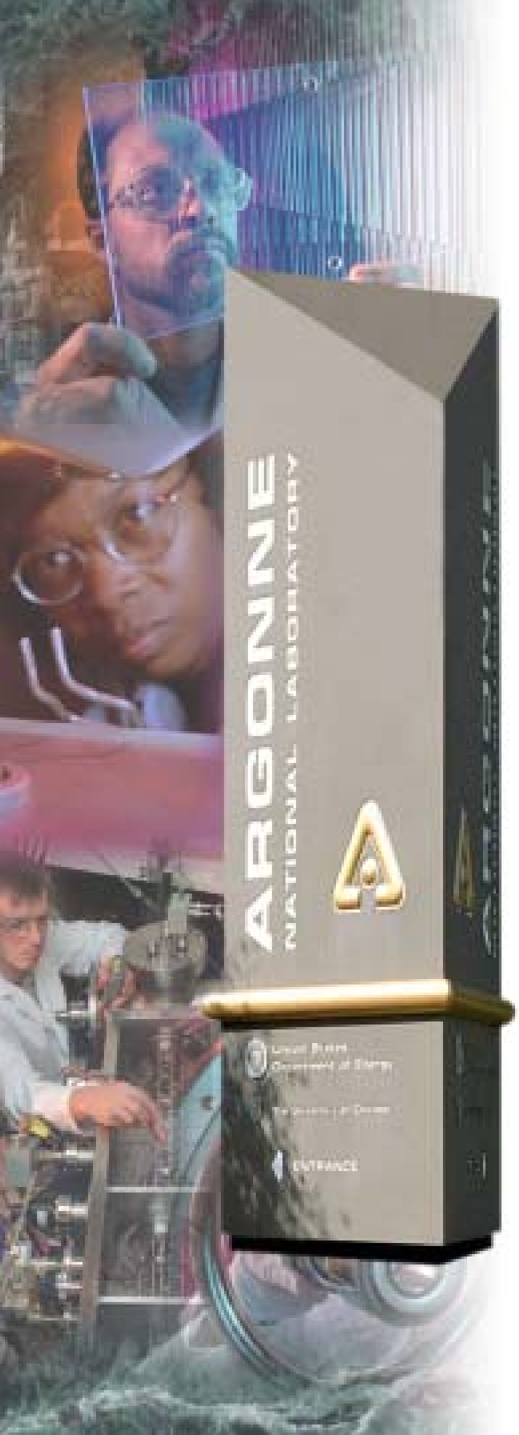

Signal to Noise ratio of XPCS using high efficiency area detectors

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Porquerolles, June 16, 2005

Argonne National Laboratory

Office of Science
U.S. Department of Energy

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Office of Science Laboratory
Operated by The University of Chicago

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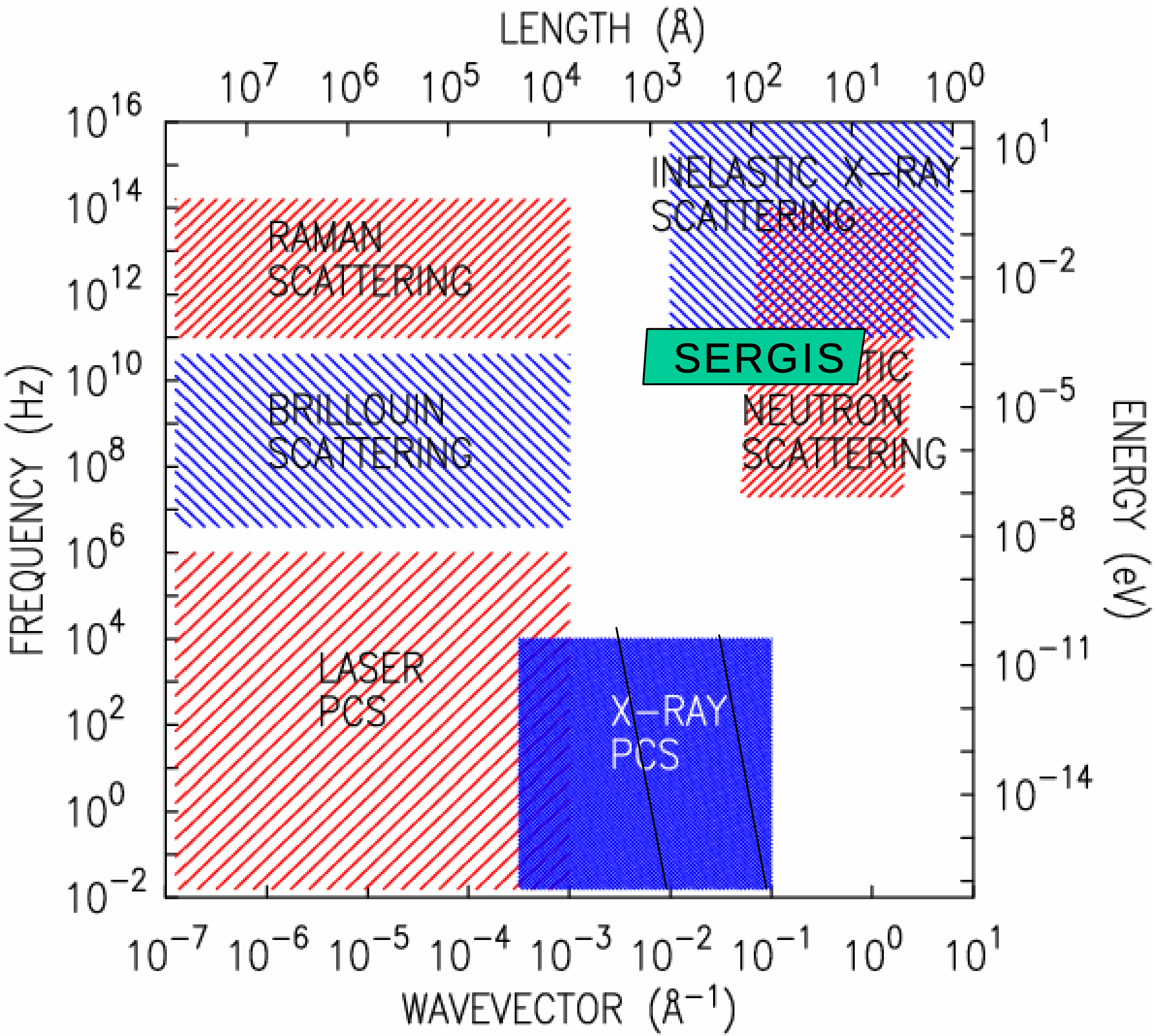
For details of 8-ID see poster 50 by M. Sprung

