Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 9	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2021		
	G. Grübel, O. Seeck, V. Markmann, F. Lehmkühler, Andre Philippi-Kobs, M. Martins		
Location	online		
Date	Tuesdays	12:30 - 14:00	(starting 6.4.)
	Thursdays	8:30 - 10:00	(until 8.7.)

DESY

Methoden moderner Röntgenphysik: Online Info

Tuesday Zoom-Meeting
https://desy.zoom.us/j/92674682486
Meeting ID: 926 7468 2486
Passcode: 144456

Thursday Zoom-Meeting
https://desy.zoom.us/j/99738625981
Meeting ID: 997 3862 5981
Passcode: 841881

Tutorial Zoom-Meeting
https://desy.zoom.us/j/95288979489
Meeting ID: 952 8897 9489
Passcode: 832350

Literature

Basic concepts:

Moderne Röntgenbeugung
Röntgendiffraktometrie für Materialwissenschaftler, Physiker und Chemiker
Authors
(view affiliations)
Lothar Spieß
Robert Schwarzer
Herfried Behnken
Gerd Teichert
https://link.springer.com/book/10.1007/978-3-663-10831-3

Elements of Modern X-Ray Physics
J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)

X-Ray Diffraction
B.E. Warren, DOVER Publications Inc., New York

Principles of Optics
M. Born and E. Wolf, Cambridge University Press, 7^{th} ed.

Soft X-rays and Extreme Ultraviolet Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/

Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996

Lecture Notes

https://photon-science.desy.de/research/research_teams/coherent_x_ray_scattering/teaching/index_eng.html

Methoden moderner Röntgenphysik: Streuung und Abbildung

Small Angle Scattering, and Soft Matter
Introduction, Form Factor, Structure Factor, Applications, ...

Anomalous Diffraction
Introduction into Anomalous Scattering, ...

Introduction into Coherence
Concept, First Order Coherence, Spatial Coherence, Second Order Coherence, ...

Coherent Scattering
Imaging and Correlation Spectroscopy, ...

The Concept of Coherence: Classical Light

First Order Coherence

Coherence and Emission Spectrum

Spatial Coherence

Second Order Coherence

Chaotic Light

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)

Coherence: Applications

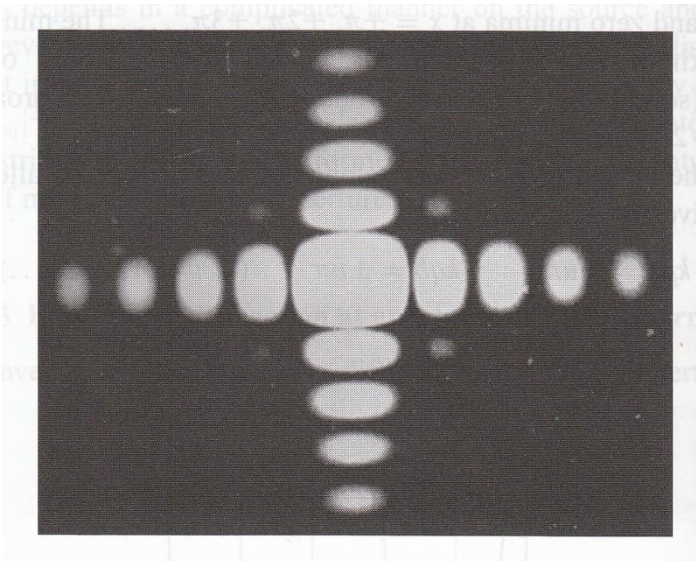
Interference Patterns

X-ray Speckle

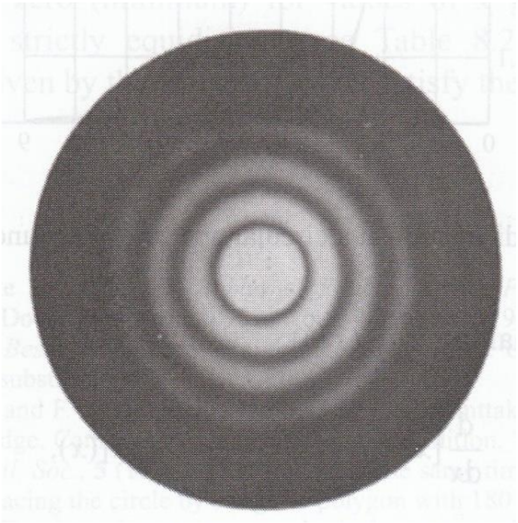
(Imaging)

