XPCS at XFEL
or
How to measure S(q,t) at XFEL sources

Christian Gutt

DESY, Notke-Str. 85, 22607 Hamburg

Outline

- Speckles
- XPCS Modes at XFEL sources
- Split-Pulse technique
- Speckle sizes, signal to noise ratio and some implications for detectors
- Beam damage – are non-destructive single shot measurements possible ?
- Single shot coherence – implications from the SASE process

Scientific Agenda

Measure

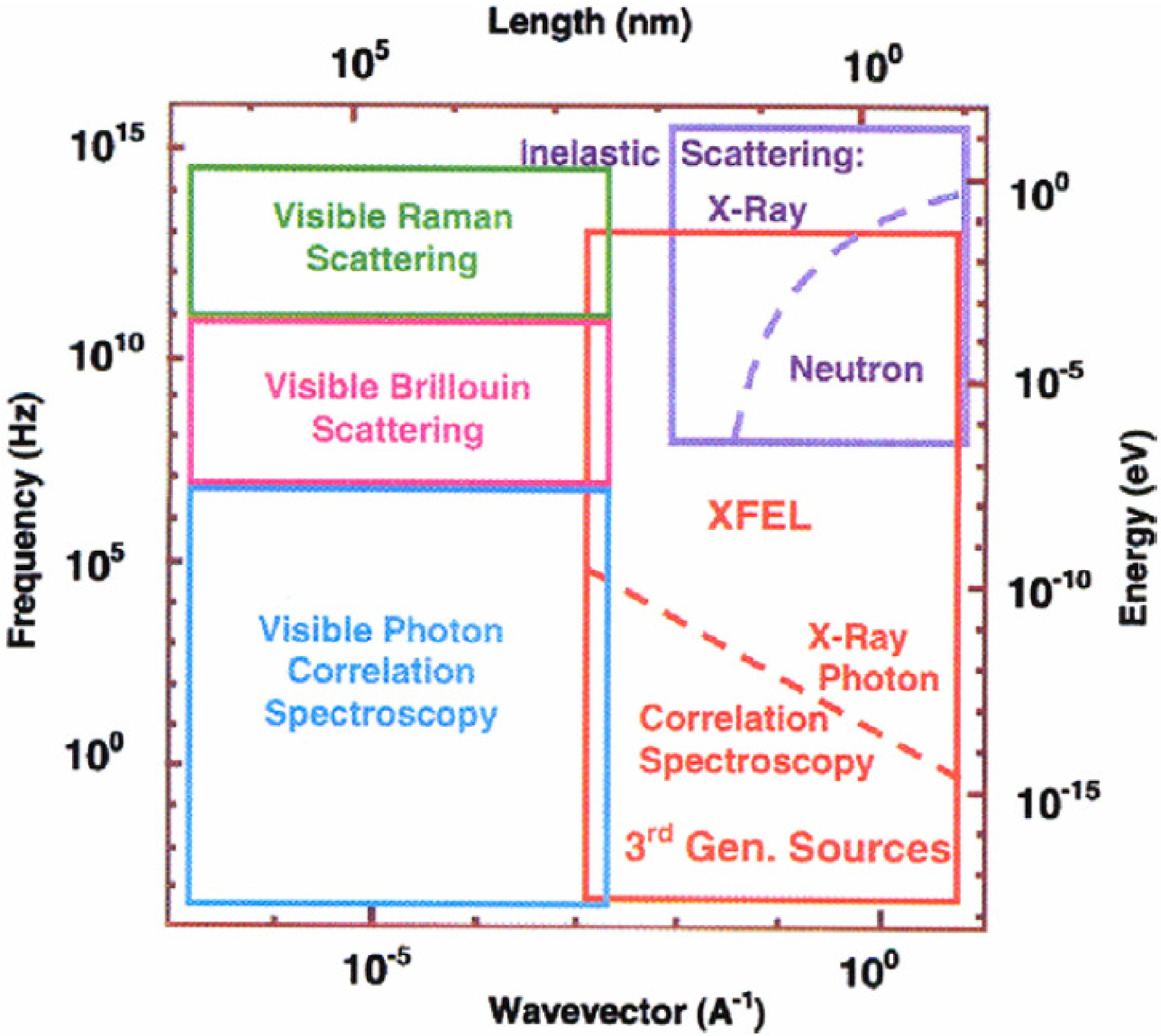
- S(q,t)
- local symmetries
- higher order correlations in time and space
- non-equilibrium processes
- rotational dynamics...

Systems

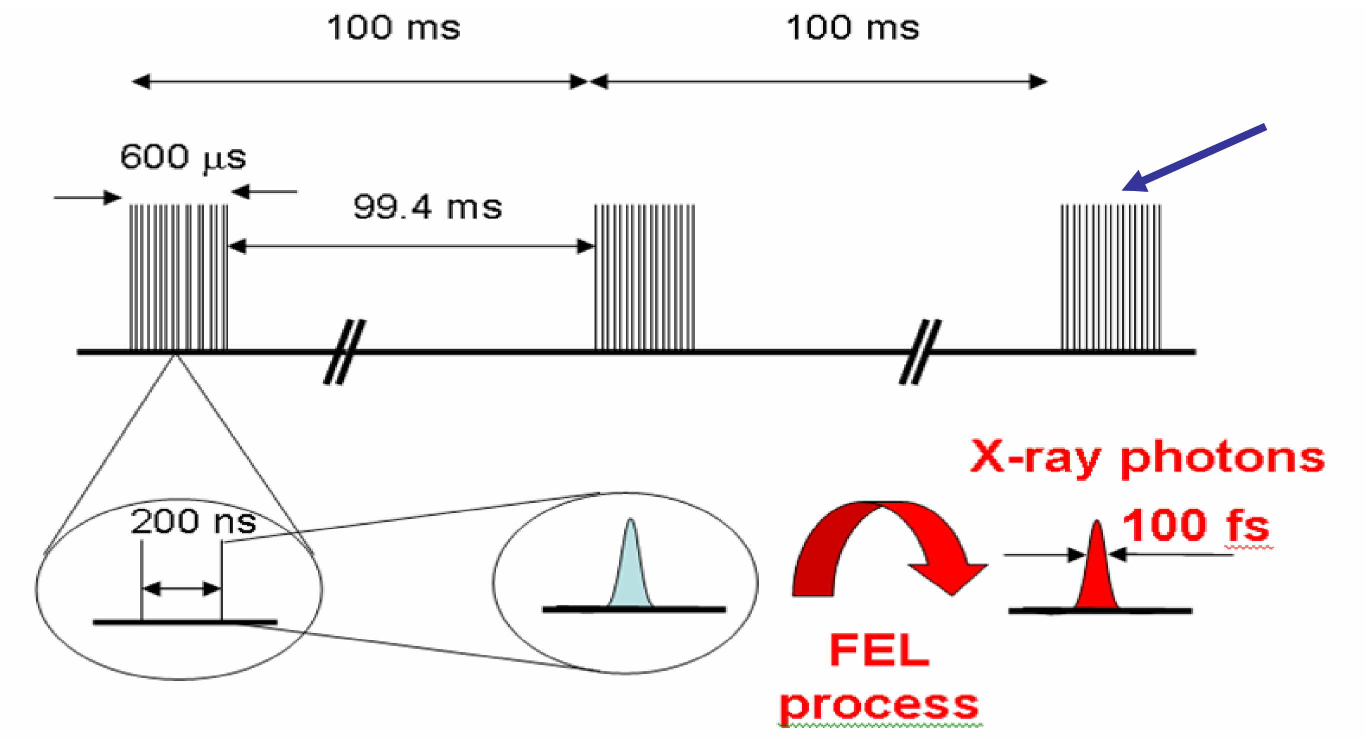
- magnetization dynamics
- structure and dynamics of fluids (e.g. water)
- phonon anomalies in low dimensional systems
- nucleation and phase transitions
- (slow) molecular scale dynamics in supercooled liquids
- short-lived, metastable fluctuations
- atomic scale diffusion in solids
- dynamics of biomolecules

