Discussion of Design and Instrumentation Priorities for XPCS and microbeam SAXS at NSLS-II

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XPCS and microbeam SAXS at NSLS-II workshop
Brookhaven National Laboratory
January 11, 2008

Crucial points for a state-of-the-art XPCS beamline

→ Storage ring, hutches and beamline geometry

→ Energy tunability vs. Brilliance

→ Coherence preserving optics

→ Focusing capabilities

→ Detectors and instrumentation

→ On-line data reduction/data analysis

→ Circumvent beam damage

Crucial points for a state-of-the-art XPCS beamline

→ Storage ring, hutches and beamline geometry

Example: ESRF ~850 m circumference, 6 GeV, 32 straight sections

Modes:

Uniform (200mA, lifetime >70 hrs)	(Very good for XPCS)
7/8+1 (200mA, lifetime ~60 hrs)	(OK for slow XPCS)
Hybrid (200mA, lifetime ~45 hrs)	(OK for slow XPCS)
16 bunch (90mA, lifetime ~10hrs)	(Peak in $g^{(2)}(t)$ at 176 ns)
4 bunch (40mA, lifetime <10hrs)	(Peak in $g^{(2)}(t)$ at 704 ns)

Future plans:

- Ramp-up of current 200→250→?mA (~2-? years)
- New lattice with decreased vertical emittance
- Maybe top-up ?

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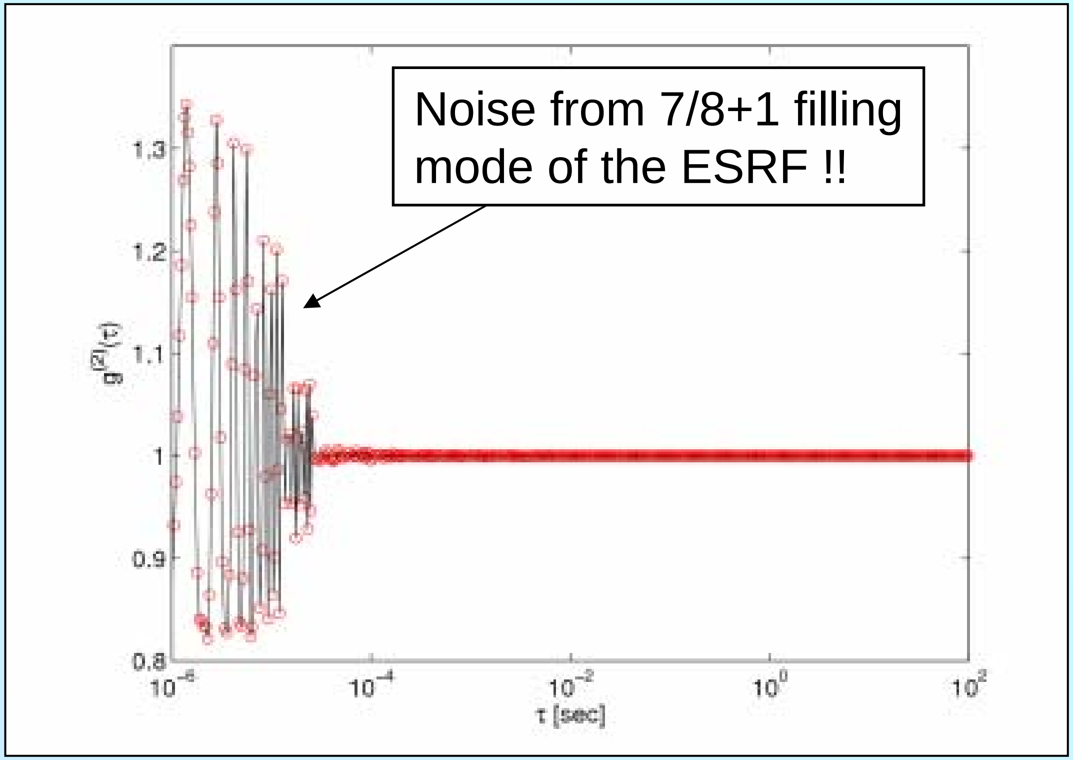


Fast XPCS benefits from a (quasi) DC source
Slow XPCS benefits from a long lifetime (top-up)

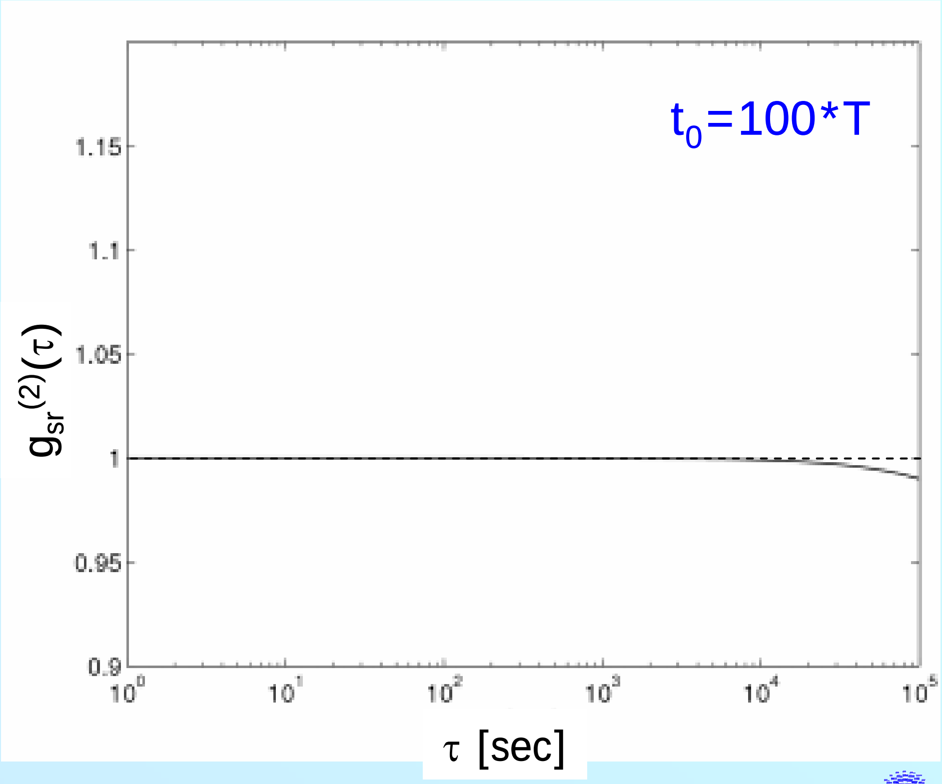
Crucial points for a state-of-the-art XPCS beamline

