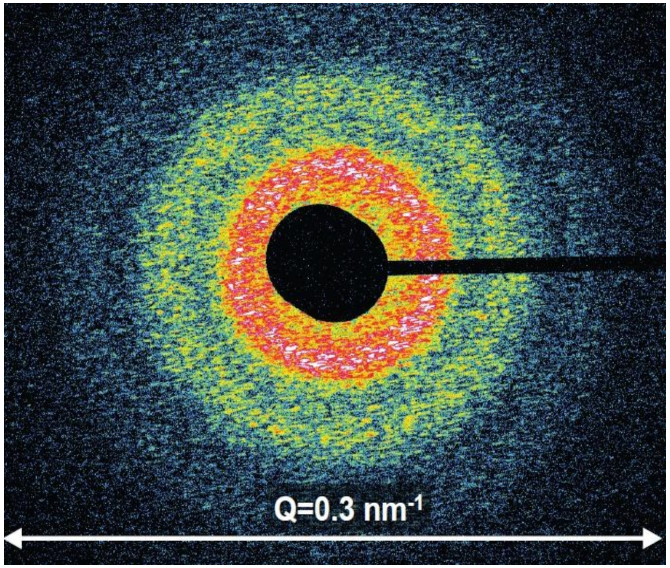

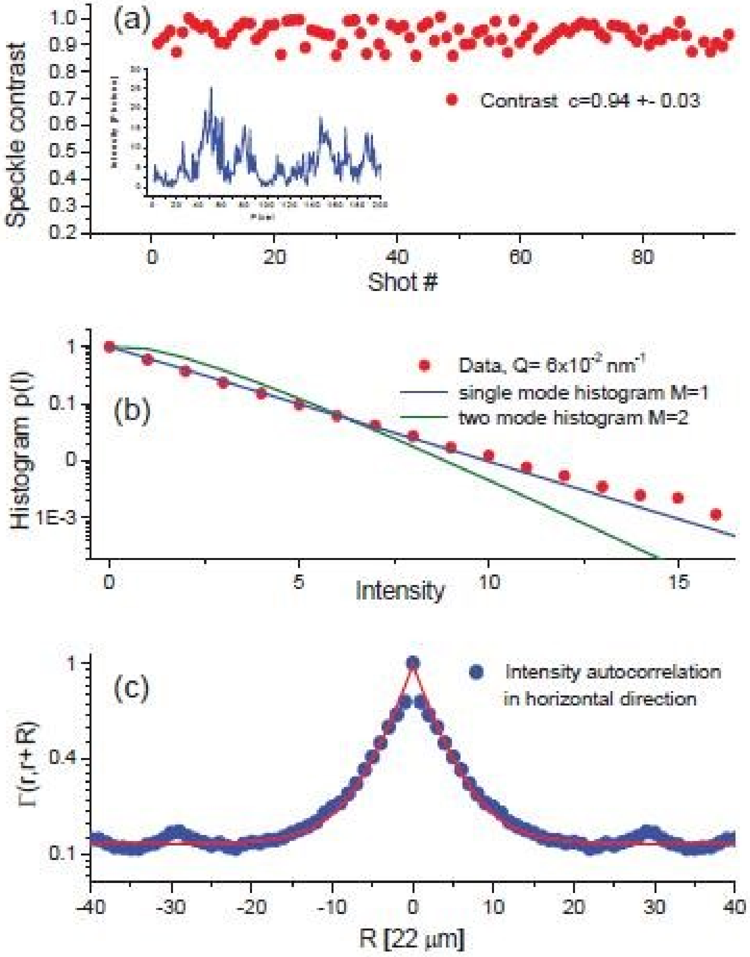

Single pulse hard X-ray speckle pattern captured from nano-particles in a colloidal liquid (photon wave-length λ= 1.37 Å

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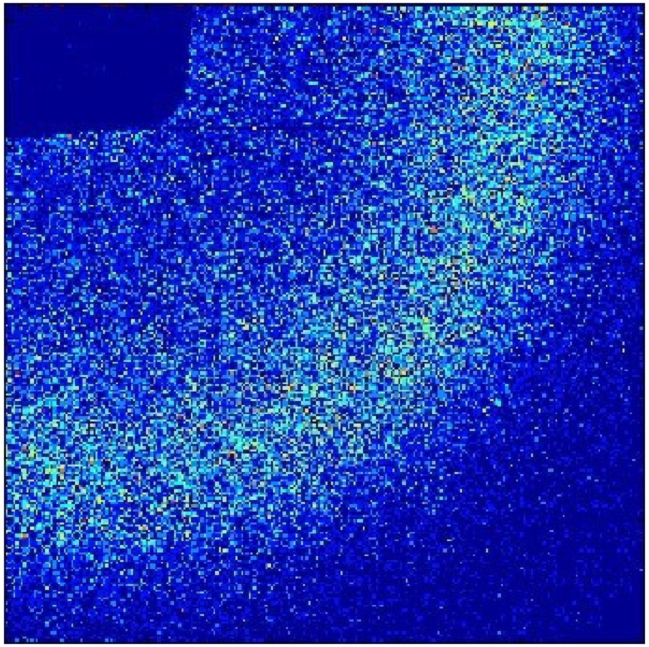


j in coherence volume $c = \xi_t^2 \xi_l$

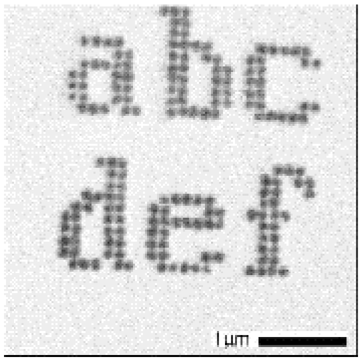
<u>Incoherent Light:</u>

$S(Q,t) = \langle S_c(Q,t) \rangle_{V>>c}$

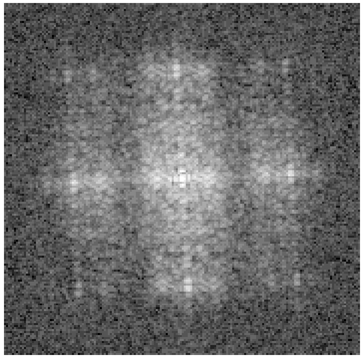
ensemble average

Introduction: Speckle Reconstruction

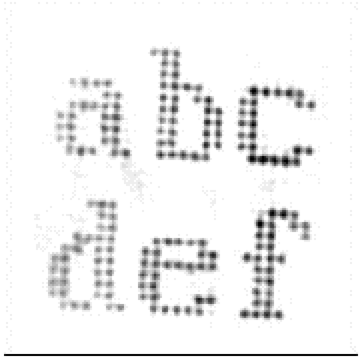
Reconstruction (phasing) of a speckle pattern: **"oversampling" technique**



gold dots on SiN membrane (0.1 µm diameter, 80 nm thick)