See talks of

P. Wochner, B. Stephenson, L. Cipelletti, B. Sepiol, H.Sinn, A. Madsen


Length (nm)
10^5
10^0
10^15
10^10
10^5
10^0
Frequency (Hz)
Inelastic Scattering:
X-Ray
Neutron
Visible Raman Scattering
Visible Brillouin Scattering
Visible Photon Correlation Spectroscopy
XFEL
X-Ray Photon Correlation Spectroscopy
3rd Gen. Sources
10^0
10^-5
10^-10
10^-15
Energy (eV)
10^-5
10^0
Wavevector (A^-1)

XPCS at a FEL source:

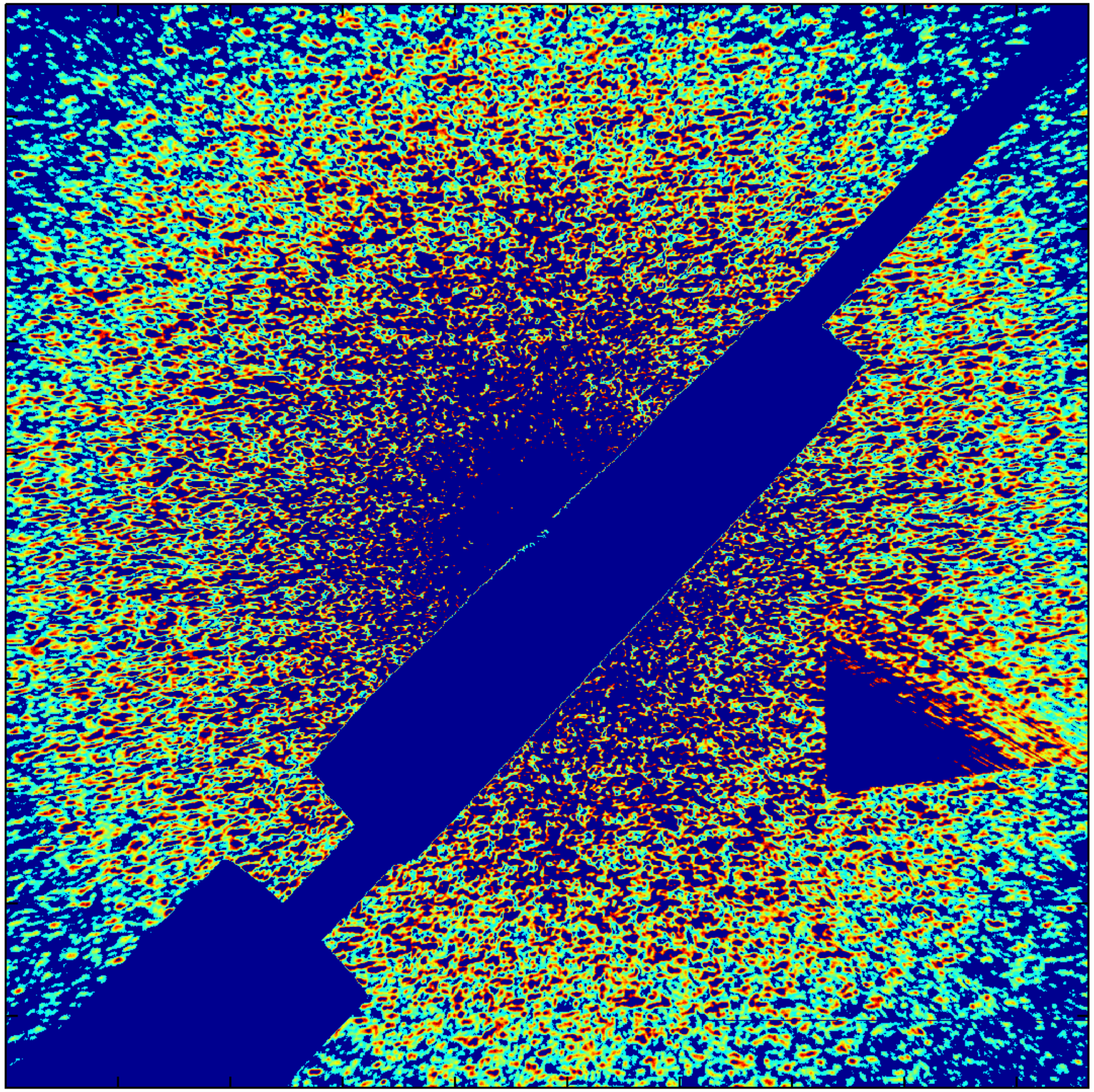


200ns < t < 600 µs — "movie" mode

1ps < t< 10 ns: — "delay-line" mode

for "all" times: — "pump-probe" mode

Speckle pattern