Outline

1. Introduction to XPCS
2. How to optimize your beamline to your detector
3. How to fit your detector to your beamline
4. What did we use our new detector for

Scattering phase-space



$$SNR = AI\sqrt{T\tau}$$

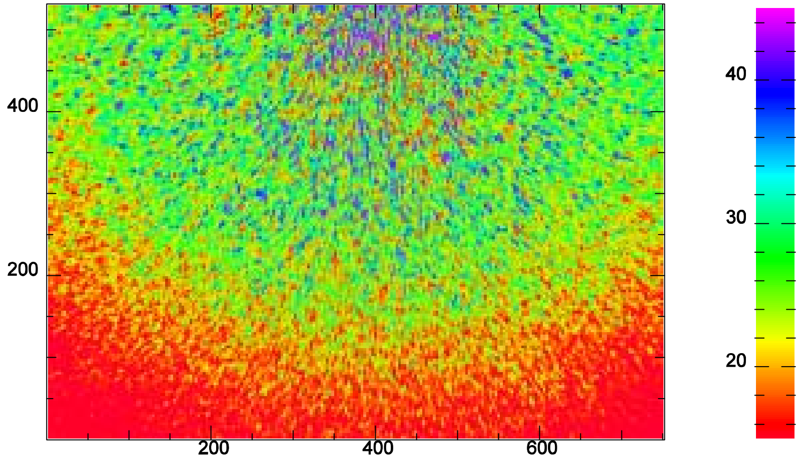
$$T \propto \tau^{-1}$$

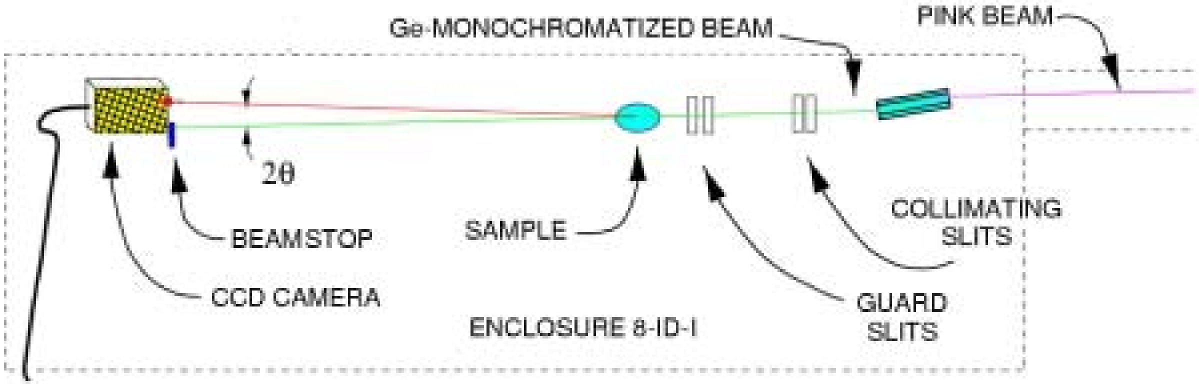
$$I \propto Q^{-4}, \tau \propto Q^{-2}$$

$$T \propto Q^{10}!!!!$$

How is XPCS done ?

- XPCS requires coherent X-rays
- Detects the movement of speckles
- Without X-ray lasers we use collimated synchrotron beam



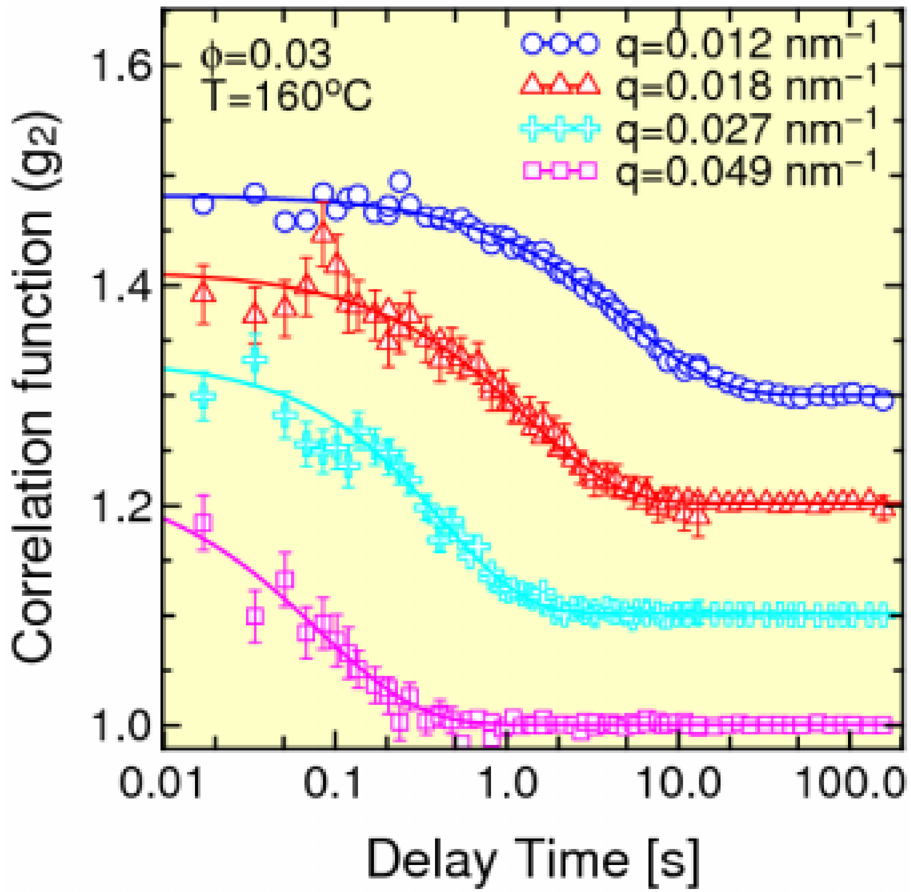


XPCS measures the time auto-correlation function of the scattered intensity g2:

