

Scientific Trends and Opportunities from the Perspective of 8-ID

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Outline

- 8-ID experiment categories
- Historical trends
- Future directions
- Ancillary items

8-ID Experiment Categories

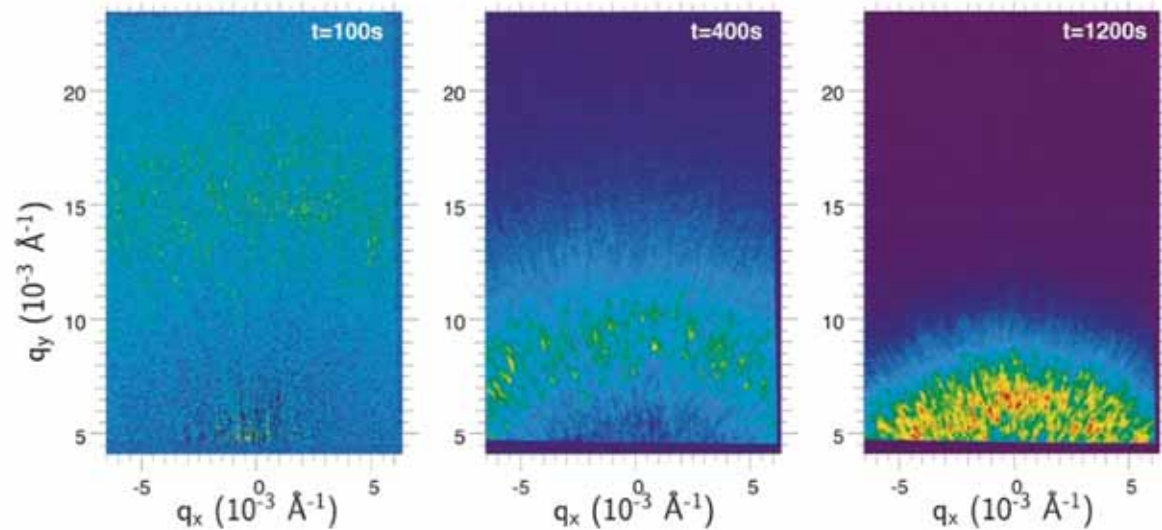
1. Noteworthy successes
2. Bleeding-edge, marginal and jury-still-out experiments
3. Failures and too-hard and too-scary to try experiments



ERL Experiments?

