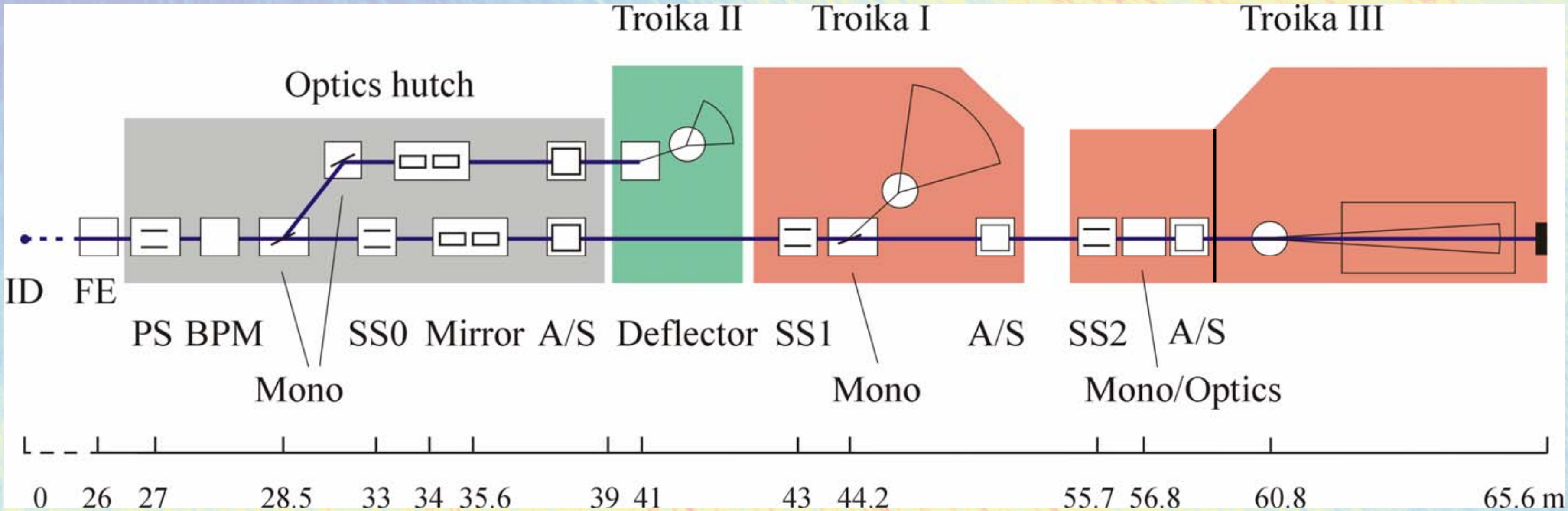
Status and Perspectives for XPCS

New Possibilities for XPCS at the ERL ?

Towards The Ultimate XPCS Beamline

- Is (focusing) optics useful ?
- Can beam induced sample damage be avoided ?
- Which detector could we dream about (and what is available) ?
- Time structure ?
- How can the s/n ratio of XPCS be improved ?

The TROÏKA beamline



ID10A (open undulator beamline) comprises two stations: **TROÏKA I** and **TROÏKA III**

TROÏKA I in user mode since 1994, TROÏKA III in operation since ~2002

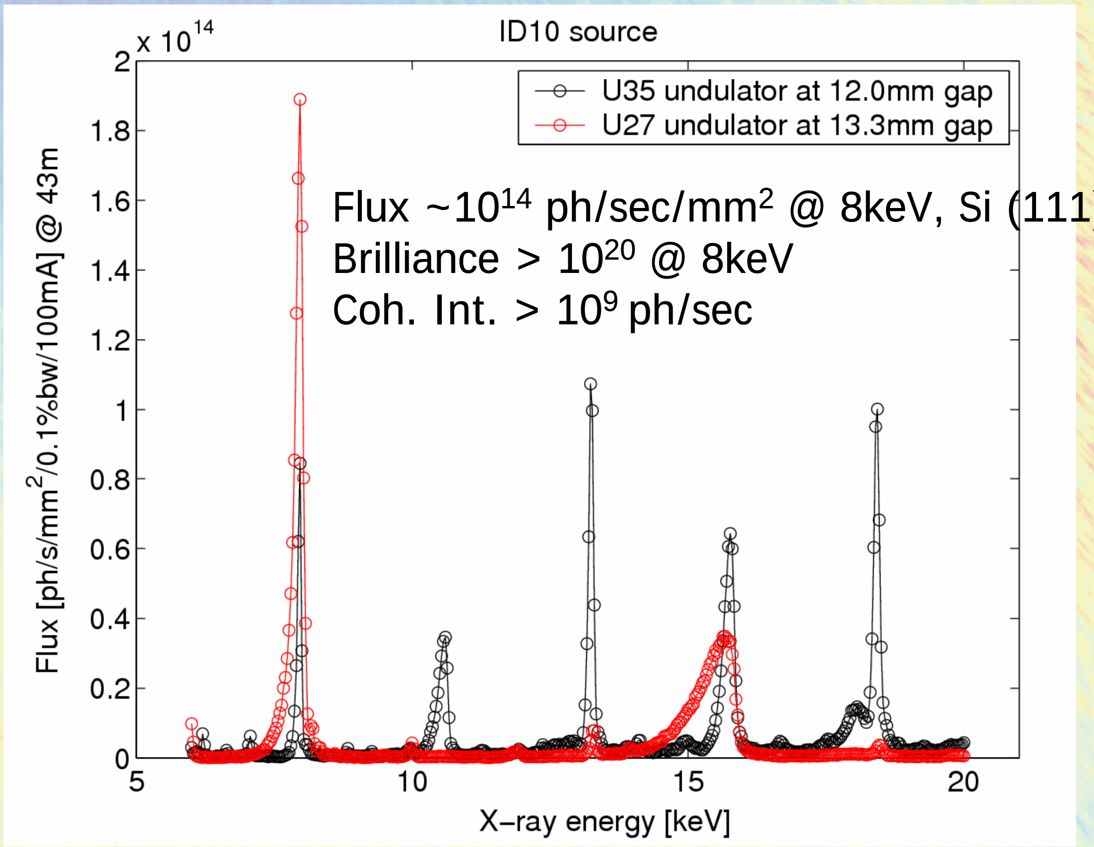
Techniques:

TROÏKA I : High resolution diffraction and surface scattering with coherent X-rays, XPCS

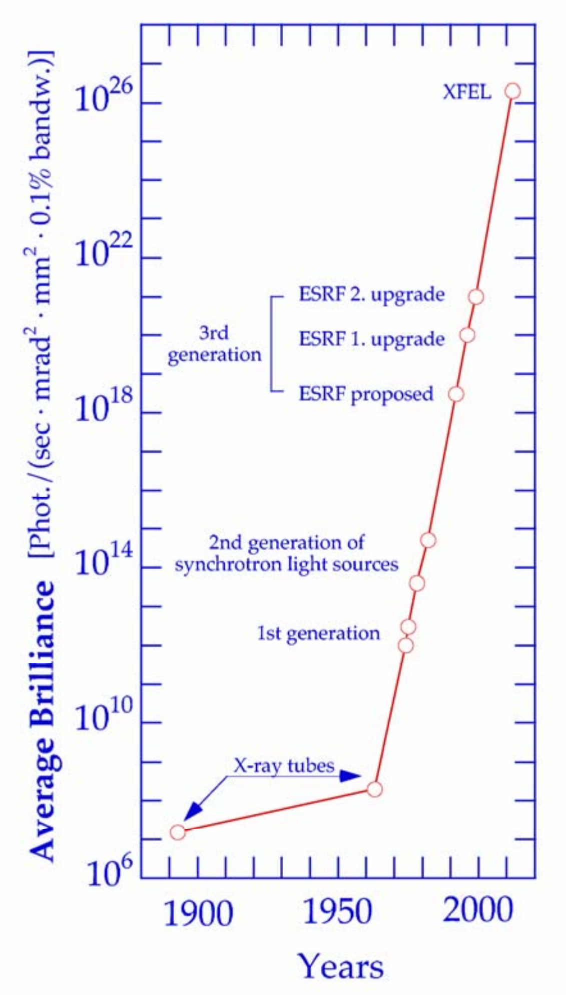
TROÏKA III : Small Angle X-ray Scattering, XPCS, Pink and White beam options

The ID10 undulator source

- U27 undulator (27 mm period), U35 undulator (35mm period), min. gap 11mm
- Revolver unit U27/U35, in-situ exchangeable



Flux ~10^{14} ph/sec/mm^2 @ 8keV, Si (111)
Brilliance > 10^{20} @ 8keV
Coh. Int. > 10^9 ph/sec

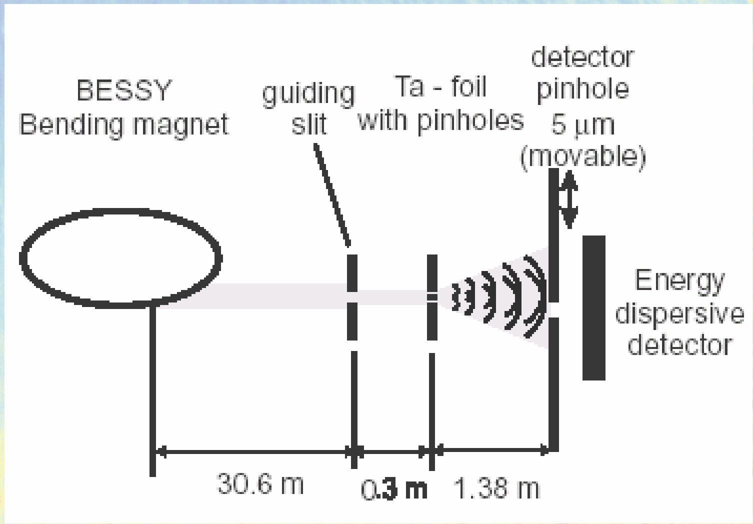


- Source size (FWHM): 23(v) x 928(h) μm (high-β)
- Beam divergence (FWHM): 17(v) x 28(h) mrad

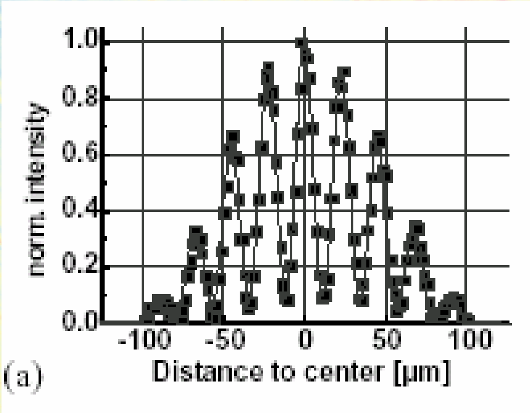
ESRF

Partially coherent light: Coherence lengths

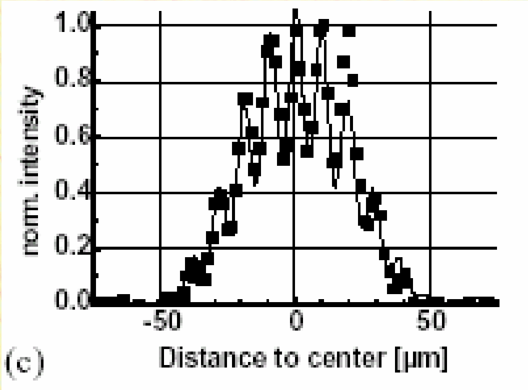
Example: Young's double slit experiment with X-rays