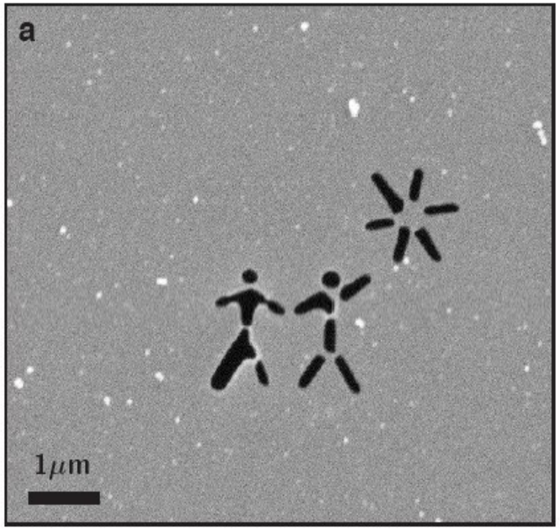
λ=17Å coherent beam at X1A (NSLS), $1.3 \cdot 10^9$ ph/s 10µm pinhole 24 µm x 24 µm pixel CCD

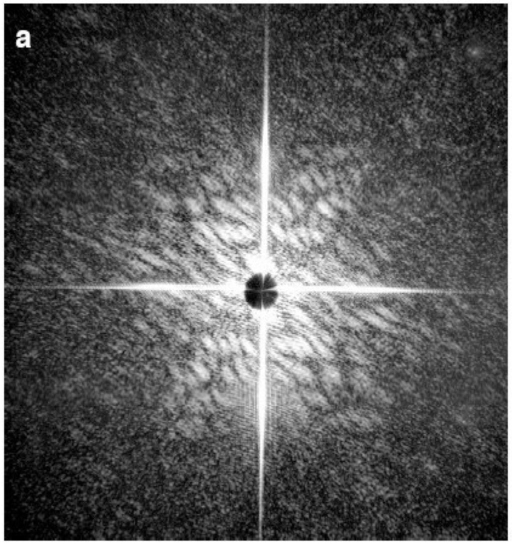


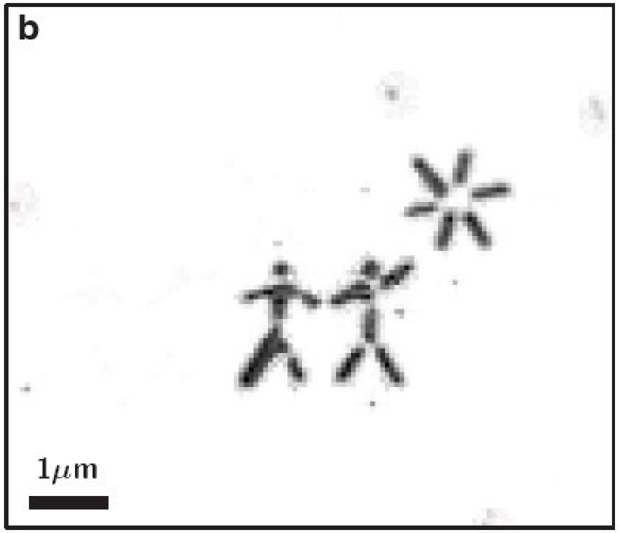
reconstruction "oversampling" technique

Miao, Charalambous, Kirz, Sayre, Nature, 400, July 1999

Reconstruction of "oversampled" data





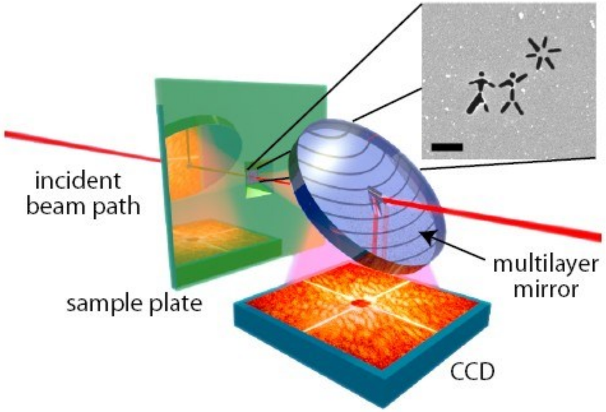


Model structure in 20 nm SiN membrane

Speckle pattern recorded with a single (25 fs) pulse

Reconstructed image

Incident FEL pulse:
25 fs, 32 nm,
4 x 10^{14} W cm^{-2} (10^{12} ph/pulse)