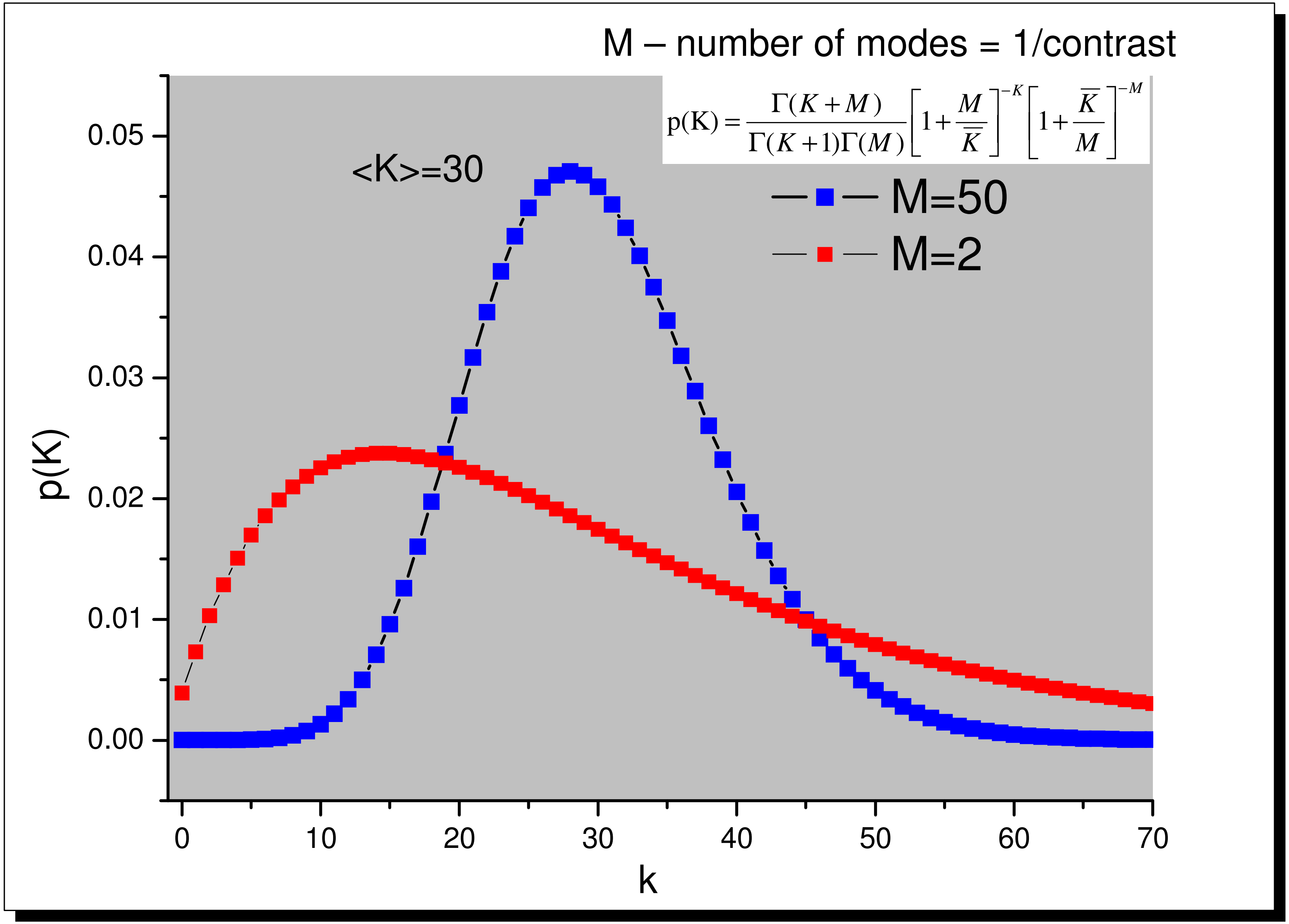


Speckle size $S = \frac{\lambda L}{D}$

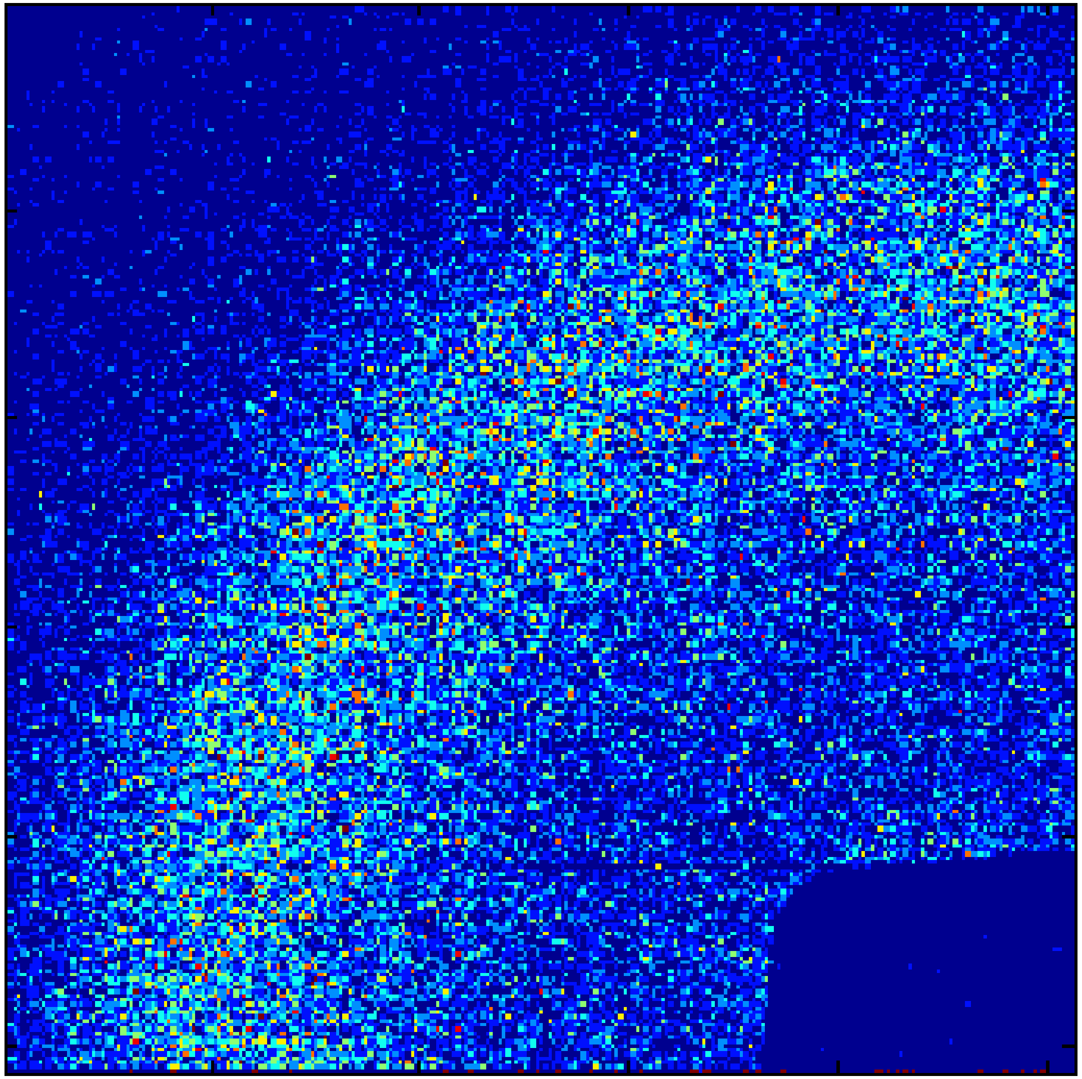
Contrast (visibility) $\beta(Q) = \frac{\sqrt{\langle I^2 \rangle - \langle I \rangle^2}}{\langle I \rangle}$

Influence of detector pixel size on contrast $\beta_{eff} = \beta \times \frac{1}{1 + (P/S)^2}$

Counting statistics of a speckle pattern

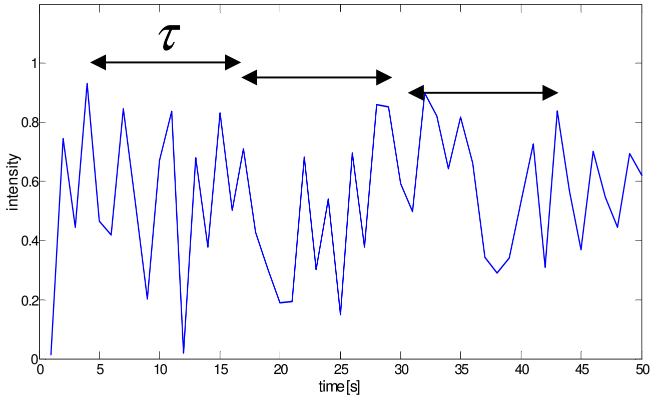


Fluctuating Speckle Pattern



ID10 A

Intensity Autocorrelation Function



$$\left\langle I(q,t_1)I(q,t_1+\tau)\right\rangle = \left\langle \rho(q,t_1)\rho^*(q,t_1)\rho(q,t_1+\tau)\rho^*(q,t_1+\tau)\right\rangle$$