→ Storage ring, hutches and beamline geometry

$$I_{SR} \propto \exp(-t/t_0) \quad \text{lifetime } t_0 \text{ (ESRF: 10-80 hrs)}$$

$$g_{sr}^{(2)}(\tau) = \frac{\langle I_{sr}(t) I_{sr}(t+\tau)\rangle_T}{\langle I_{sr}\rangle^2}$$

$$g^{(2)} = g_{sr}^{(2)} \times g_{sample}^{(2)}$$



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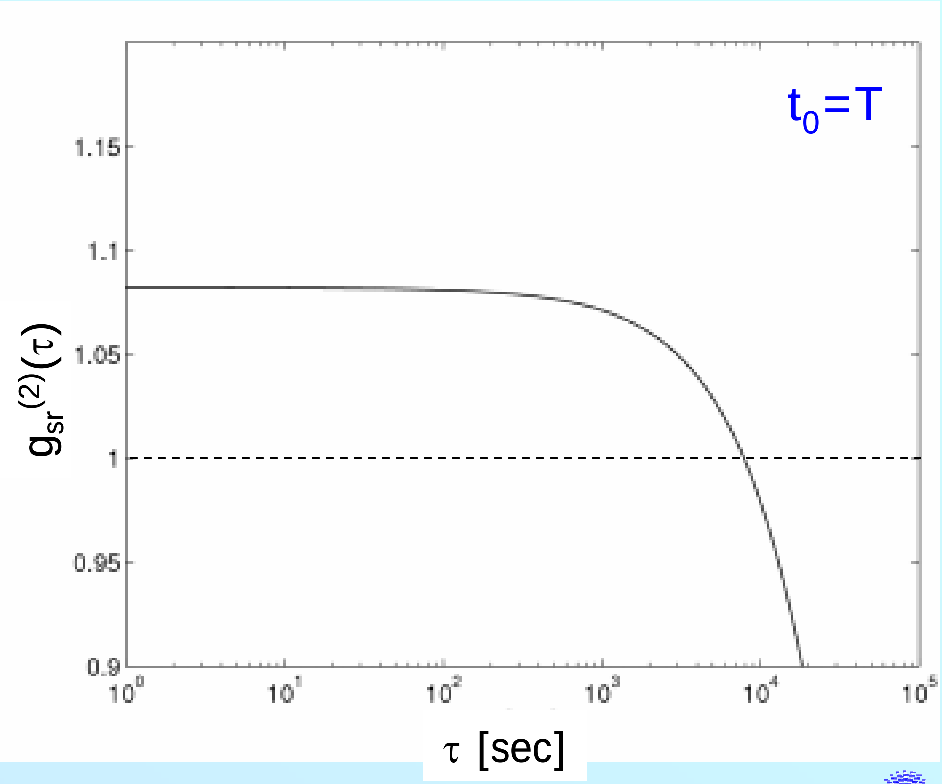

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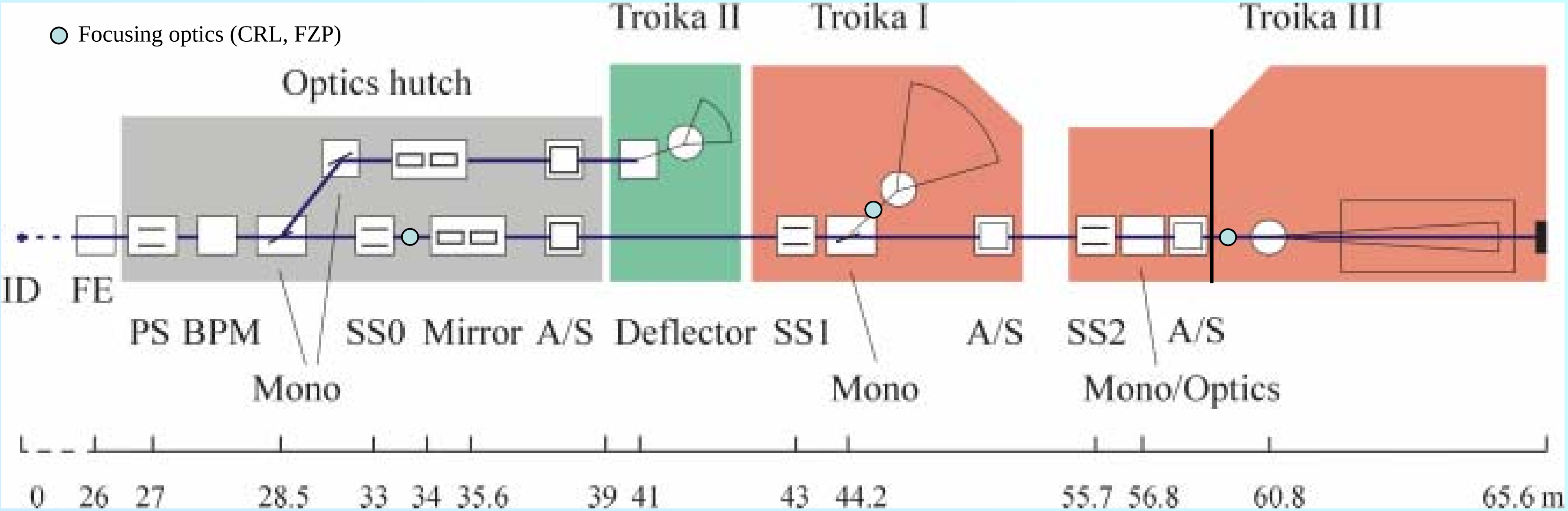
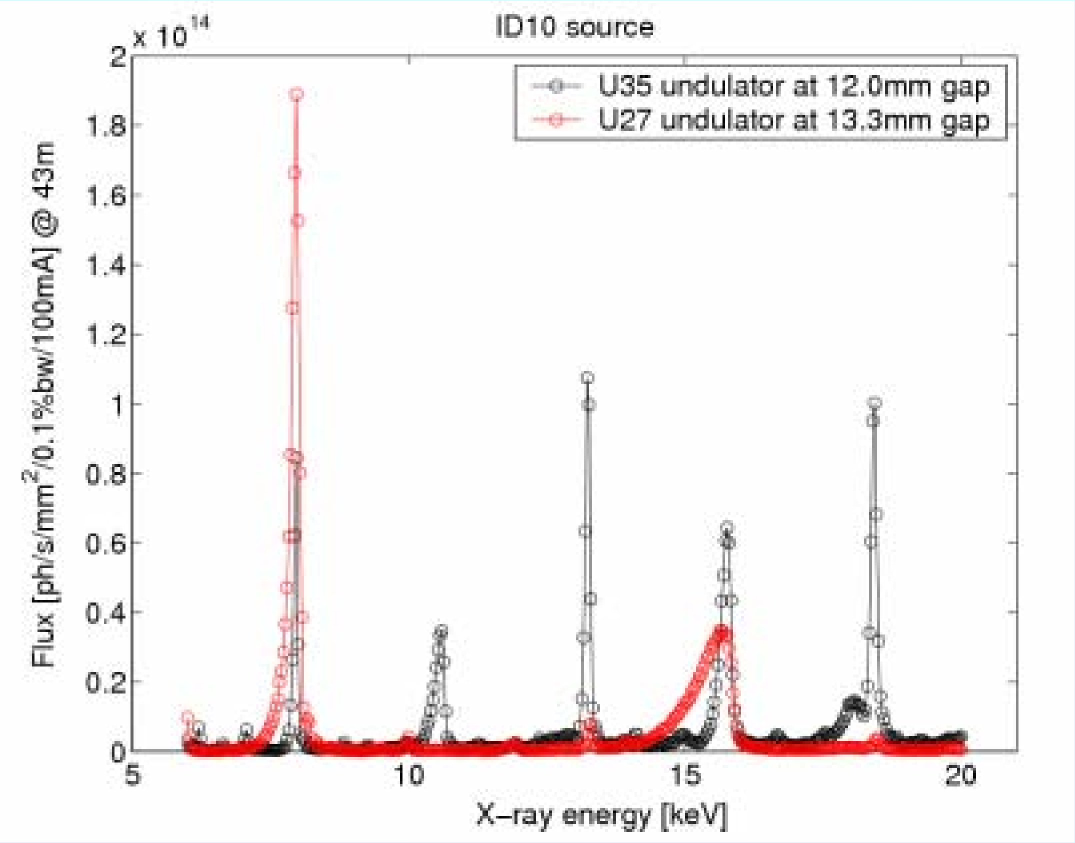