$$g_2(\tau) = \frac{\langle I(t+\tau)I(t)\rangle_t}{\langle I(t)\rangle_t}$$

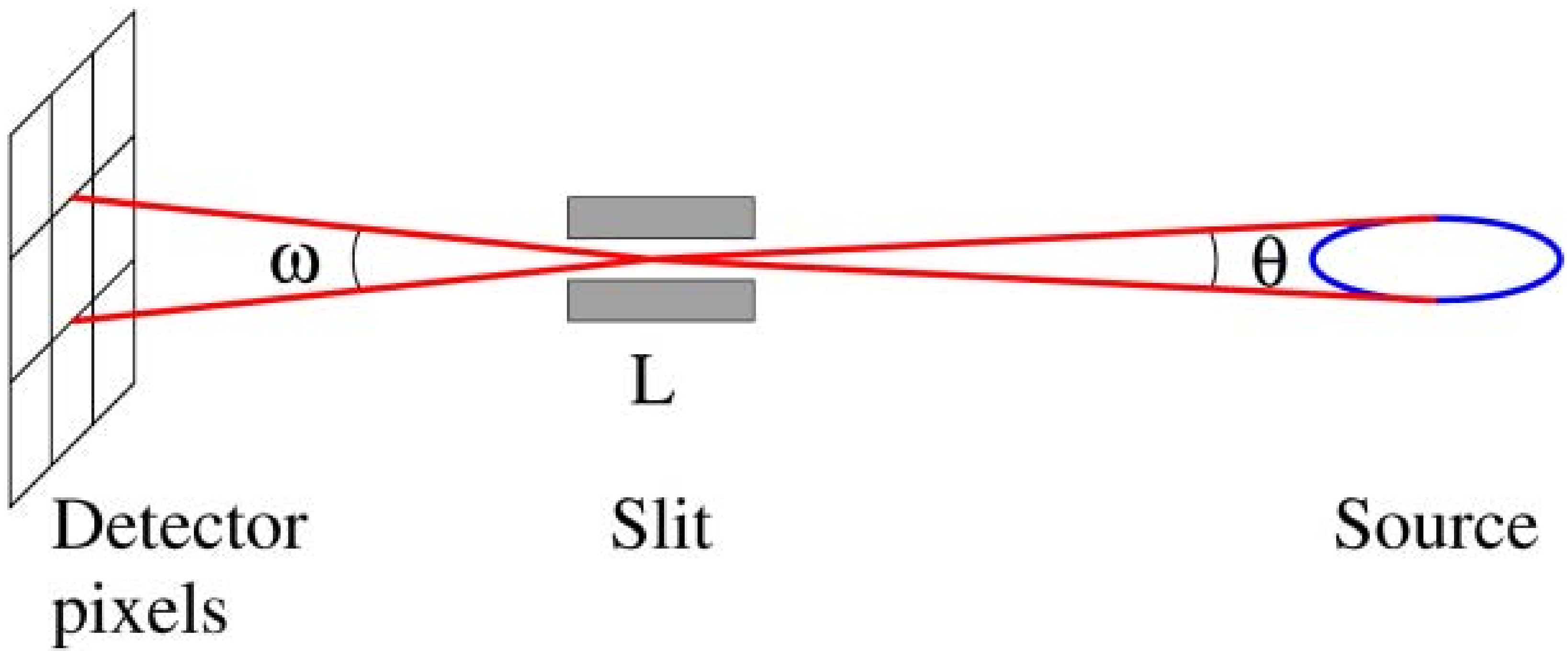
Which is connected to the intermediate scattering function *f* (ISF) via the Siegert relation:

$$g_2(Q,\tau) = 1 + \beta f(Q,\tau)^2$$
$$f(Q,\tau) = \langle \rho(-Q,t)\rho(Q,\tau)\rangle$$



A typical line shape is the stretched exponential

$$f(\tau) = e^{-\left(\tau/\Delta t\right)^{\alpha}}, \quad \Delta t \propto Q^{-z}$$



$$\omega_x = U_x / R_{det}$$

$$\theta_x = \sqrt{6}\sigma_x / R'$$

$$\xi_x = \frac{\sqrt{6}}{2\pi}\frac{\lambda}{\theta_x}$$

$$\Xi_x = \frac{\sqrt{6}\lambda}{2\pi}\frac{1}{\sqrt{\omega_x^2 + \theta_x^2}}$$

SNR ‘calculation’

