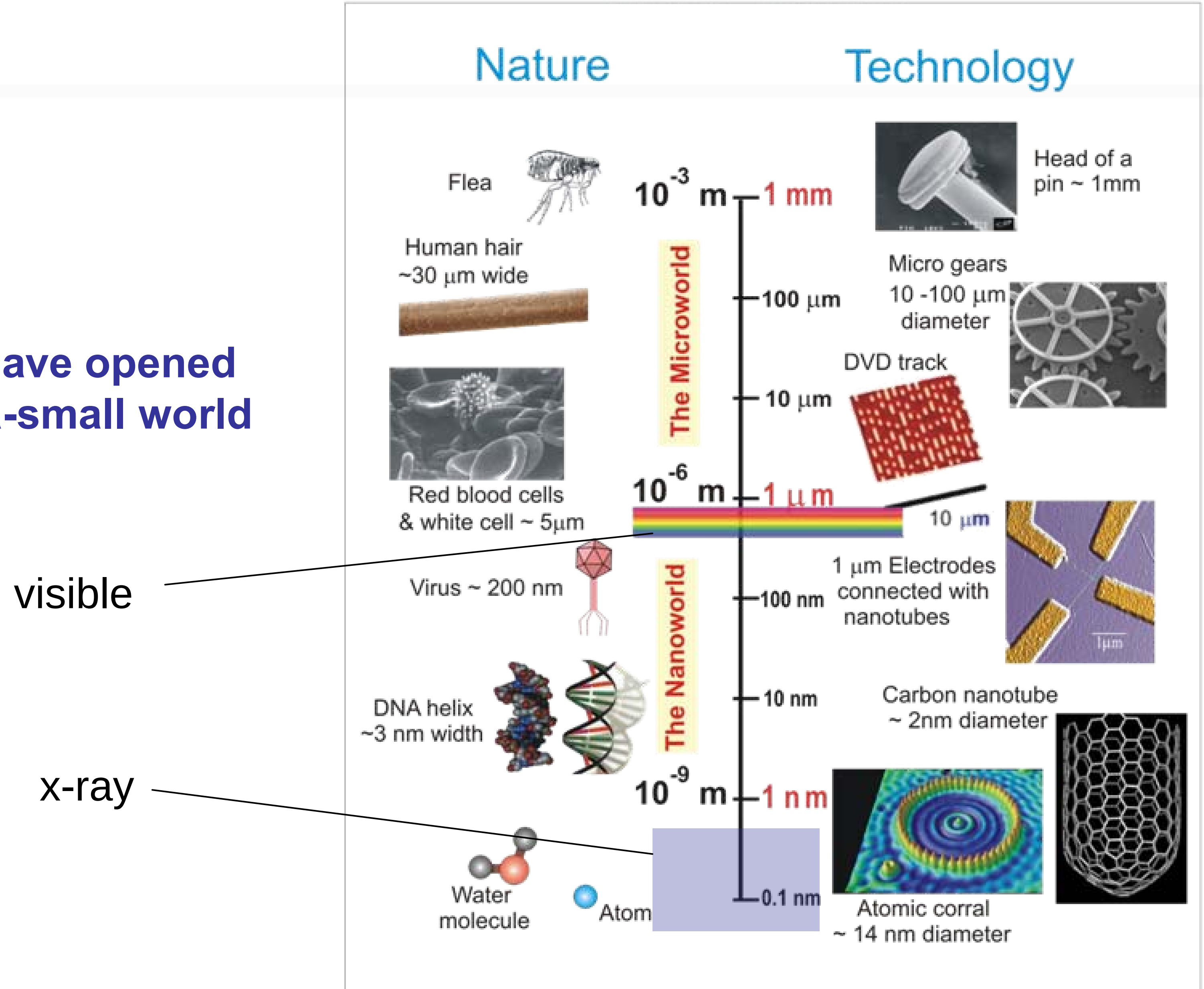
Detectors for the LCLS Science Program

J. B. Hastings
Stanford Synchrotron Radiation Laboratory
Stanford Linear Accelerator Center
Dec 8, 2005

X-rays have opened the ultra-small world

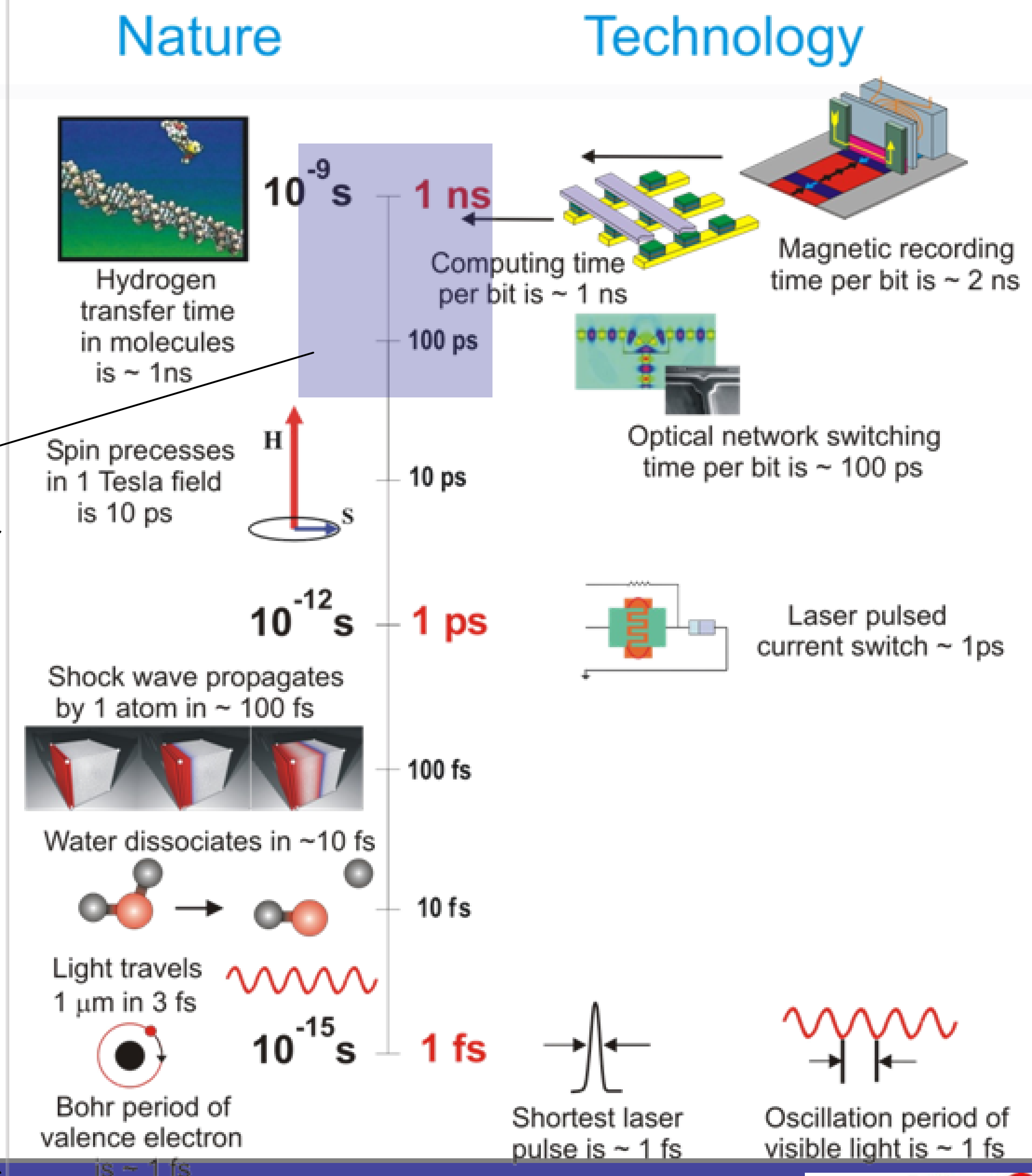


jbh@slac.stanford.edu
Jerry Hastings

In addition to the Ultra-Small world, we'd like to explore the *Ultra-Fast*

synchrotron source

new territory



Expected LCLS characteristics

Fundamental FEL Radiation Wavelength	1.	15	Å
Electron Beam Energy	14.3	4.5	GeV
Normalized RMS Slice Emittance	1.2	1.2	mm-mrad
Peak Current	3.4	3.4	kA
Bunch/Pulse Length (FWHM)	230	230	fs
Relative Slice Energy Spread @ Entrance	<0.01	0.025	%
Saturation Length	87	25	m
FEL Fundamental Saturation Power @ Exit	8	17	GW
FEL Photons per Pulse	1.1	29	10^{12}
Peak Brightness @ Undulator Exit	0.8	0.06	10^{33} *
Transverse Coherence	Full	Full	
RMS Slice X-Ray Bandwidth	0.06	0.24	%
RMS Projected X-Ray Bandwidth	0.13	0.47	%