Advantages: simultaneous operation of several stations (GID, XPCS, SAXS)
Drawbacks: beamsplitter optics, ID sharing

An optimized XPCS/coherent scattering beamline should **not** be multiplexed

Crucial points for a state-of-the-art XPCS beamline

→ Energy tunability vs. Brilliance



ID10 (ESRF):

U27 undulator (27 mm period, min. gap 10mm)
U35 undulator (35mm period, min. gap 10mm)
Revolver unit U27/U35, in-situ exchangeable

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

3x1.6m (~5m) in total, upgrade plan: go to 7m

Many experiments could benefit from >8keV operation (beam damage, anomalous/resonance effects,…)

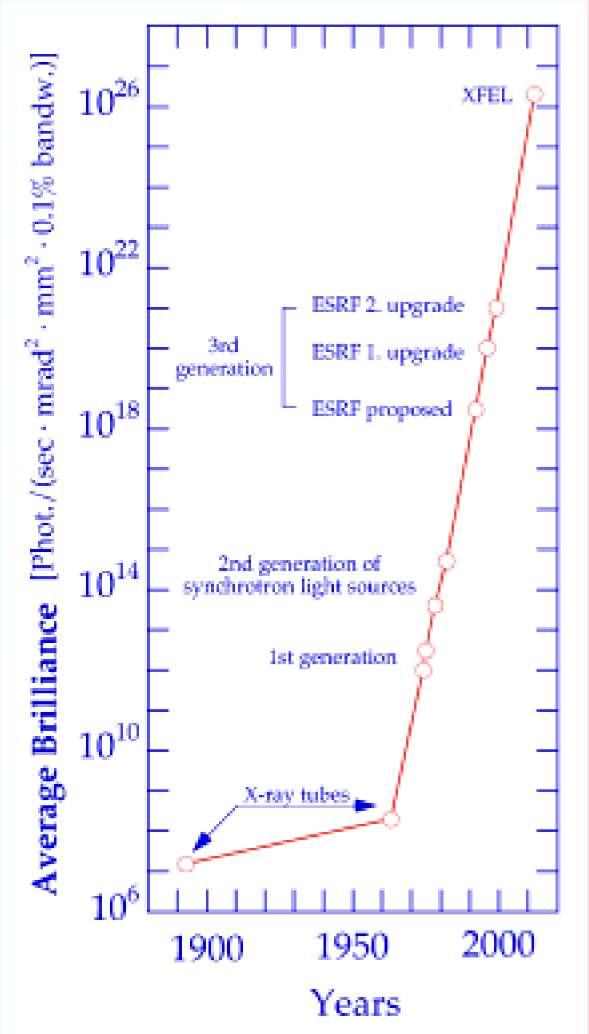
Crucial points for a state-of-the-art XPCS beamline

→ Energy tunability vs. Brilliance

Tunability vs. Brilliance, a delicate compromise….

$$I_C \propto \mathbf{B} \times \lambda^2$$

Long, in-vacuum undulators may allow the desired energy tunability and ensure $I_c > 10^{10}$ ph/s in the entire range



Crucial points for a state-of-the-art XPCS beamline

→ Coherence preserving optics

Mirrors: continuous source of problems due to the grazing incidence (phase contrast imaging). Better if one could avoid them !

However, the use of upstream mirrors may allow more gentle cooling of downstream monochromators reducing vibrations

Pink beam option with mirror is interesting for SAXS XPCS

→ Specs for slope errors must be <1μrad
→ Think carefully about the scattering geometry (horizontal/vertical)
→ Avoid thermal deformations (cooling, illumination profile,..)
→ Use the mirror in “flat” configuration (no bender)

Crucial points for a state-of-the-art XPCS beamline

→ Coherence preserving optics

Monochromators: Match angular acceptance to beam divergence

Match the longitudinal coherence length to the needs (SAXS, WAXS)

Diamond would be the best monochromator material but for the moment the quality is not sufficient for coherent scattering purposes (dislocations, surface quality)

Si based mono technology is well established (symmetric Bragg, single bounce, channel cut,…)

Pre-collimation before mono allows gentle cooling (He gas, H2O)

Larger bandwidth (1%) monochromators is an interesting option; similar beam characteristics may be obtained by mirrors.

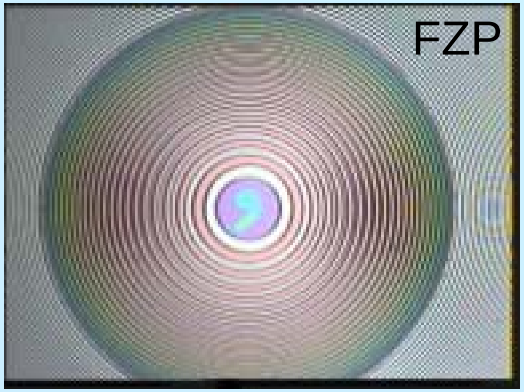
Crucial points for a state-of-the-art XPCS beamline

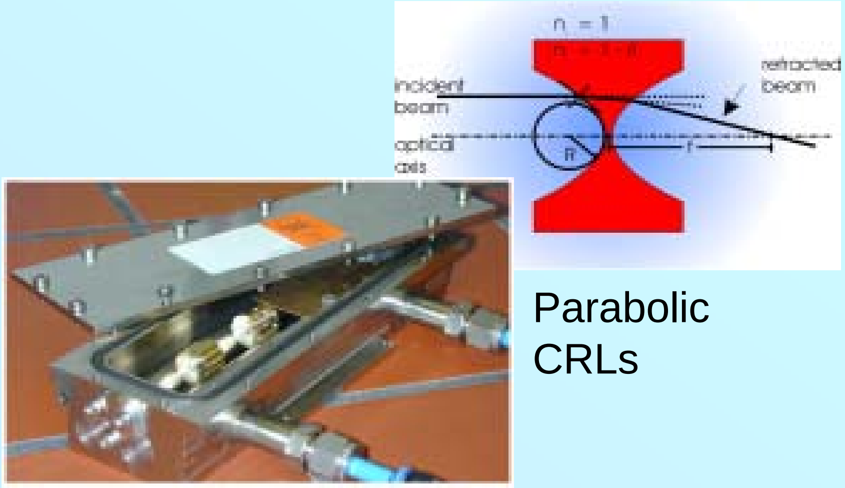
→ Focusing capabilities

Focusing is necessary for optimized XPCS operation.