The original Jakeman formula:

$$R_{sn} = A\bar{I}\sqrt{T\tau n_x n_z}$$

$$R_{sn} = \sqrt{T\tau\ \Omega_x\Omega_z\eta}\ \Sigma W\, e^{-W/\Lambda}\,\tilde{B}\,(\Delta E/E)\, r_{snx}\, r_{snz}$$

detector sample source

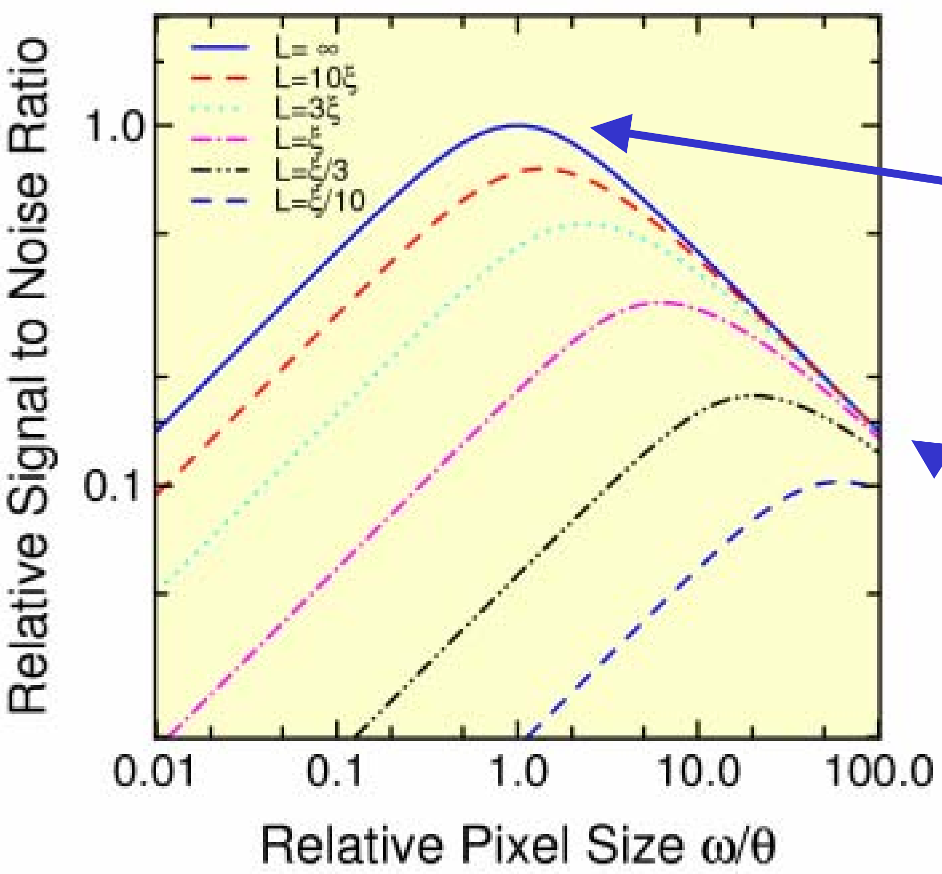
$$r_{snx} = F\left(\frac{L_x}{\Xi_x}\right)\sqrt{\omega_x}\theta_x L_x$$

$$F(x) = \frac{1}{x^2}\left[x\sqrt{\pi}\,\mathrm{erf}\,(x) + e^{-x^2} - 1\right]$$

- **We will optimize** $r_{snx} \cdot r_{snz}$
- **Horizontal and vertical direction are separated**
- **Dependent only on** ω, θ, L

Lumma et al RSI v71 p 3274 (2000), Falus et al. JSR submitted

Optimum pixel size



- SNR Depends on slit size
- There IS an optimum size
- For large slits the optimum is

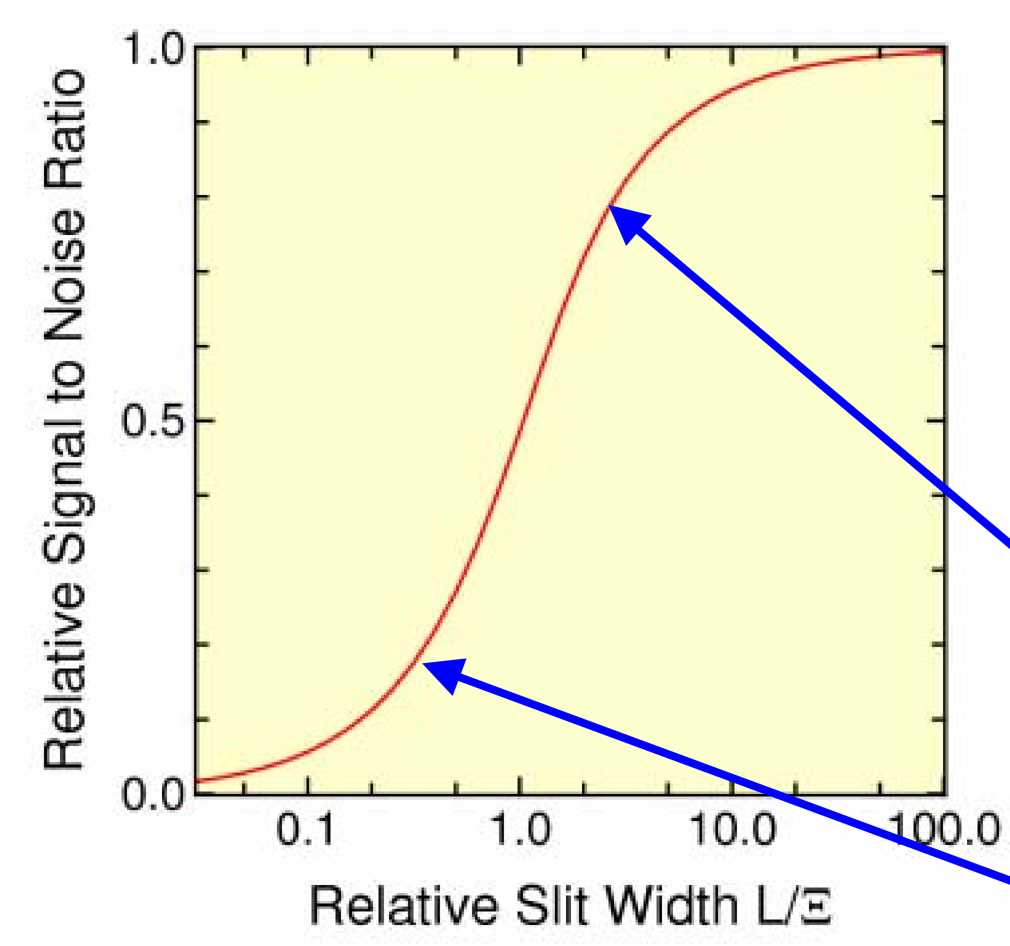
$$\omega = \theta$$

- For large pixel sizes measurement time increases as

$$T \propto \left(\omega / \theta \right)^2$$

Go far, have small pixels

How wide the slits should be ?