*** photons/sec/mm^2/mrad^2/ 0.1%-BW**

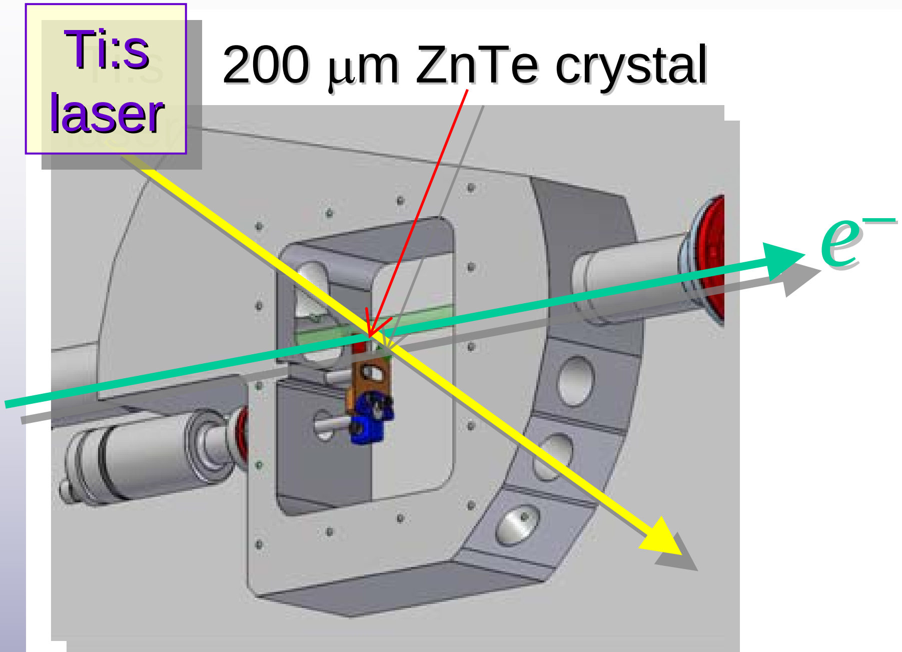
jbh@slac.stanford.edu
Jerry Hastings
Stanford Linear Accelerator Center
SSRL

All the x-rays come at once

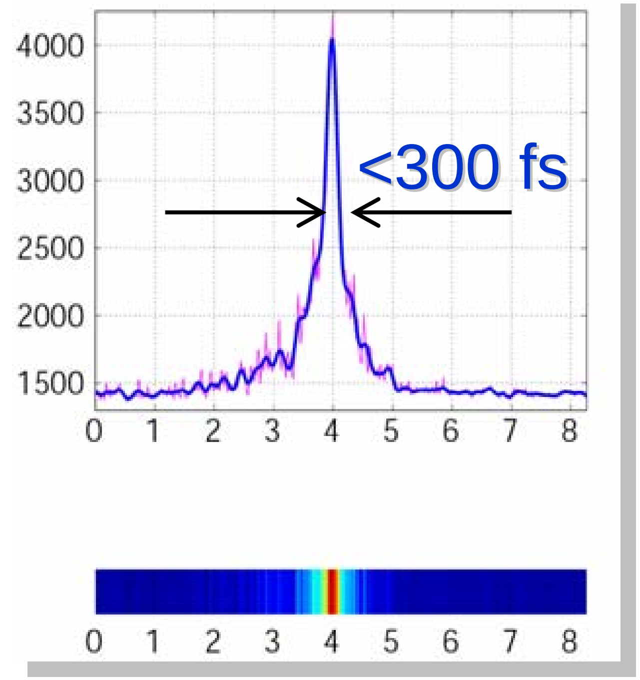
- Each pulse is 'a new experience': pulse by pulse diagnostics will be critical
  - Pulse energy (number of photons)
  - Central wavelength
  - Position
  - Spot size
  - Pulse width (time)
  - Pulse arrival time

jbh@slac.stanford.edu
Jerry Hastings

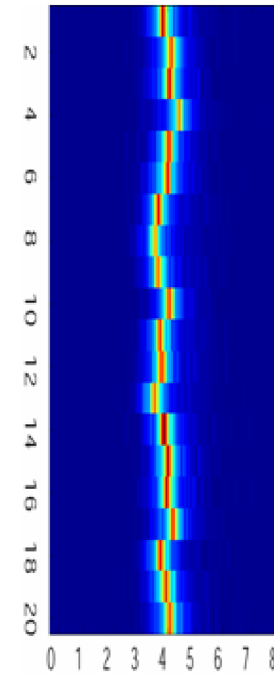
Electro-Optical Sampling: arrival time



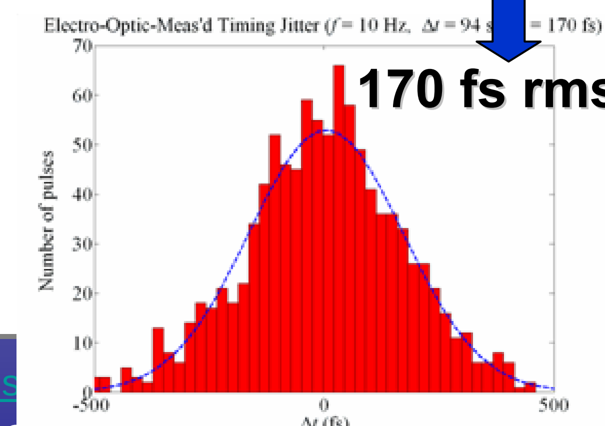
Single-Shot



Timing Jitter (20 Shots)



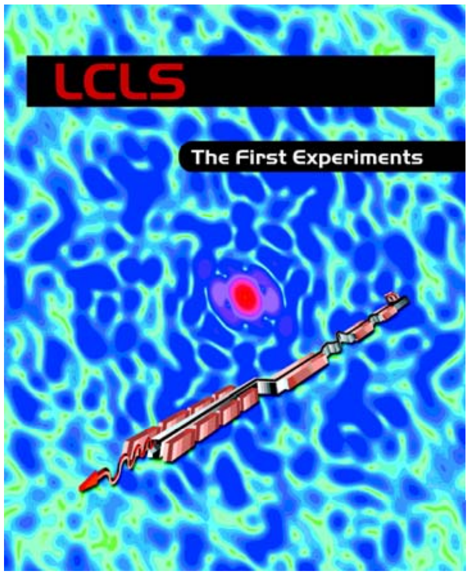
e^- temporal information is encoded on transverse profile of laser beam



Sub-Picosecond Pulse Source

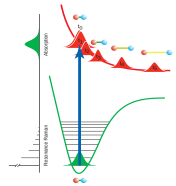
Adrian Cavalieri et al., *U. Mich.*

SLAC Report 611

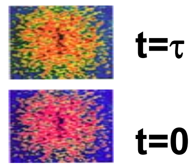


Program developed by international team of scientists working with accelerator and laser physics communities

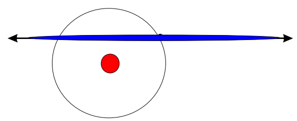
“the beginning.... not the end”



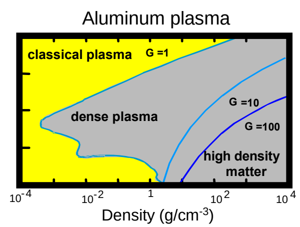
Femtochemistry



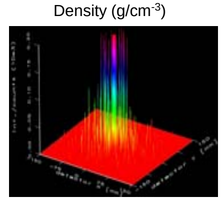
Nanoscale Dynamics in Condensed matter



Atomic Physics



Plasma and Warm Dense Matter



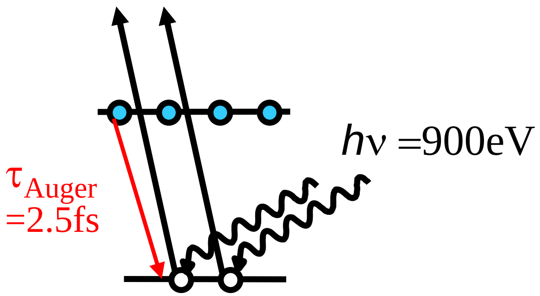
Structural Studies on Single Particles and Biomolecules

jbh@slac.stanford.edu
Jerry Hastings

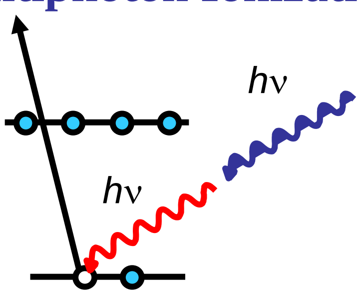
LCLS applications: *Atomic Physics*

Most basic LCLS experiments, aimed at understanding the physics of interaction of intense, ultra-fast pulse with atoms

Formation of Hollow Atoms:



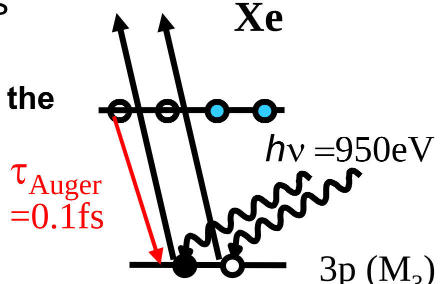
Multiphoton Ionization:



Giant Coulomb explosions of Xe clusters

10^9 atoms

Understanding is central to the imaging of biomolecules



jbh@slac.stanford.edu
Jerry Hastings

LCLS Ultrafast Science: AMOS

Workshop Objective:

Advertised Workshop broadly (Synchrotron & Laser Community)

Solicit input & participation from the AMOS community for the LCLS project

- Shape the scientific program: Gather Community Ideas
- Help define the critical XFEL machine parameters
- Help define the designs of AMOP end-stations
    instrumentation, detectors, hutch requirements
- Interaction of the five collaborative teams

Charge:

1) Review/Refine Scientific case as input for CD

2) Identify critical R&D needs
    - -Feasibility calculation
    - -Detectors specifications
    - -Space specifications
    - -Laser specifications

jbh@slac.stanford.edu
Jerry Hastings

AMOS Need Three type of Detectors

- **2D X-ray detector** to be used for small-angle elastic scattering (same as Imaging Group).