H. Chapman et al., Nature Physics, 2,839 (2006)

Introduction: Scattering with coherent X-rays

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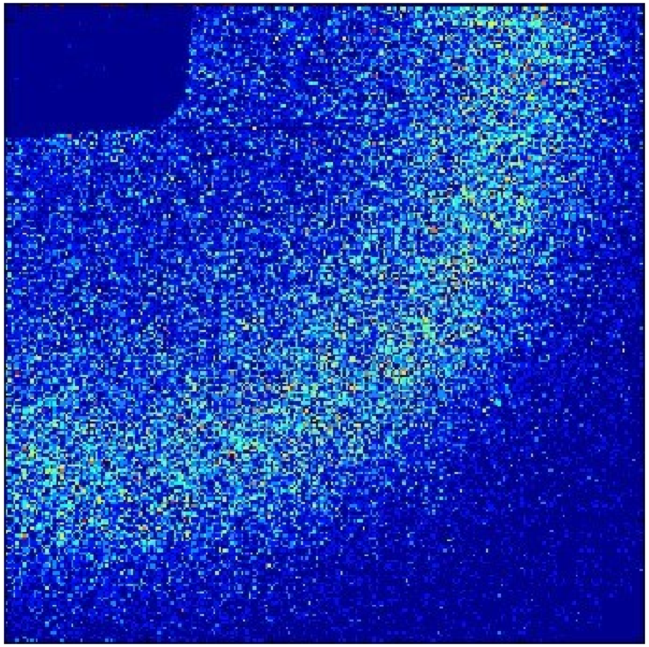


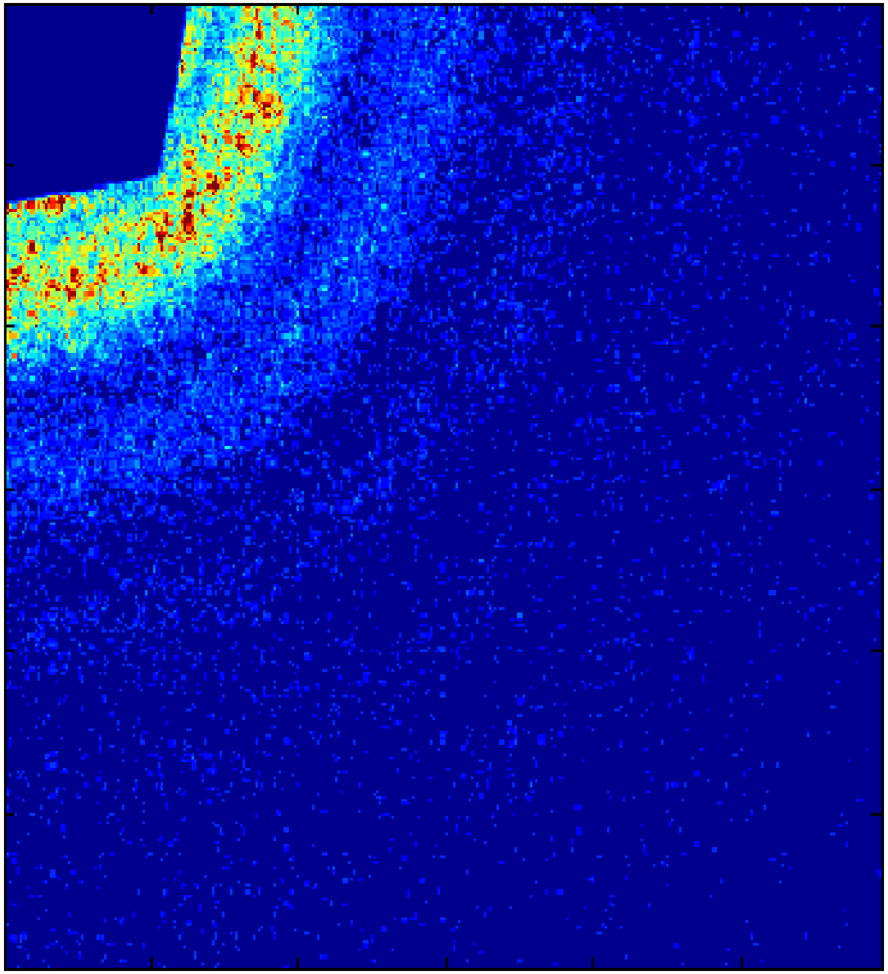
j in coherence volume $c = \xi_t^2 \xi_l$

<u>Incoherent Light:</u>

$S(Q,t) = < S_c(Q,t)>_{V>>c}$

ensemble average

▪ Introduction: X-ray Photon Correlation Spectroscopy (XPCS)



colloidal silica particles undergoing Brownian motion in high viscosity glycerol

V. Trappe and A. Robert

- quantify dynamics in terms of the intensity correlation function $g_2(Q,t)$:

$I(\mathbf{Q},t) = |\mathbf{E}(\mathbf{Q},t)|^2 = |\sum b_n(\mathbf{Q}) \exp[i\mathbf{Q}\bullet\mathbf{r}_n(t)|^2$

Note: $\mathbf{E}(\mathbf{Q},t) = \int d\mathbf{r}' \rho(\mathbf{r}') \exp[i\mathbf{Q}\bullet\mathbf{r}'(t)]$ $\rho(\mathbf{r}')$: *charge density*

$g_2(\mathbf{Q},t) = <I(\mathbf{Q},0) \bullet I(\mathbf{Q},t)> / <I(\mathbf{Q})>^2$

if $\mathbf{E}(\mathbf{Q},t)$ is a zero mean, complex gaussian variable:

$g_2(\mathbf{Q},t) = 1 + ß(\mathbf{Q}) <\mathbf{E}(\mathbf{Q},0)\mathbf{E}^*(\mathbf{Q},t)>^2 / <I(\mathbf{Q})>^2$

<> ensemble av.; ß(**Q**) contrast

$g_2(\mathbf{Q},t) = 1 + ß(\mathbf{Q}) |f(\mathbf{Q},t)|^2$ with $f(\mathbf{Q},t) = F(\mathbf{Q},t) / F(\mathbf{Q},0)$