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



λ=2.1Å, d=11μm
Visibility(β) ~ 80%



λ=0.9Å, d=11μm
Visibility(β) ~ 30%

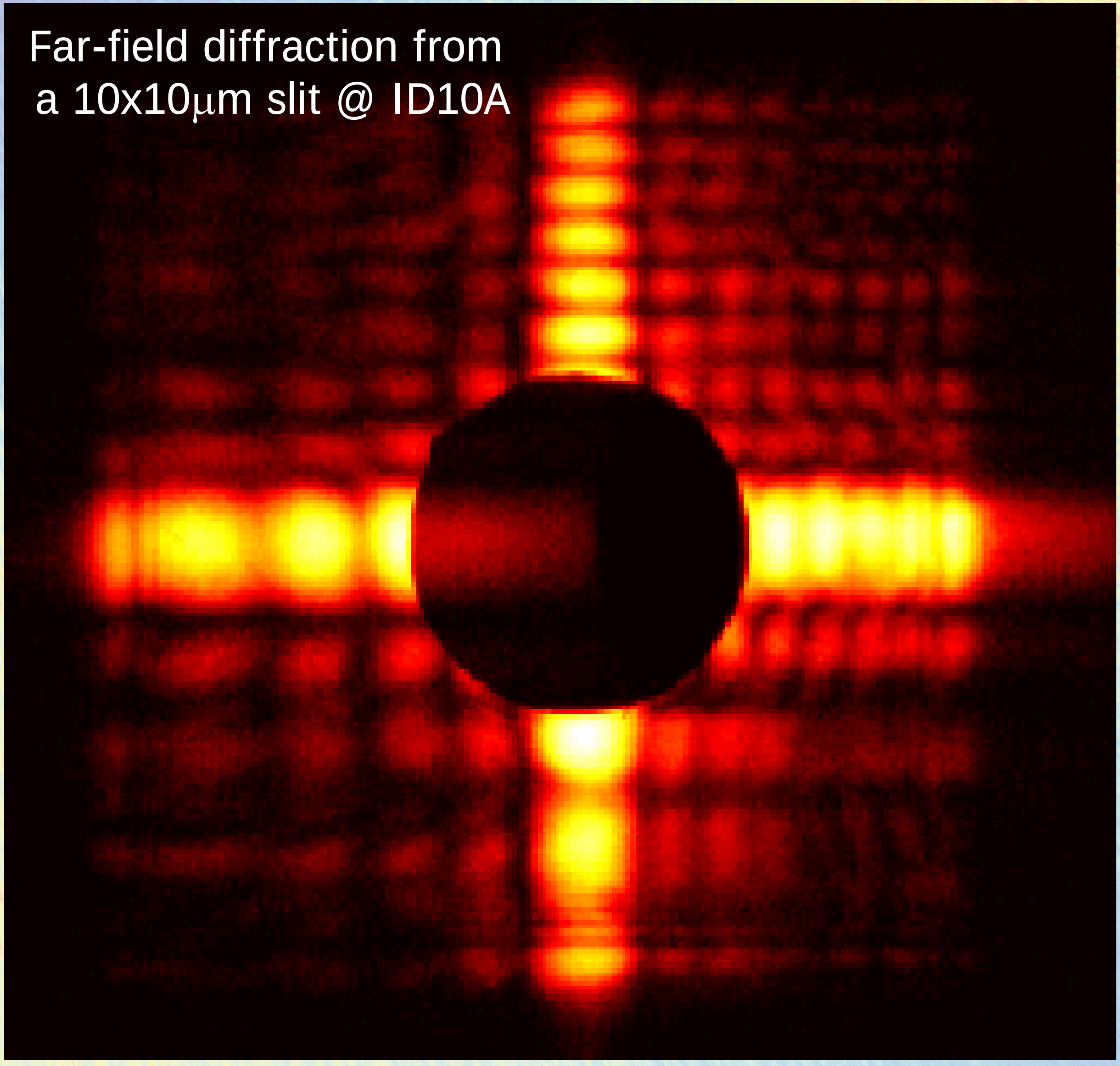
$\Delta y = \lambda L/d$

Transverse coherence length (v,h) : $l_{v,h} = \lambda L/\pi d_{v,h}$ (~2-150 μm)

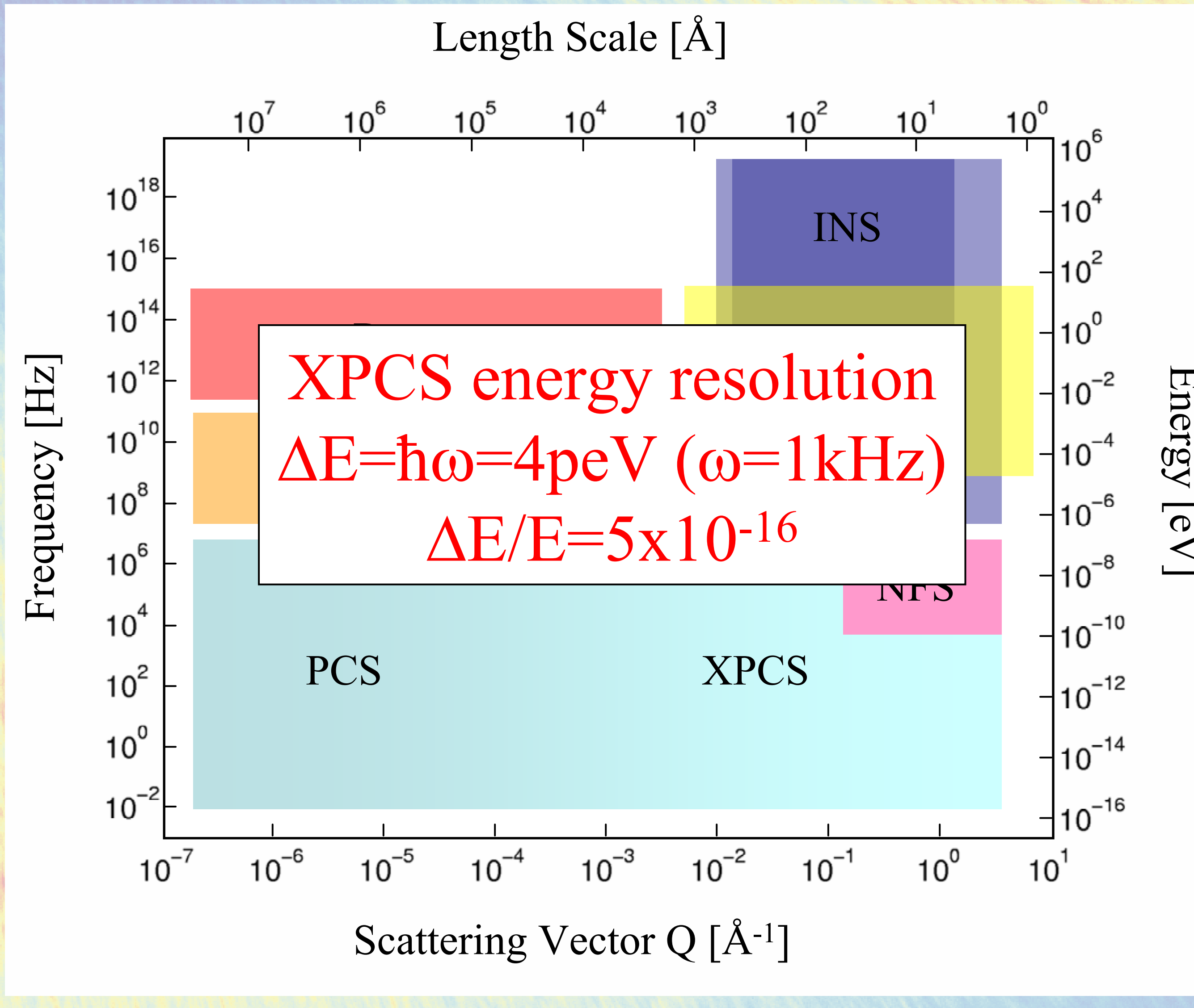
Longitudinal coherence length $l_l = \lambda/(\pi\Delta\lambda/\lambda)$ (~1μm)

$\beta \approx Vc/Vs$

Diffraction imaging with partially coherent X-rays



XPCS vs. other “dynamic” scattering techniques



ESRF

Important source parameters

Brilliance B = photons/sec / [source area × solid angle × bandwidth]

Lateral coherence area $A_t = \pi l_h l_v / 4 = (\lambda L)^2/(4\pi d_h d_v)$ (~200 μm^2)

N_c=photons in V_c ($V_c = A_t \times l_l$)

Coherent solid angle $\Omega_C = A_t/L^2 = \lambda^2/(4\pi d_h d_v) = \lambda^2/16A_s$

$N_c = B \times \tau_0 \times A_s \times \lambda^2/16A_s \times \Delta\nu/\nu = B\,\lambda^3/(16\pi c)$ $\tau_0 = l_l/c$ (10^{-15}-10^{-14} s)

Coherent intensity $I_c = (N_c/V_c) \times c \times A_t$

$= B \times (\lambda/4)^2 \times (\Delta\lambda/\lambda)$ (~10^9-10^{10} ph/s)

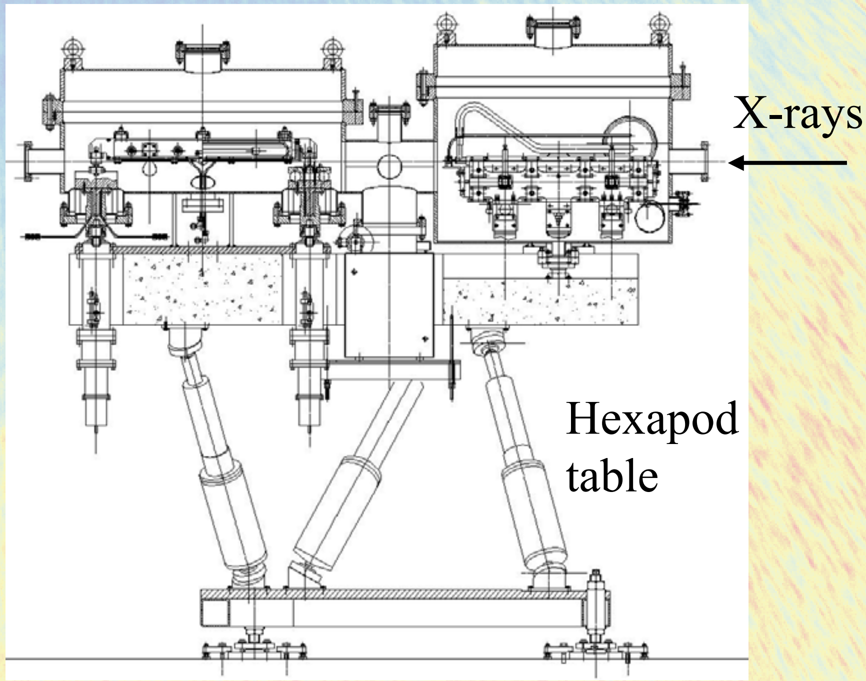
Coherent intensity decreases with decreasing λ (increasing energy) !

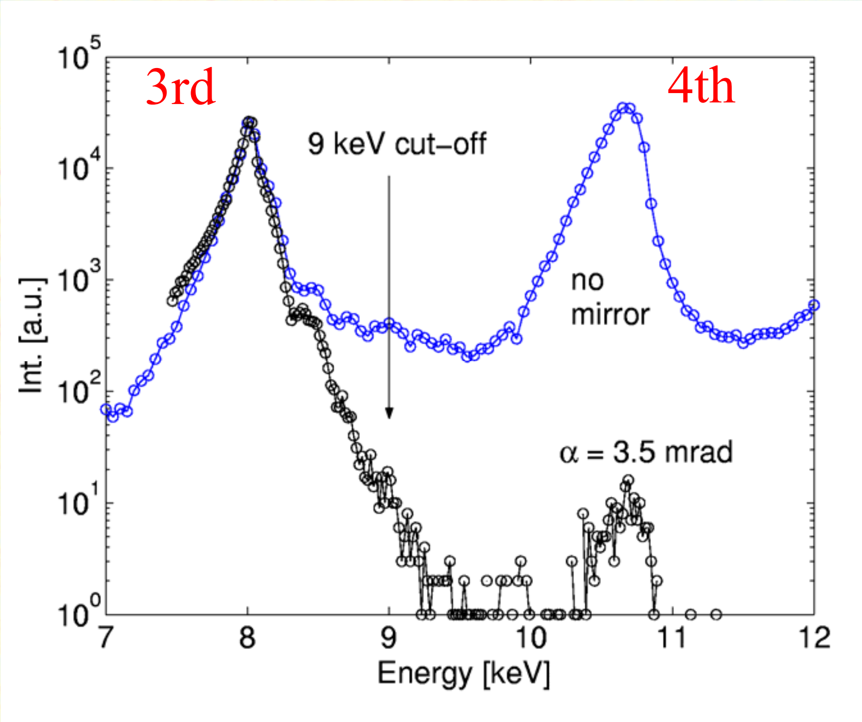
Coherent scattering is very Brilliance-hungry !