- **Electron detectors**, time and position sensitive area, 50 ps time resolution, 50 micron spatial resolution, 50 mm diameter, 120 Hz readout time.

jbh@slac.stanford.edu
Jerry Hastings

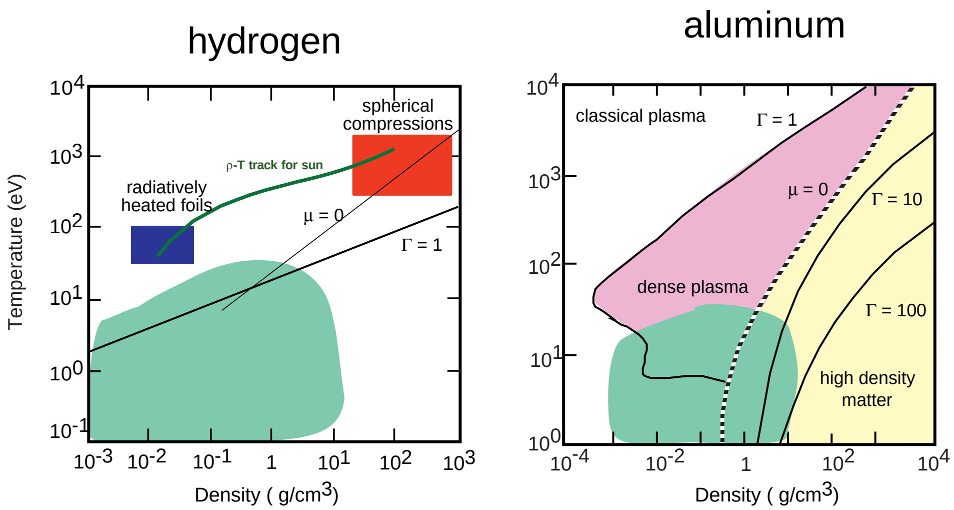
Ion Detectors continued,

- **Ion detector for momentum measurement**, Energy resolution: better than 5µeV (need a supersonic beam. Spatial resolution: better than 50µm (we expect 20µm). Temporal resolution: better than 100ps (we expect 50 ps). Detector area: 80 mm or 120 mm diameter, multihit capability: 3 events / 50 nsec (30 events / 50 nsec in future)
- **Detector for ion imaging**: spatial resolution: 50µm, frame rate 100Hz, 2000 x 2000 pixels

jbh@slac.stanford.edu
Jerry Hastings

LCLS applications: *Studies of Warm Dense Matter*

"...that part of the density-temperature phase space where the standard theories of condensed matter physics and/or plasma statistical physics are invalid."



Γ = ratio between electric and thermal potential energy
μ = chemical potential (atom interaction potential)

Astrophysical and weapons-related studies lie in the area of warm dense matter. Largest uncertainties in many applied research areas of chemistry and physics come in the warm dense regime

jbh@slac.stanford.edu
Jerry Hastings

Improvements of the x-ray detector will allow scattering with $<10^{12}$ photons

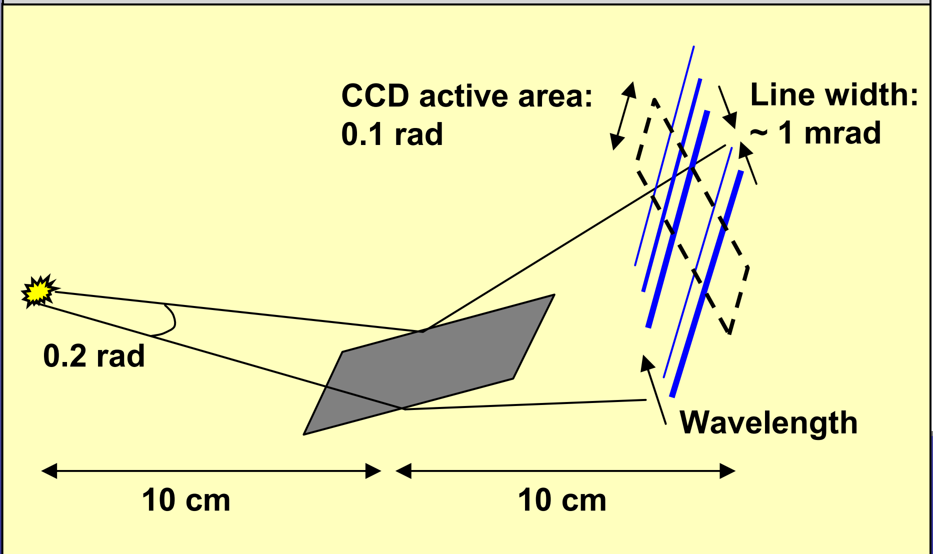
IV. Collected fraction:
0.1 rad × 1 mrad × 1% / 4π ≈ 10^{-7}

Solid angle along spectral line | Solid angle of spectral line | CCD efficiency

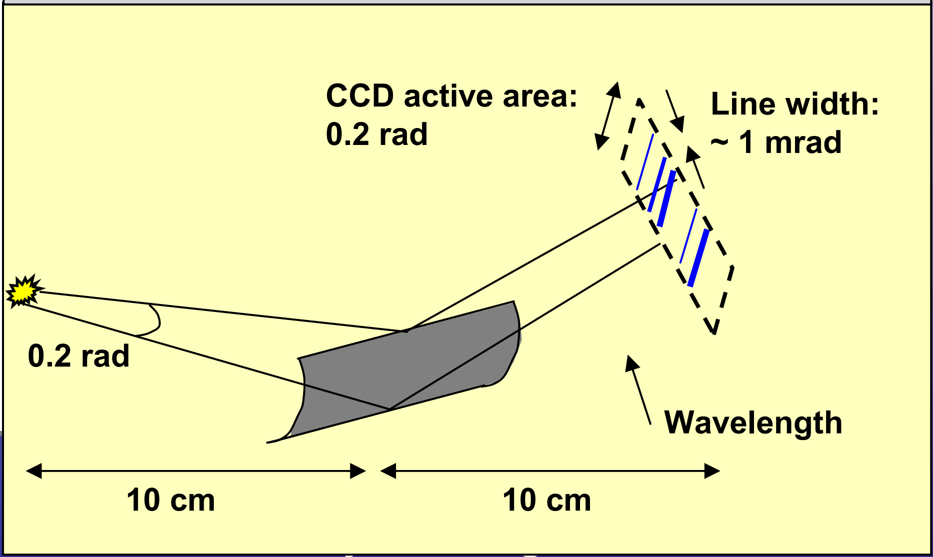
- Improve collection fractions with efficient CCD [1% → 60%]
- Improve solid angle using Van Hamos crystal [0.1 rad → 0.2 rad]

- Photons collected: $10^{12} \times 3 \times 10^{-3} \times 10^{-5} \approx$ 30,000
- Assume 10^{12} photons at the sample [1/300]

Flat crystal spectrometer

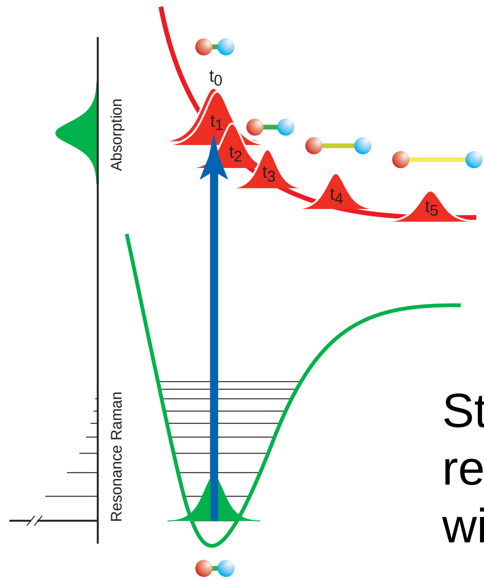


Van Hamos crystal spectrometer [curved]



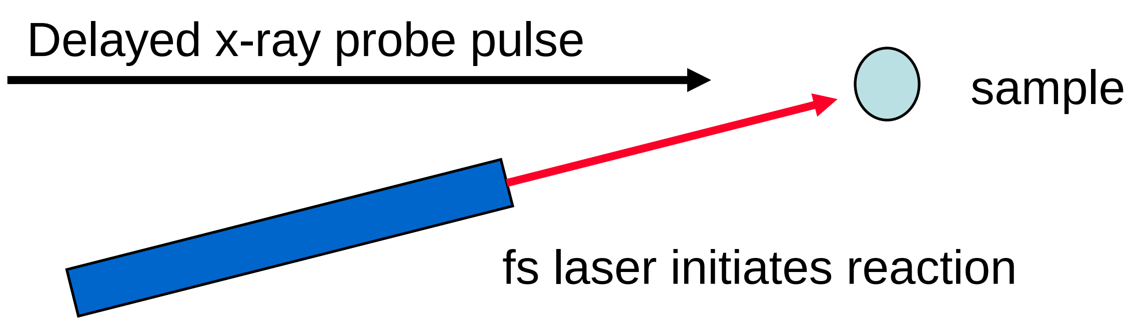
LCLS applications: *Femtosecond Chemistry*

X-ray FEL offers the ability to follow the motions of atoms on a femtosecond time scale



Studies of small system reactions can be compared with theory

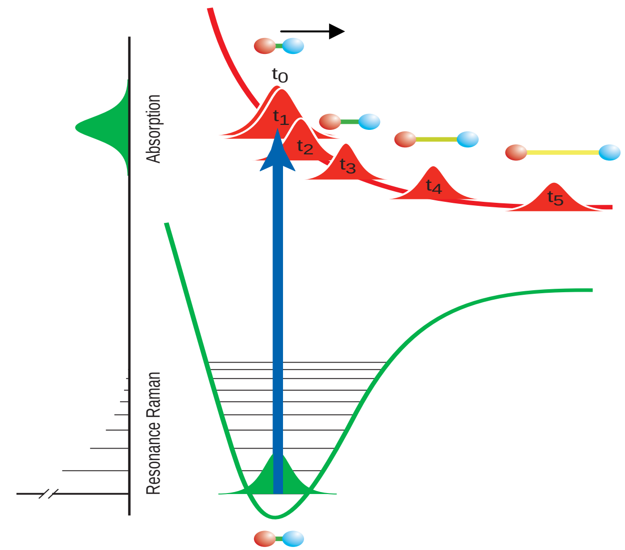
Combine single-pulse x-ray diffraction with fast laser excitation



jbh@slac.stanford.edu
Jerry Hastings

Femtosecond Chemistry

Lasers probe charge dynamics
Electron Diffraction limited to ps range
LCLS will probe 200 ⟶ 10 fs range
Chemical dynamics happens in fs - ps range