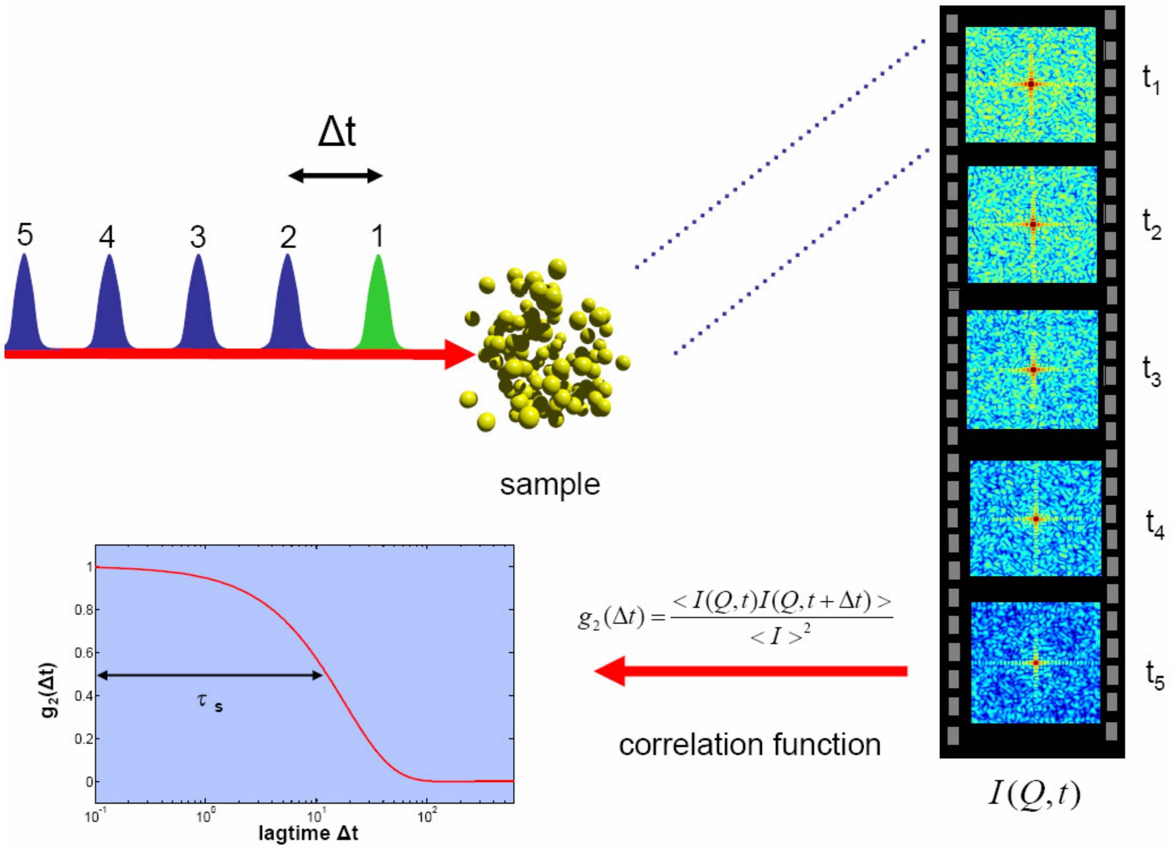
$$< I(q,0)I(q,\tau) >= \frac{1}{T}\int_0^T I(q,t)I(q,t+\tau)$$

$$g_2(q,\tau) = \frac{\left\langle I(q,0)I(q,\tau)\right\rangle}{\left\langle I(q,0)\right\rangle^2} \approx 1+\beta\left|f(q,\tau)\right|^2$$