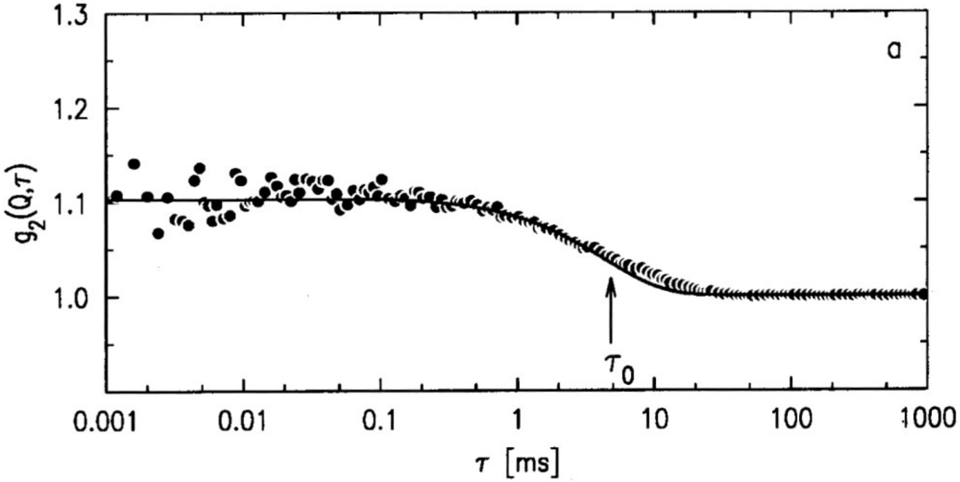
F(Q,0): static structure factor

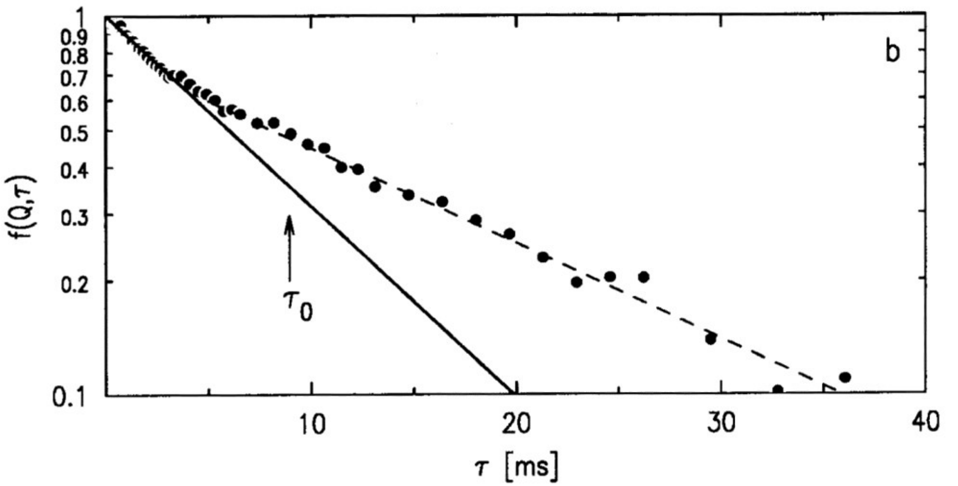
N: number of scatterers

$F(\mathbf{Q},t) = [1/N\{b^2(\mathbf{Q})\} |\sum^N_{m=1}\sum^N_{n=1} <b_n(\mathbf{Q})b_m(\mathbf{Q})\bullet\exp\{i\mathbf{Q}[\mathbf{r}_n(0)-\mathbf{r}_m(t)]\}>$

- # Time correlation function $g_2(Q,t)$

$g_2(Q,t) = 1 + \beta(Q)\,|f(Q,t)|^2$ and $f(Q,t) = \exp(-\Gamma t) = \exp(-t/\tau)$





Coherence based X-ray techniques:

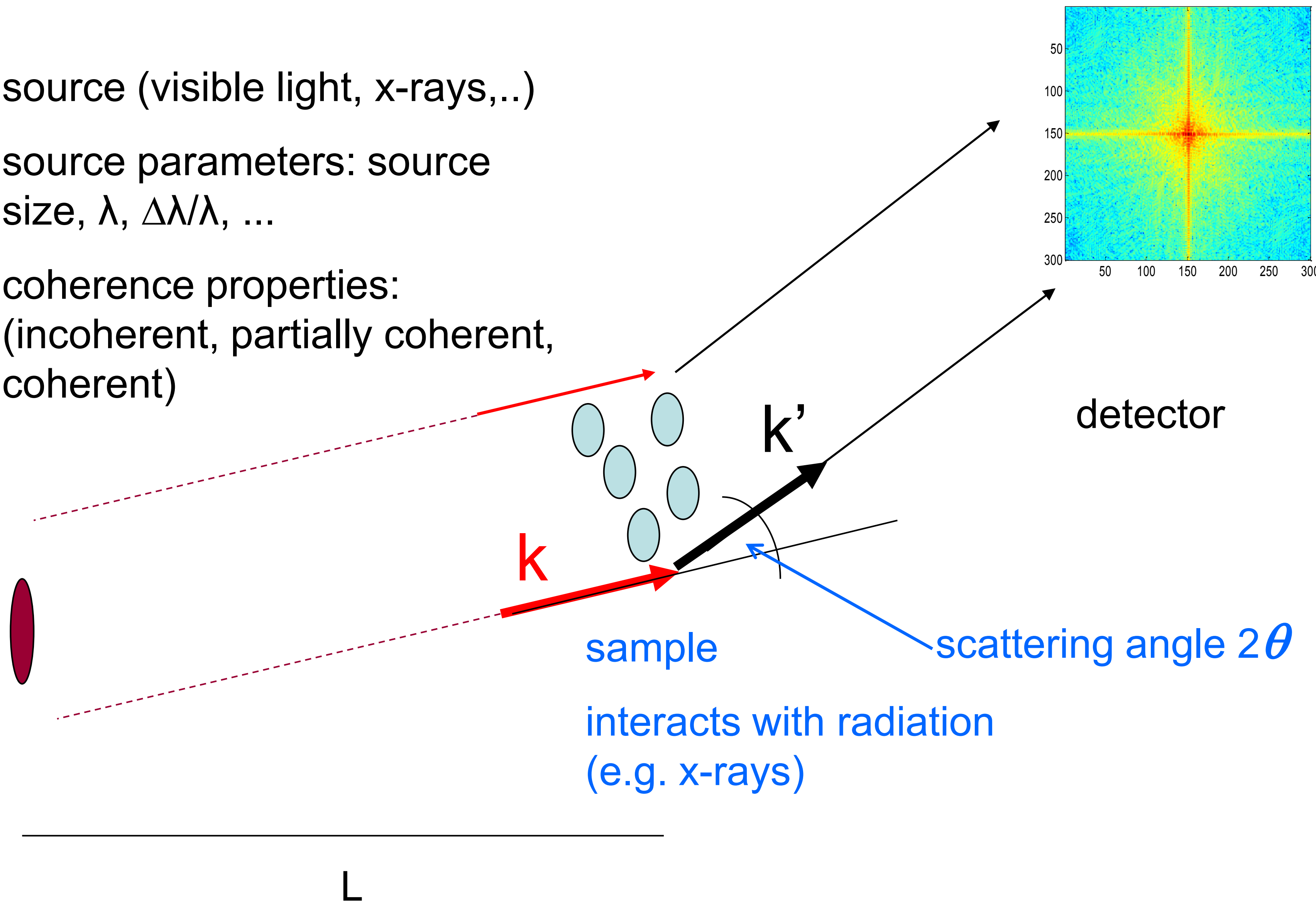
An X-ray Scattering Primer

Experimental Set-Up for Scattering Experiments

source (visible light, x-rays,..)

source parameters: source size, λ, $\Delta\lambda/\lambda$, ...

coherence properties: (incoherent, partially coherent, coherent)



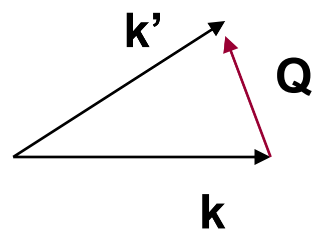
Scattering of X-rays: A primer

consider a monochromatic plane (electromagnetic) wave with wavevector k:

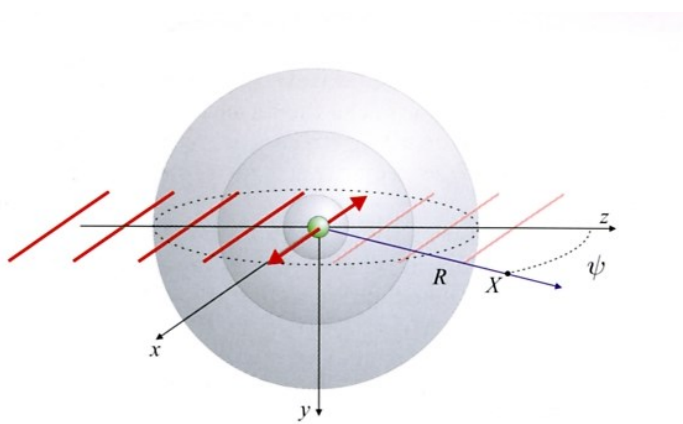
$\mathbf{E}(\mathbf{r},t) = \boldsymbol{\varepsilon}\, E_o \exp\{i(\mathbf{kr}-\omega t)\}$ with $|\mathbf{k}|=2\pi/\lambda$, $\lambda[\text{Å}]=hc/E$, $\omega=2\pi/\nu$

elastic scattering:

$\hbar\, \mathbf{k'} = \hbar\, \mathbf{k} + \hbar \mathbf{Q}$



Scattering by a single electron:



$E_{rad}(R,t)/E_{in} =$

$-(e^2/4\pi\varepsilon_o mc^2)\exp(ikR)/R \cos\psi$

spherical wave

thomson scattering length r_o

($=2.82*10^{-5}$ Å)

▪

<u>scattered intensity:</u>

$I_S/I_o = |E_{rad}|^2 R^2 \Delta\Omega \,/\, |E_{In}|^2 A_o$ $R^2\Delta\Omega$: solid angle seen by detector

A_o incident beam size

$$I_s = (d\sigma/d\Omega)\,(I_o/A_o)\,\Delta\Omega$$

with the differential cross section (for Thomson scattering)

$$(d\sigma/d\Omega) = r_o^2 P \qquad P = \begin{cases} 1 & \text{vertical} \\ \cos^2\psi & \text{horizontal} \\ \tfrac{1}{2}(1+\cos^2\psi) & \text{unpolarized} \end{cases}$$

note: $\sigma_{total} = \int (d\sigma/d\Omega) = (8\pi/3)\, r_o^2$

▪

scattering by a single atom:

phase factor

scattering amplitude by an ensemble of electrons

$$-r_o f^o(Q) = -r_o \sum_{r_j} \exp(iQ \cdot r_j)$$

(atomic) formfactor — position of scatterers

$$f^o(Q \rightarrow 0) = Z, \quad f^o(Q \rightarrow \infty) = 0$$

form factor of an atom:

$$f(Q,\hbar\omega) = f^o(Q) + f'(\hbar\omega) + i f''(\hbar\omega)$$

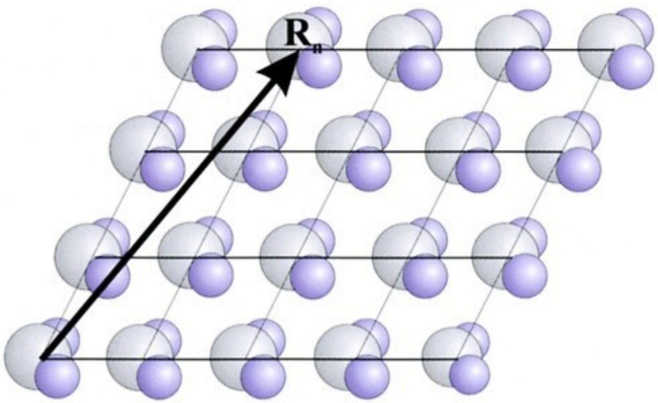
dispersion corrections: level structure, absorption effects

scattering intensity:

$$I_s = r_o^2 f(Q) f^*(Q) P$$

▪

scattering by a crystal:



$r_{j'} = R_n + r_j$

lattice vector + atomic position in lattice

$$F^{crystal}(Q) = \Sigma_{rj} f_j(Q)\exp(iQr_j)\Sigma_{Rn}\exp(iQR_n)$$

unit cell structure factor — lattice sum

$$I_s = r_o^2 F(Q) F^*(Q) P$$

lattice sum ≡ phase factor of order unity or N (number of unit cells) if

$$Q \bullet R_n = 2\pi \text{ x integer} \quad (\$)$$

▪

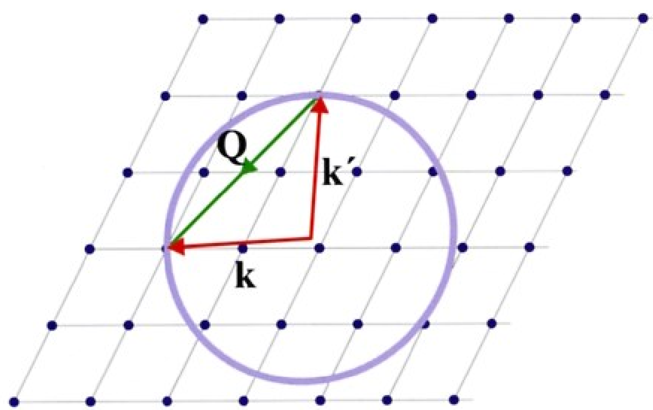
<u>evaluation of lattice sums:</u>

construct reciprocal space such that: $a_i \bullet a_j^* = 2\pi\ \delta ij$

with a_i defining a

reciprocal lattice *such that* $G = h\ a_1^* + k\ a_2^* + l\ a_3^*$

and G fullfills ($) for Q = G (Laue condition)



k + Q = k'

Ewald sphere

$\sin(\theta/2) = (Q/2) / k$

Laue condition ≡ Bragg's law

<u>lattice sum:</u> $|\Sigma_{Rn} \exp(iQR_n)|^2 \rightarrow N\ v_c^*\ \delta\ (Q\text{-}G)$

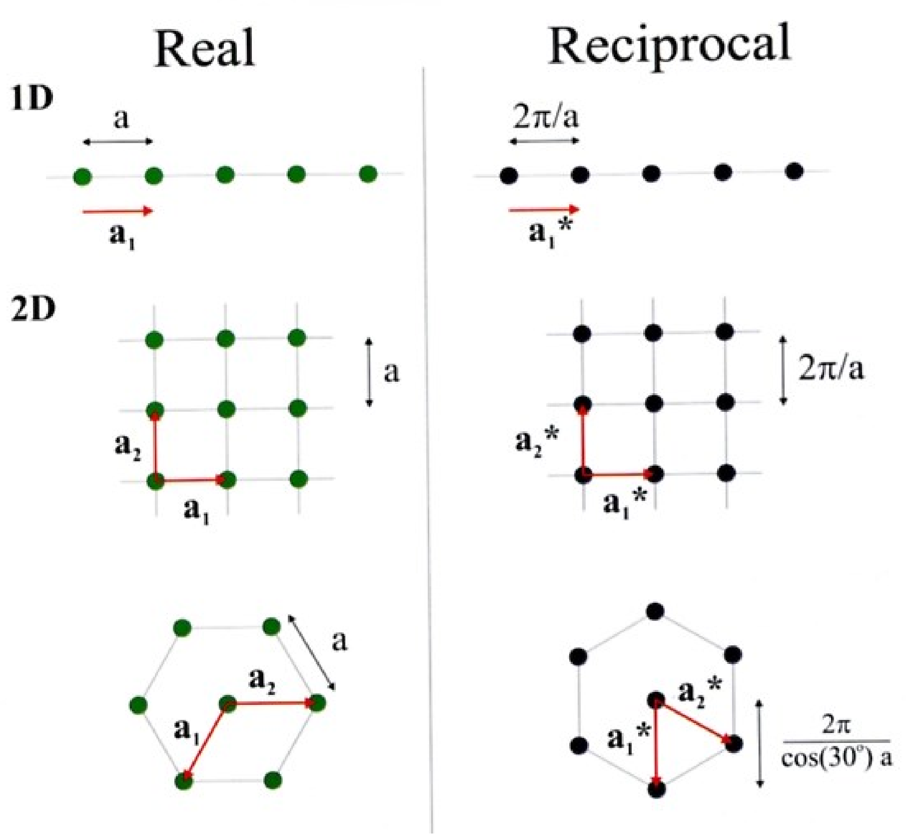
N number of unit cells; v_c^* unit cell volume in reciprocal space

▪

construction of reciprocal space:

(real space lattice constants a_1, a_2, a_3); $v_c = a_1 \bullet (a_2 \times a_3)$

$a_1^* = 2\pi/v_c\,(a_2 \times a_3)$ $a_2^* = 2\pi/v_c\,(a_3 \times a_1)$ $a_3^* = 2\pi/v_c\,(a_1 \times a_2)$



▪

unit cell structure factor:

$$\sum_{r_j} f_j(Q)\exp(iQr_j)$$

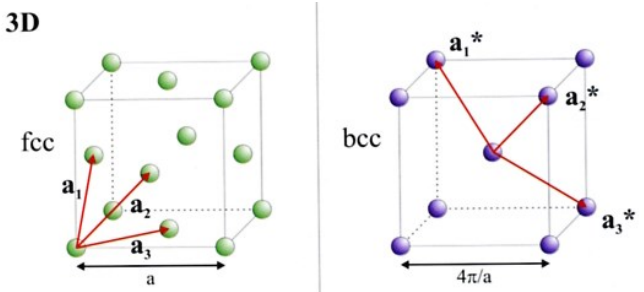
e.g. fcc lattice

$r_1 = 0$

$r_2 = ½\,(a_1+a_2)$

$r_3 = ½\,(a_2+a_3)$

$r_4 = ½\,(a_3+a_1)$



$$F_{hkl}^{fcc} = f(Q)\sum \exp(iQr_j) \qquad \text{with } Q = G = h\,a_1^* + k\,a_2^* + l\,a_3^*$$

$$= f(Q)\,\{1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)}\}$$

$$= f(Q) \times \begin{cases} 4 & \text{if h,k,l are all even or odd} \\ 0 & \text{otherwise} \end{cases}$$