Beam size on the sample larger than 10-50μm is not desirable. Lenses are used to match the coherence length to the desired beam size and increase the intensity

s/n ratio in XPCS is proportional to intensity and coherence





Parabolic CRLs

Crucial points for a state-of-the-art XPCS beamline

→ Focusing capabilities

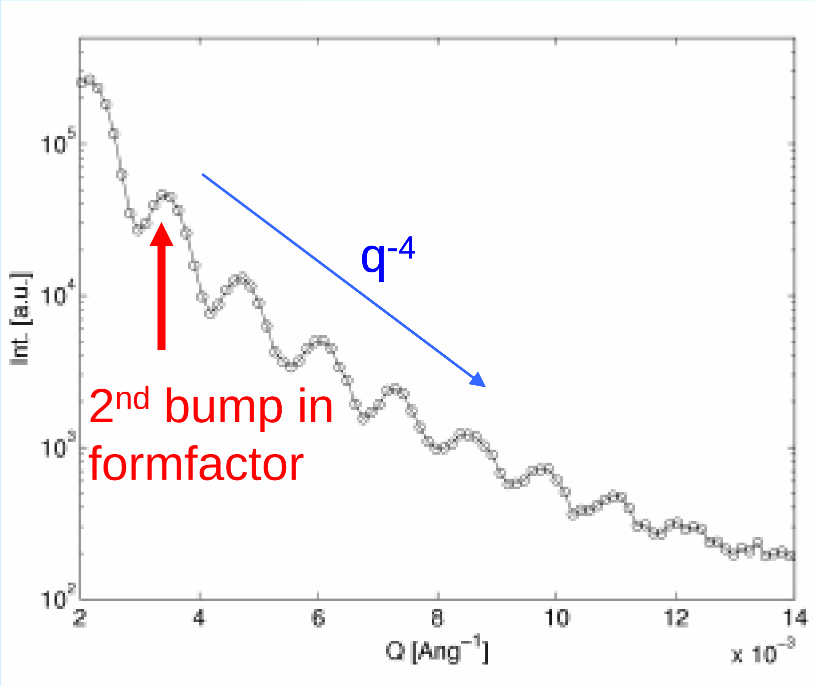
Sample: PMMA (HS) colloids in cis-decaline,
Radius ≈ 1500 Å

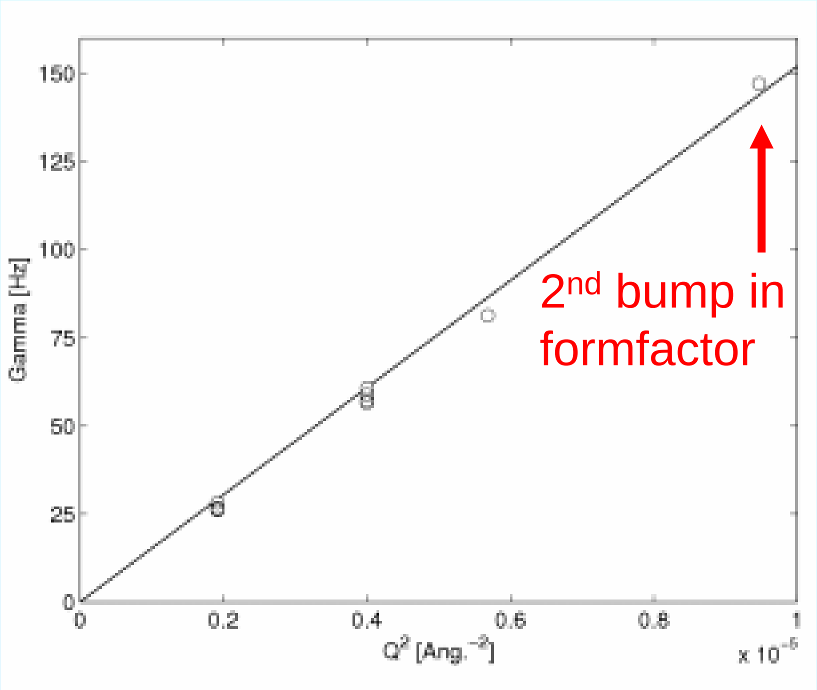
Incident flux: $1x10^9$ ph/sec/$10\times10\mu m^2$
(200mA, 8keV, no focusing)