X-Ray Photon Correlation Spectroscopy (XPCS)

Fraunhofer Diffraction

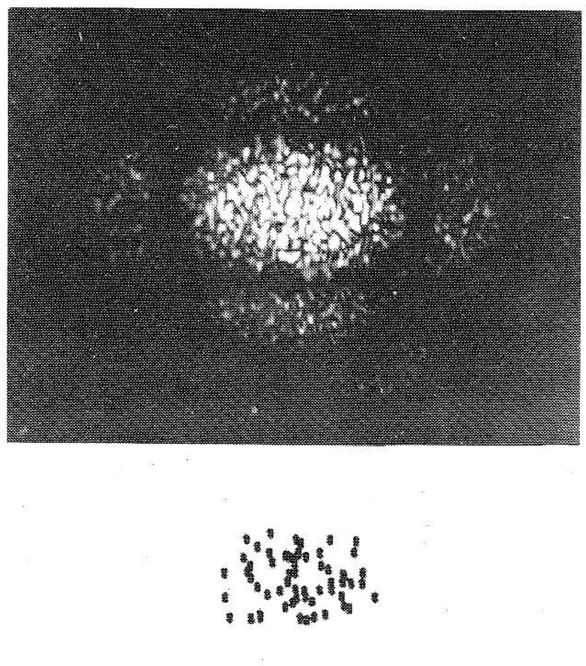


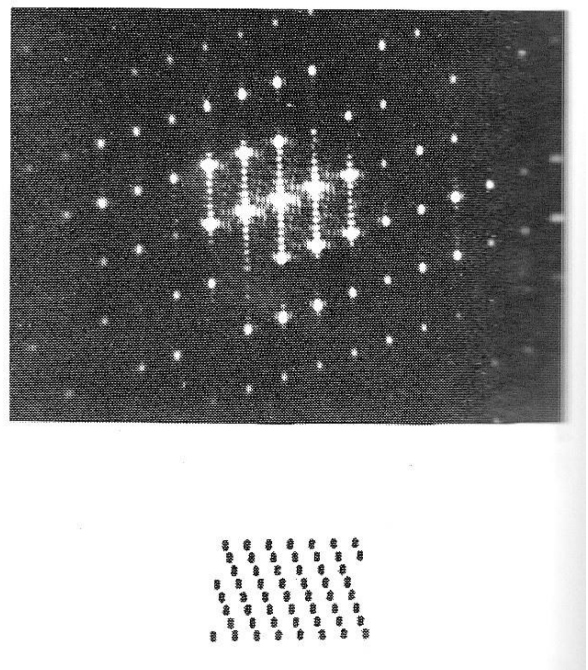
Fraunhofer diffraction of a rectangular aperture 8 x 7 mm^2, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)