Double mirror/thermal bender

Location: optics hutch 35m from source, 25m from sample (Troika III)

Typical working parameters:
α=3.5 mrad (cut 4th harmonics)





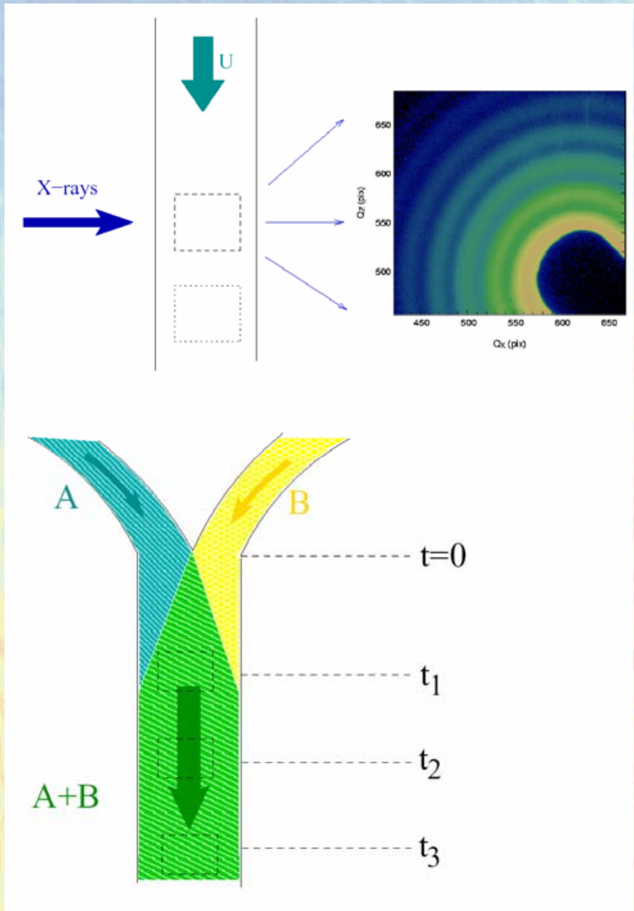
1st mirror (500x50x115 mm), top cooled three stripes: Pd, Pt and Si. Thermal bender
2nd mirror: Piezo actuator to correct beam position via an ion-chamber BPM

Pink beam with $\Delta E/E$=1.5%
Pink flux >1x10^{11} ph/sec/100μm^2

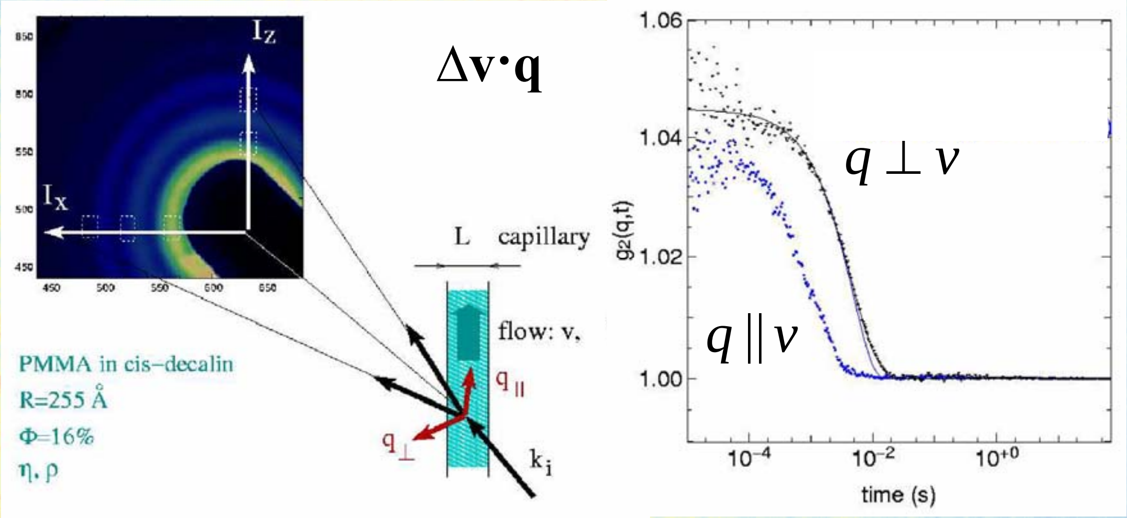
BEAM DAMAGE !!

A flowcell for XPCS applications

Flow/mixing cell: mixing kinetics, Protein folding kinetics, etc..



Flowcell: To avoid beam-damage.
How are XPCS results influenced by the flow ?



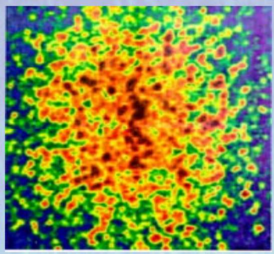
$q \perp v : g^{(2)} \sim 1 + \exp(-2\Gamma t)$

$q \| v : g^{(2)} \sim 1 + G(t)\exp(-2\Gamma t)$; G(t) some Bessel function

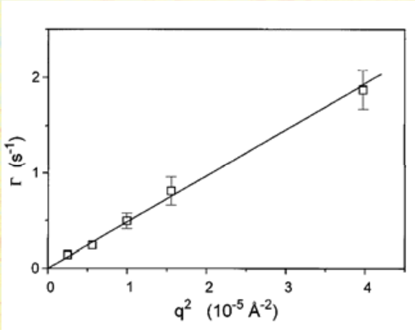
work in progress……..

(Fluerasu, Moussaid, Falus & Madsen)

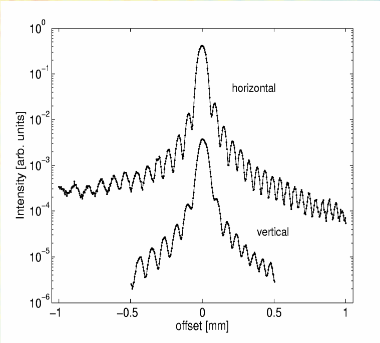
XPCS Highlights

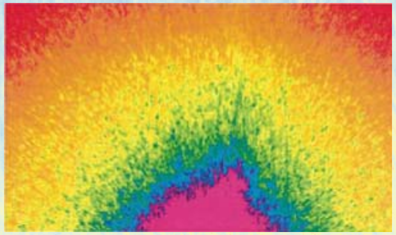


Critical dynamics in Fe_3Al
S. Brauer et al. PRL (1995)



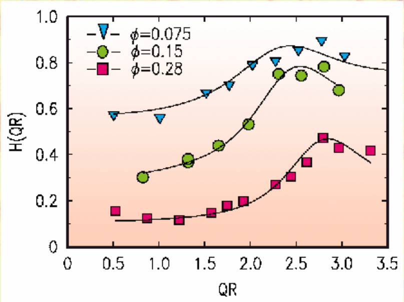
Diffusion of colloidal Pd
T. Thurn-Albrecht et al. PRL (1996)



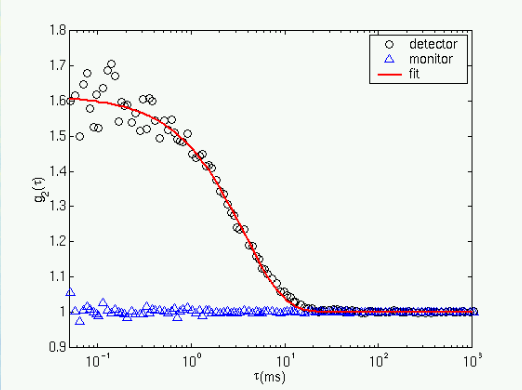


Dynamics of Block Copolymers micelles
S. G. J. Mochrie et al. PRL (1997)

Hydrodynamic screening of charge-stabilized colloids
D. O. Riese et al. PRL (2000)



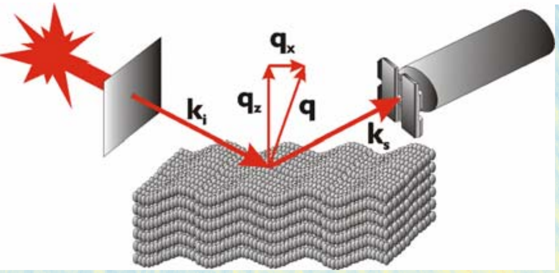
Freezing of surface capillary waves
T. Seydel et al. PRB (2001)



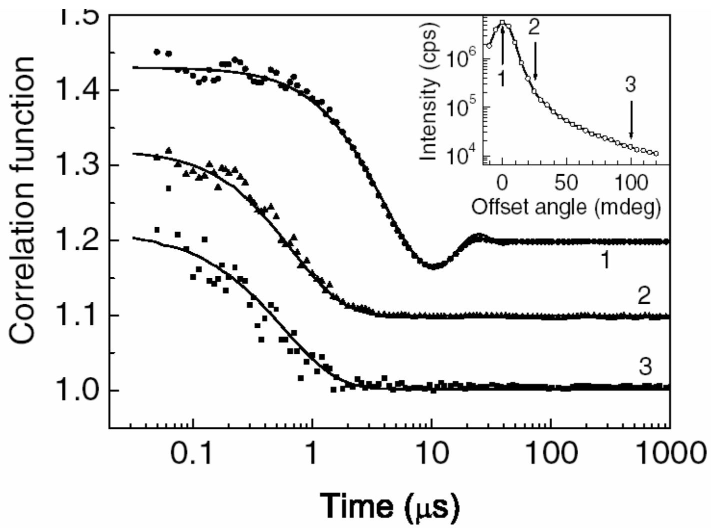
VOLUME 88, NUMBER 11 PHYSICAL REVIEW LETTERS 18 MARCH 2002

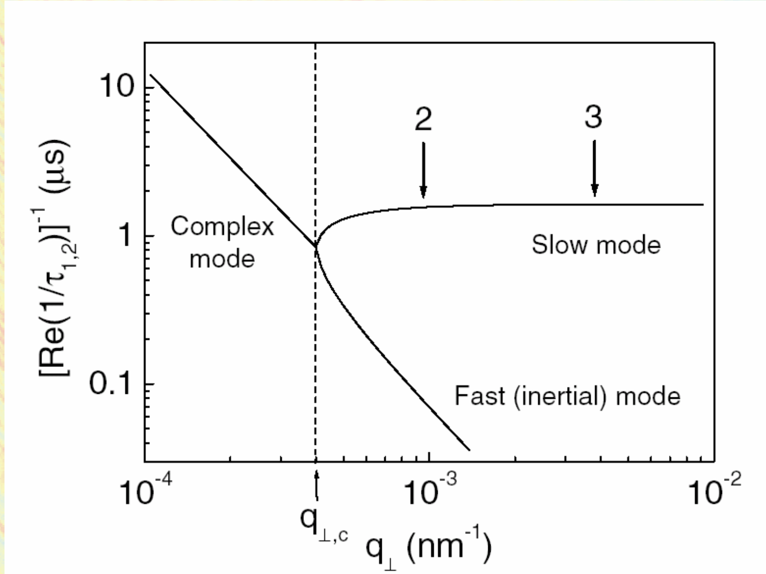
Smectic Membranes in Motion: Approaching the Fast Limits of X-Ray Photon Correlation Spectroscopy

Irakli Sikharulidze,[1] Igor P. Dolbnya,[2] Andrea Fera,[1] Anders Madsen,[3]
Boris I. Ostrovskii,[1,4] and Wim H. de Jeu[1]



XPCS data taken on FPP membranes
First point: 50 ns (APD detectors)





Surface regime

$q < q_c$:

complex “propagating” mode

$q > q_c$:

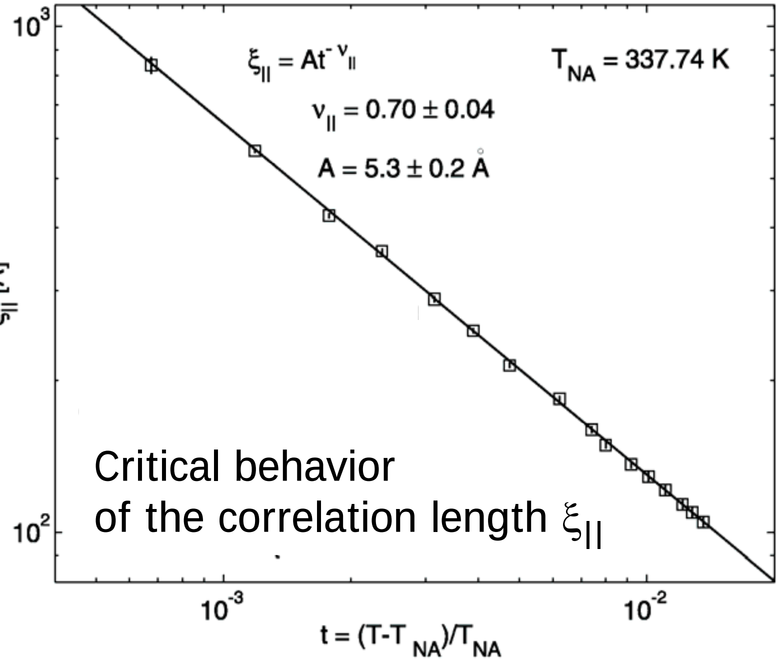
two “over-damped” modes

VOLUME 90, NUMBER 8 PHYSICAL REVIEW LETTERS week ending 28 FEBRUARY 2003

Viscosity of a Liquid Crystal near the Nematic–Smectic *A* Phase Transition

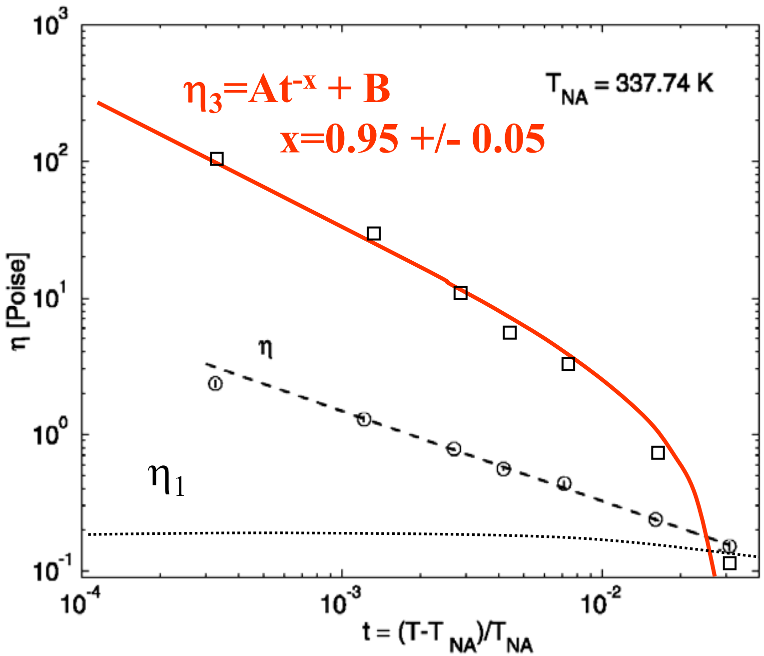
Anders Madsen,[1,*] Jens Als-Nielsen,[2] and Gerhard Grübel[1]

Static, critical scattering



Critical behavior
of the correlation length $\xi_{||}$

Critical, diverging viscosity



XPCS is signal-to-noise limited

signal-to-noise ratio of $g^{(2)}(\tau)$

$$s/n = C\,I\sqrt{N}\sqrt{T/F}$$

C: Contrast (Coherence factor)
I: Intensity
N: Number of detectors (1 for 0D, number of pixels for CCD)
T: Acquisition time
F: Frame rate (varies with lag-time τ)

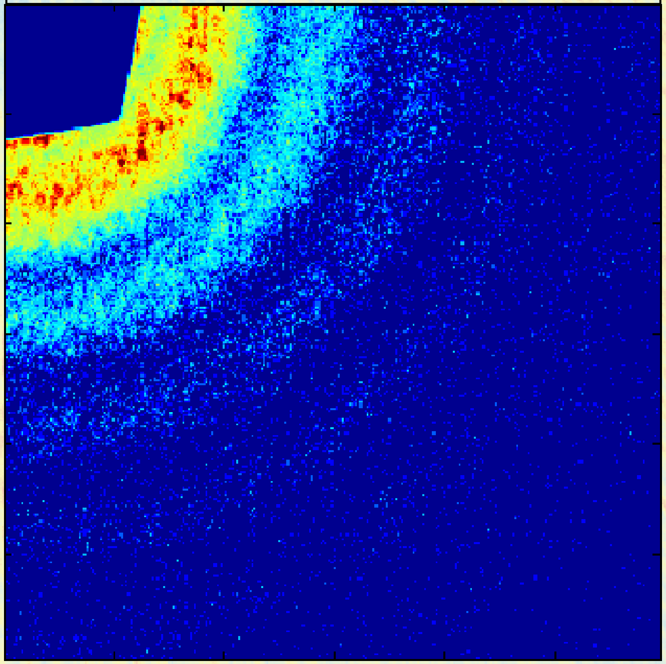
2D detection is the way to go !!!

2D-detection and XPCS

Good idea, BUT

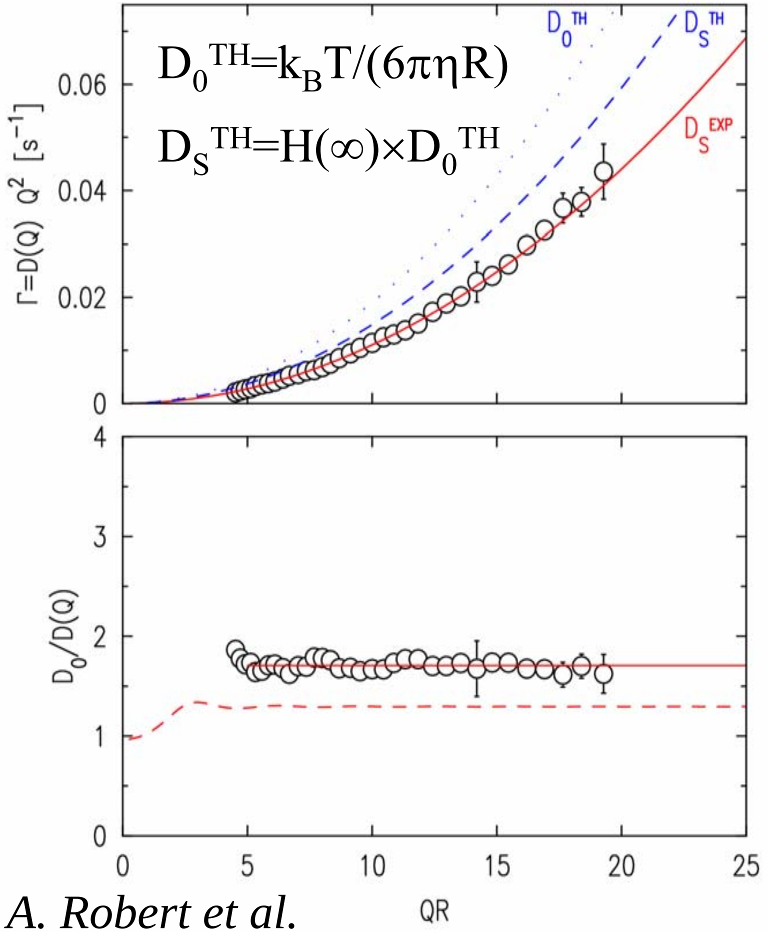
- Only a big advantage if the scattering is “2D” (e.g. transmission SAXS)
- Direct illumination CCDs are fragile (not user friendly)
- Limited by 2D detector speed

R=2610Å, δ=3%
ϕ = 10% vol. in glycerol
T = -14°C, η=560 Poise



$D_0^{TH}=k_BT/(6\pi\eta R)$

$D_S^{TH}=H(\infty)\times D_0^{TH}$



A. Robert et al.

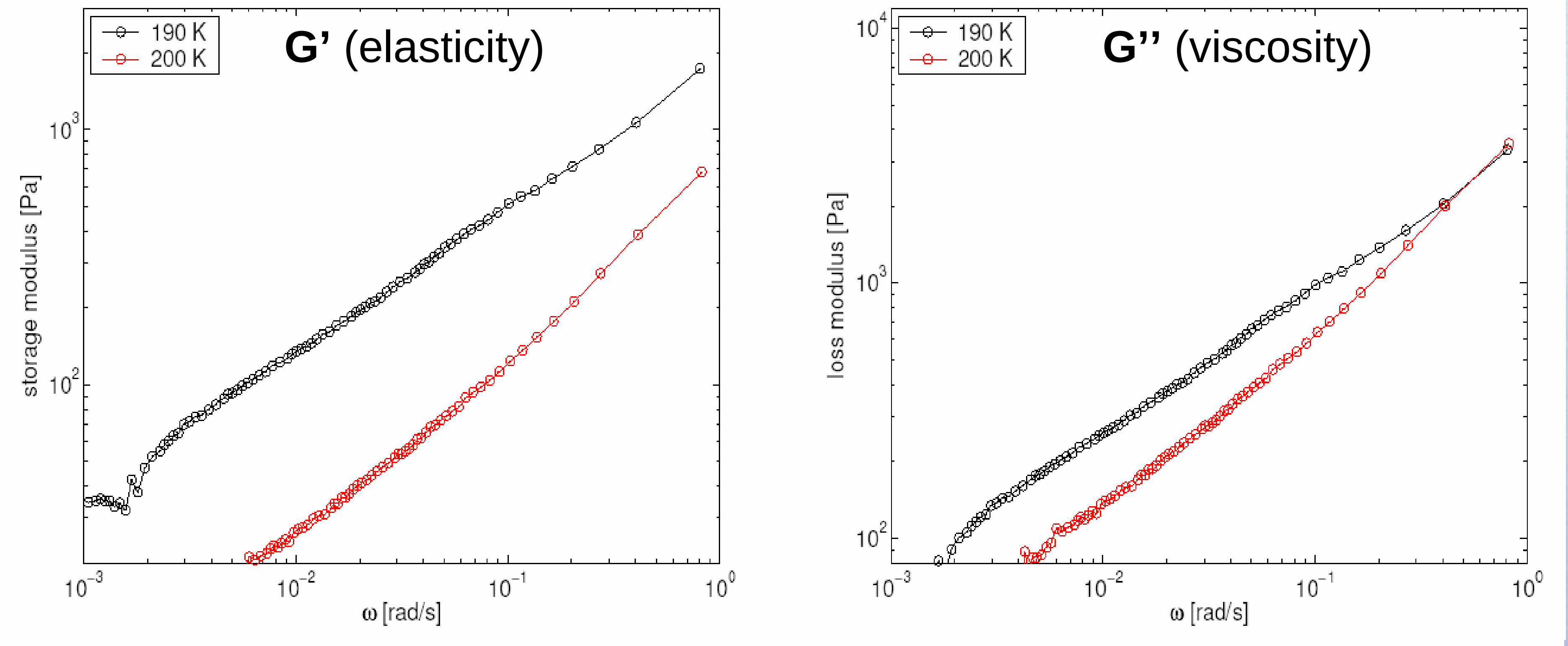
A. Madsen, Soft Materials and Nanoscience ERL Workshop, Cornell Univ. NY, June 19-20, 2006

2D-detection and XPCS

Scientific case: Micro- and nano rheology. Comparison of bulk and surface glass dynamics

Mason & Weitz, PRL (1995) ; Papagiannopoulos et al, JPCM (2005)

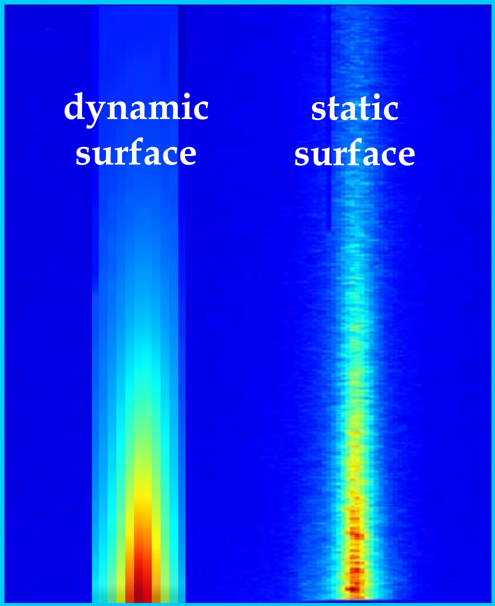
SiO_2 nano-particles (18nm) in a glass forming polymer solvent