Siegert relation

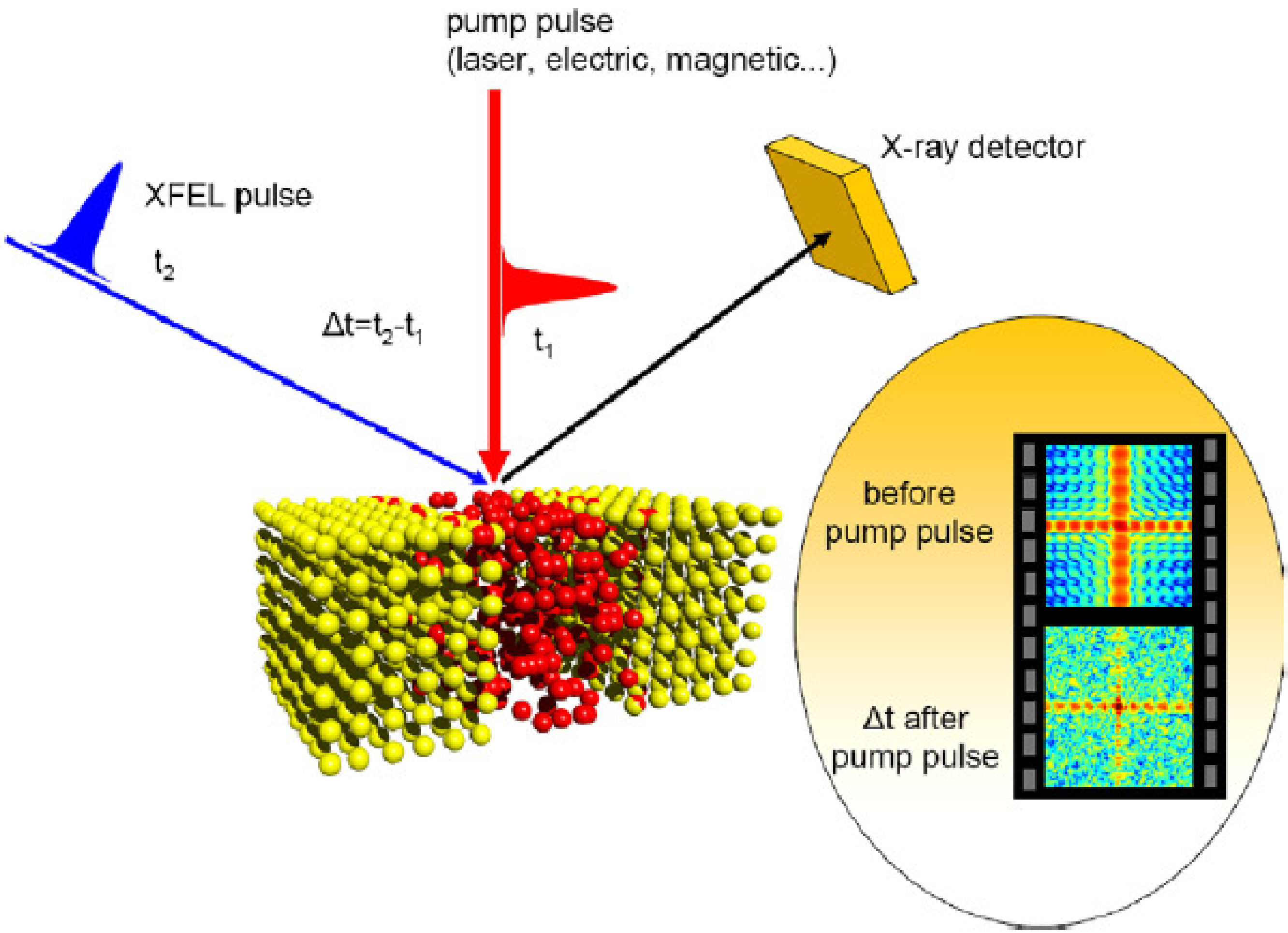
f(q,t) Intermediate scattering function

XPCS at a FEL source: Movie Mode

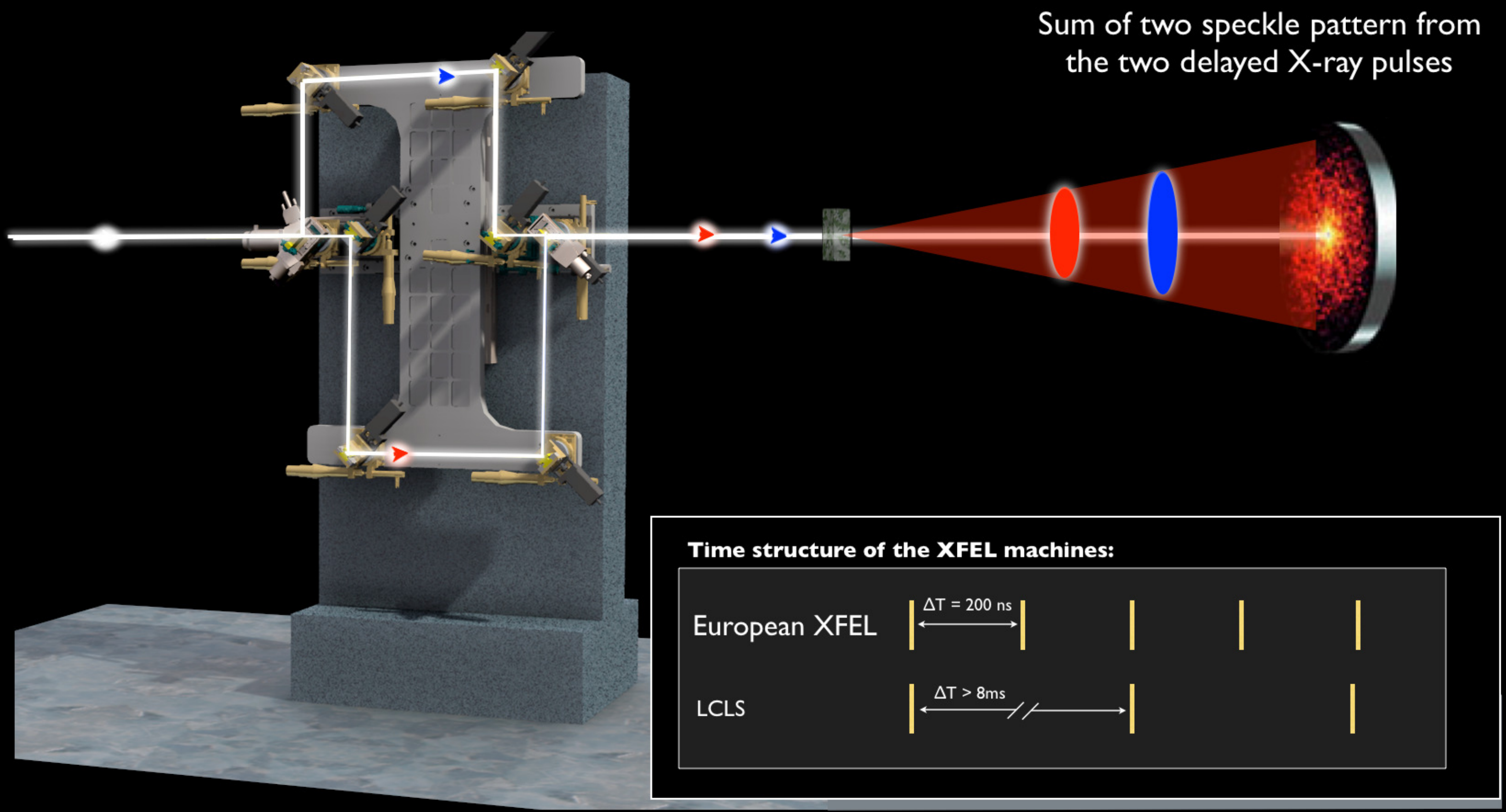


→Detectors with frame rate 200 ns

XPCS at FEL sources: pump and probe mode



Split and delay concept at XFEL sources



Concept G. Grübel, G.B. Stephenson, C. Gutt, H. Sinn, T. Tschentscher, NIM B 262, 357 (2007)
Split and delay line W. Roseker et al. Optics Letters 34, 1768 (2009)

Movie Mode

$$g_2(\tau) = \frac{\left\langle I(t)I(t+\tau)\right\rangle}{\left\langle I(t)\right\rangle^2} = 1 + \left|f(\tau)\right|^2$$