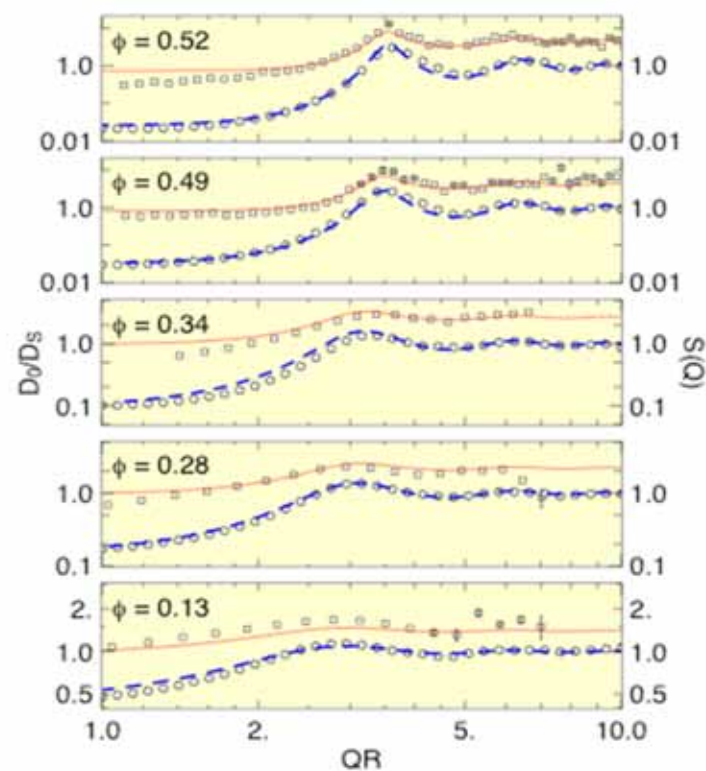
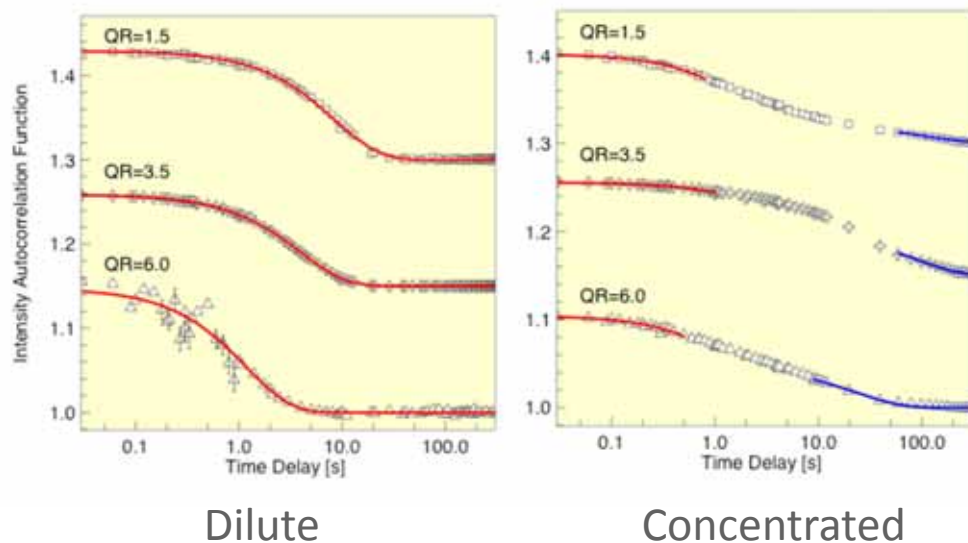
1. Noteworthy successes

- Domain coarsening in glasses
 - Fluctuations about evolution to a phase separated state in a sodium borosilicate glass [A. Malik et al., PRL 81, 5832 (1998)]
 - Dynamics measured in a non-equilibrium system
 - Pink-beam used in small-angle transmission geometry
 - One-and-only pink beam XPCS measurement from 8-ID
 - Time scales: > 1 s



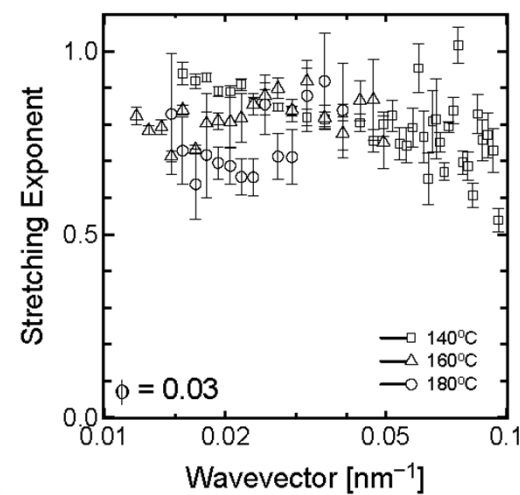
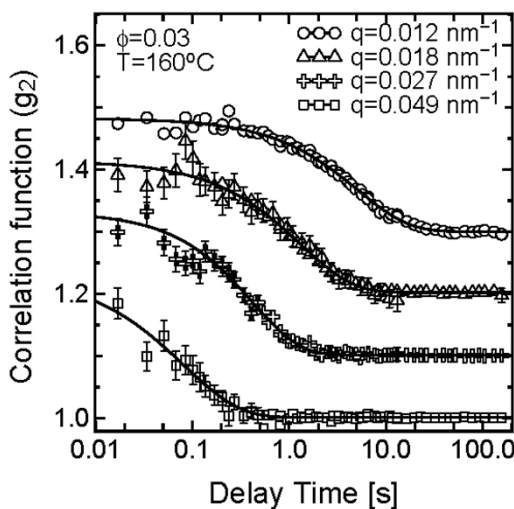
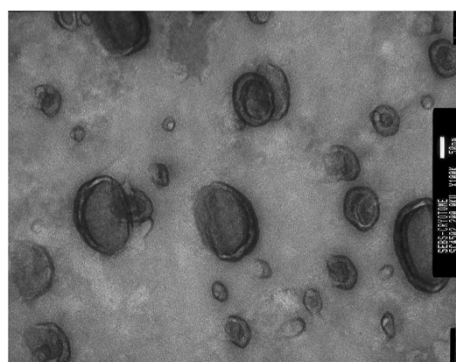
1. Noteworthy Successes