(Caronna & Madsen, unpublished)

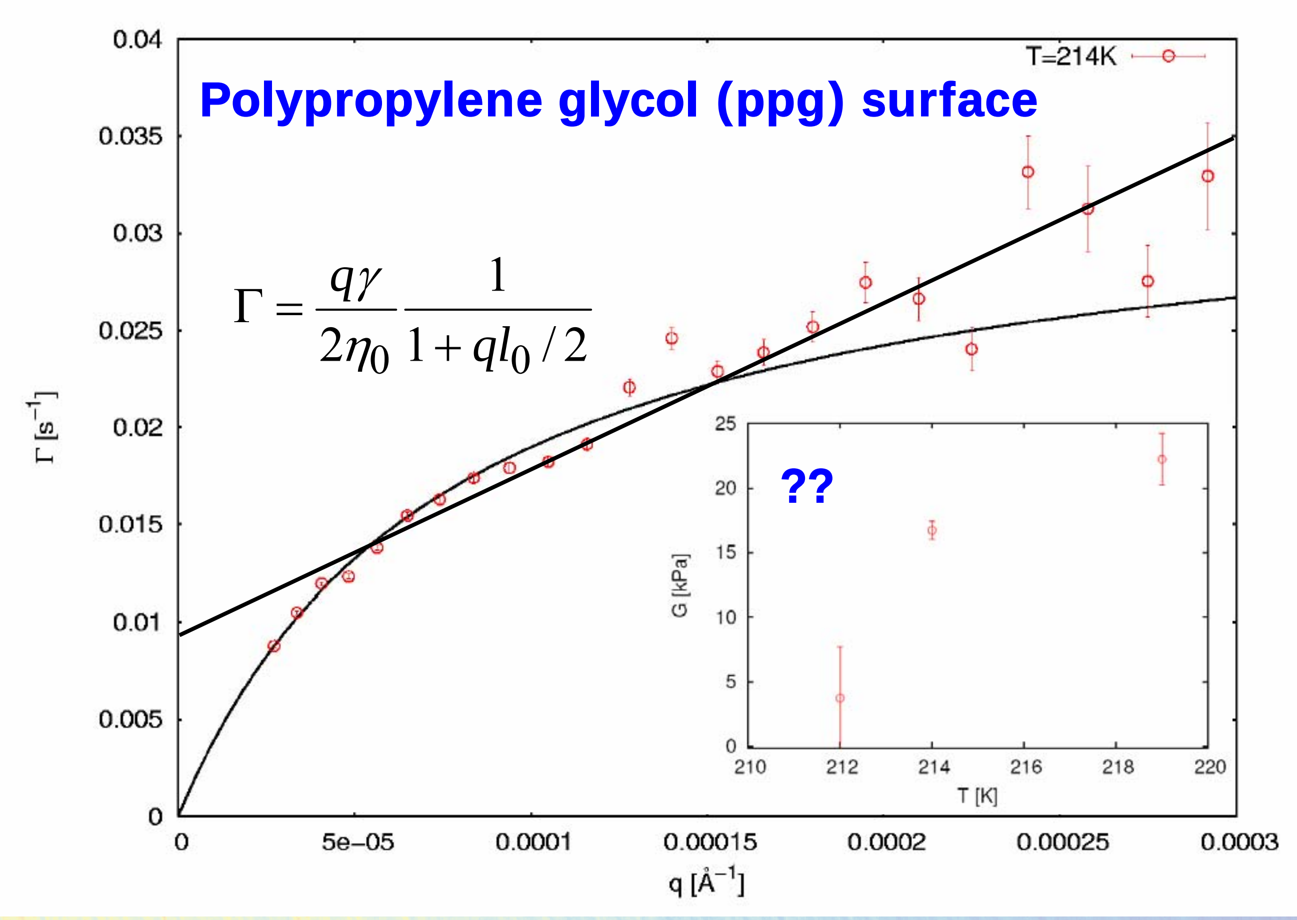
2D-detection and XPCS

Probing dynamics of a glass surface with coherent X-rays



Maxwell-Debye: $\eta(\omega) = \eta_0/(1-i\omega\tau)$

$l_0 = \gamma\tau/\eta_0$ (Jaeckle length)

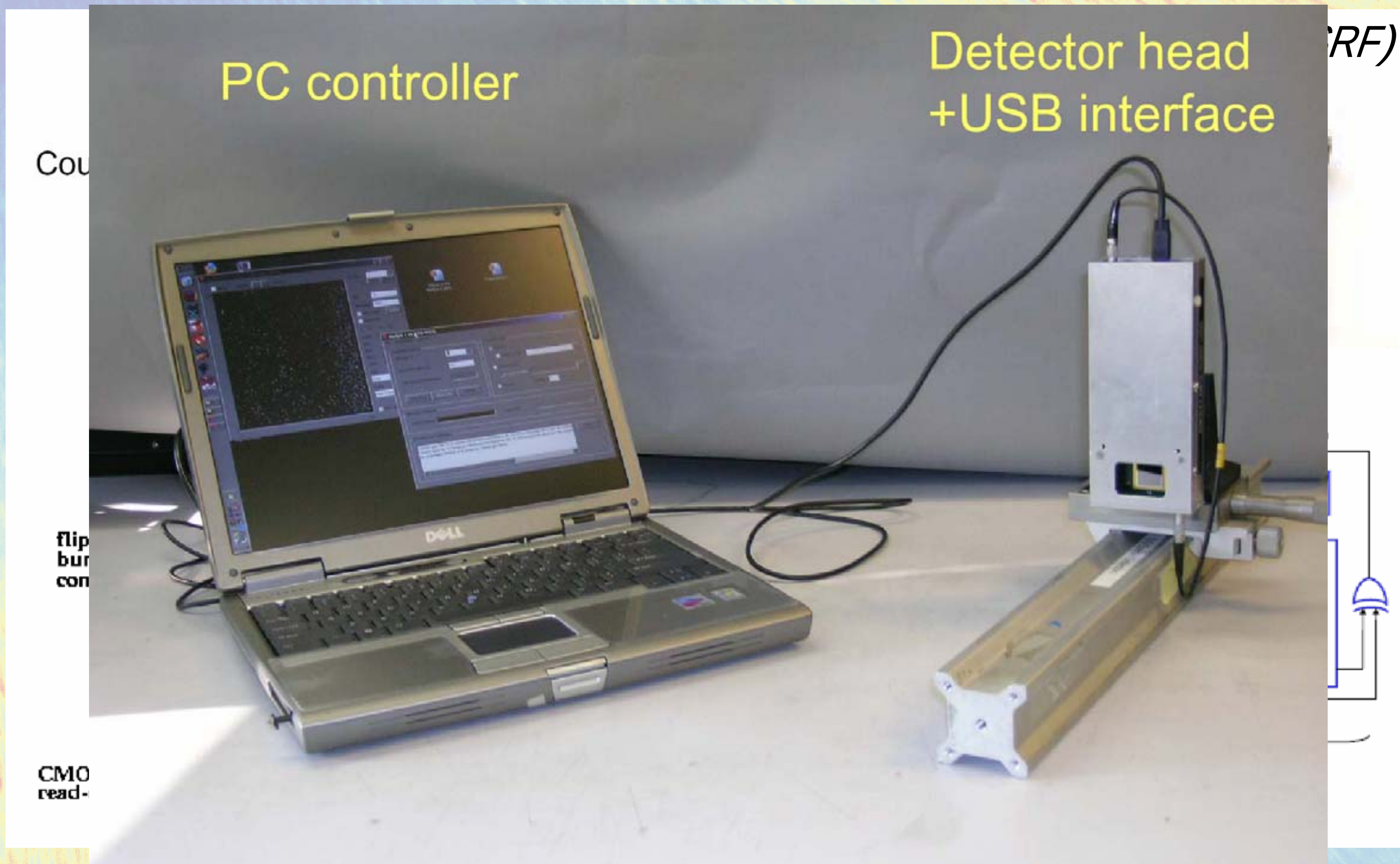


Voigt-Kelvin: $\Gamma = \frac{q\gamma}{2\eta} + \frac{E}{\eta}$

$$S(q) = \frac{k_B T}{g\rho + \gamma q^2 + 2Eq}$$

(Caronna, Sternemann, Streit, Gutt, Seydel, Tolan, and Madsen)

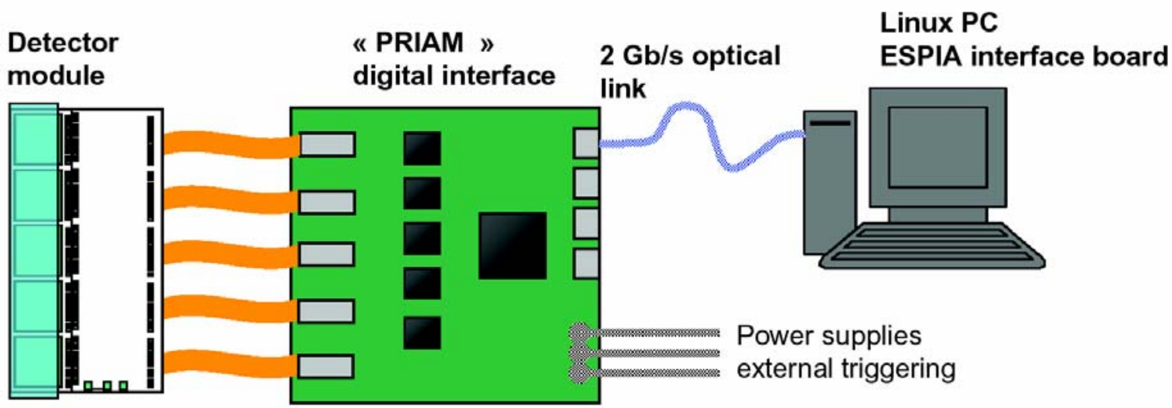
2D-detection and XPCS



(256 x 256 pixels) 55 μm pixel size
2 MHz/pixel count rate (20 bit)
Photon counting
Upper and lower energy threshold

2D-detection and XPCS

Multichip assembly for X-ray imaging based on a photon-counting pixel array



0.3 Megapixel

sub-ms readout

photon counting

- Based on Medipix-2 readout chip
- 1280 x 256 pixels (5 x 1 chips)
- **70 x 14 mm^2 detection area**
- 2 (3) sides buttable module
- 0.3 ms readout dead time
- **>1 kHz frame rate/chip frame rate**

(C. Ponchut, ESRF)

Readout speed limited by electronics.
New and faster electronics available ultimo 2006

XPCS is signal-to-noise limited

Still 2D detectors are too slow or inconvenient for certain applications
Is there a way to increase s/n by increasing the QualityFactor *CI* ?