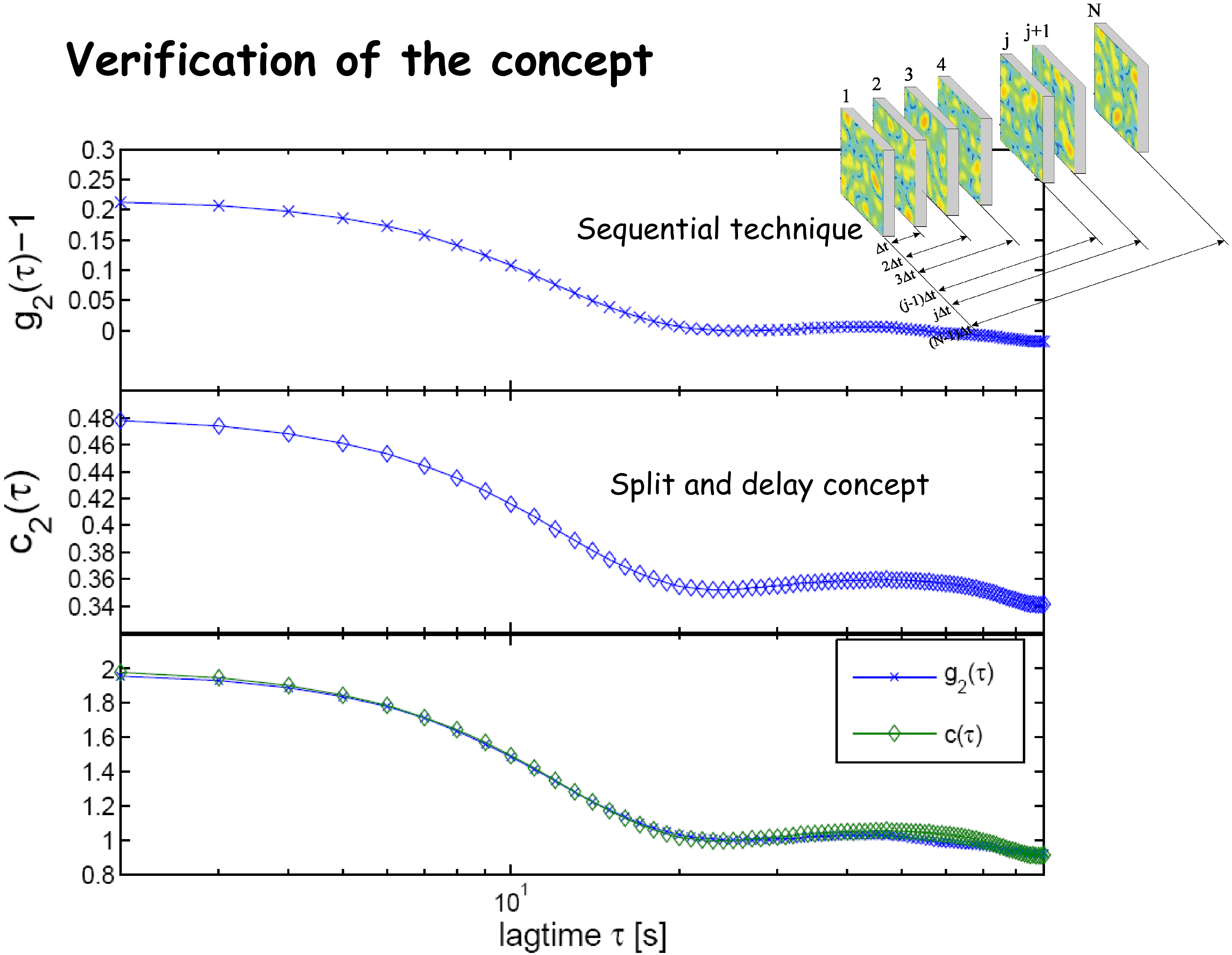
Split-Pulse technique

$$S(\tau) = I(t) + I(t+\tau)$$

$$c_2(\tau) = \frac{\left\langle S(\tau)^2\right\rangle - \left\langle S(\tau)\right\rangle^2}{\left\langle S(\tau)\right\rangle^2} = \frac{1}{2}\left(1 + \left|f(\tau)\right|^2\right)$$

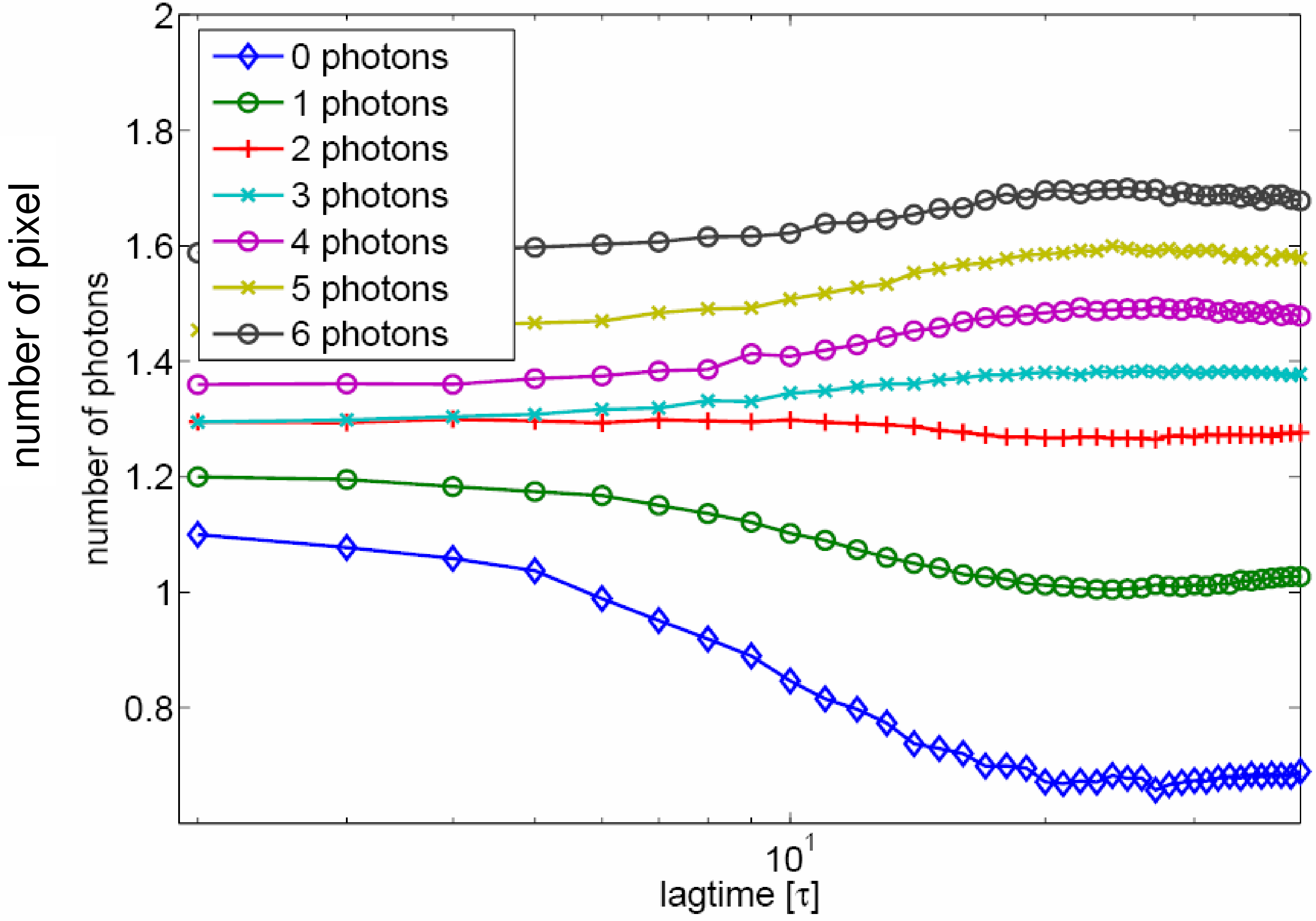
C. Gutt, L.-M. Stadler, A. Duri, T. Autenrieth, O. Leupold, Y. Chushkin, G. Grübel
Optics Express 17, 55 (2009)