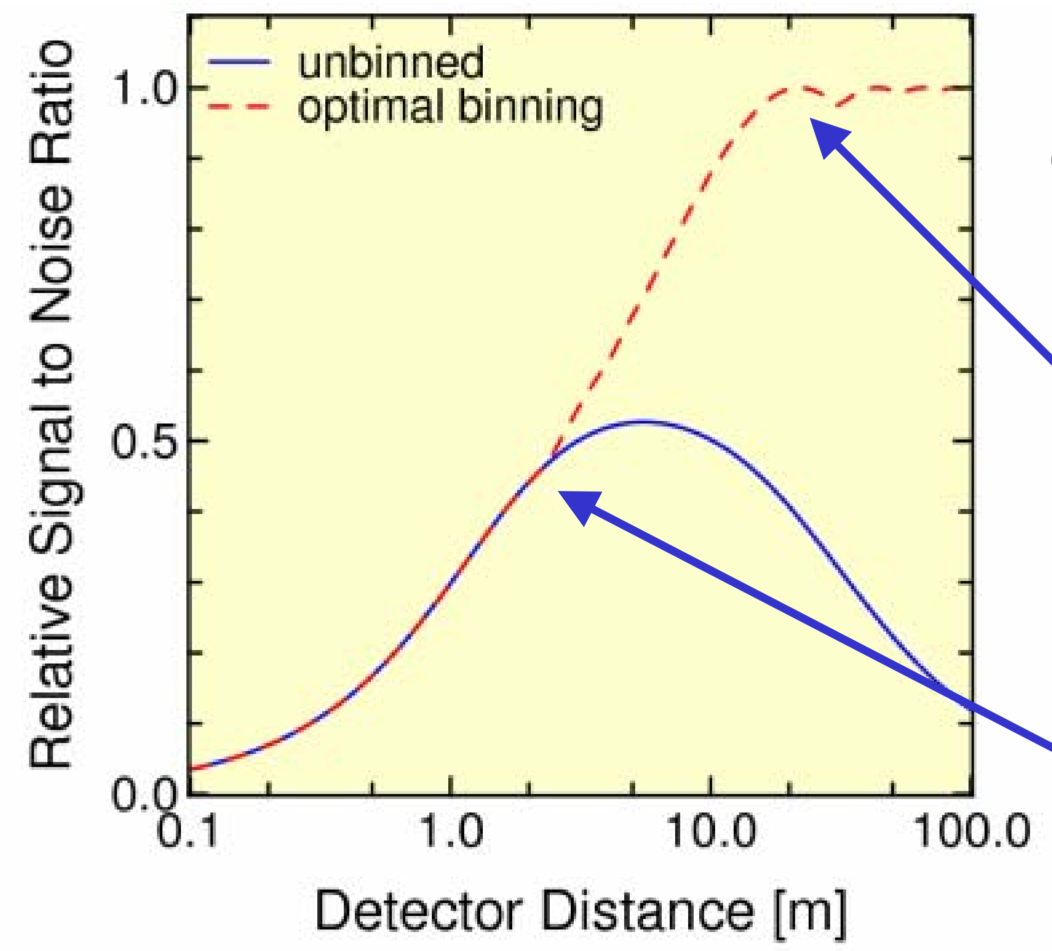
- Up to factor 100x improvement in measurement time compared to

$$L/\Xi = \sqrt{1/2} \approx L/\xi = 1$$

- Width of 4 has a contrast of 0.14 within factor of 3 of maximum (90ux90u slits at 8-ID)

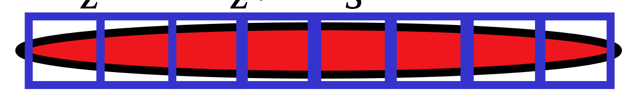
$$T \propto L^{-4}$$

Should we have square pixels ?

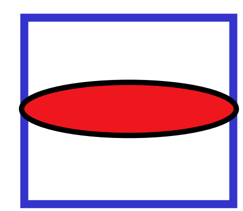


For typical 8-ID parameters:
14um pixels, 15x220um source
65 m from sample, 8keV

$$\omega_z = \theta_z, R_s = 25m$$



$$\omega_x = \theta_x, R_s = 1.7m$$



Binning helps if we go far enough !

Optimal XPCS beamline:

- **Slits are much bigger than the transverse coherence length**
- **The detector has small pixels, and the pixel shape matches the source shape**
- **The detector is far enough from the sample to match the angular pixel and source sizes at least in the horizontal direction**
- **Possibly use focusing to achieve reasonable detector source distances.**

Good XPCS detector

$$R_{SN} = AI\sqrt{T\tau} \quad \eta\sqrt{\tau fn}$$

Ideal point detector SNR $\sqrt{DQE2}$

- **Small pixels**
- **Low noise to enable photon counting**
- **Maximizes DQE2**