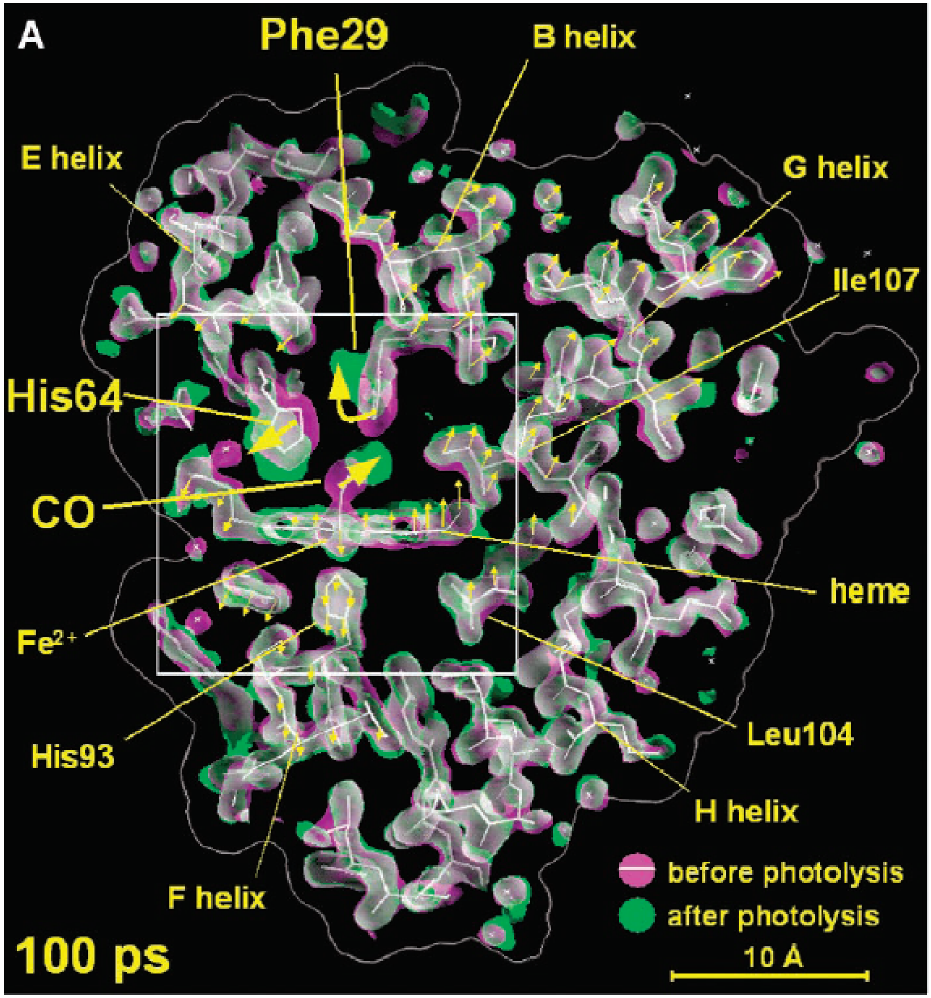
$H_2O \rightarrow OH + H$
about 10 fs

time depends on mass ⟶

$CH_2I_2 \rightarrow CH_2I + I$
about 100 fs

jbh@slac.stanford.edu
Jerry Hastings

Studies of Ultrafast Condensed Matter Structural Dynamics at the LCLS



Kelly Gaffney
SSRL
October 26, 2004

jbh@slac.stanford.edu
Jerry Hastings

Experimental Needs (3)

Feature	Protein Crystallography	Diffuse Scattering
dynamic range	1 photon to 1000	1 photon to 500
read-out rate	10 Hz	120 Hz
sensitivity	single photon	single photon
pixel number	2000X2000	500X500
pixel size	50 micron	100 micron
quantum efficiency	approaching 100%	high at 3rd harmonic

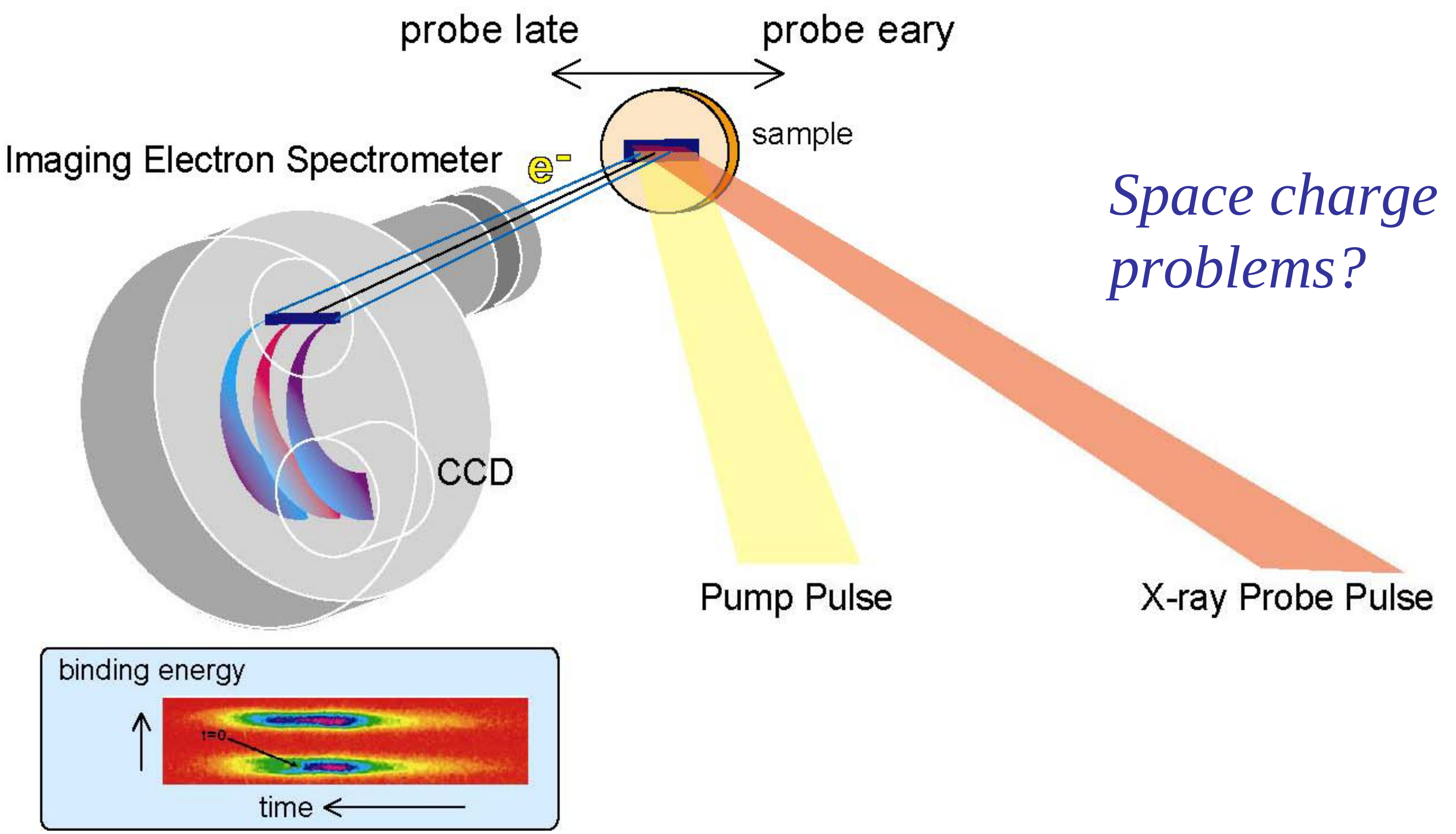
Liquid Scattering → 3rd harmonic or multiple detectors
annular detectors advantageous – Development at APS

Diffuse Scattering → will saturation of Bragg peaks make it difficult to determine width change?

jbh@slac.stanford.edu
Jerry Hastings

Measures complete time history around t=0 in single shot

SCIENTA R4000 (Spatial resolution: 9mm, Pass Energy 200 eV) gives, time resolution: ~30 fs, energy resolutiuon: ~100 meV