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

Speckle Pattern

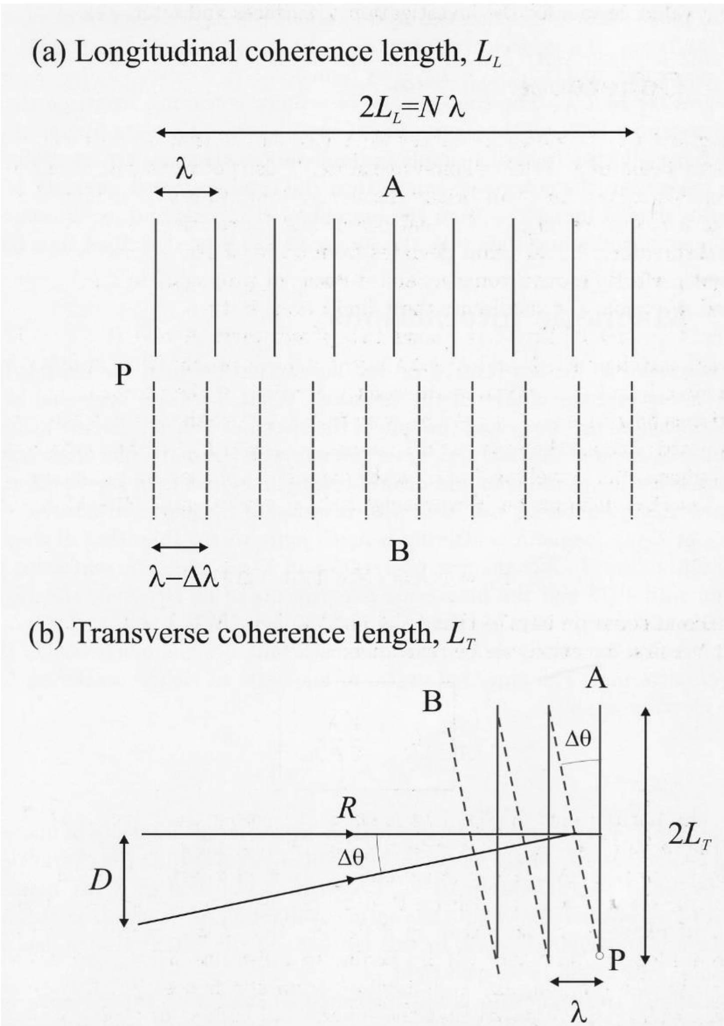




Random arrangement of apertures: speckle

Regular arrangement of apertures

Coherence Lengths (0.1 nm X-Rays)



Longitudinal coherence:

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

$$\xi_l = \left(\frac{\lambda}{2}\right)\left(\frac{\lambda}{\Delta\lambda}\right)$$

$$\lambda = 0.1\text{nm} \qquad \frac{\Delta\lambda}{\lambda} = 10^{-4} \qquad \Rightarrow \xi_l \approx 1\ \mu\text{m}$$

Transverse coherence:

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

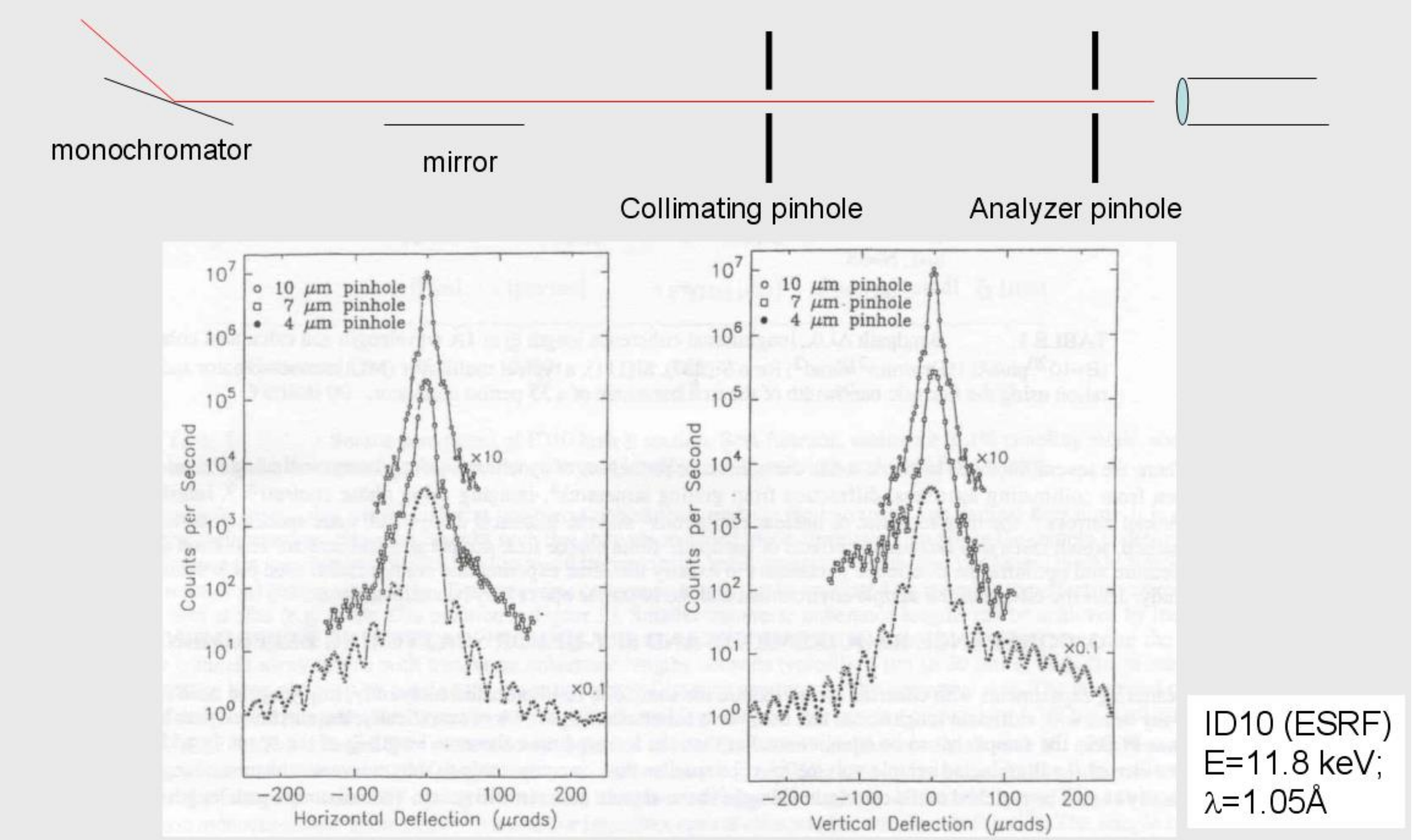
$2\xi_t\,\Delta\theta = \lambda$

$$\xi_t = \left(\frac{\lambda}{2}\right)\left(\frac{R}{D}\right)$$

$$\lambda = 0.1\text{nm}, R = 100\ \text{m}, D = 20 - 150\ \mu\text{m}$$

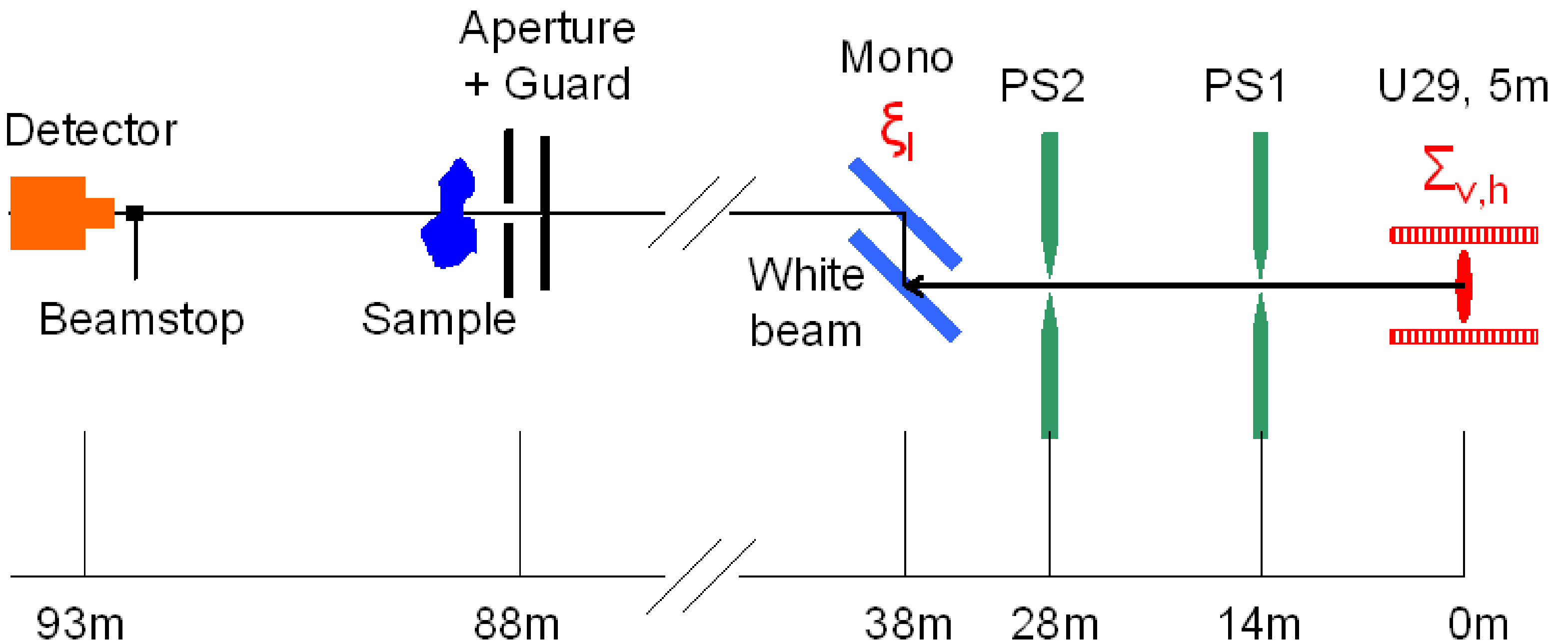
$$\Rightarrow \xi_t \approx 100\ \mu\text{m}$$