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

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

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





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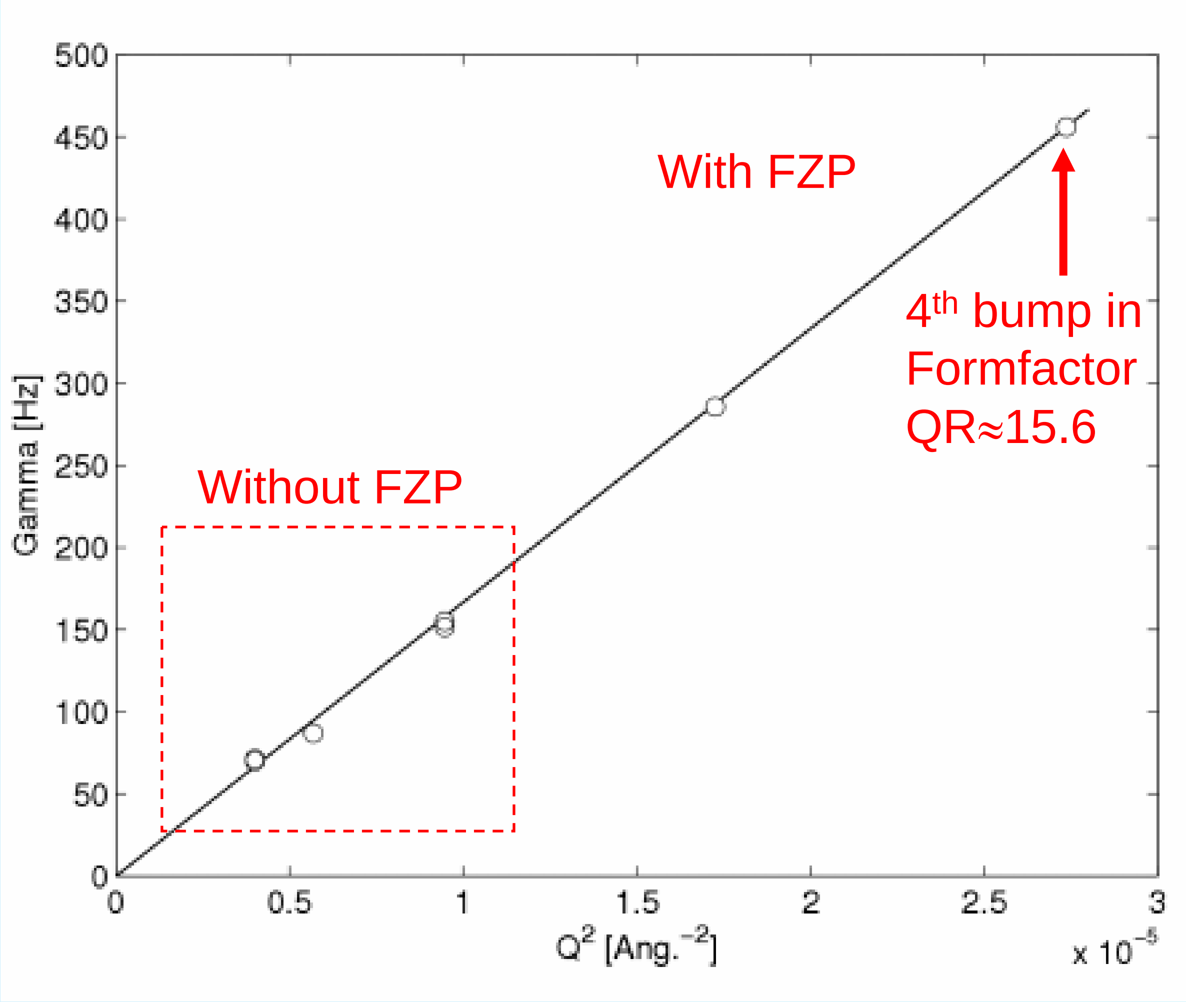
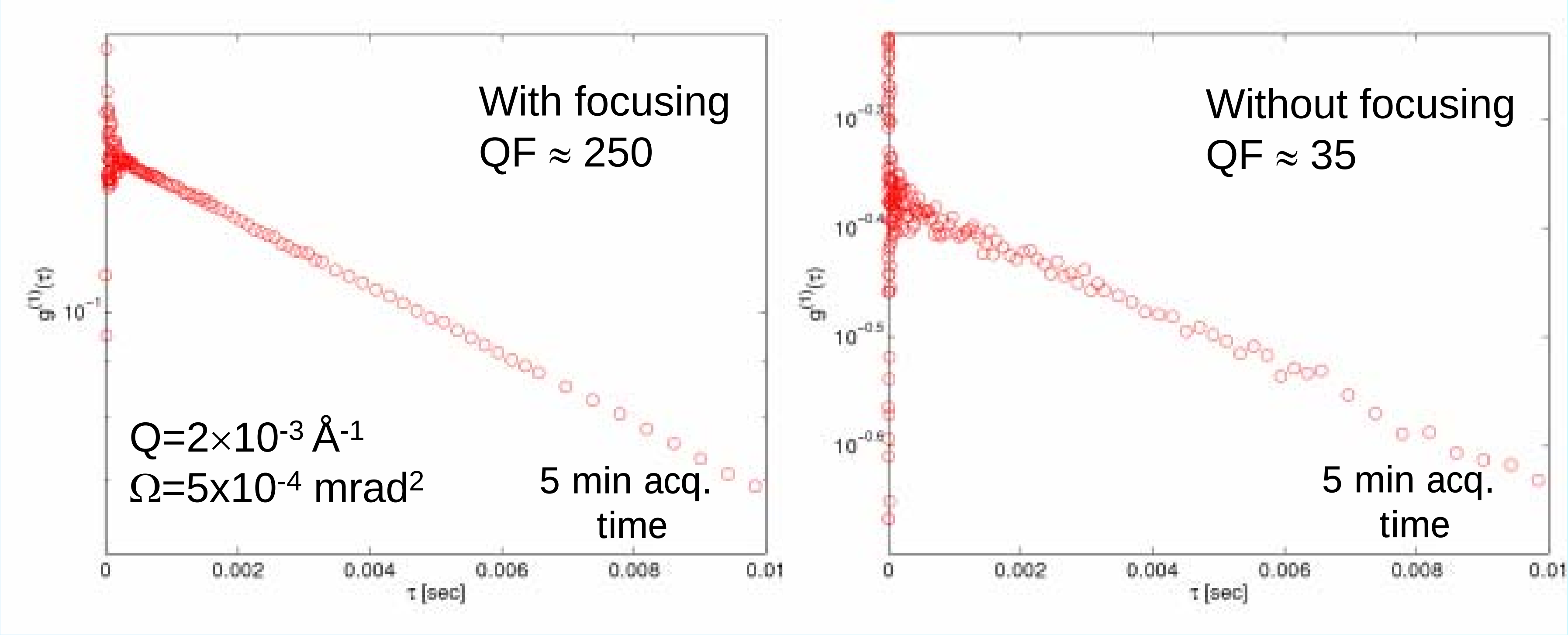