- Dynamics in concentrated hard-sphere suspensions
 - Correlation functions of sufficient quality to distinguish hydrodynamic corrections to diffusion of concentrated nanoparticles
 - [L. B. Lurio et al., PRL 84, 785 (2000)]
 - Time scales: > 50 ms (kinetics)



1. Noteworthy Successes

- Dynamics of block copolymer vesicles
 - Membrane fluctuations in a tri-block homopolymer mixture
 - Rapidly fluctuating speckle patterns
 - Correlation functions of sufficient quality to see stretched (2/3) exponential decays
 - Home-built SMD/Dalsa fast direct-detection detector
 - [P. Falus et al., PRL 94, 016105 (2005) and P. Falus et al., RSI 75, 4383 (2004)]
 - Time scales: > 10 ms



1. Noteworthy Successes

- Fluctuations about the evolution to equilibrium
 - Fluctuations in a phase ordering system [A. Fluerasu et al., PRL **94**, 055501 (2005)]
- Aging at the nanoscale
 - Nanoscale dynamics versus aging time vis-à-vis structure (Leheny et al., several publications)
- Heterodyne XPCS
 - Heterodyne methods to track flow and fluctuations within flow at the nanoscale [F. Livet et al., J. Synch. Rad **13**,453 (2006)]
- Polymer surface and interface experiments of increasing sophistication
 - Thick films, thin films, buried interfaces, wave-guide enhancements, temperature $\approx T_g$ (Z. Jiang, H. Kim, J. Lal, L. Lurio, S. Narayanan, S. K. Sinha)
- Re-entrant glass
 - Dynamics of repulsive and attractive glass phases and a novel “liquid” phase in between [X. Lu et al., PRL **100**, 045701 (2008)]
- Metal surface fluctuations
 - Dynamics in the reconstruction of Au(001) versus temperature [M. Pierce et al., PRL **103**, 165501 (2009)]



Trends and Future Directions

- Observations
 - Temperature and sample composition have been the main independent variables
 - Area detectors have enabled quantitative g_2 measurements
 - Non-equilibrium
 - Aging, jamming
 - Results to-date have been achieved with
 - Essentially no increase in effective brilliance (no focusing)
 - Little change in detector throughput
 - SMD/Dalsa detector is an exception
 - 8-ID science cases have largely been ignored

- For the future examine
 - Variables other than temperature and sample composition
 - Bleeding-edge experiments
 - Too-hard or too-scary experiments
 - 8-ID sciences cases
 - Large wave-vector transfer XPCS
 - Largely untapped - over last 12 years: 3 publications, 1 in press and 2 under review
 - Flux levels make for very challenging experiments
 - High resolution (coherent) beam reveals new features in the diffraction pattern



Future Directions: Bleeding Edge and Too-Hard

- Variables other than temperature or composition

- Shear

- Connection between nanoscale dynamics and bulk rheology

- [W. Burghardt](#), S. Narayanan, M. Sikorski, ...