(signal-to-noise ratio of $g^{(2)}$)

$$s/n = C\,I\sqrt{N}\,\sqrt{T/F}$$

C: Contrast (Coherence factor)
I: Intensity
N: Number of detectors (1 for 0D, number of pixels for CCD)
T: Acquisition time
F: Frame rate (varies with lag-time τ)

Optimizing the setup for XPCS

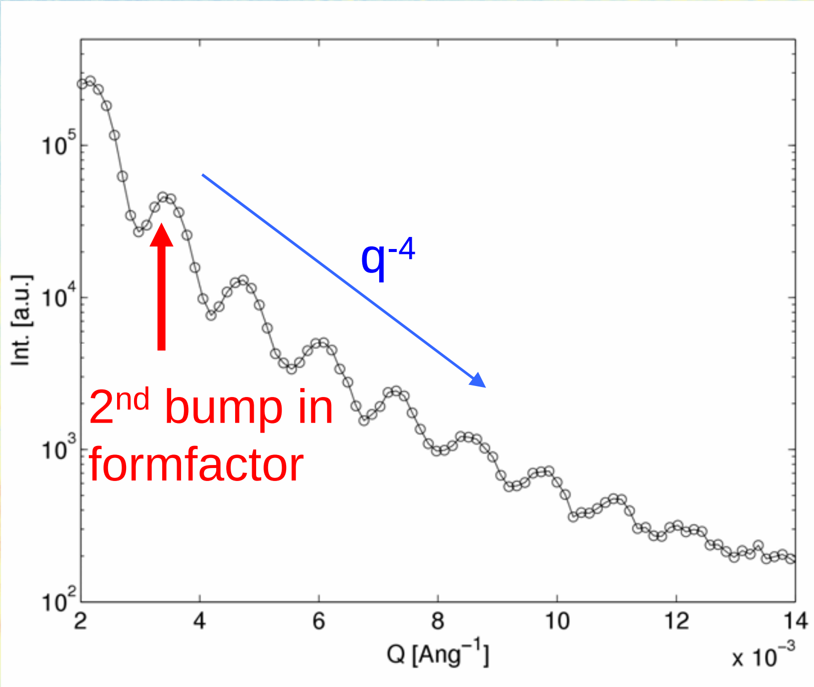
Sample: PMMA (HS) colloids in cis-decaline,
Radius ≈ 1500 Å

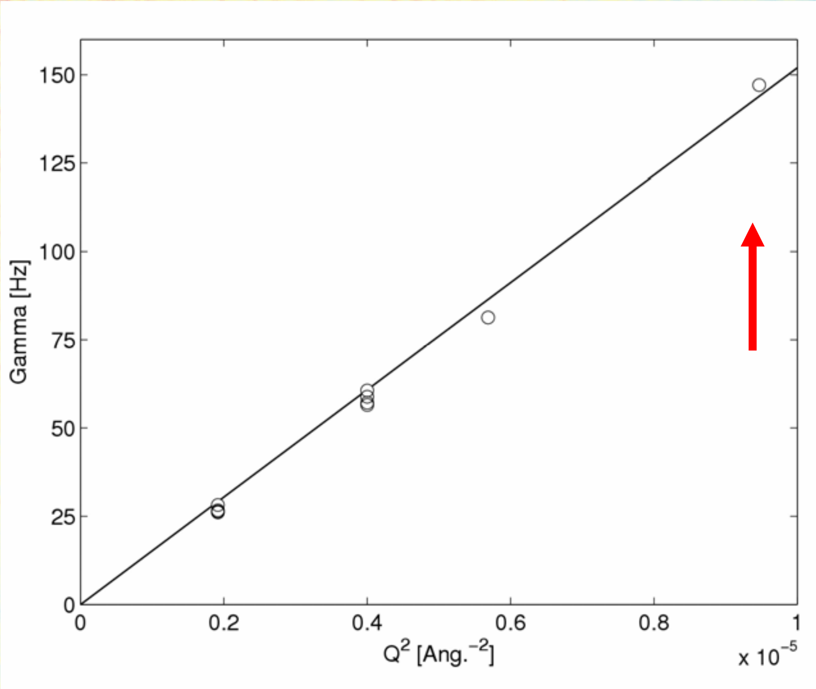
Incident flux: $6\text{x}10^8$ ph/sec/100µm^2
(100mA, 8keV, no focusing)

$$\Gamma = D(Q)Q^2$$

$$D(Q) = H(\infty)D_0$$

$$D_0 = k_B T/(6\pi\eta R)$$



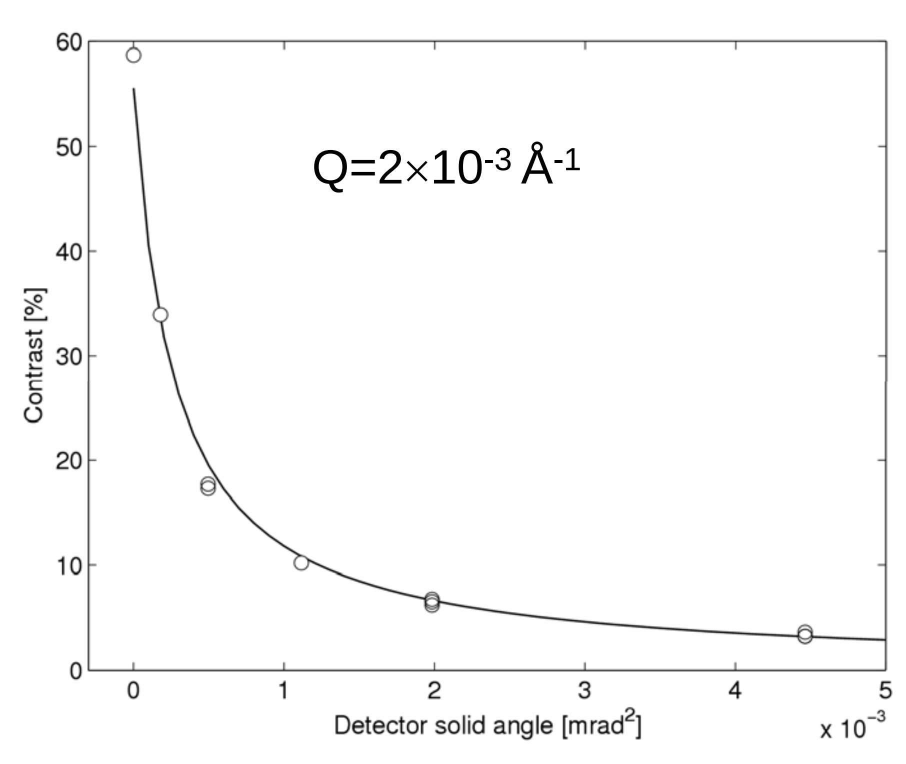


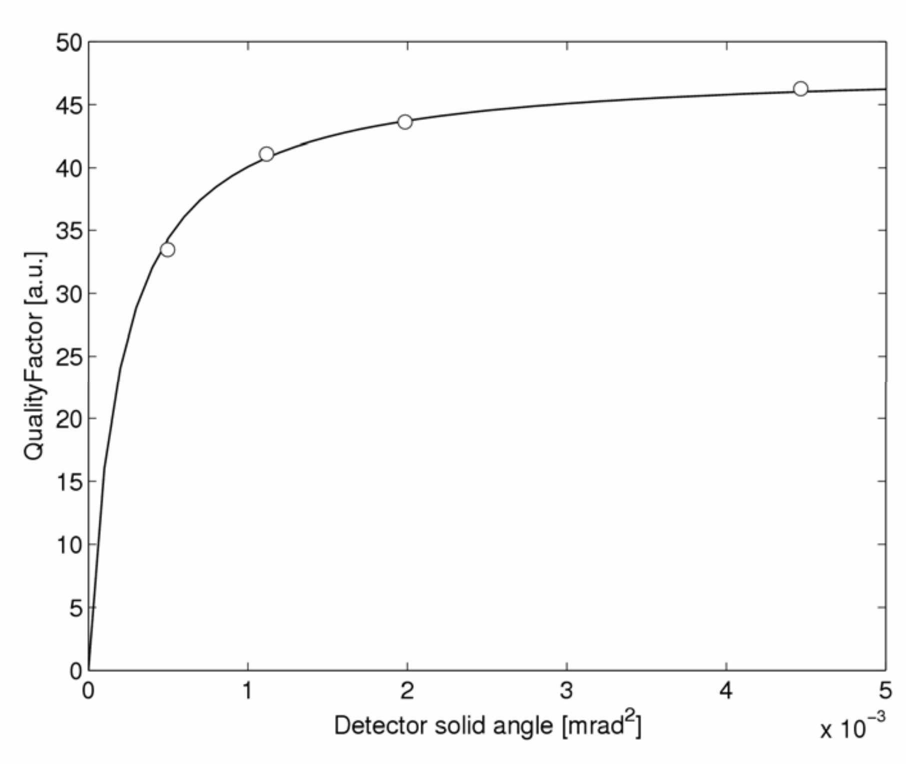
Optimizing the setup for XPCS

Is it possible to increase the QualityFactor on the detector side?

$$C(\Omega) \approx \frac{C_0}{\Omega + \Omega_0} \qquad I(\Omega) = I_0\Omega$$

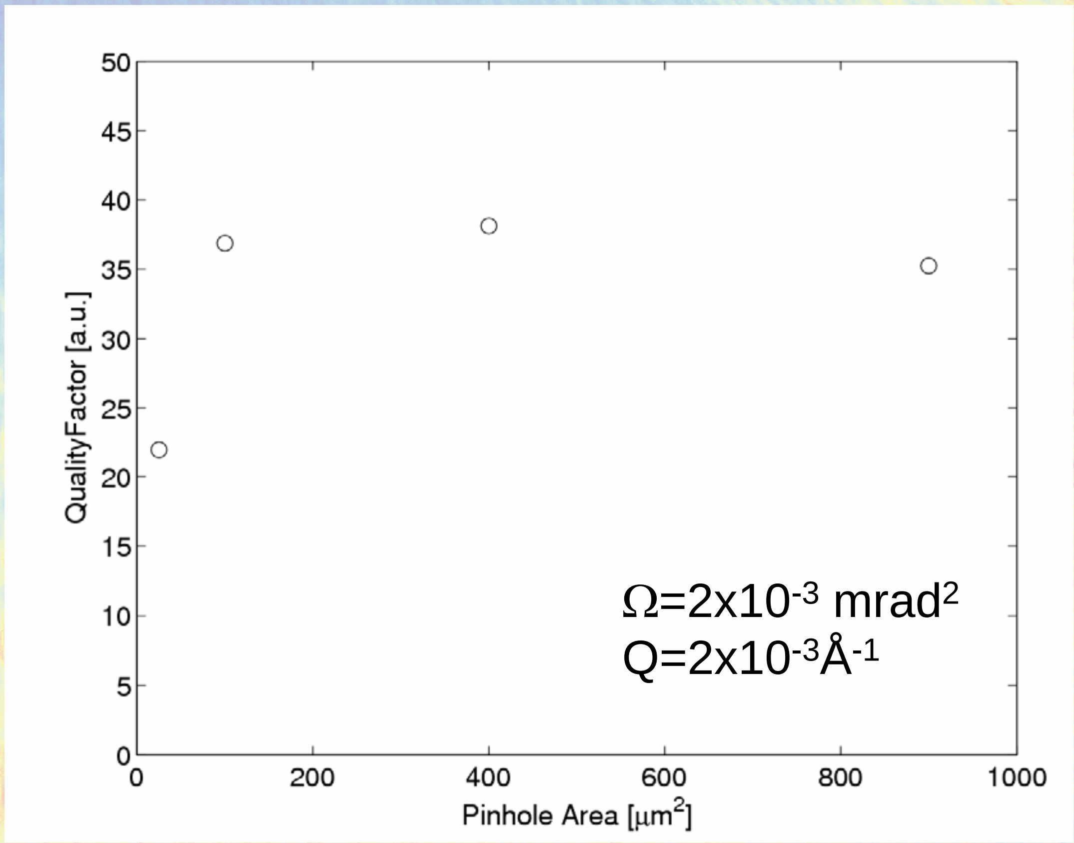
$$QF = CI = C_0 I_0 \frac{\Omega}{\Omega + \Omega_0} \rightarrow C_0 I_0 \;\; for\ \Omega >> \Omega_0$$



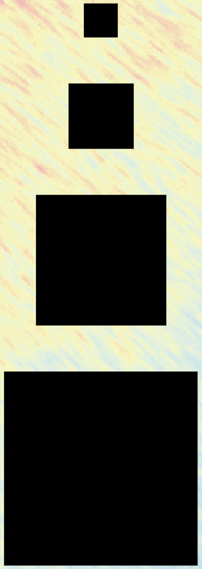


Optimizing the setup for XPCS

Is it possible to increase the QualityFactor on the incident side ?