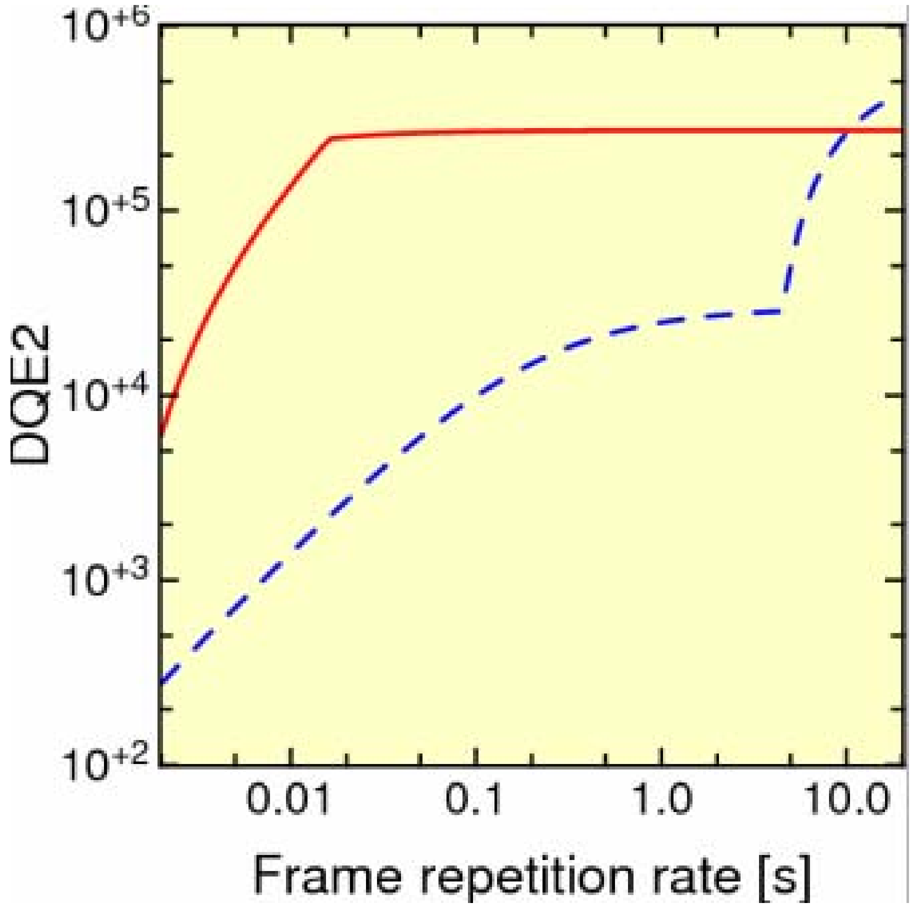
Practical example

We need 16ms time resolution:

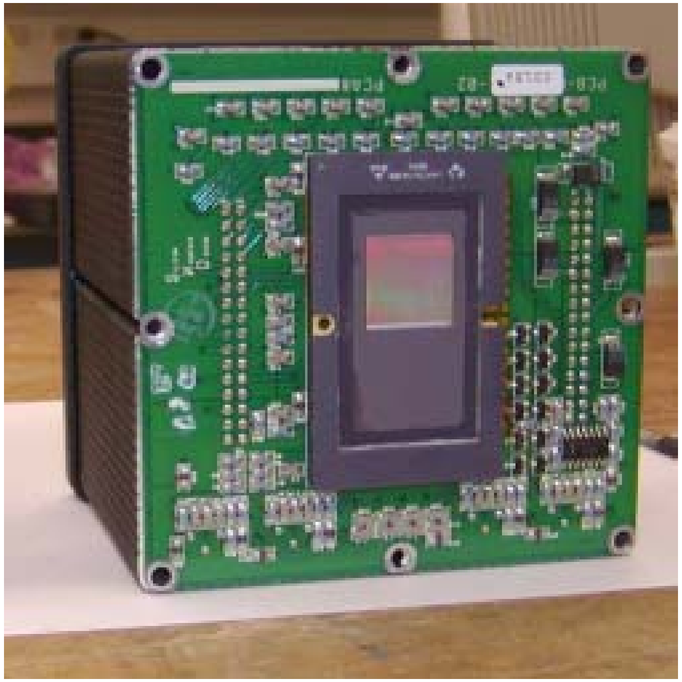
SMD Camera
- 14ux14u pixel size
- 15.2ms exposures
- 1024x1024 pixels
- Continuously
- 49% efficiency
- Noise 0.08 Photon RMS
- 12 bit resolution

Princeton Instruments camera:
- 22ux22u pixel size
- 16ms exposures
- 64x1242 pixels
- 240ms exposure then 3600ms dead time
- 68% efficiency (6.4 keV)
- Noise: 0.003 Photon RMS
- 16 bit ‘resolution’

New detector reduced measurement time 100x

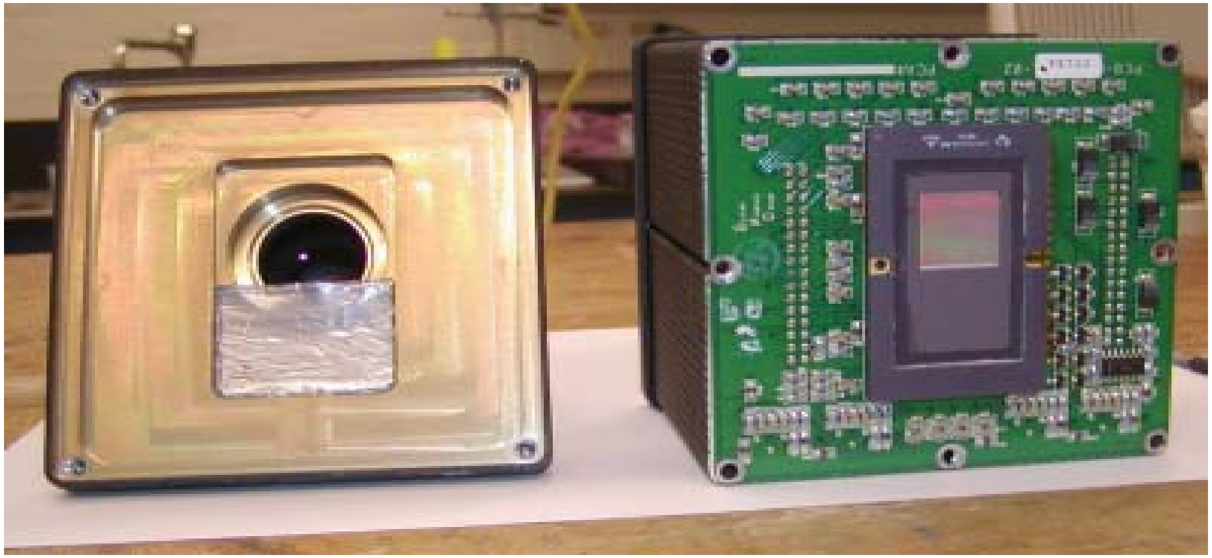


$$DQE\,2 = \eta^2 \tau f n_x n_y$$



Tomography: DiMichiel et al. Rev. Sci. Instrum. 76 043702 (2005)