- Pressure

- Pressure-driven structure fluctuations

- W. Yang

- Environment

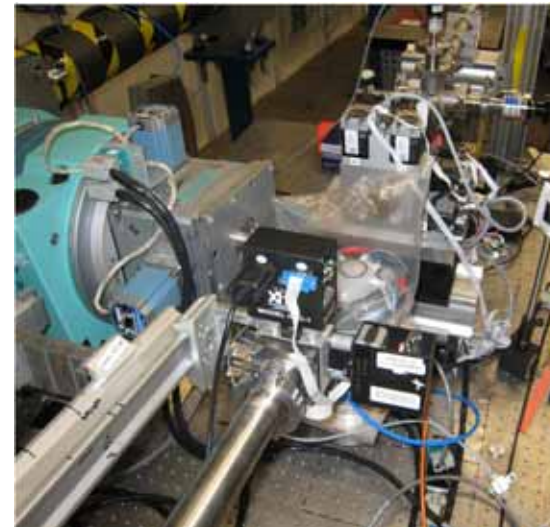
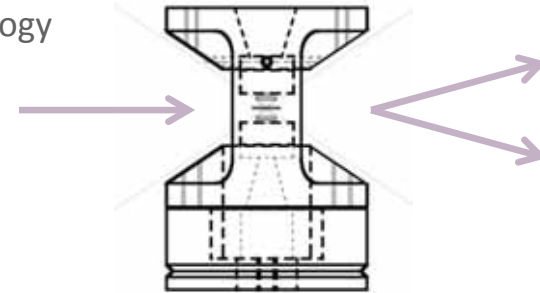
- Electrochemistry, catalysis

- [M. Pierce](#), H. You

- Confinement

- Biophysics

- [A. Fluerasu](#), L. Lurio, S. G. J. Mochrie



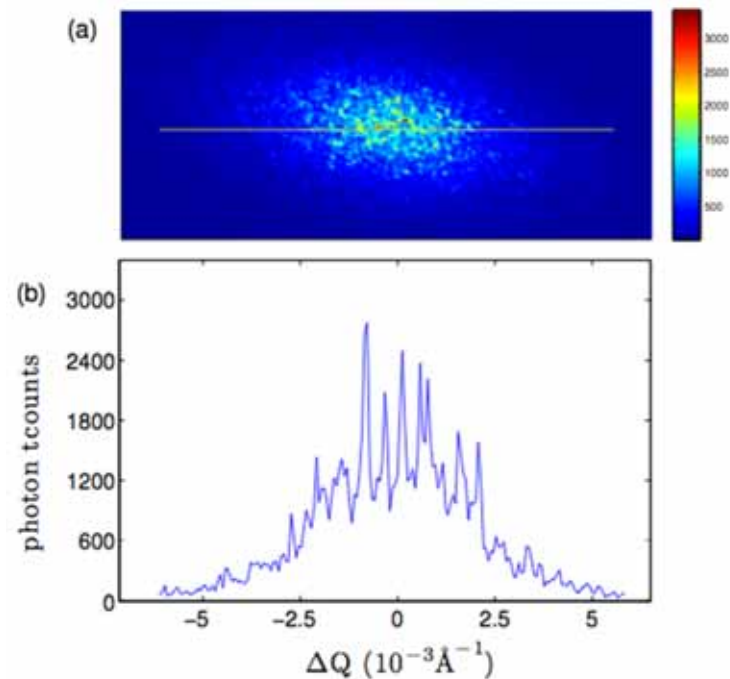
- Above experiments benefit from higher x-ray energies and require considerably more brilliant sources: $F_c = B(\lambda/2)^2$