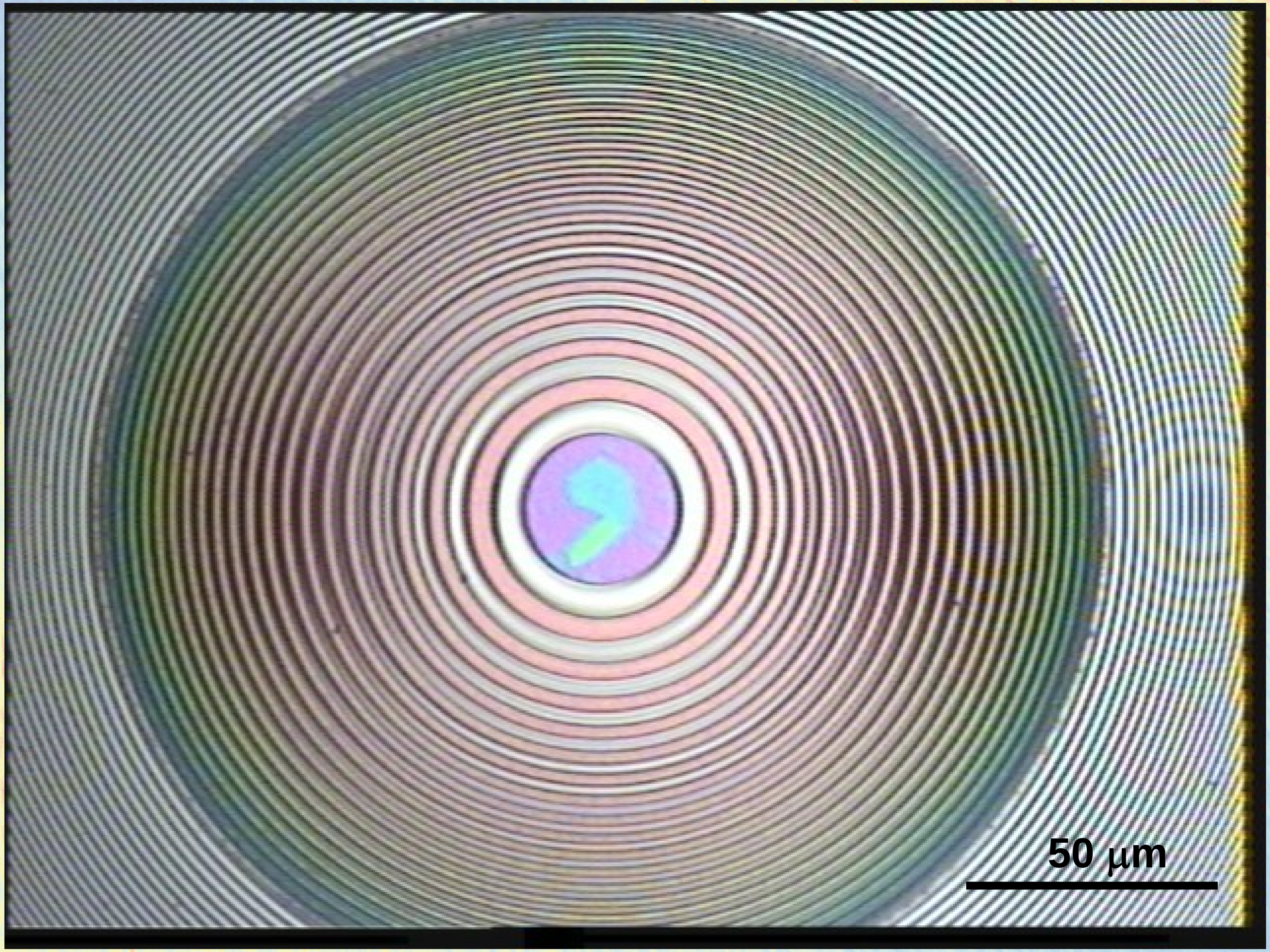
Incident beam



☝ Let’s insert some focusing optics ☝

Optimizing the setup for XPCS

Fresnel Zone Plate, pure Si (phase object)
f=1.5 m @ 8keV, OD=580μm, Δr_n=400nm. Efficiency ~25%

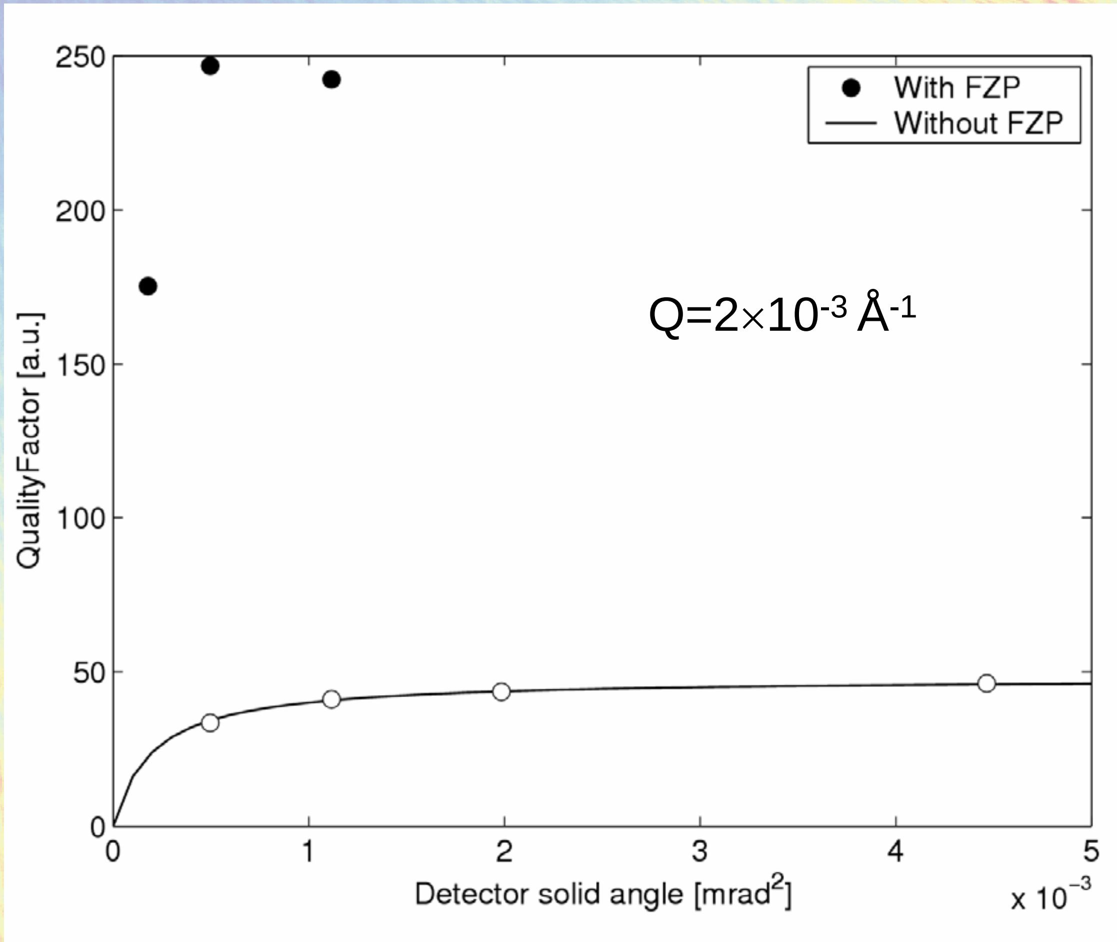


Upstream slit to define horizontal sec. source

Beamsize ~1 x 1 μm

Intensity ~10^{11} ph/sec

Optimizing the setup for XPCS

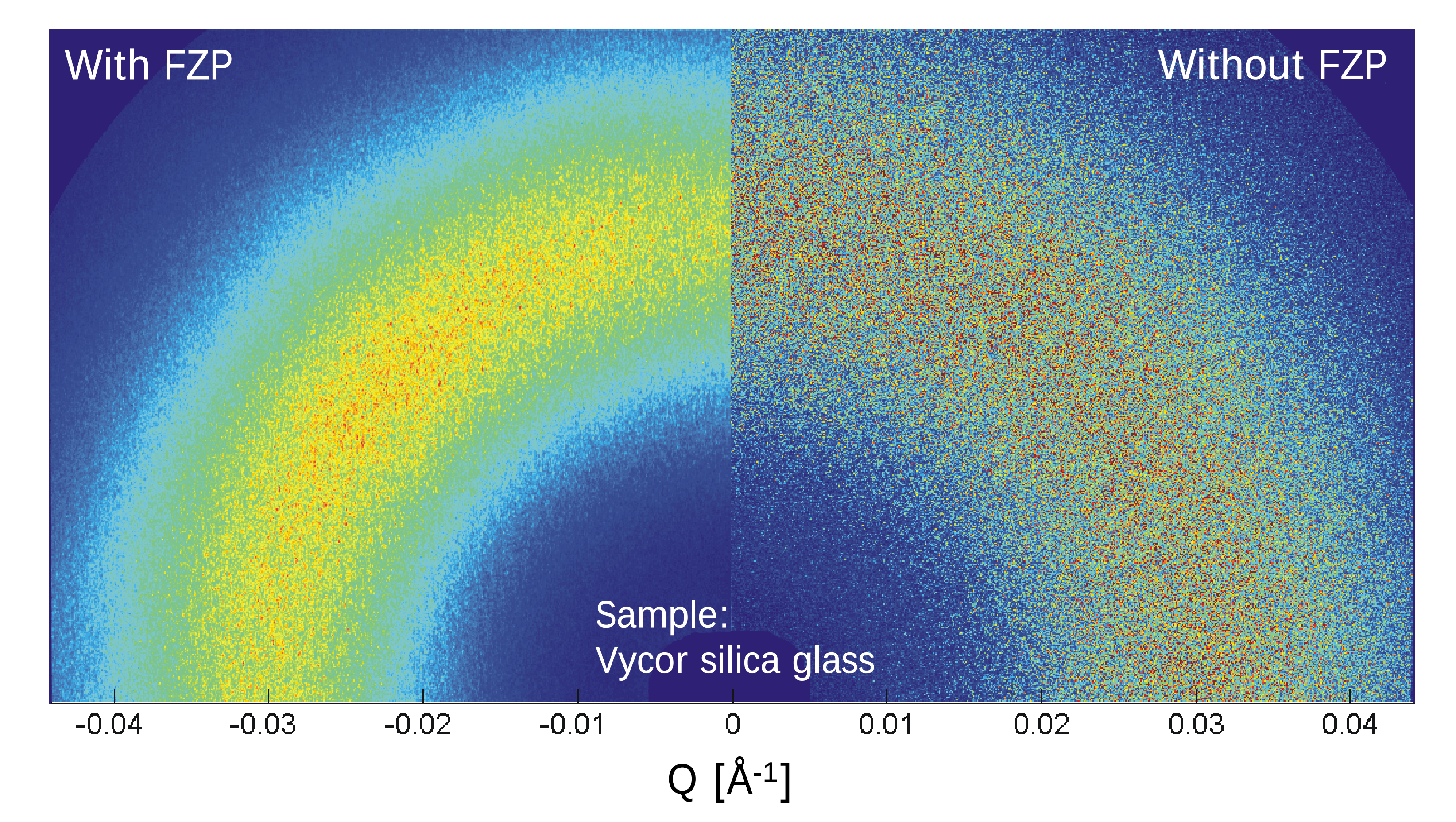


Gain in QF with FZP: ~**5-10**, depending on Q

Same effect as going from 10 min to 17 hrs acquisition time

Theoretical explanation: In progress.........