Fraunhofer Diffraction (λ = 0.1nm)



ID10 (ESRF)
E=11.8 keV;
λ=1.05Å

Coherence Lengths of a Storage Ring Beamline



$$\Sigma_v \approx 5 - 10\mu m$$

$$\frac{\Delta\lambda}{\lambda} = 10^{-4}$$

$$\Sigma_h \approx 100 - 200\mu m$$

Speckle

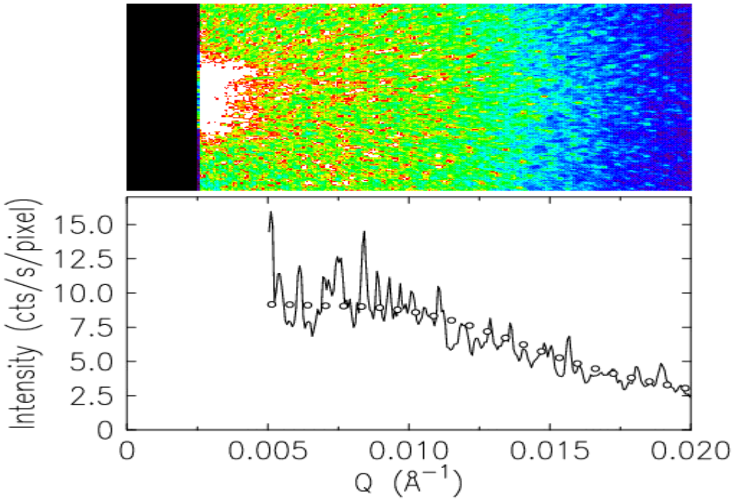
If coherent light is scattered from a disordered system it gives rise to a random (grainy) diffraction pattern, known as "**speckle**". A speckle pattern is an interference pattern and related to the exact spatial arrangement of the scatterers in the disordered system.

$$I(Q,t) \propto S_C(Q,t) \propto \left| \sum e^{iQR_j(t)} \right|^2$$

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

<u>Incoherent Light:</u> $S(Q,t) = < S_c(Q,t) >_{V \gg Vc}$ ensemble average

Aerogel
λ=1Å
CCD (22 μm)



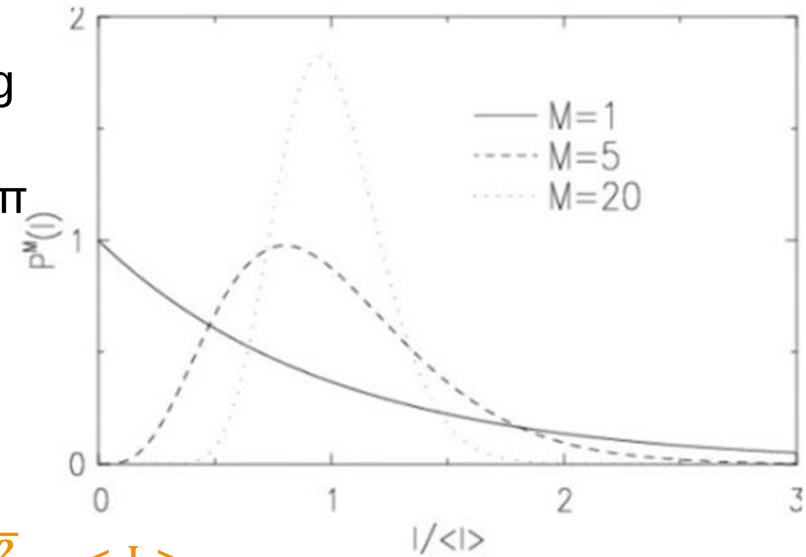
Abernathy, Grübel, et al.