XDL XPCS Workshop - Alec Sandy 6-30-11



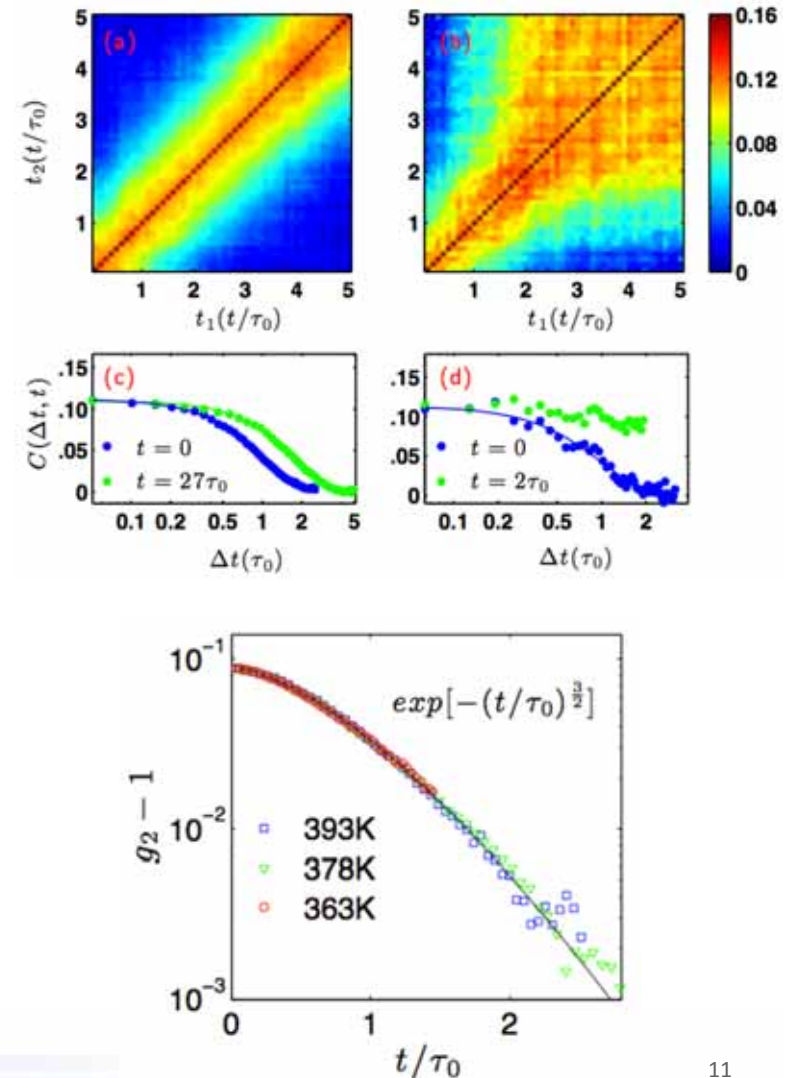
Future Directions: Bleeding Edge and Too-Hard

- Large wave-vector XPCS
 - Charge-density waves
 - Charge-density wave peak studied in incommensurate phase of $1T$ -TaS₂ in pure and Ti doped samples [J. Su, A. Sandy (ANL), M. Sutton (McGill)]
 - CDW speckle patterns from properly annealed samples are static meaning no spontaneous phase fluctuations (phasons)



Future Directions: Bleeding Edge and Too-Hard

- Charge-density waves
 - Charge-density wave peak studied in incommensurate phase of $1T\text{-TaS}_2$ in pure and Ti doped samples ...
 - Annealing deeply-quenched (freshly-prepared) samples yields transient dynamic speckle patterns
 - Transient effects are damped out more rapidly in more strongly doped samples
 - Correlation functions are compressed exponentials suggestive of collective re-arrangement of CDW phase domain walls
 - ERL would enable
 - » Wave-vector- and spatially-resolved motion of phase domains
 - » Other CDW's