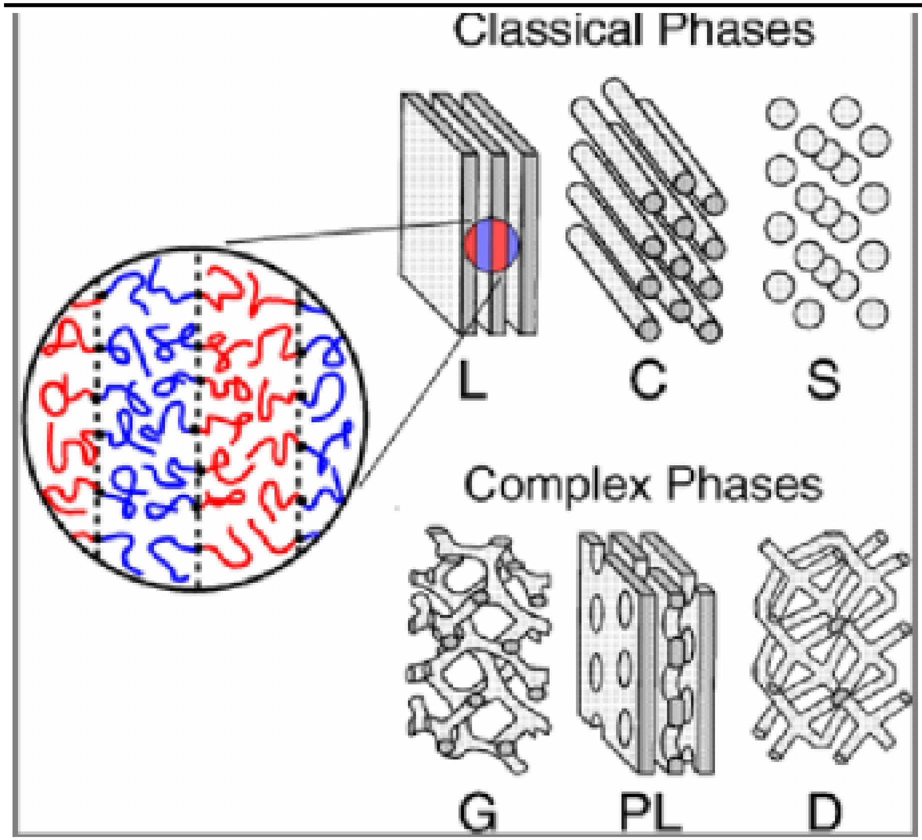
How to modify a visible light camera



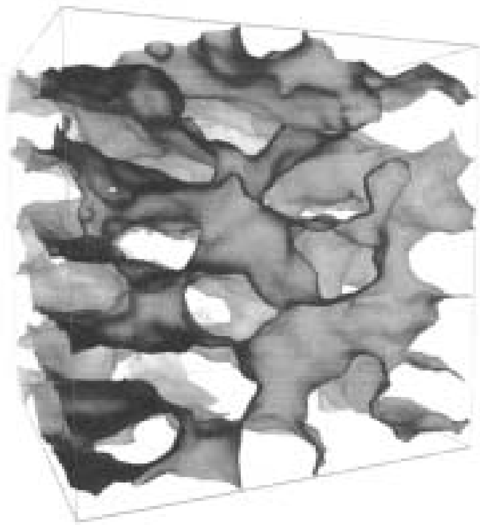
- Choose a ‘frame transfer’ camera
- ‘Scalp’ the CCD
- Shield the transfer region from X-rays
- Make sure you can save the data real time

Robert Flughum: All I really need to know I learned in kindergarten (1988)

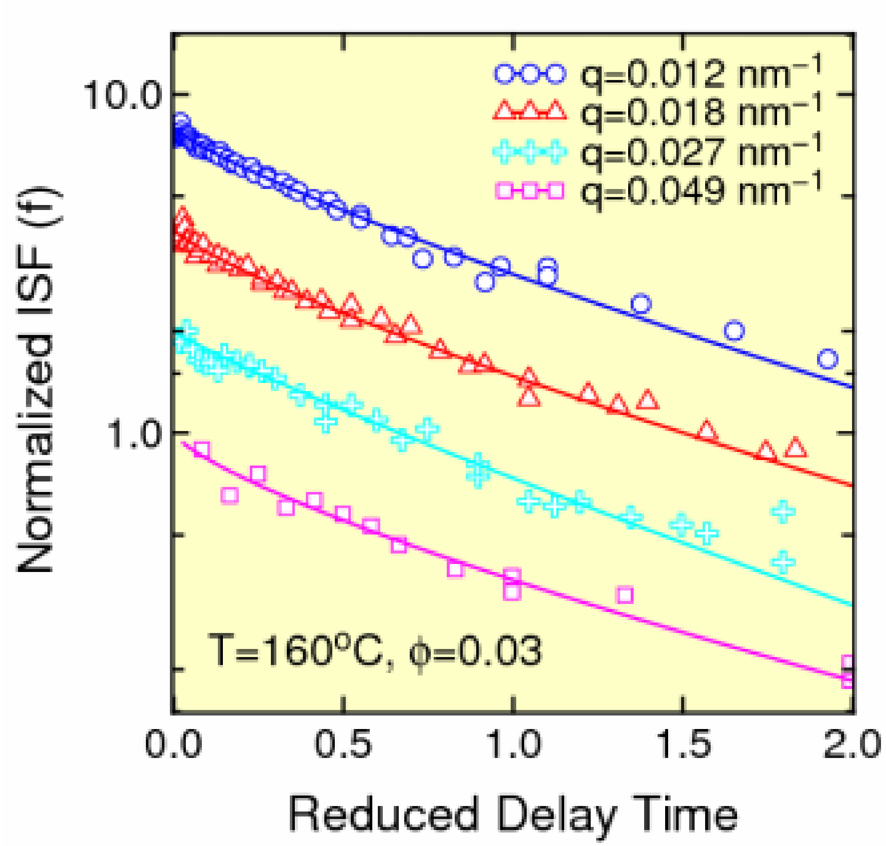
Why Study block copolymer vesicles with XPCS ?