Verification of the concept

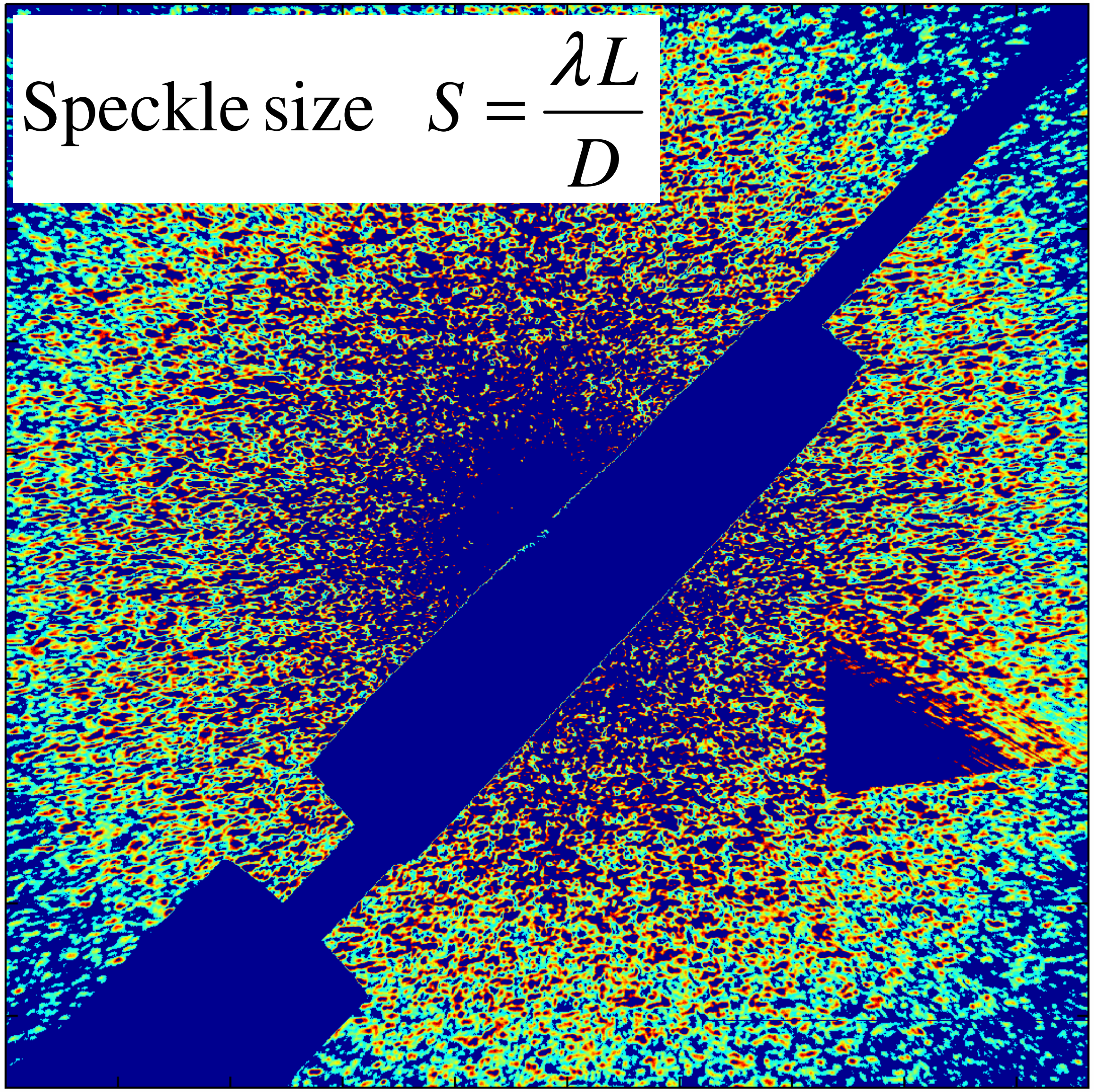


C. Gutt, L.-M. Stadler, A. Duri, T. Autenrieth, O. Leupold, Y. Chushkin, G. Grübel Optics Express 17, 55 (2009)

Analysis of the photon statistics



Speckles



- No need to oversample speckle pattern

- Need to put beam twice on the same sample spot

-> reduce heat load via unfocussed beam sizes

-> need to detect beam damage, e.g. as today via fluctuations in S(q,t)

Consequence of beam sizes

Detector distance [m]	Sample size [microns]	Speckle size [microns]
2	40	5
4	20	20
20	25	80
20	40	50
20	80	25

Signal to noise ratio in XPCS

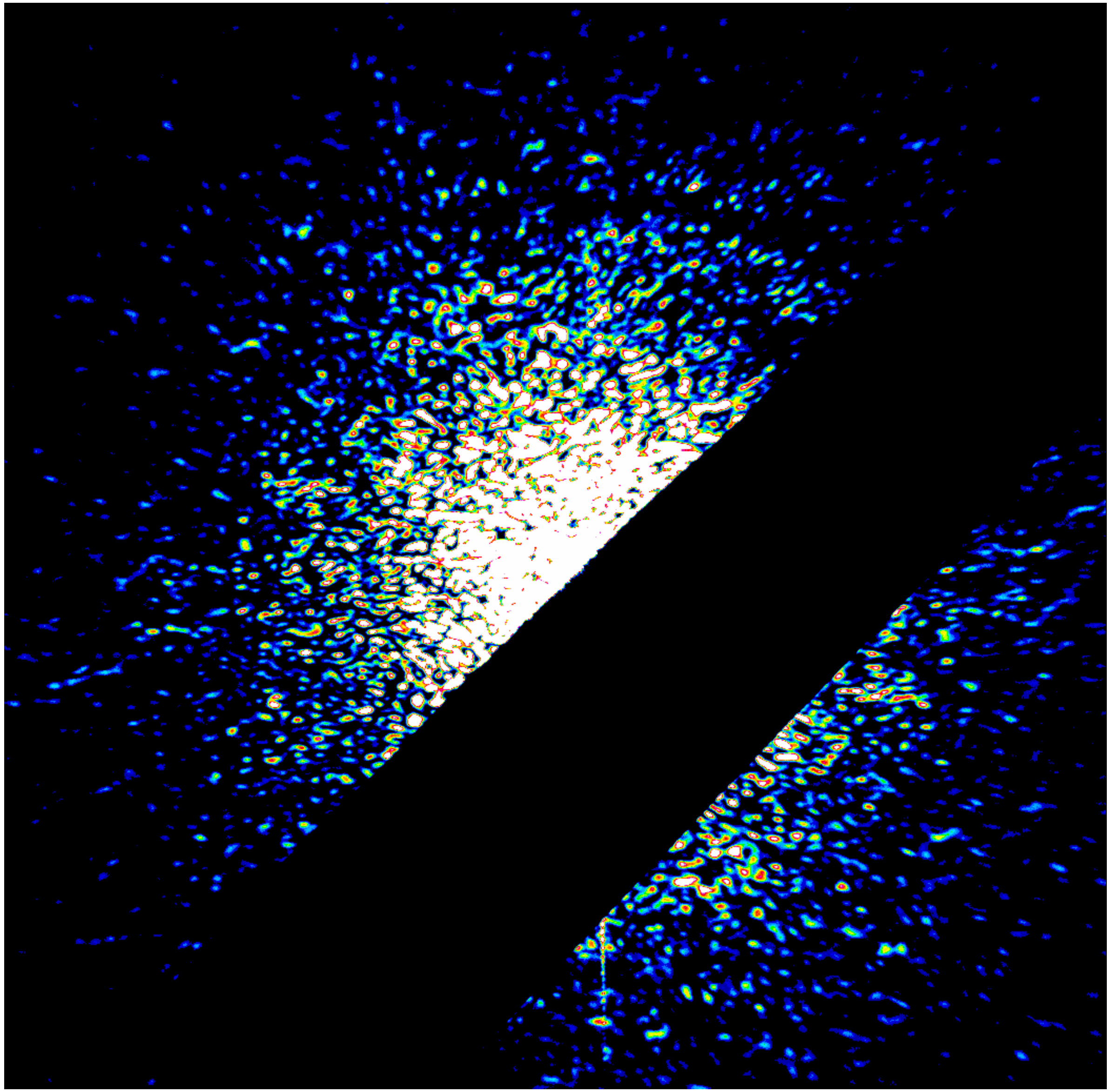
$$SNR \propto \beta(Q)\frac{N_{Pulses}}{1+(P/S)^2}$$