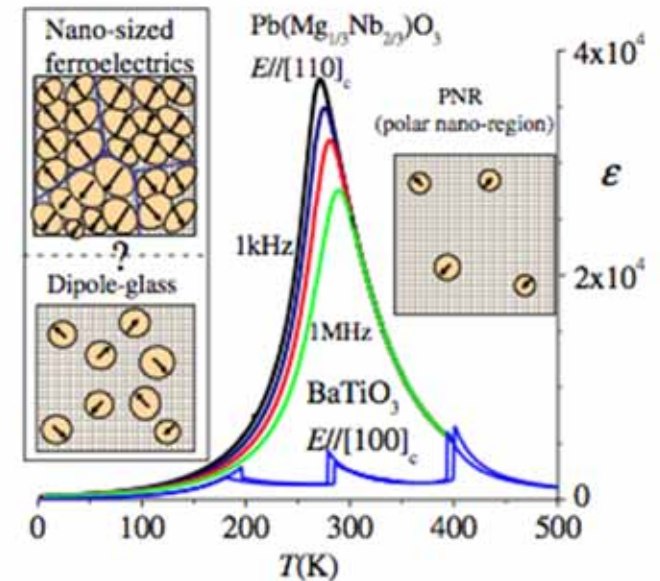


Future Directions: Bleeding Edge and Too-Hard

■ Large wave-vector XPCS

– Relaxor Dynamics

- Ferroelectric material that displays a large dielectric response to an applied field
 - Response to driving fields is large and temperature and frequency dependent
 - Origin of response has been studied for decades but remains controversial
 - $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ (PMN) is a prototypical example
 - » Polar nano-regions (PNR's) believed to exhibit either a static dipole glass at low temperature or nano-sized ferroelectric domains



Fu et al., PRL 103, 207601 (2009)

Future Directions: Bleeding Edge and Too-Hard

- Additional large Q possibilities
 - Glassy condensed matter
 - Spin ice (S. K. Sinha)
 - Frustrated ferromagnetic state with glassy behavior at low temperatures
 - Orientational glasses
 - I.e., $(\text{KBr})_{1-x}(\text{KCN})_x$ or $(\text{KCl})_{1-x}(\text{KCN})_x$
 - KCN molecules orient locally and freeze their orientations low temperatures
 - » Use XPCS to examine this transition

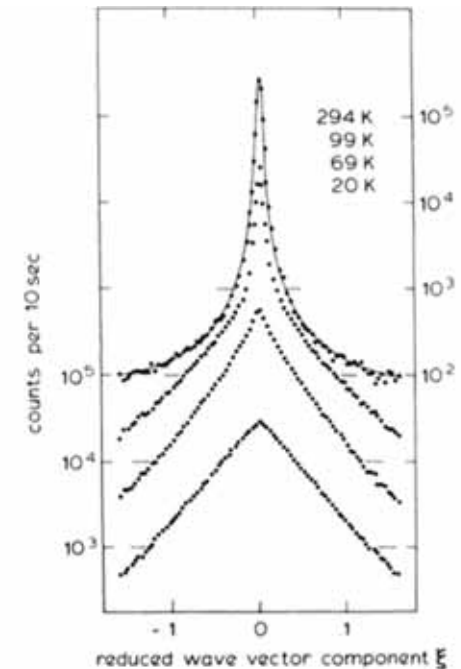


FIG. 1. The $(2\xi 0)$ profiles of $(\text{KCl})_{0.2}(\text{KCN})_{0.8}$ shown on a logarithmic intensity scale. The left scale refers to the 20-K data, and the right one to the 294-K data. The profiles are shifted by one order of magnitude with respect to each other. The ticks mark the 10^3 level for each run. The solid line of the high-temperature profile results from the superposition of a δ -like Bragg spike and diffuse intensity $I \sim \xi^{-2}$, folded with the experimental resolution and fitted to the data. The linewidth at 294 K is 0.0057 in ξ or 0.17° in the rocking angle (FWHM).