J. Synchroton Rad. 5, 37, 1998

Speckle Statistics

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:

$$P(I) = \left(\frac{1}{<I>}\right) e^{\frac{-I}{<I>}}$$



Mean: $< I >$ **Std. Dev. σ:** $\sqrt{< I^2 > - < I >^2} = < I >$

Contrast: ß = σ²/ $< I >^2$ **= 1**

Partially coherent illumination: the speckle pattern is the sum of M independent speckle patterns

$$\mathbf{P_M(I) = M^M \bullet \frac{\left(\frac{1}{<I>}\right)^{M-1}}{\Gamma(M)<I>} \bullet e^{-\frac{MI}{<I>}}}$$

Mean: $< \mathbf{I} >$; $\boldsymbol{\sigma} = \frac{\mathbf{<I>}}{\sqrt{\mathbf{M}}}$ ß = 1/M

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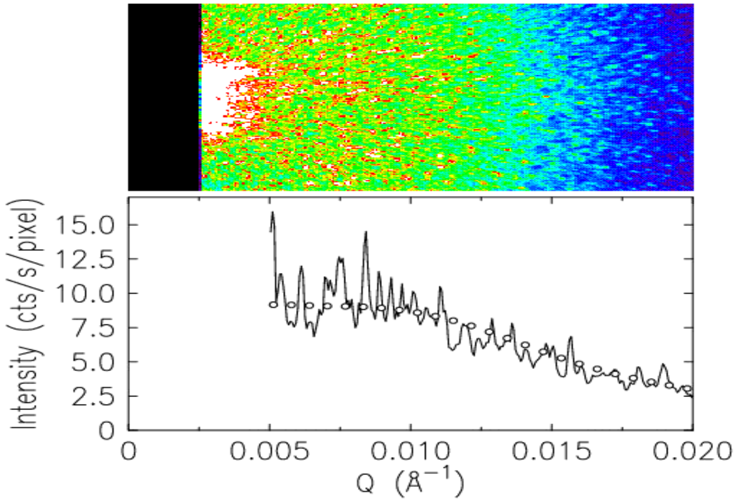
j in coherence volume $V_c = \xi_t^2 \xi_l$

Incoherent Light: $S(Q,t) = \langle S_c(Q,t) \rangle_{V \gg V_c}$ ensemble average

Aerogel
λ=1Å
CCD (22 μm)