P pixel size
S speckle size

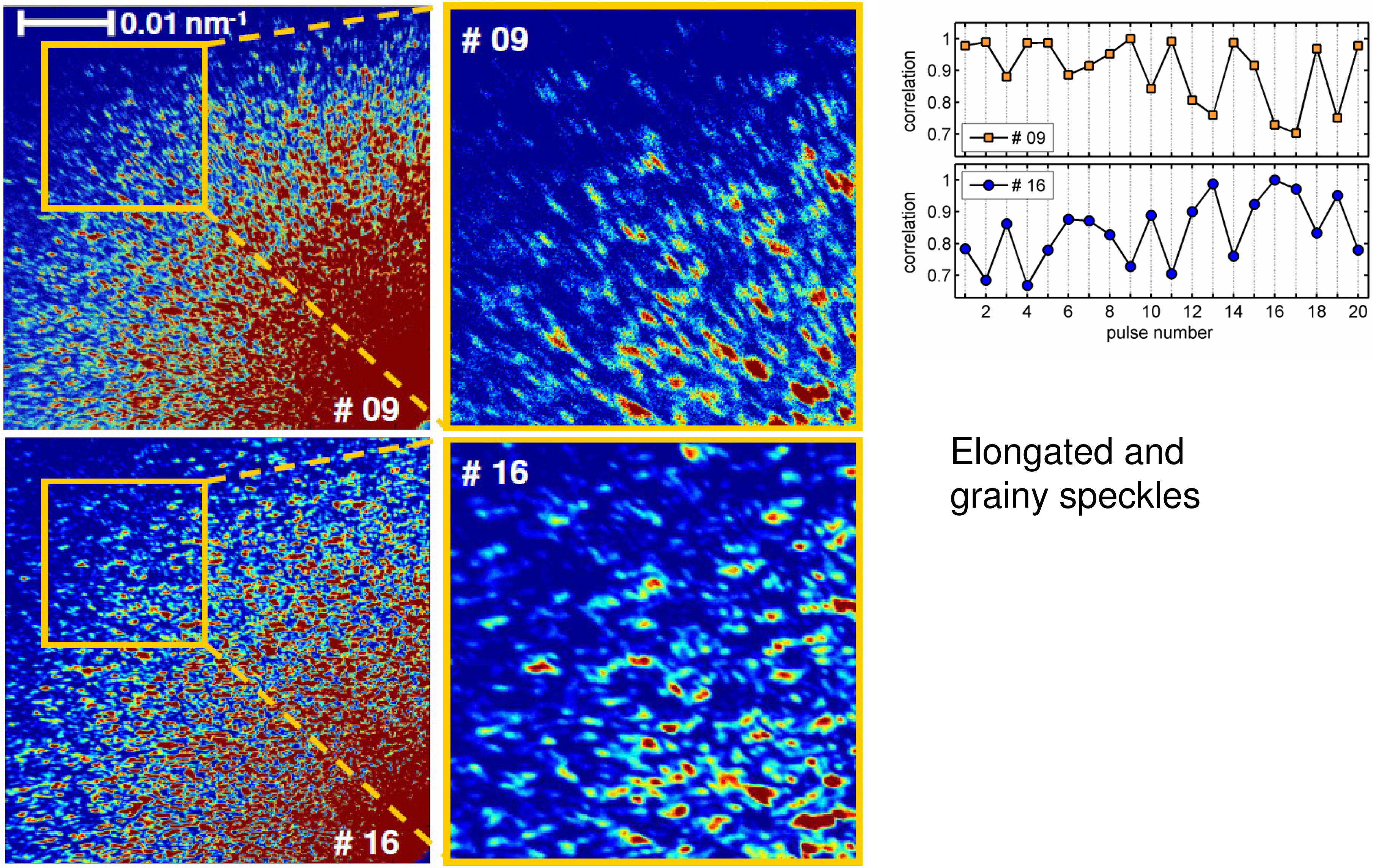
Wanted: high contrast <u>and</u> many pixels =>
pixel size similar to speckle size

Can we record single shot pattern without frying the sample ?

Series of 30 fs single shot images
FLASH @ 20.8 nm



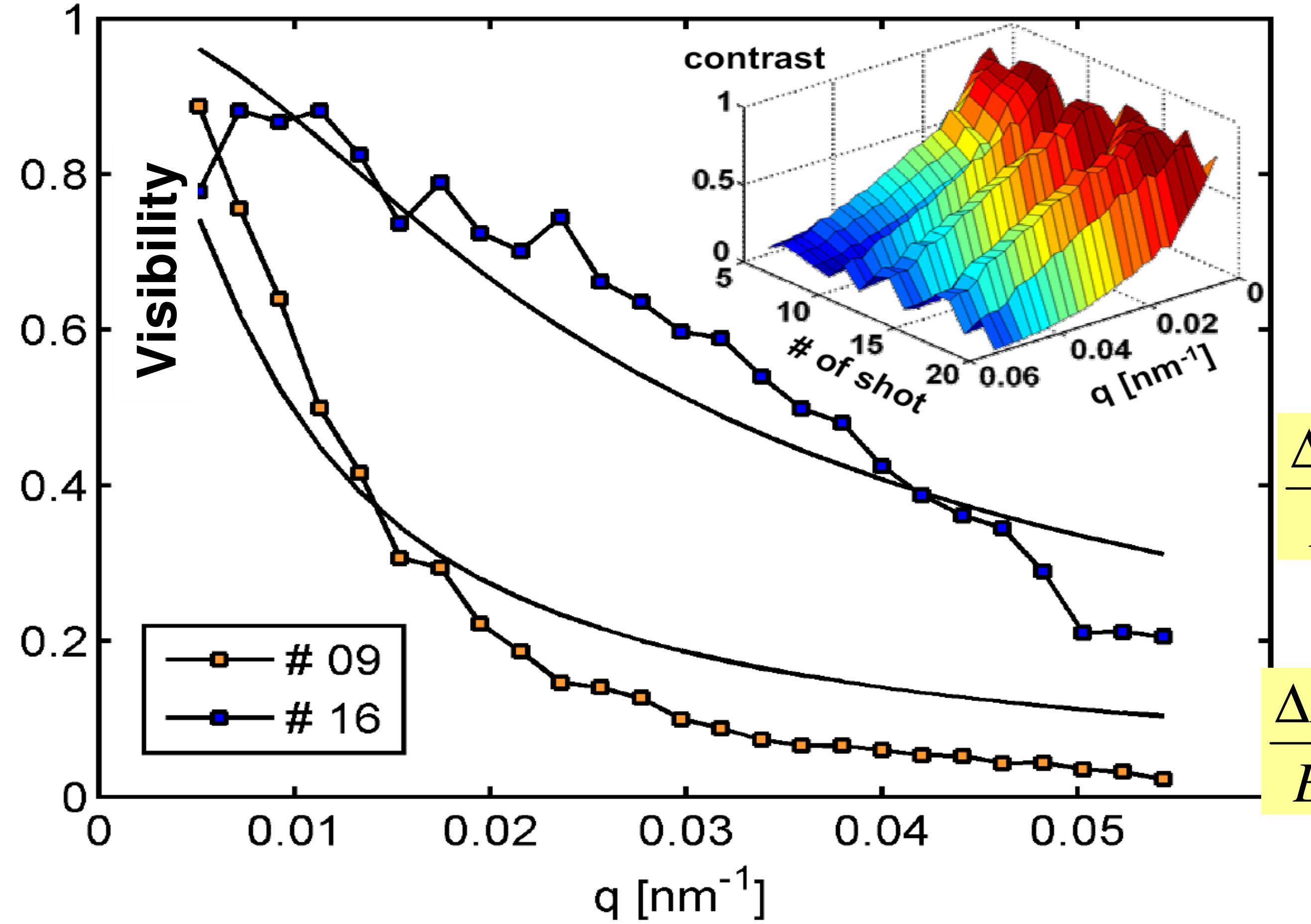
Destruction-free single shot speckles at FLASH



Elongated and grainy speckles

Speckle visibility and the SASE process

$$V = \frac{1}{1 + W^2 q^2 \left(\frac{\Delta E}{E}\right)^2}$$



$$\frac{\Delta E}{E} \approx 0.3\%$$

$$\frac{\Delta E}{E} \approx 1.0\%$$

Conclusion

XPCS schemes at XFEL

Delay line is existing and tested at synchrotron sources

XPCS experiments at XFEL are limited by SNR ->
pixel size of detectors will be a of central importance

beam damage is a function of energy density – strongly
dependent on sample composition and beam size