K. Knorr and A. Loidl, PRL 57, 460 (1986)



Future Directions: Bleeding Edge and Too-Hard

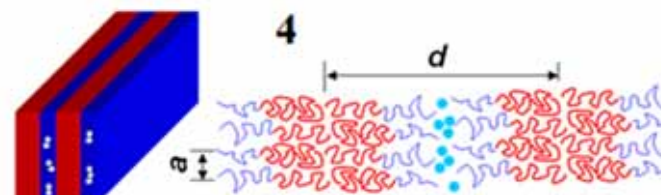
■ “Nanoparticle” dynamics

– Confinement

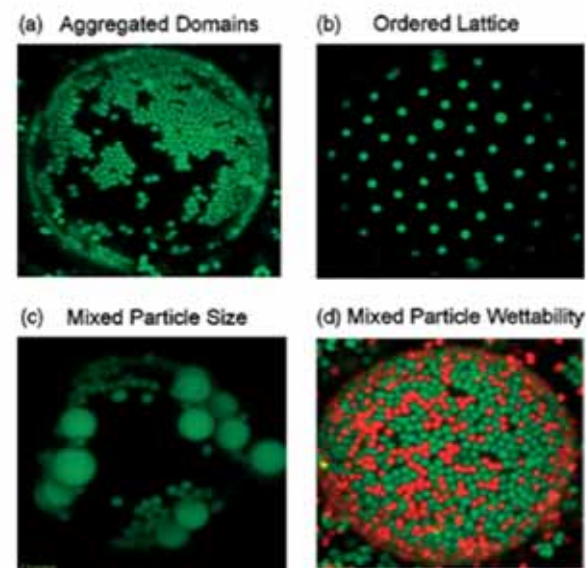
- Nanoparticles segregated at interfaces
 - Block copolymers
 - Pickering emulsions
 - Liquid surfaces or interfaces (doped lamellar phases)
- ERL high brilliance to overcome weak scattering contrast

– Biophysics

- Protein solutions
 - Eye-lens protein (L.B. Lurio and G. Thurston)
 - Protein gelation
- ERL high brilliance extended to higher energies mitigates damage and probes fast dynamics



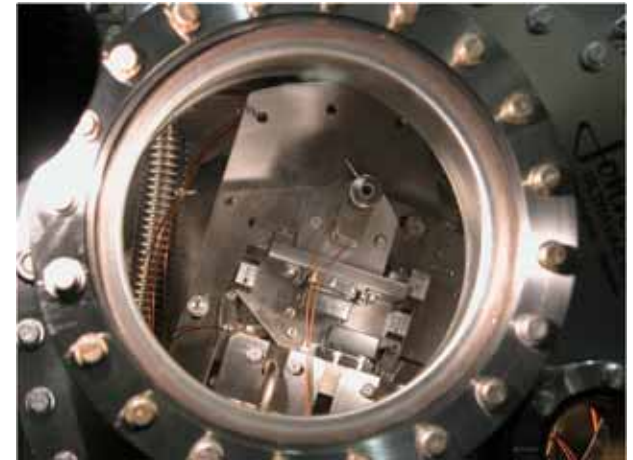
B. Lee et al., unpublished



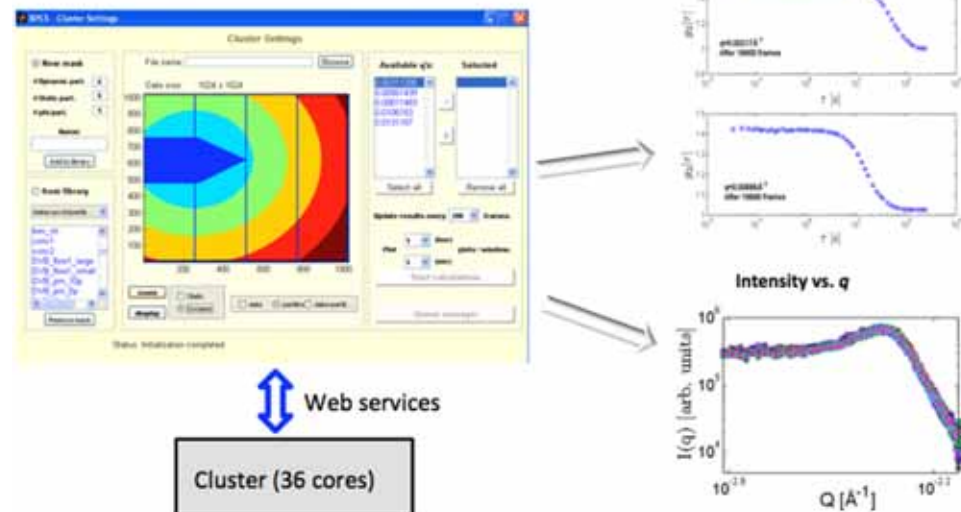
L. Dai et al., Scanning 30, 87 (2008)