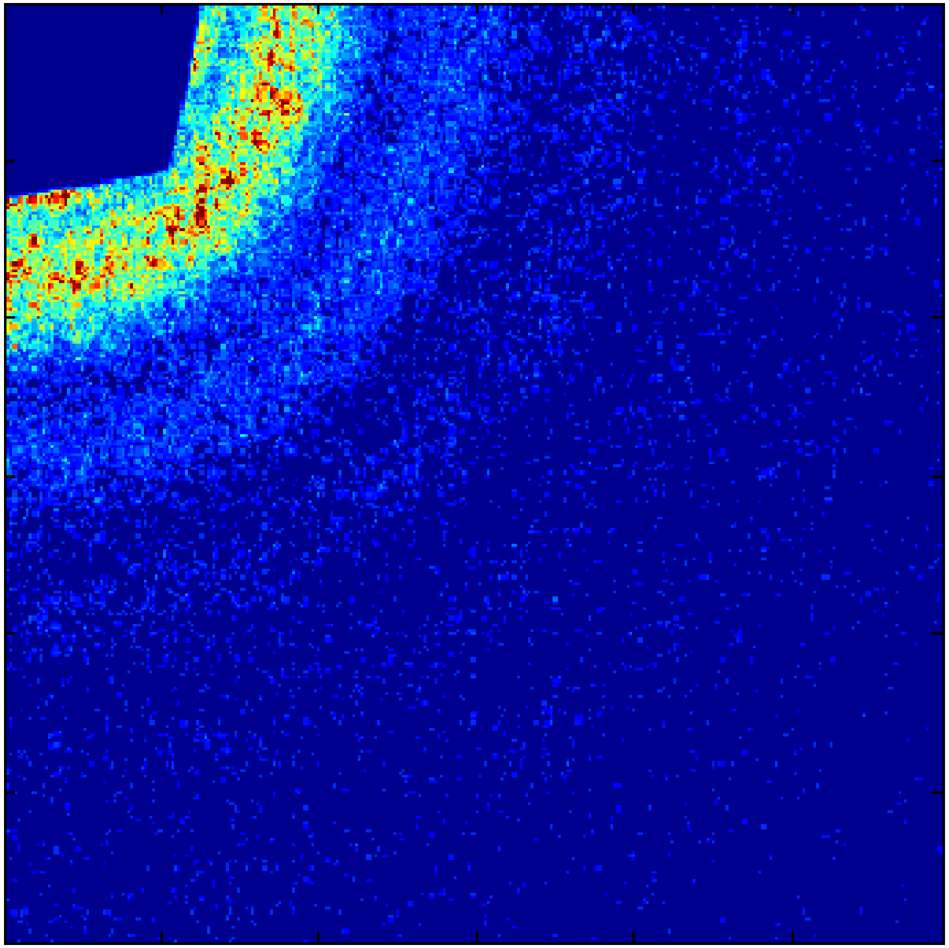


Abernathy, Grübel, et al.

J. Synchroton Rad. 5, 37, 1998

Fluctuating Speckle Patterns

Silica: 2610 Å, $\frac{\Delta R}{R} = 0.03$, 10 vol% in glycerol, $T = -13.6$ °C, $\eta \approx 56000$ cp



V. Trappe
& A. Robert

X-Ray Photon Correlation Spectroscopy (XPCS)

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

$$I(Q,t) = |E(Q,t)|^2 = \left| \sum b_n(Q) e^{iQ \bullet r_n(t)} \right|^2$$

<u>Note:</u> E(Q,t) = ∫ dr' ρ(r') $e^{iQ \bullet r'(t)}$ ρ(r'): charge density

If E(Q,t) is a zero mean, complex Gaussian variable:

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

<>: ensemble av.; ß(Q): contrast

$g_2(Q,t) = 1 + ß(Q)\,|f(Q,t)|^2$ with f(Q,t) = S(Q,t)/S(Q,0)

S(Q,0): static structure factor N: number of scatterers

$$S(Q,t) = \frac{1}{N\{b^2(Q)\}} \Sigma_{m=1}^{N} \Sigma_{n=1}^{N} < b_n(Q) b_m(Q) e^{iQ[r_n(0) - r_m(t)]} >$$

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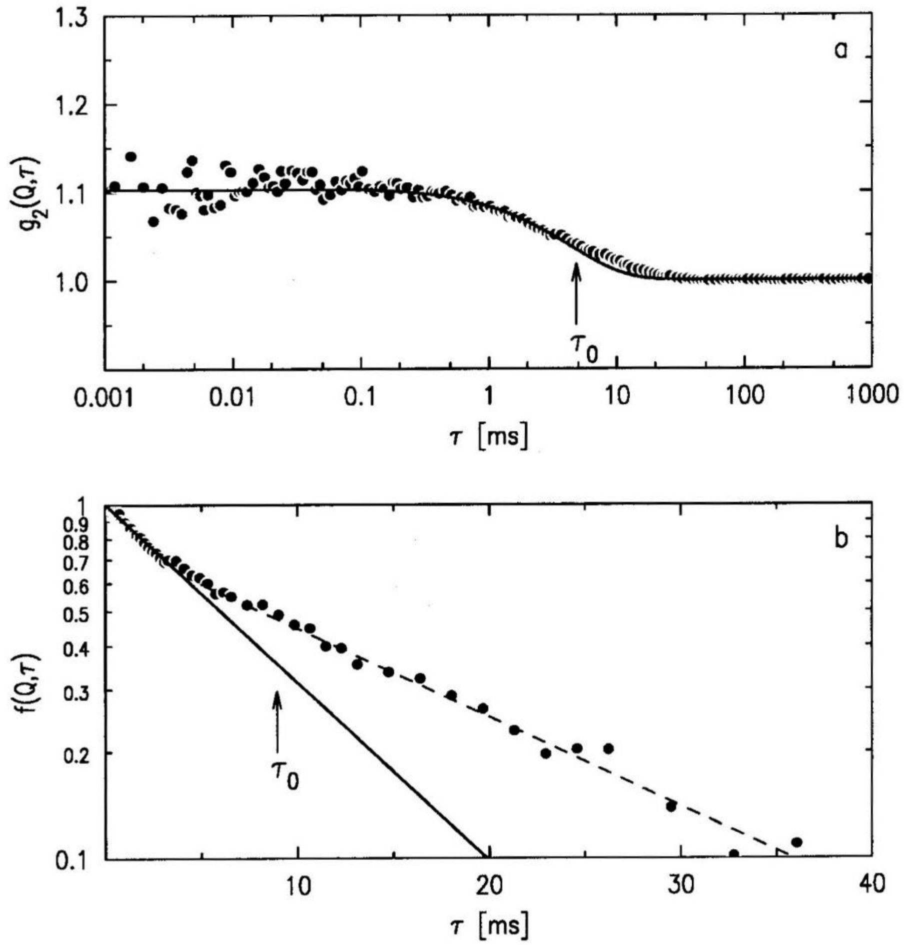
Time Correlation Function $g_2(Q,t)$