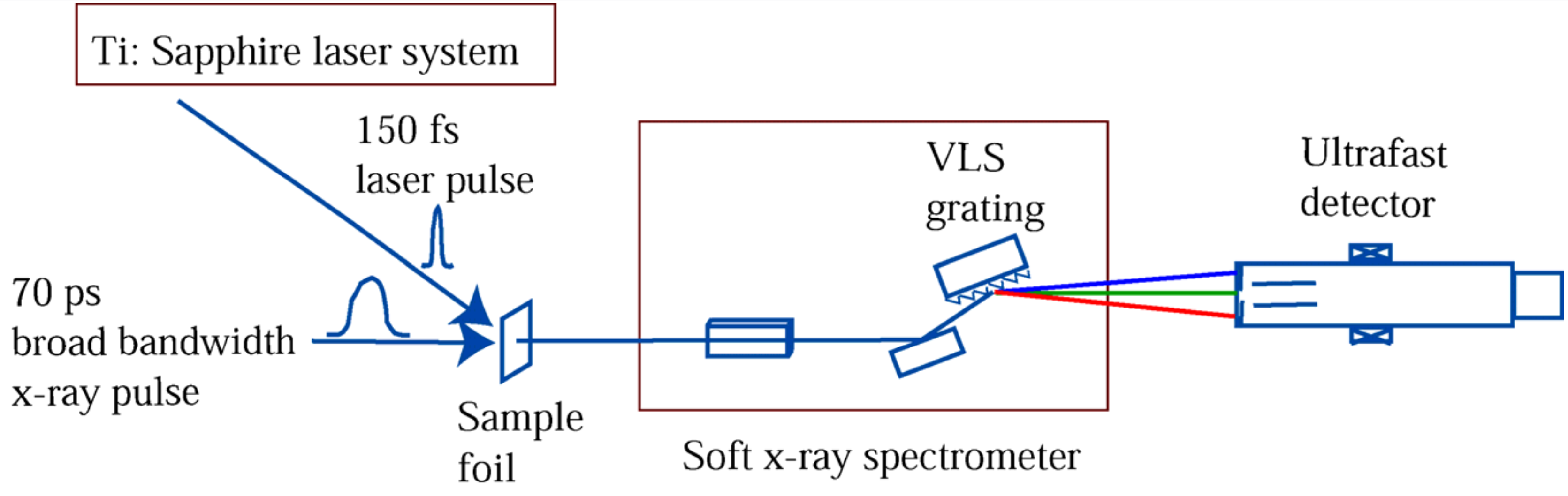


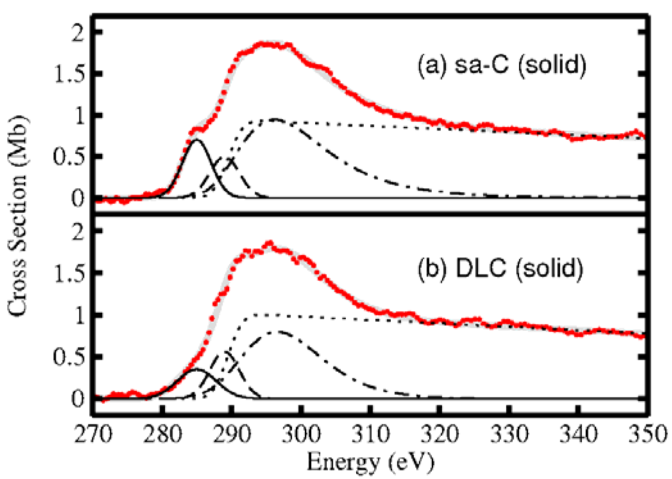
Space charge problems?

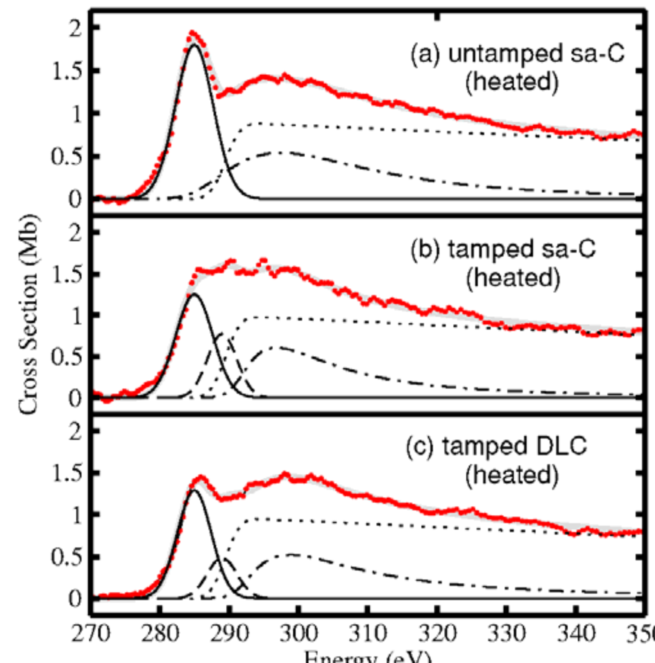
courtesy Anders Nilsson

jbh@slac.stanford.edu
Jerry Hastings

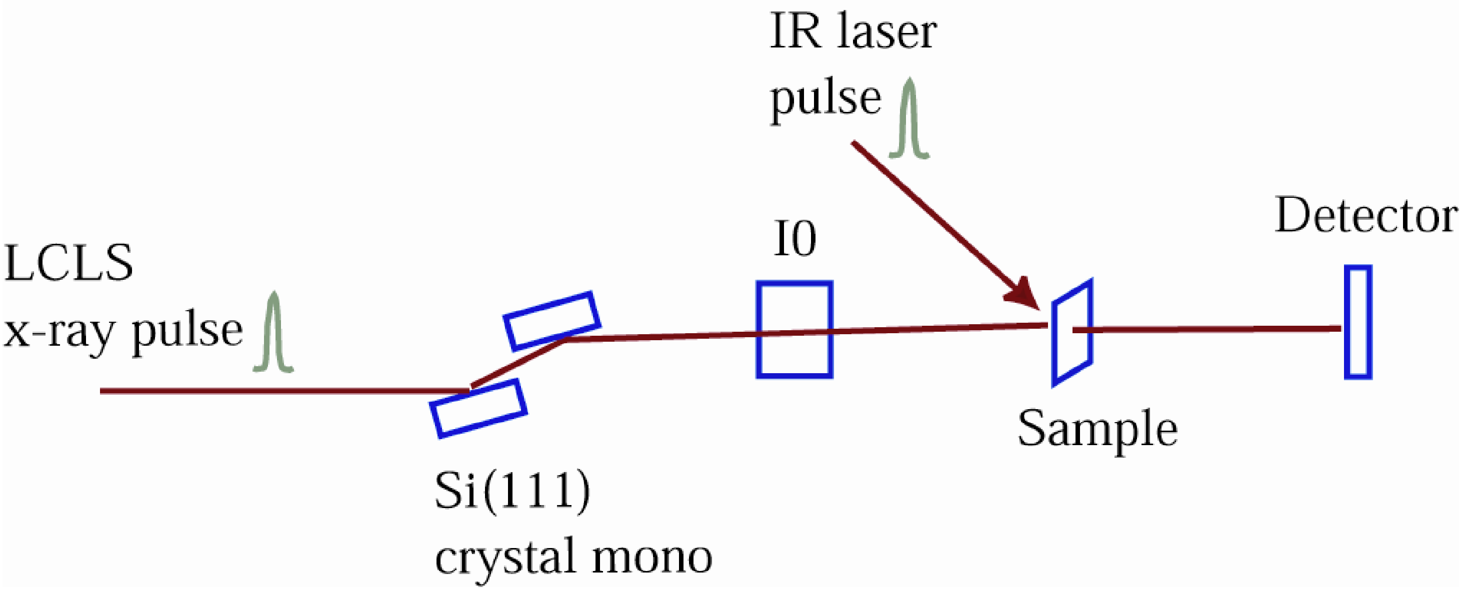
Time-resolved x-ray absorption spectroscopy







Schematic of the LCLS experiment and Requirements



- Requirements
  - Attenuate LCLS beam by ~ 1/100 -> < 0.1 J/cm^2 so that x-rays do not modify sample
  - Need good I0 normalization
  - Tunability of photon energy100 eV for XANES, 1000 eV for EXAFS
  - Alternatives: Inelastic x-ray Raman scattering, Crystal spectrometer

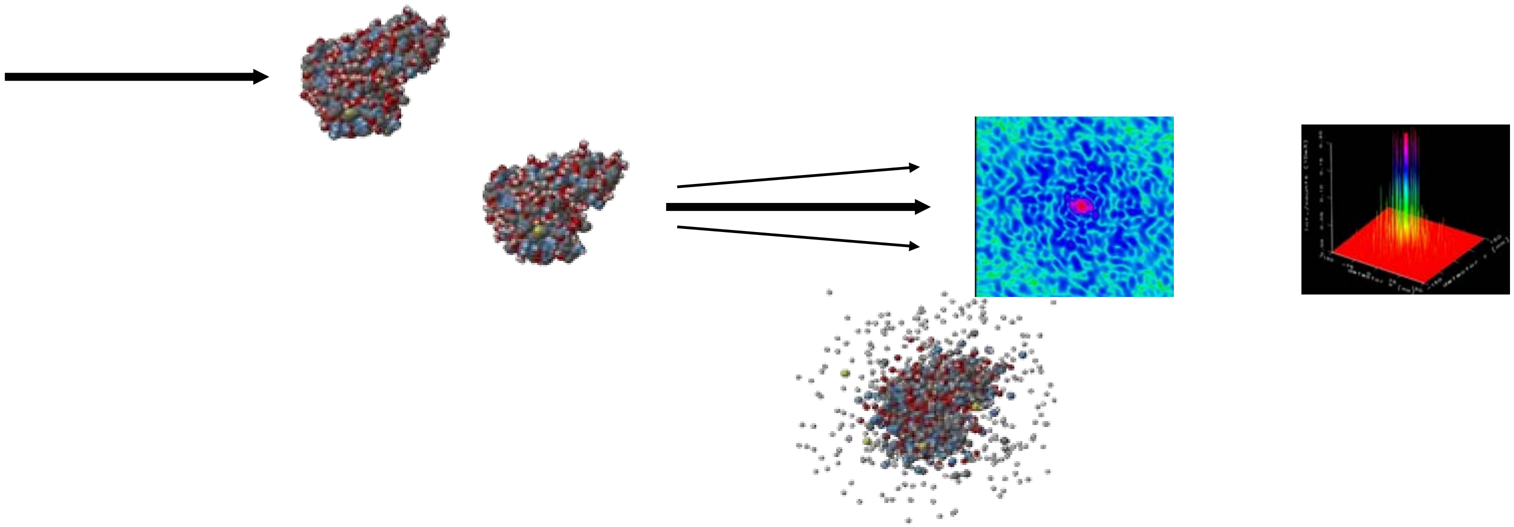
jbh@slac.stanford.edu
Jerry Hastings

LCLS applications:

X-Ray Diffraction from a Single Protein Molecule

Avoids radiation damage problem by taking diffraction data before damage occurs

Would allow much broader range of biological structures to be determined



jbh@slac.stanford.edu
Jerry Hastings

LOW FLUENCE INSTRUMENT

SCIENCE: Imaging of nanocrystalls and non-periodic nanomaterials, using multiple exposures

- Pulse length not critical for imaging,
- Large diameter beam (150 micron-1 micron) with large transverse coherence length,
- Semi-macroscopic samples,
- Automatic sample changer,
- Semi-conventional sample environment (Cryo-EM sample holder/diffractometer),
- Monochromator (delta lambda/lambda = 10^{-4}),
- Medium high vacuum (~10^{-4} mbar) or wet He atmosphere,
- Lasers for reaction initiation,
- Video microscope for sample alinement, looking down the beam.