Ancillary Items

- Stable, brilliance-preserving beamline optics
 - APS → LCLS → ERL
 - (S. Narayanan et al., J. Synch Rad. 15, 12 (2008)).
- User-friendly and powerful XPCS data discrimination and reduction tools
 - Makes XPCS facilities accessible to users



XPCSGUI – CLUSTER

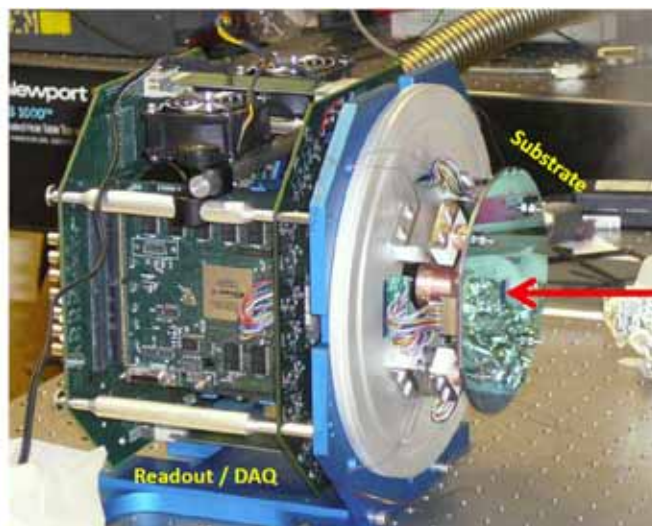
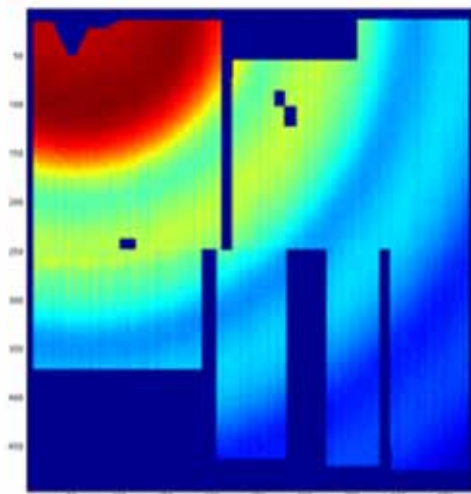


M. Sikorski, Z. Jiang, M. Sprung, S. Narayanan, A. R. Sandy, and B. Tieman, "A graphical user interface for real-time analysis of XPCS using HPC", Nucl. Instr. And Meth. A (in press).



Ancillary Items

- Stable and long-term support for detector development to support advanced x-ray sources (and XPCS) is a critical need!



LBL-ANL Fast CCD v. 1.0 (2004-2010)

- 140 (0.25 Mpix) fps digitization
- (v2.0 soon? – 200 (1 Mpix) fps

Maxipix (2010)

- 1400 (0.06 Mpix) fps digitization

SMD (2004)

- 60 (1 Mpix) fps digitization



Acknowledgements

- 8-ID staff and post-docs
 - Zhang Jiang
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