Crucial points for a state-of-the-art XPCS beamline

→ Focusing capabilities

QF=C×I

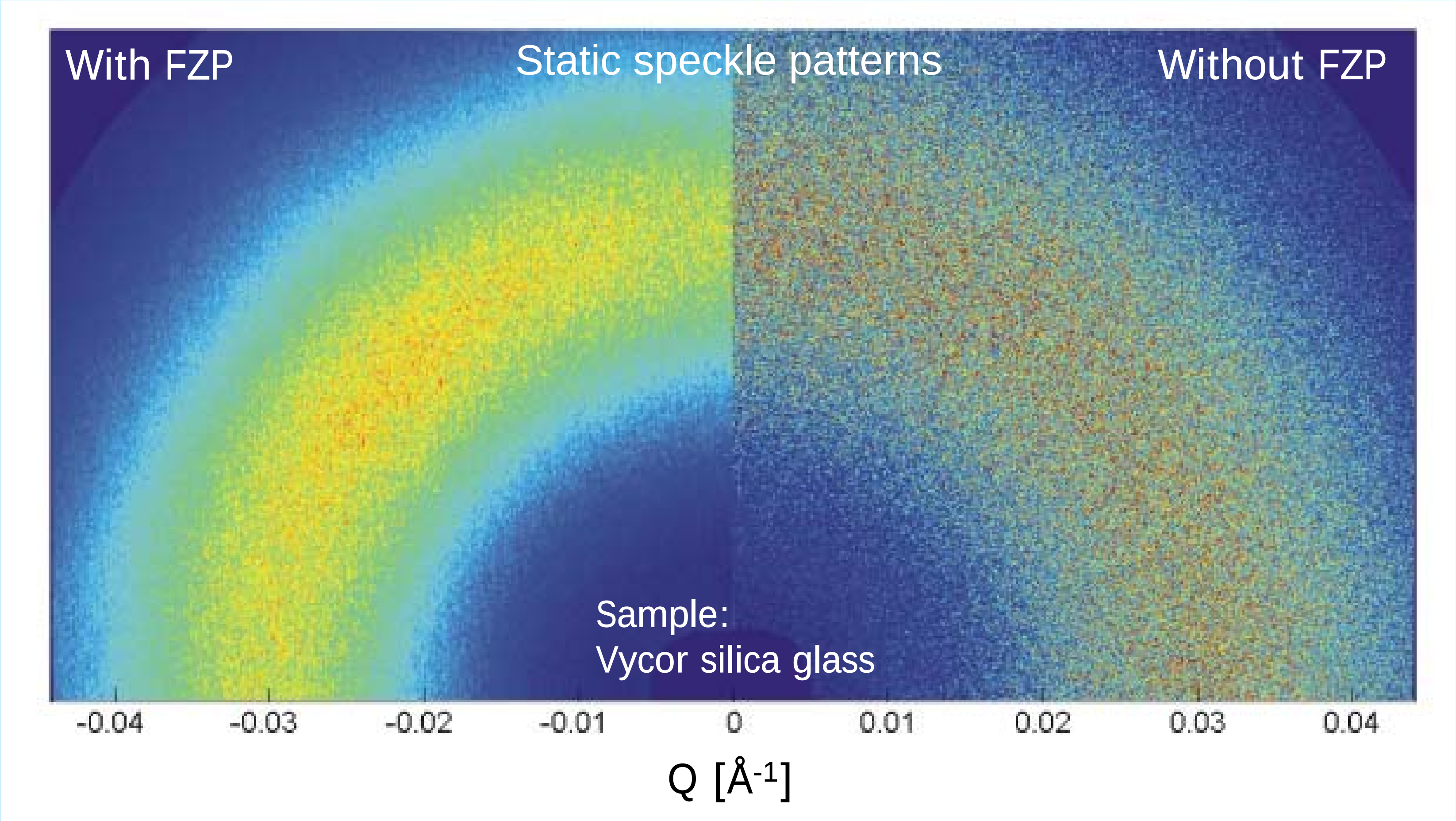


Intensity is often the limiting factor for XPCS

ESRF

Crucial points for a state-of-the-art XPCS beamline

→ Focusing capabilities



Large, intense speckles are good for XPCS

Crucial points for a state-of-the-art XPCS beamline

→ Detectors and instrumentation

Detectors (photon counting):

2D detectors (pixelated cmos detectors: medipix, pilatus,..)
Medipix: speed > 1kHz full frame, 256x256 pixels, 55μm
Goal: approach 1MHz, larger panels (maxipix)

0D detectors (avalanche photo diode, APD)
Speed ~1GHz
Goal: APD arrays (2d)

Match sample-detector distance to the pixel size to resolve the speckles

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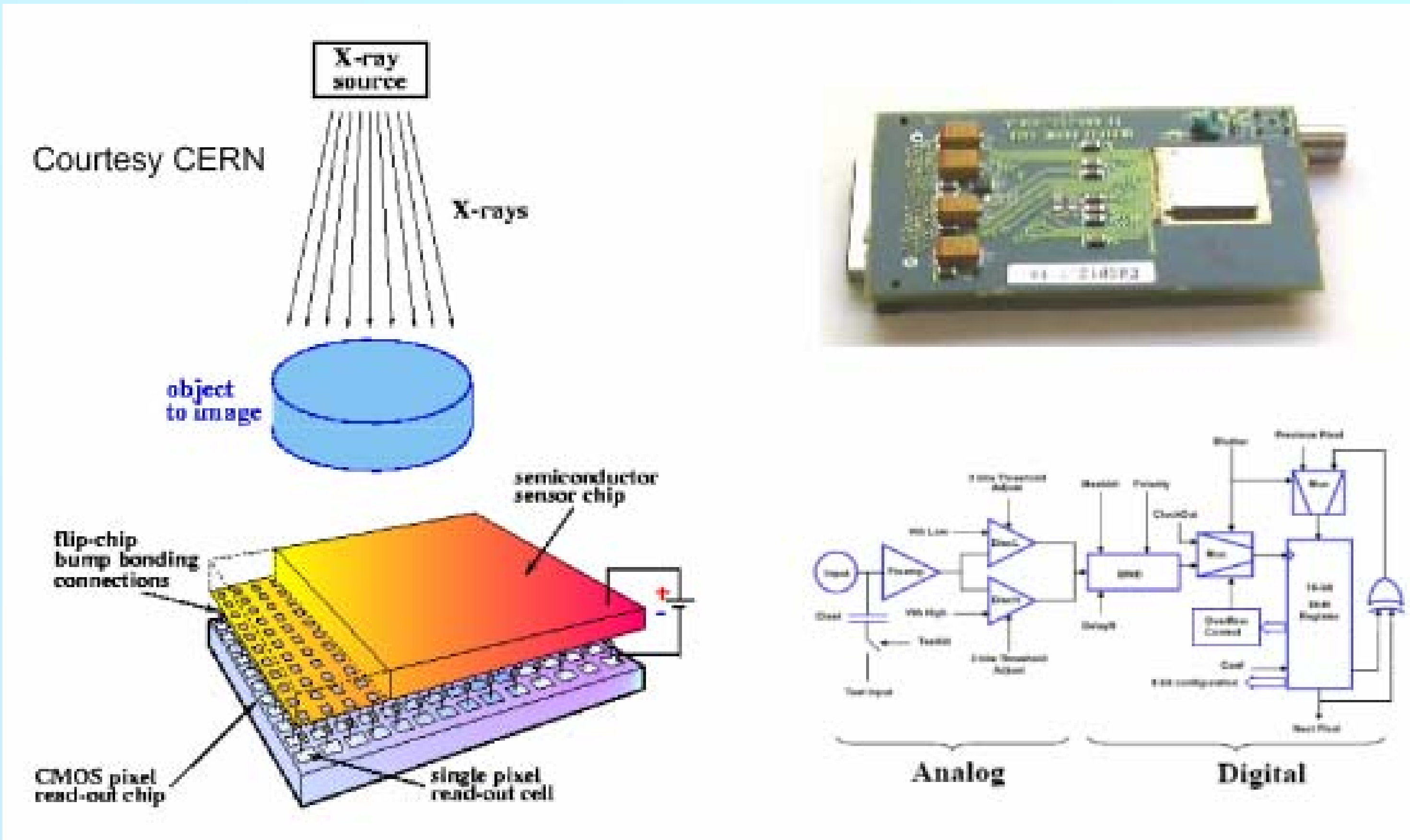
→ Detectors and instrumentation