Detectors:

- **1/ Area detector (2k x 2k, ~100 mm x 100 mm), 50-100 micron pixels, (dynamic range >10^4),**
- **2/ Large area detector (commercial, ~300 mm x 300 mm), 50-100 micron pixels, (dynamic range ~10^5),**

LOCATION in the far hall: large and highly coherent beam (need large optics)

jbh@slac.stanford.edu
Jerry Hastings

HIGH FLUENCE INSTRUMENT

Single shot experiments

- Extremely short pulses (1-50 fs),
- Tightly focused beam (100-5000 nm Ø),
- Single shot experiments on nanocrystals, particles and biomolecules,
- Small area detector near the sample (dynamic range $>10^4$),
- Sample injector and cryo-EM sample holder,
- High vacuum (10^{-6}-10^{-8} mbar),
- Extended diagnostics (mass spec, ion and electron spectrometer, fluorescence detector)
- Lasers sample manipulation, reaction initiation

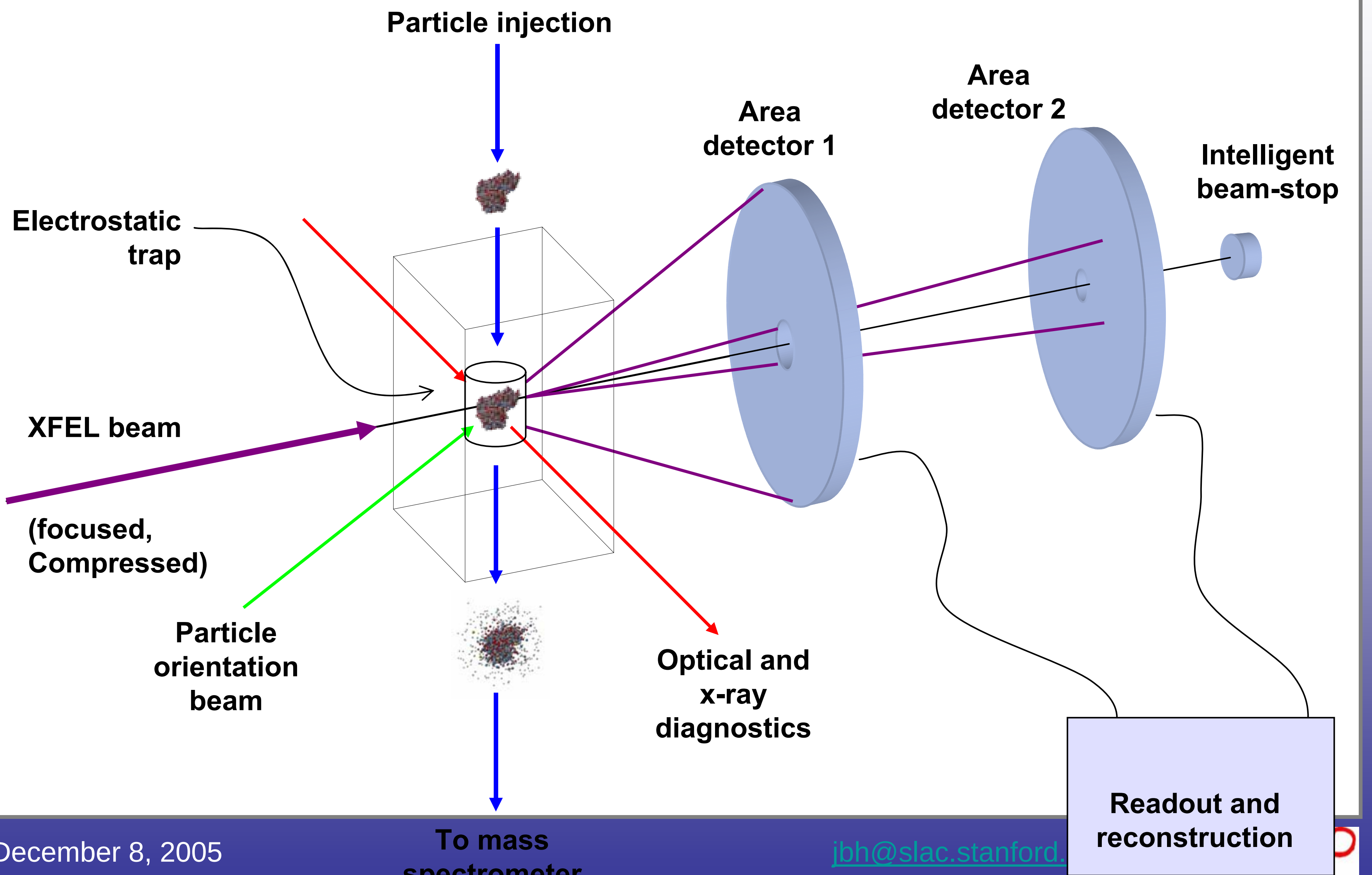
Detectors:

- Dual Area detector (≥ 1k x 1k, ~50 mm x 50 mm), 50-100 micron pixels, (dynamic range $\geq 10^4$ per detector)

LOCATION in the near hall: intense beam, small beam size, small optics (low Z)

jbh@slac.stanford.edu
Jerry Hastings

SINGLE PARTICLES AND BIOMOLECULES
Interaction chamber and detector arrangement



jbh@slac.stanford.
Jerry Hastings

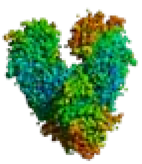
Divergence of the beam

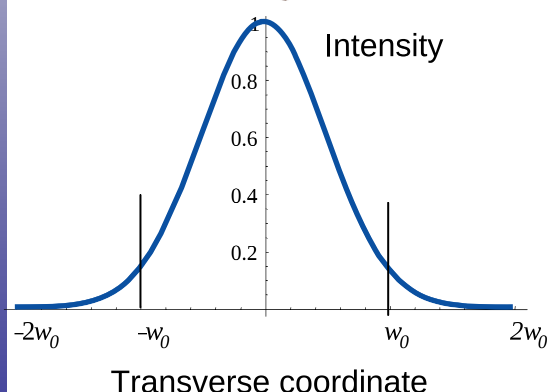
The single-Gaussian-mode will be focussed to ~0.1 micron
The beam will diverge and lead to an effective PSF of the detector
(equivalently, the effect of a CCD PSF is to limit the reconstruction field)

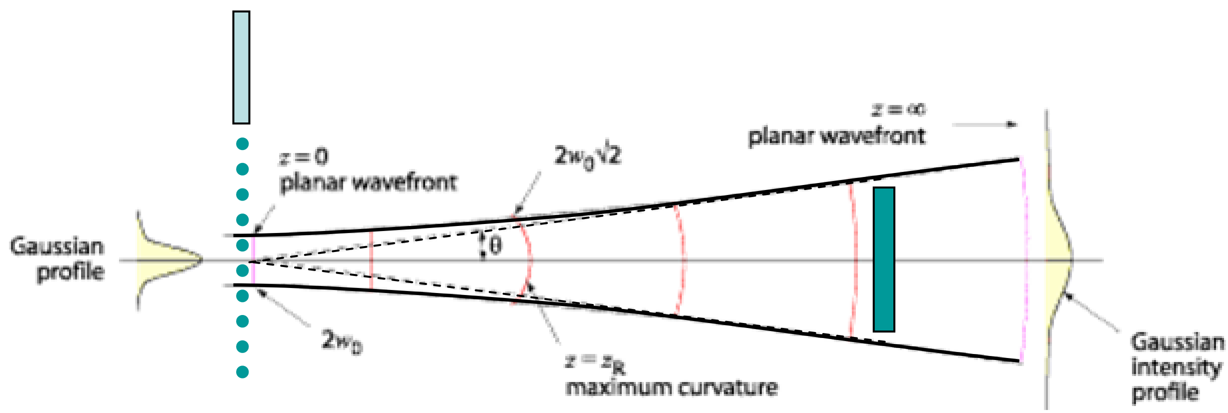
E.g. for 0.1 micron:

Divergence: $$\Delta\theta = \frac{\lambda}{\pi w_{0f}} = 0.52 \text{ mrad}$$

detector pixel angle: $$\Delta\vartheta_{\text{pix}} = \lambda/(D\,s) = 0.75 \text{ mrad}$$