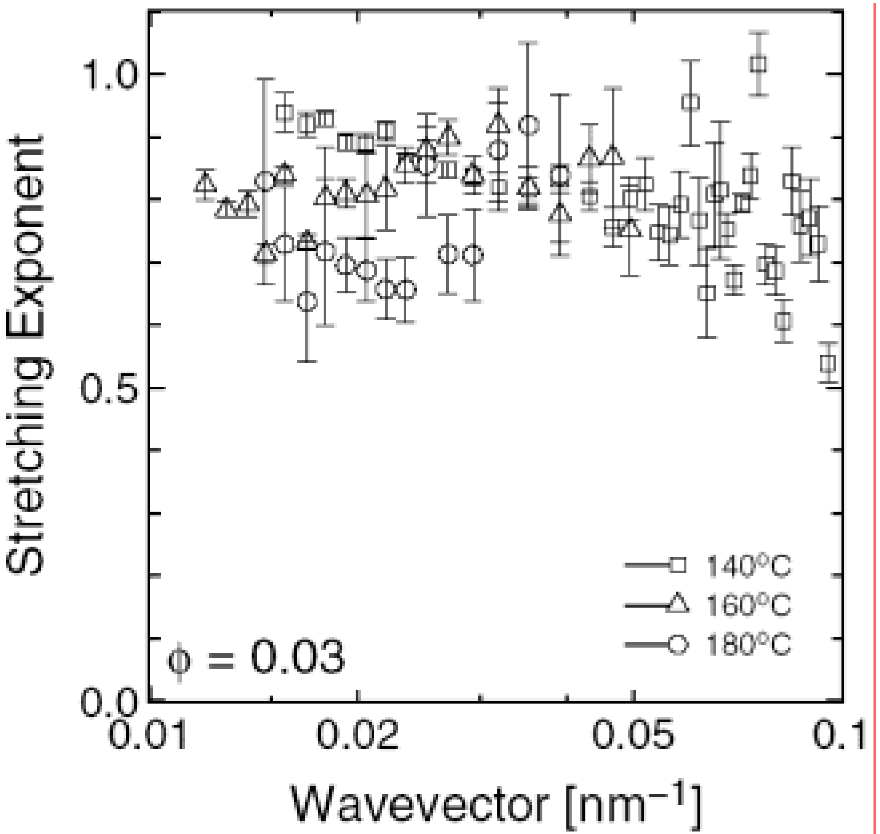


oNo hard to measure material parameters, easy comparison with theory
oMatching time- and lengthscale
oNo multiple scattering



Falus et al. PRL 94 016105 (2005)
Falus et al. PRL 93 145701 (2004)





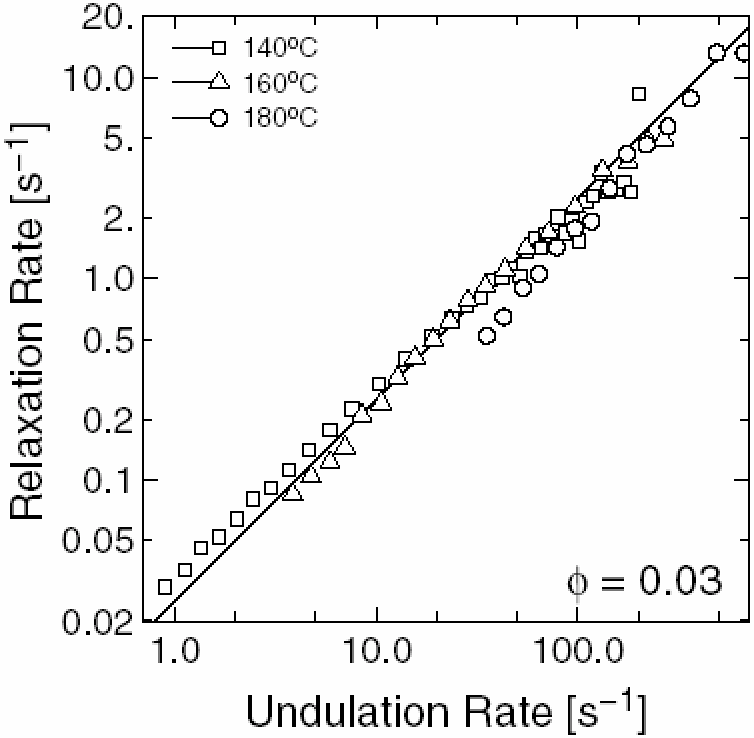
$$Diffusion: \alpha = 1, z = 2, \quad Membranes \quad \alpha = 2/3, z = 3$$

Zilman&Granek predicts data collapse versus the undulation rate:

$$k_B T q^3 / \eta$$

For soft lamellae $\kappa \approx k_B T$

$$\Gamma = 1/\Delta t \approx 0.025 k_B T q^3 / \eta$$



Remarkable agreement with A. G. Zilman and R. Granek, Chem. Phys. **284**, 195(2002).

Conclusion

- XPCS is a signal to noise limited technique
- XPCS is needs dedicated beamline designs and new detectors
- We can build great XPCS detectors by modifying visible light cameras. We can measure 100 times faster !
- XPCS is proven to be useful even for weakly scattering systems like polymer vesicles