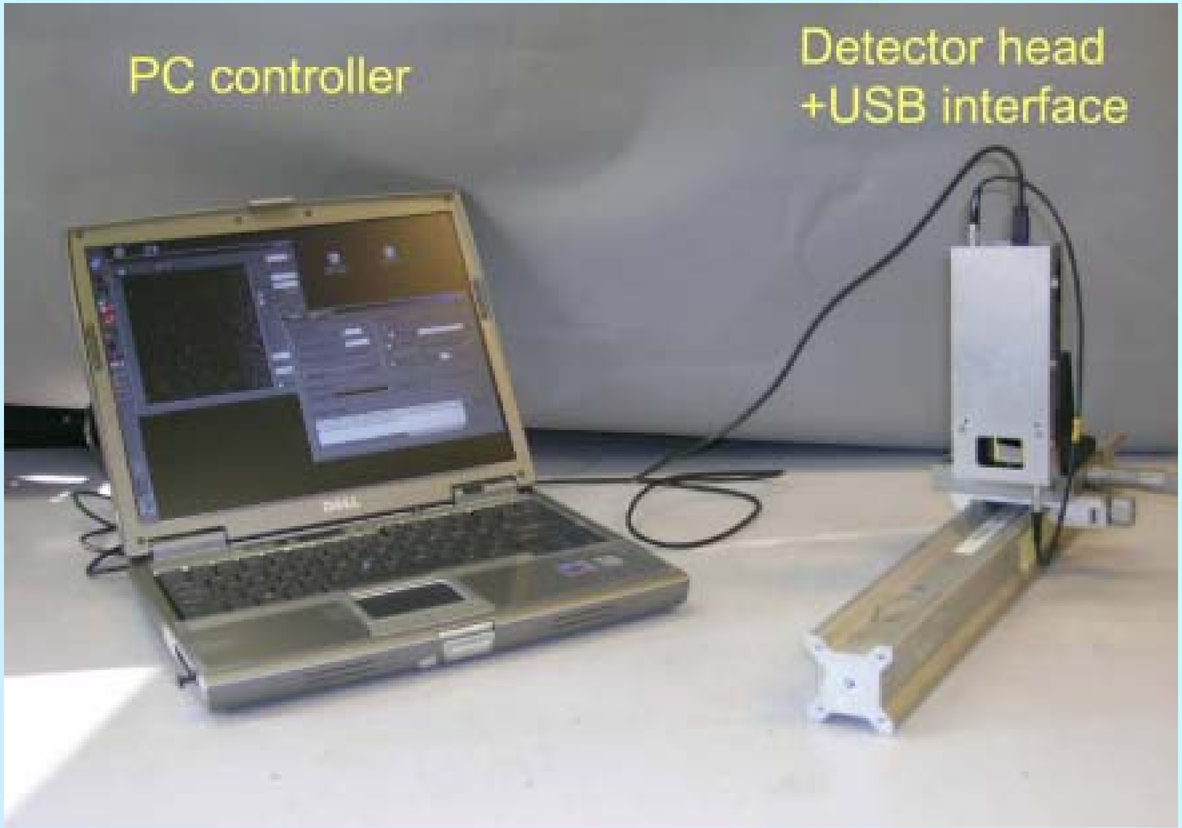


(C. Ponchut, ESRF)

Medipix detector: 256 x 256 pixels, 55 μm pixel size, 2 MHz/pixel (20 bit)
Photon counting, Upper and lower energy threshold

Crucial points for a state-of-the-art XPCS beamline

→ Detectors and instrumentation



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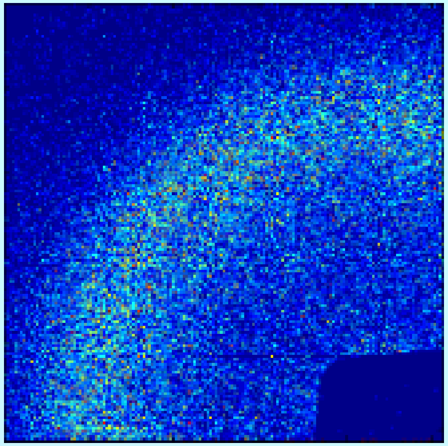
SAXS pattern



up to ~1000 frames/s

Crucial points for a state-of-the-art XPCS beamline

→ Detectors and instrumentation

Instrumentation:

Versatile, SAXS, WAXS, GID options

No vibrations

Clean electrical environment (shielding & grounding)

Enough sample-detector distance

Crucial points for a state-of-the-art XPCS beamline

→ Data reduction/data analysis

With increasing data-rates on-line calculation of correlation functions becomes challenging but very important

The multi-tau algorithm (K. Schätzel) can be "parallelized" to run in multiple processor environments

Ensemble averaging (non-ergodic samples);
equilibrium(one-time) or non-equilibrium (two-time) correlation functions

Speed can be increased by use of FPGAs (intelligent detector)

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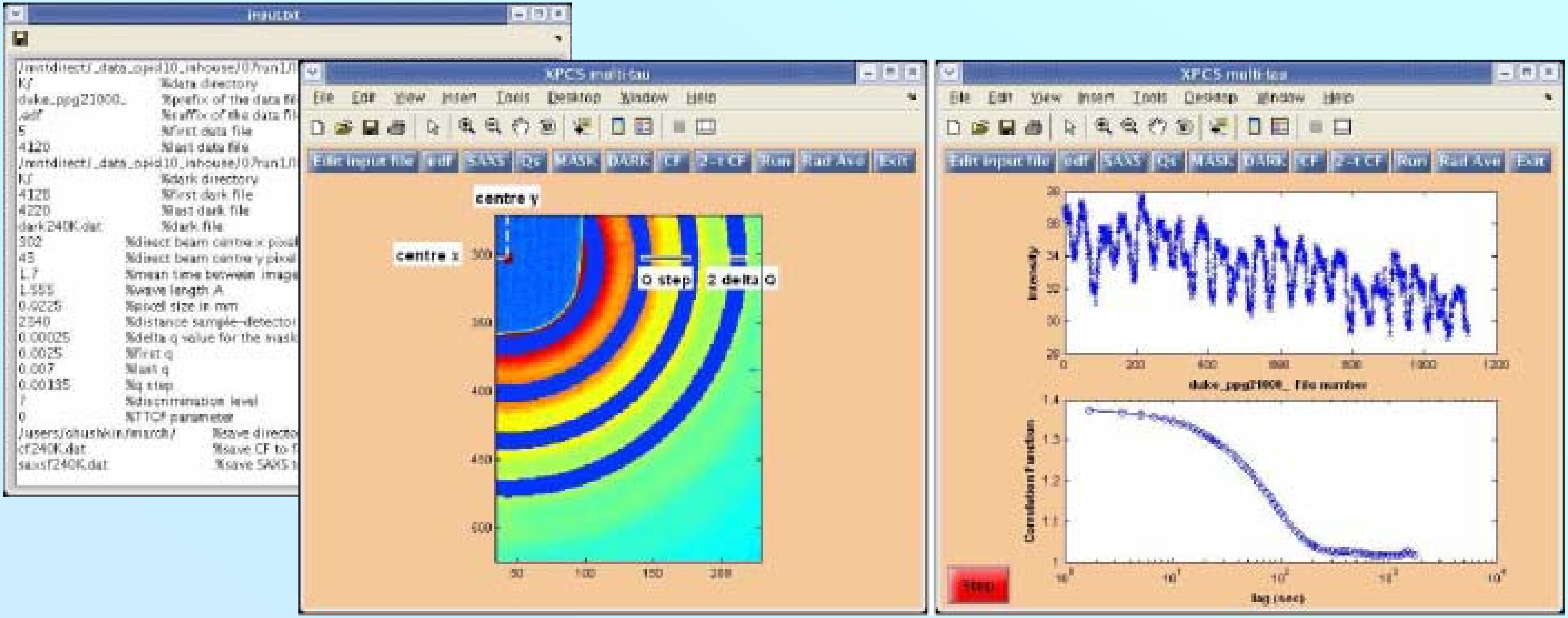

$$g^{(2)}(Q,\tau)=\frac{\left\langle\left\langle I_p(Q,t)I_p(Q,t+\tau)\right\rangle_\phi\right\rangle_t}{\left\langle\left\langle I_p(Q,t)\right\rangle_\phi\right\rangle_{0\le t\le T-\tau}\left\langle\left\langle I_p(Q,t)\right\rangle_\phi\right\rangle_{\tau\le t\le T}}$$