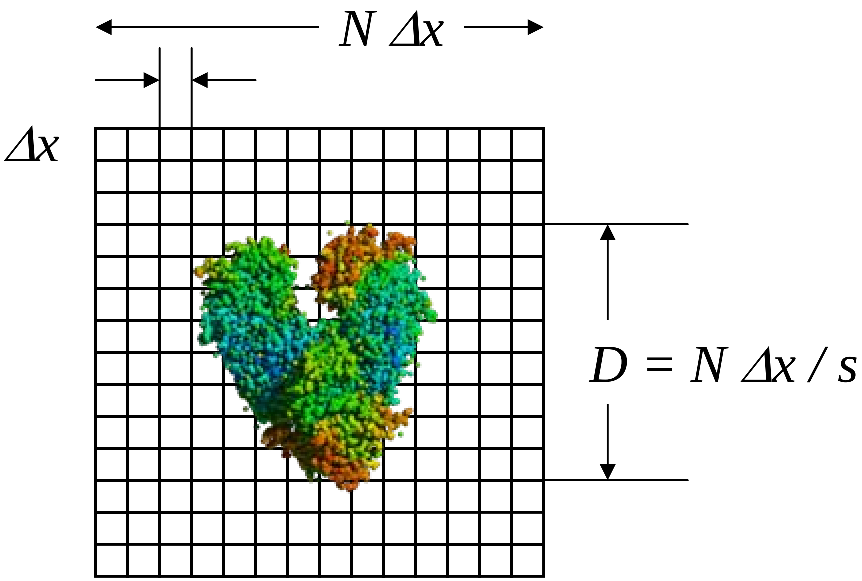


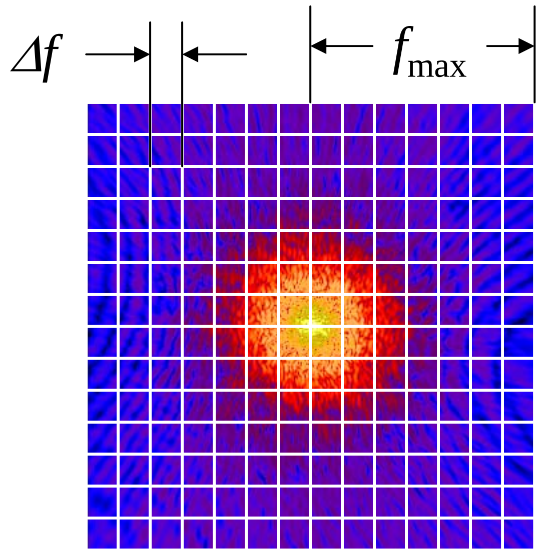
Particles

Crystals, arrays

jbh@slac.stanford.edu
Jerry Hastings
Stanford Linear Accelerator Center
SSRL

The number and solid angle of the detector elements are dependent on particle size and resolution





Real space samples: Δx
Smallest period sampled: $2\Delta x = d$ or $f_{max} = 1/d$
Oversampling (per dimension): s

Array size: $N = D\,s / \Delta x = 2\,D\,s / d$

$$\Delta f = 2\,f_{max} / N$$
$$= 1/(D\,s)$$
$$\Delta \vartheta_{pix} \approx \lambda \Delta f$$
$$= \lambda / (D\,s)$$

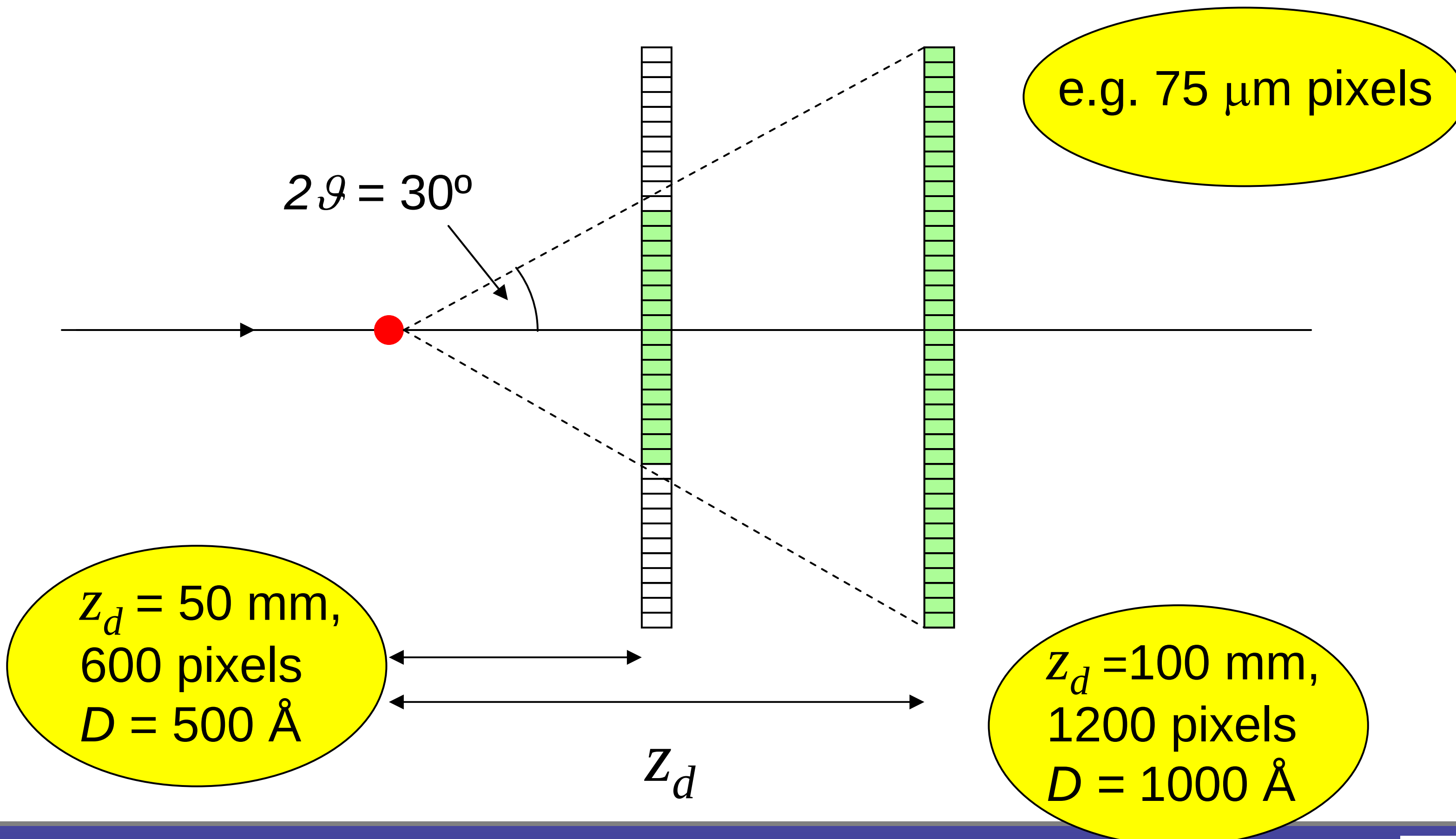
E.g. $D = 1000$ Å, $d = 3$ Å, $s = 2$ $\Rightarrow$ $N = 1200$
$\lambda = 1.5$ Å $\quad$ $\Delta\vartheta_{pix} = 0.75$ mrad

jbh@slac.stanford.edu
Jerry Hastings

Smaller particles require fewer pixels

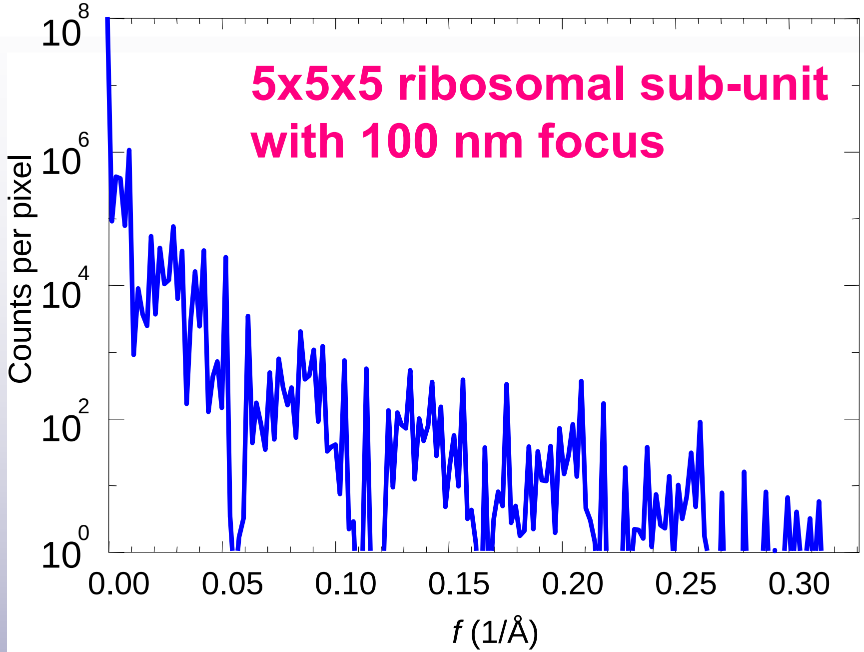
E.g. $D = 1000$ Å, $d = 3$ Å, $s = 2$ $\Rightarrow$ $N = 1200$

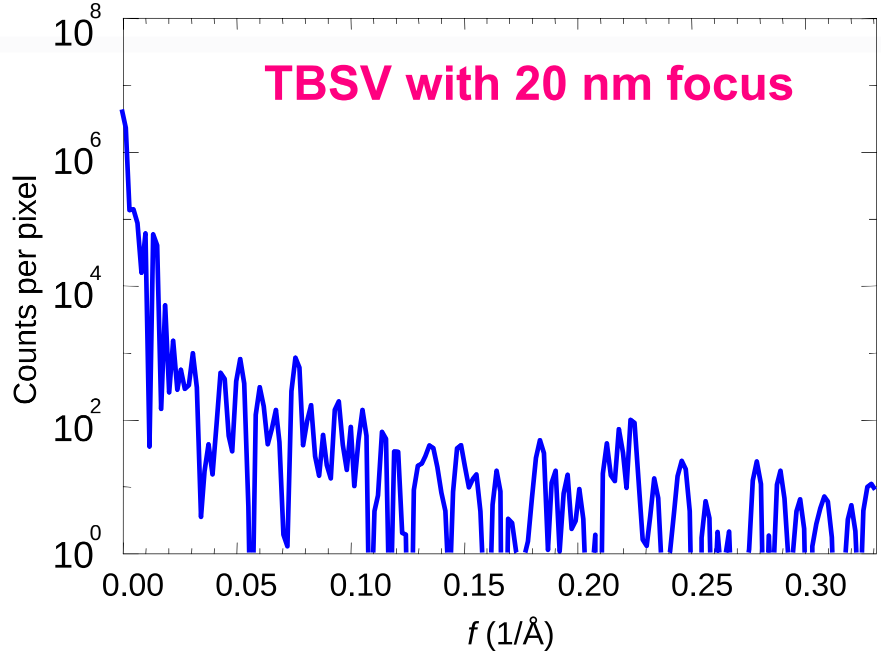
$\lambda = 1.5$ Å $\Delta\theta_{pix} = 0.75$ mrad



jbh@slac.stanford.edu
Jerry Hastings

Expected detector signals





$$I(\mathbf{q}) = \Omega r_e^2 I_0 \left| \sum_j f_j(\mathbf{q}) \exp\{i\mathbf{q}\cdot\mathbf{x}_j\} \right|^2$$

$$\approx \Omega r_e^2 I_0 \, N \left| f(\mathbf{q}) \right|^2$$

For a particle of diameter D:		Array $n \times n$:
Number of scatterers	$N \sim D^3$	$N \sim (n^2)^2$
Pixel solid angle	$\Omega \sim 1/D^2$	$\Omega \sim 1/n^2$ or 1
Incident fluence	$I_0 \sim 1/D^2$	$I_0 \sim 1/n^2$
Counts per pixel:	$\sim 1/D$	~ 1 or n^2