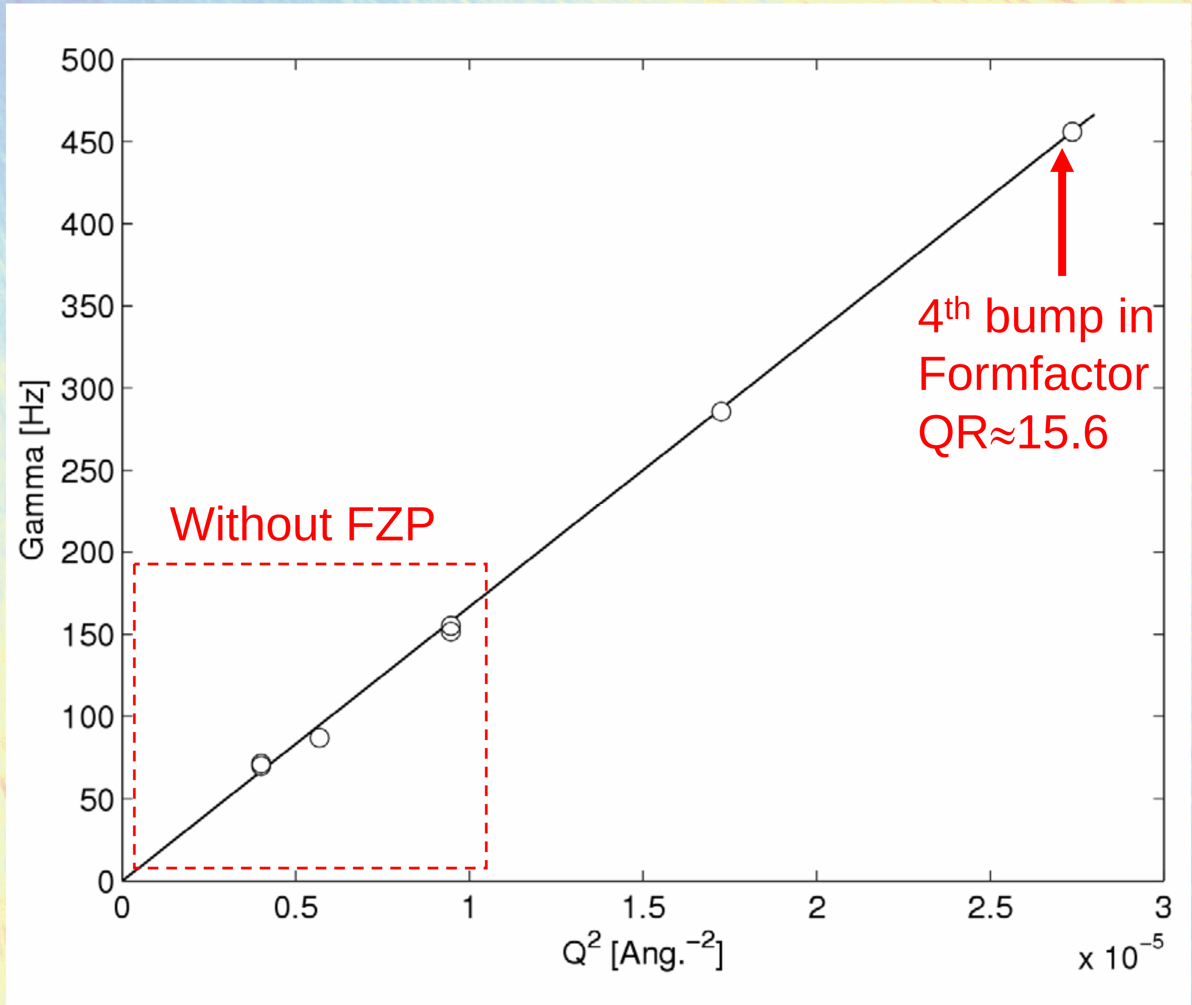
Influence of the speckle size



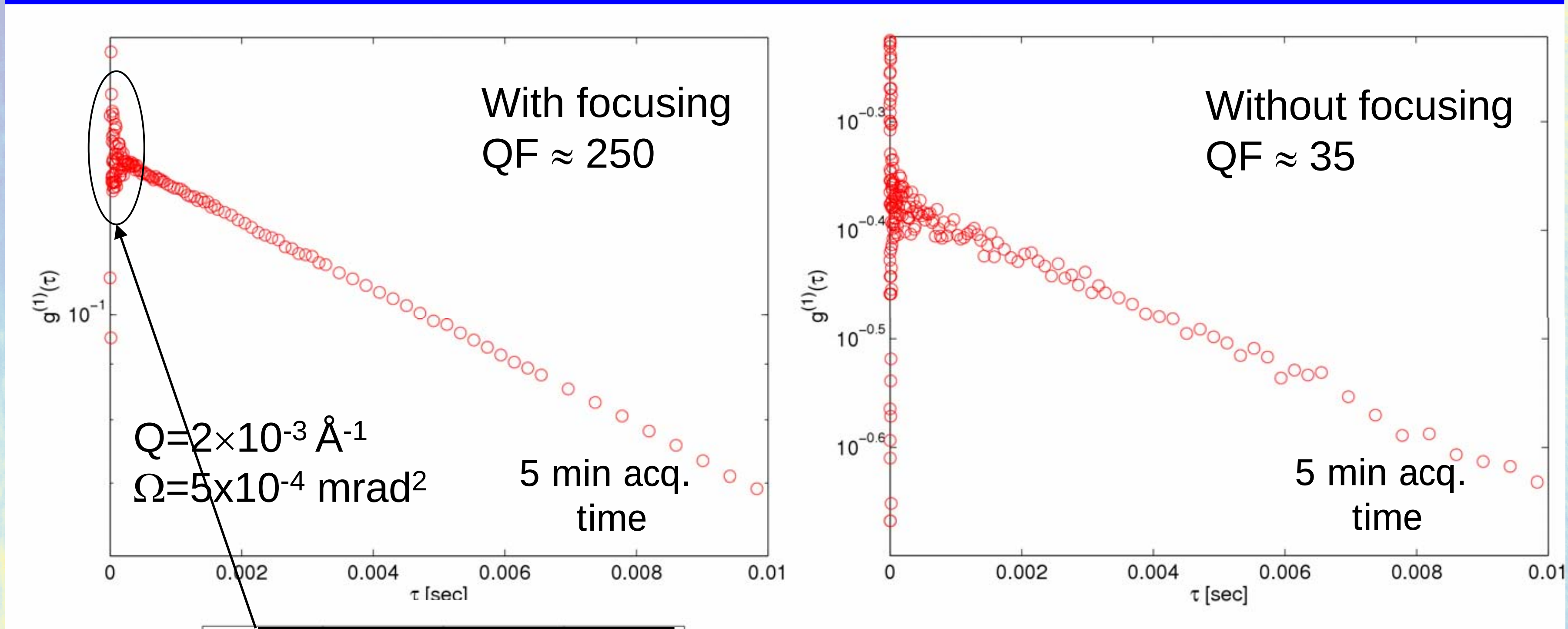
Large, intense speckles are good for XPCS

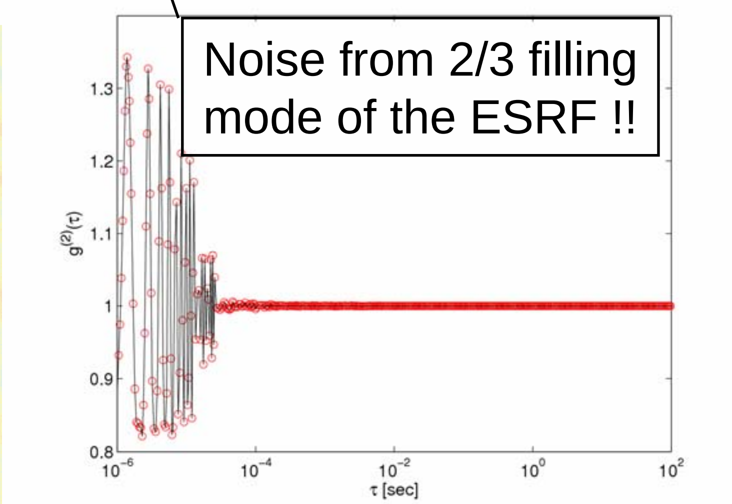
Optimizing the setup for XPCS

Diffusion in a colloidal suspension probed using a FZP



Optimizing the setup for XPCS





- Fast detectors
- Improved s/n ratio:

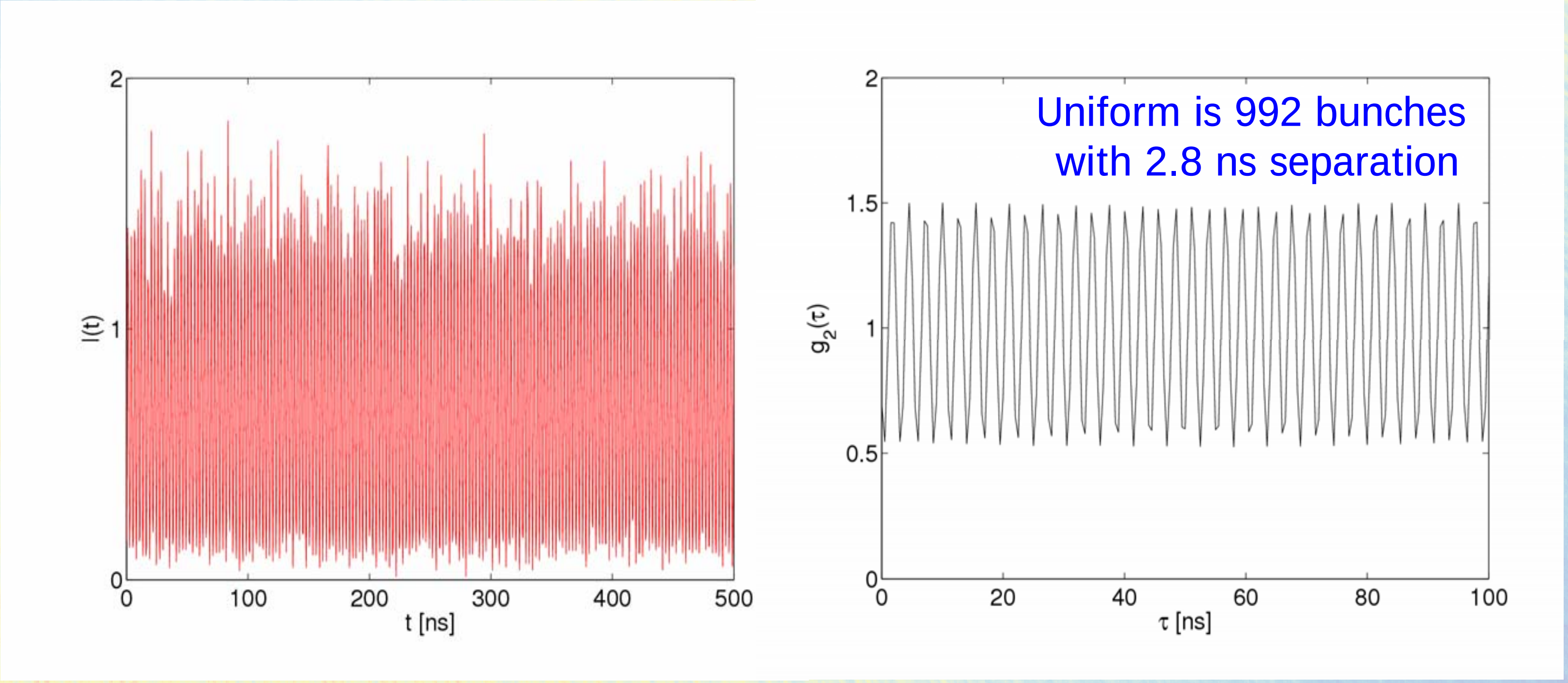
☝ **The time-structure of the ring becomes the limiting factor**

The ESRF Storage Ring: Limitations for fast XPCS

~850 m circumference, 6 GeV, 32 straight sections

Modes:

Uniform (200mA, lifetime >70 hrs) (Very good for XPCS)



Data taken with APD detector and 2GHz scaler board

……….and with the ERL one could dream about

XPCS from non-crystalline, amorphous materials
i.e. systems without long range correlations (Thomson scattering)

Scientific case:

- nano-scale hydro-dynamics in supercooled liquids and glasses
  (surface tension and viscosity in the nano-world)
- unique possibility to measure q-dependent dynamics

Minimum requirements:

- two-three orders of magnitude in coherent flux
- slow dynamics (glass transition)

Challenges (headaches):

- Detectors
- Beam damage

Concluding remarks

The ERL will offer:

- A quasi DC source with infinite lifetime (advantage for XPCS)
- 2-3 orders of magnitude more in coherent intensity than ESRF/APS
- Possibility to perform XPCS at high E (>25keV, buried interfaces...)
- Too large coherence lengths for some applications → focusing

One has to think about:

- Beamline design
- Flexible, focusing optics build in from the beginning
- Optimized use of detectors (pixel detectors/APD detectors)
- How to avoid beam damage (high E?)
- Everyone needs to think about coherence
  (ensemble averaging may be needed for certain experiments)

The End