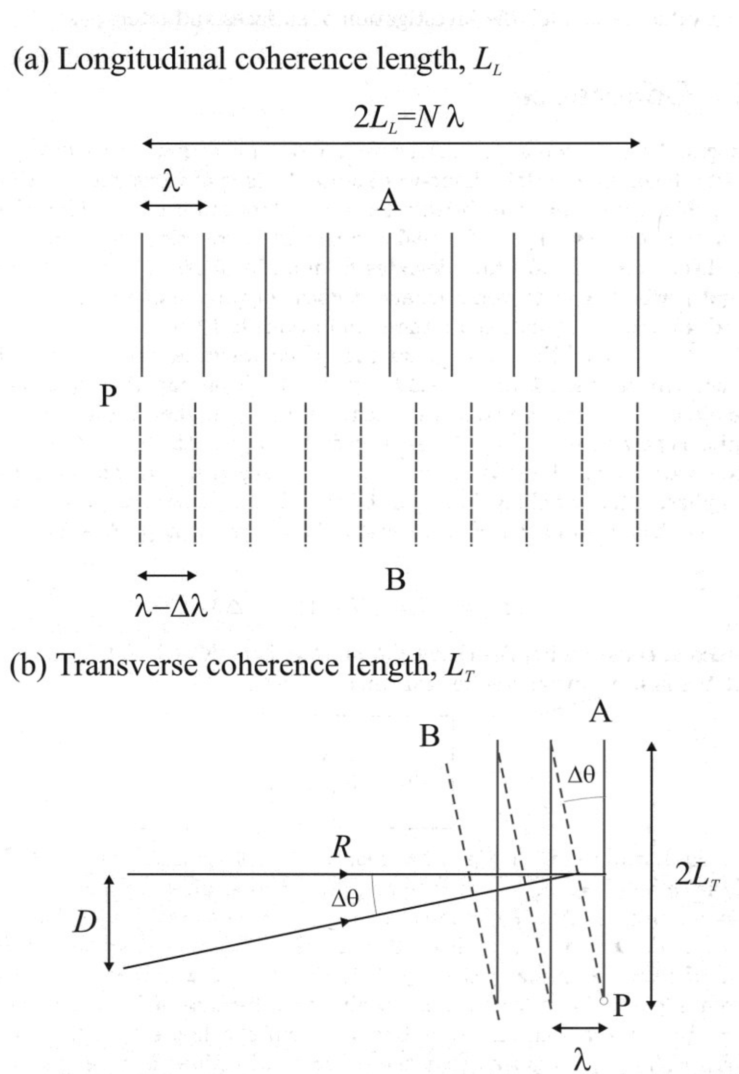
- From a measurement of a (large) set of crystal reflections $|F_{hkl}|^2$ it is possible to deduce the positions of the atoms in the unit cell.

<u>Limitations:</u>

phaseproblem: $| F(Q)| = | F(-Q) |$

$$| F(Q) | = | F(Q)e^{i\Phi} |$$

Coherence



<u>Longitudinal coherence:</u>

Two waves are in phase at point P. How far can one proceed until the two waves have a phase difference of π:

$$\xi_l = (\lambda/2)\ (\lambda/\Delta\lambda)$$

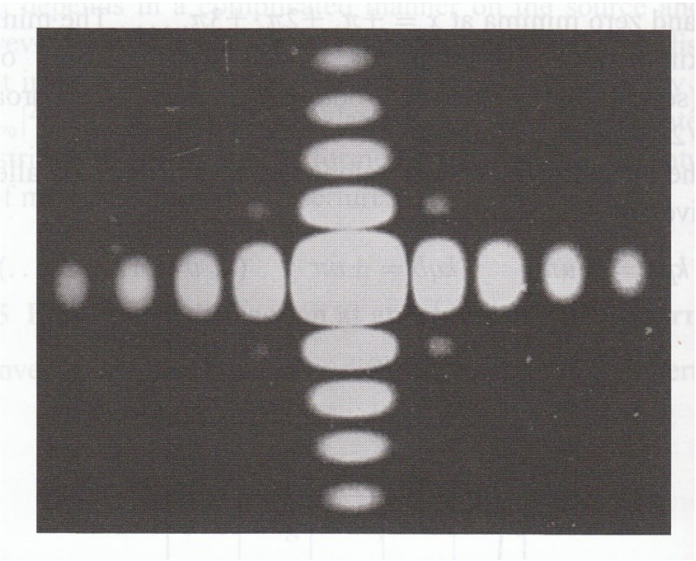
<u>Transverse coherence:</u>

Two waves are in phase at P. How far does one have to proceed along A to produce a phase difference of π:

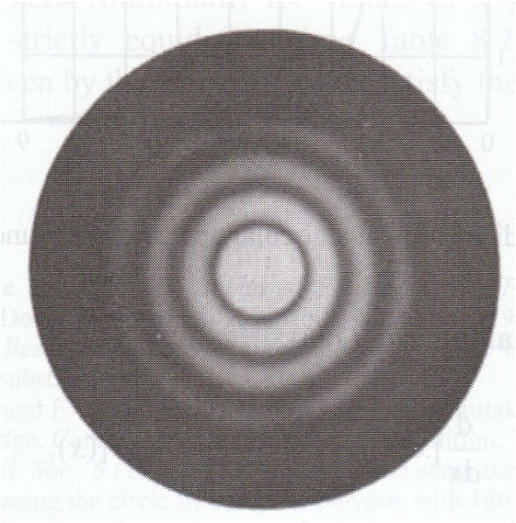
$$2\xi_t\ \Delta\theta = \lambda$$

$$\xi_t = (\lambda/2)\ (R/D)$$

Fraunhofer Diffraction

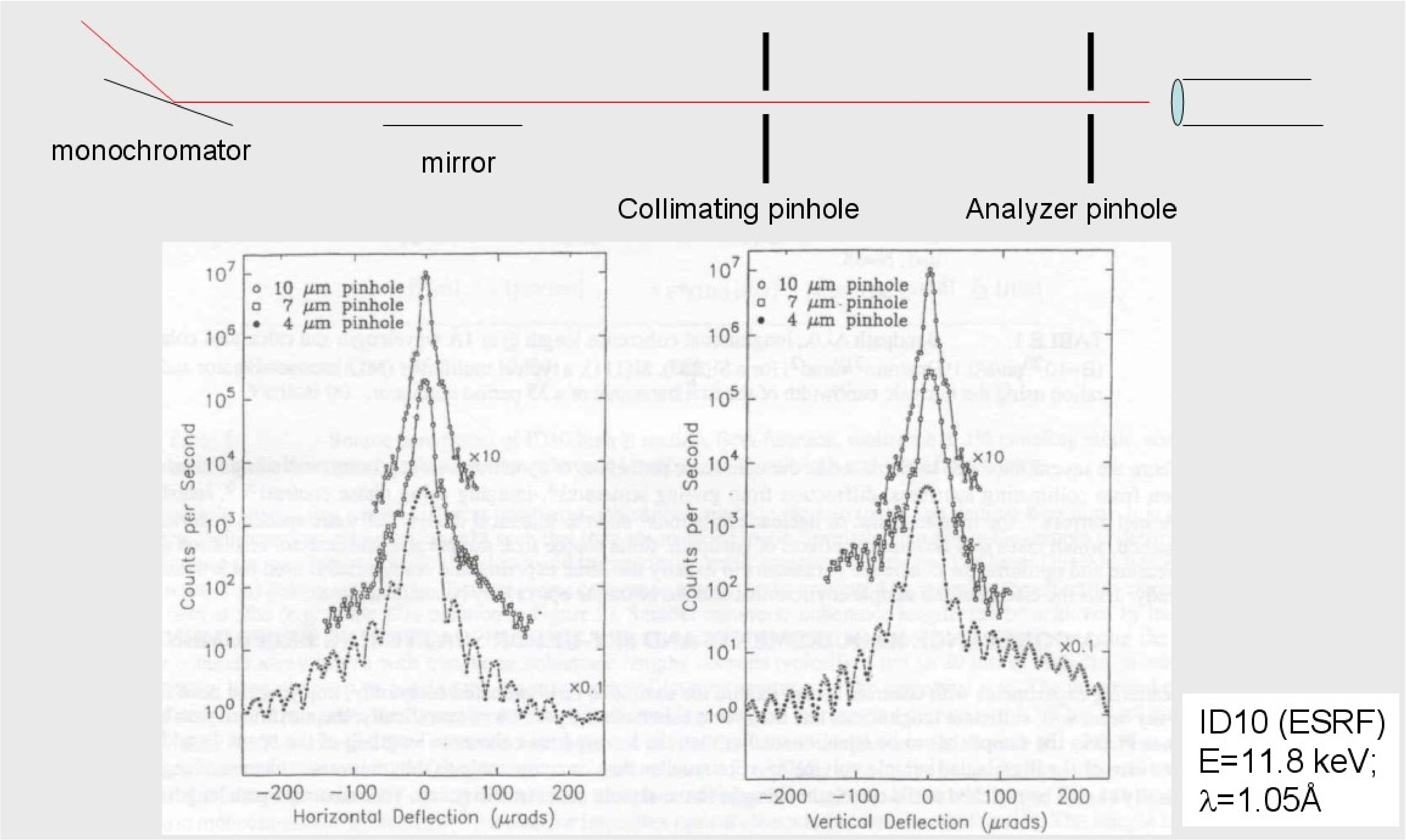


Fraunhofer diffraction of a rectangular aperture 8 x 7 mm^2, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)

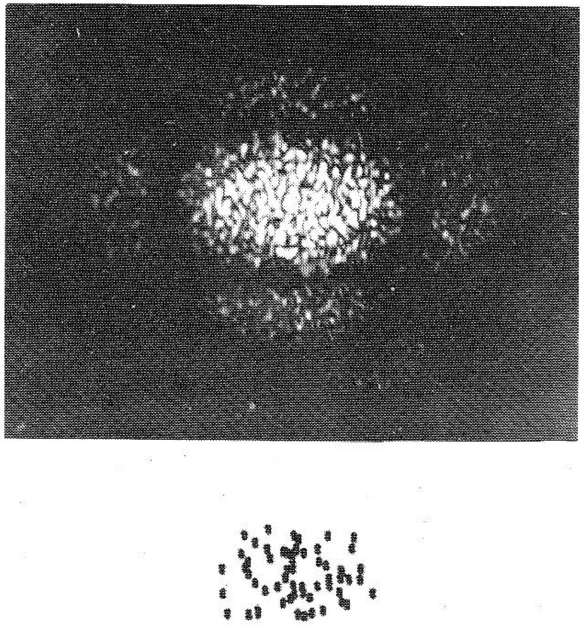


Fraunhofer diffraction of a circular aperture, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)

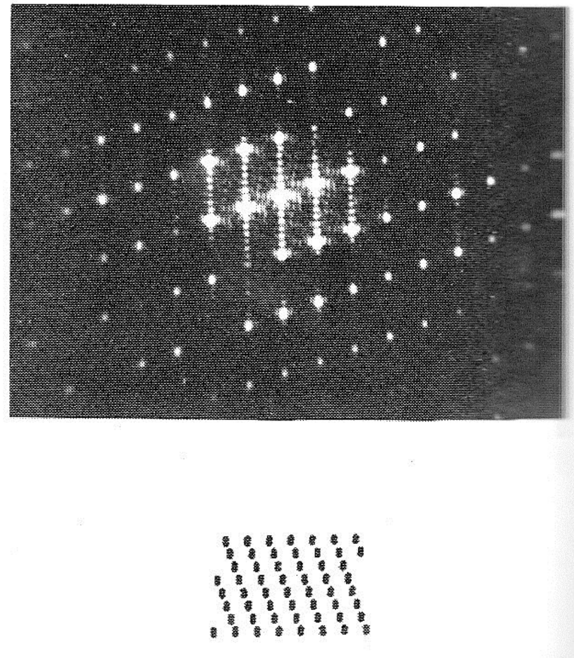
Fraunhofer Diffraction (λ=0.1nm)



▪ Speckle pattern



random arrangement of apertures: speckle



regular arrangement of apertures