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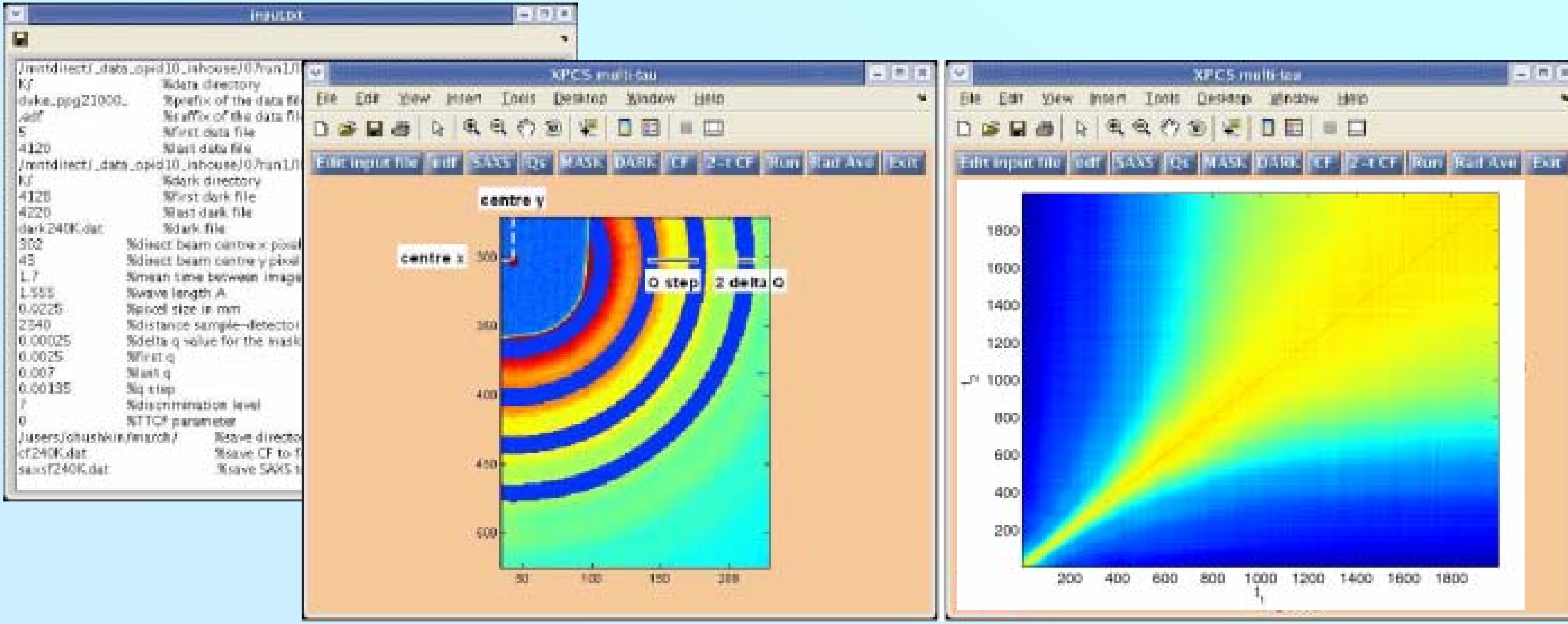


$$G(Q,t_1,t_2) = \frac{\left\langle I_p(Q,t_1) I_p(Q,t_2) \right\rangle_\phi}{\left\langle I_p(Q,t_1) \right\rangle_\phi \left\langle I_p(Q,t_2) \right\rangle_\phi}$$

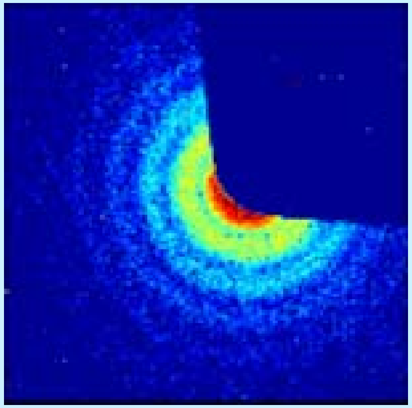
Higher order correlation functions?

Crucial points for a state-of-the-art XPCS beamline

→ Beam damage

Huge problem for soft condensed matter, increasing problem with higher flux

Possible ways to minimize beam damage:
- → Right choice of X-ray energy
- → 2D detection (shutter in front of sample!)
- → Intelligent sample environment (flowing liquid samples)
- → Working in a low-flux mode (large sample-source distance)



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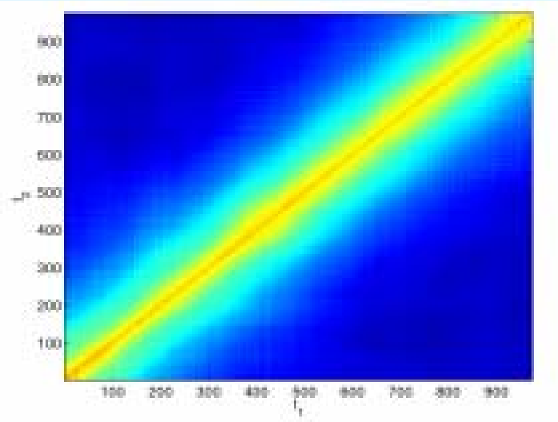
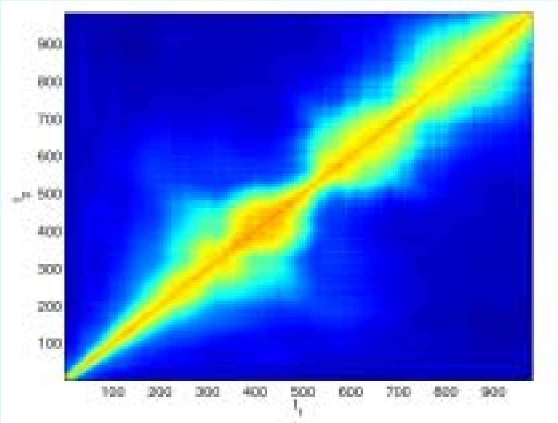
But in some cases the problem persists, and may create effects that mimic e.g. aging in soft glasses and gels





Thank you for your attention

The floor is open for discussion