$$g_{2}(Q,t) = 1 + ß(Q)|f(Q,t)|^2 \text{ and } f(Q,t) = e^{(-\Gamma t)} = e^{\left(\frac{-t}{\tau_0}\right)}$$



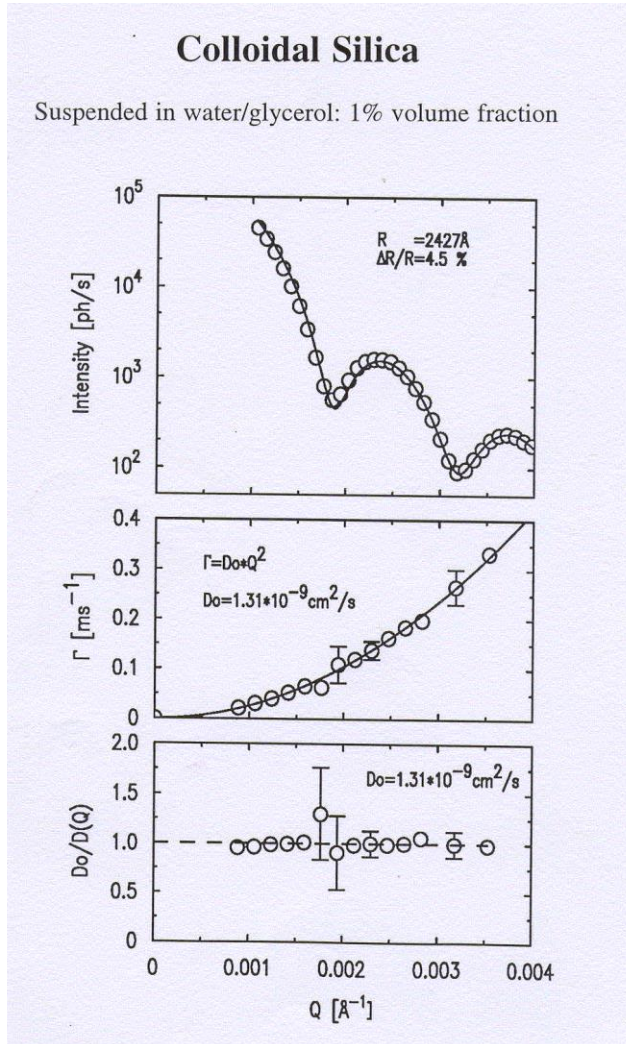
Dynamics in a Dilute, Non-interacting System

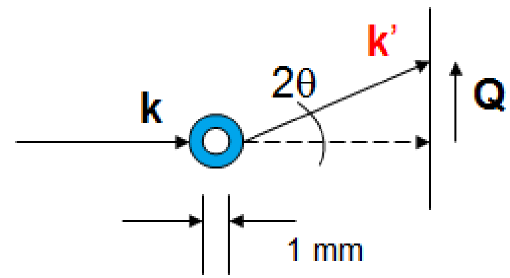
$$I \sim |F(Q)|^2 S(Q)$$

$$\sim \left[\frac{\sin QR - QR\cos QR}{(QR)^3}\right]^2$$

$$\Gamma = D_0\, Q^2$$

$$D_0 = \frac{k_B T}{6\pi\eta R}$$





Q = k'- k

Q = 2k sinθ

k = 2π/λ

G. Grübel, A. Robert, D. Abernathy
8th Tohwa University International
Symposium on "Slow Dynamics in
Complex Systems", 1998, Fukuoka, Japan

Outlook

Imaging Holographic Imaging, Ptychography,….

Impact of FEL sources……

XPCS Equilibrium, non-equilibrium dynamics delay line techniques at FEL sources…..