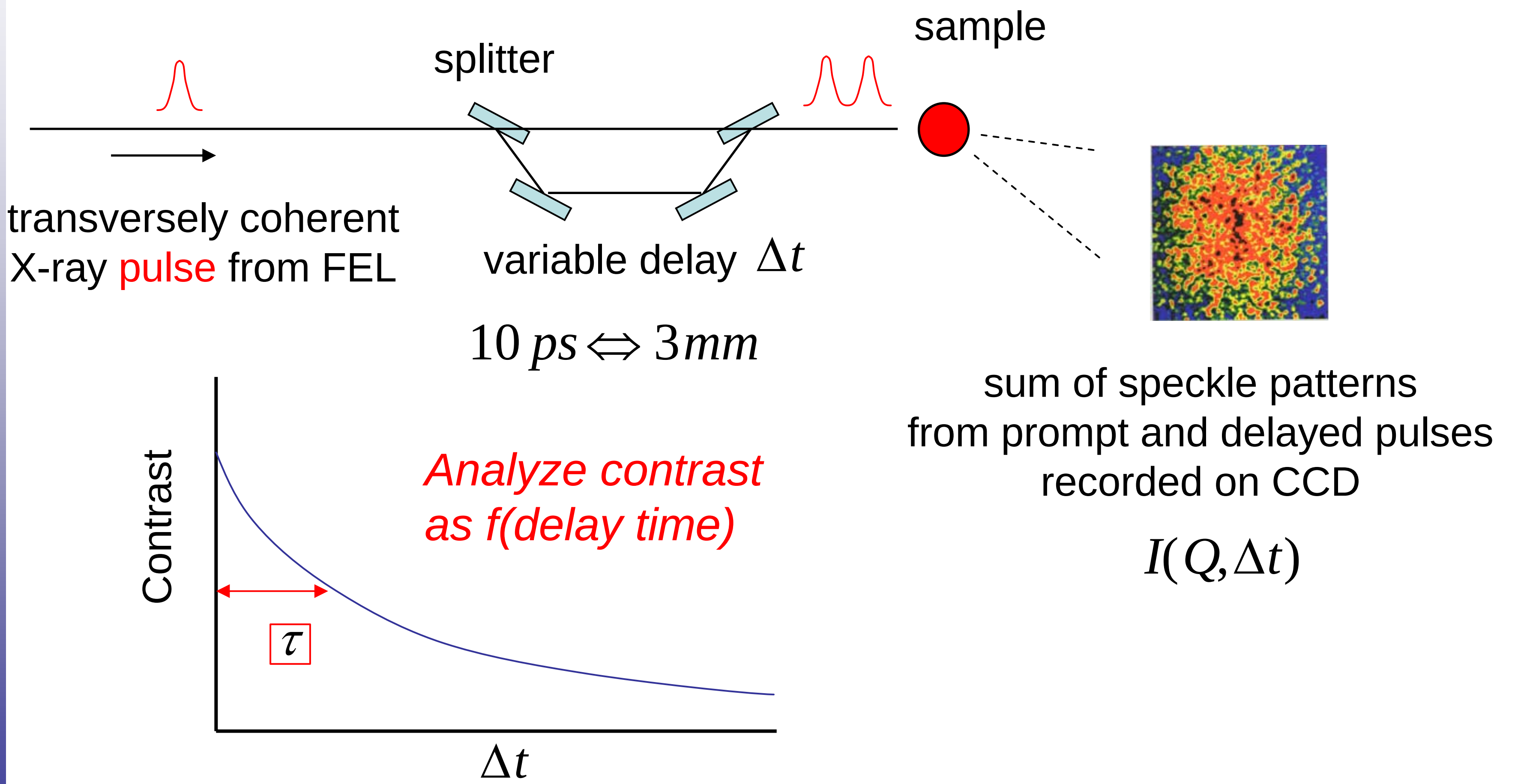
Crystallographic sampling

There will be stronger signals for higher-*Z* materials

jbh@slac.stanford.edu
Jerry Hastings

XPCS at LCLS using "Split Pulse" Mode

Femtoseconds to nanoseconds time resolution
Uses high *peak* brilliance



jbh@slac.stanford.edu
Jerry Hastings
Stanford Linear Accelerator Center
SSRL

Sample Heating and Signal Level

Is there enough signal from a single pulse?
Is sample heating by x-ray beam a problem?

Maximum available photons per pulse:

$$N_{AVAIL} = f(E, \Delta E, A)$$

Minimum required photons per pulse to give sufficient signal:

$$N_{MIN} = \frac{2\pi A E^2 \sigma_{abs}}{h^2 c^2 \sigma_{el} M_{corr}} N_{MIN}^{SPECKLE}$$

Maximum tolerable photons per pulse due to temperature rise:

$$N_{MAX} = \frac{3k_B A}{E\sigma_{abs}} \Delta T_{MAX}$$

See analysis in LCLS: The First Experiments

jbh@slac.stanford.edu
Jerry Hastings

XPCS: Beam Size

How much of the unfocused beam can be used?

Limited by ability to resolve speckle pattern in reasonable size sample-to-detector distance

Beam size = pixel size = speckle size = d = $(\lambda L)^{1/2}$

For L = 5 m, get d = 20 microns, 8 keV; d = 12 microns, 24 keV

Full beam size at 8 keV is ~400 microns

A new idea discussed at workshop: doing heterodyne detection using reference beam

jbh@slac.stanford.edu
Jerry Hastings

XPCS: Detector Specifications

Optimum pixel size:
1 to 10 'speckles'

Optimum Pixel Size, Noise Level

Speckle characterized by negative binomial distribution

Mean counts per pixel $\bar{k}$

Inverse contrast M

Probability of k counts:

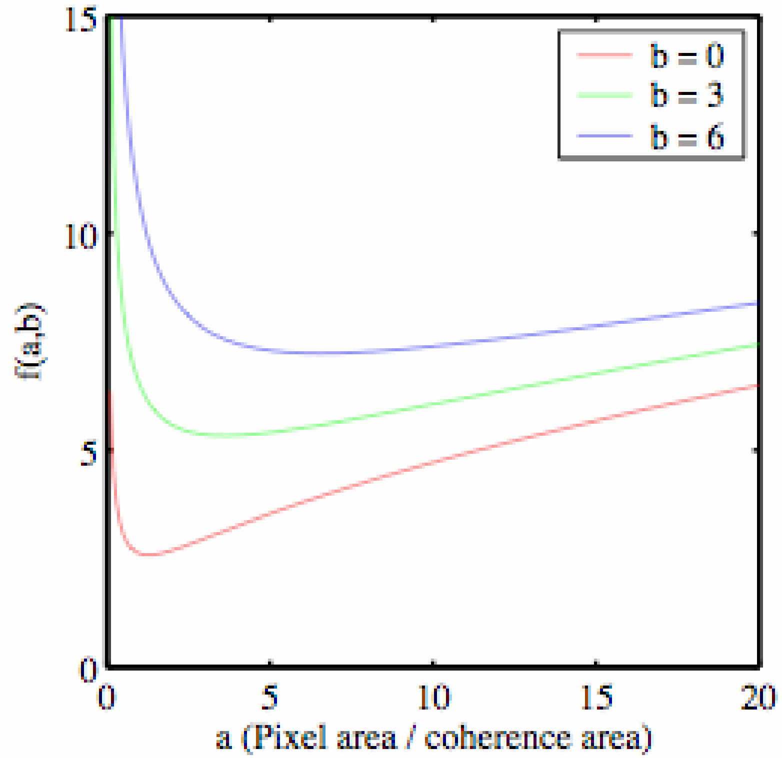
$$P_k = \frac{\Gamma(k+M)}{\Gamma(M)\Gamma(k+1)}\left(1+\frac{M}{\bar{k}}\right)^{-k}\left(1+\frac{\bar{k}}{M}\right)^{-M}$$

Low count rate limit $\bar{k} \approx 0.01$

$$P_1 = \bar{k}$$

$$P_2 = \frac{M+1}{2M}\bar{k}^2$$

$$1/M = 2P_2/P_1^2 - 1$$



Optimum noise level:
determine P_2 to a few %

Optimum number of pixels at "same" Q: ~10^6

jbh@slac.stanford.edu
Jerry Hastings

XPCS: Detector Specifications

Detector #1: 6 - 12 keV (monochromatic)

Angular resolution: 4 microradians

Sample to detector: 5 m (depends on hutch)

Pixel size/spatial resolution: 20 microns

Area: ~100 modules each of ~10^6 pixels; small dead space between modules in one dimension

DQE: >0.5

Typical signal rate: average 0.01 count per pixel per pulse

Noise: Need to discriminate pixels with one photon, two photons, and more photons. Error rate in determining double hits less than a few percent.

Pre-processing: Algorithm to locate photon positions

Max signal rate: ~100 photons per pixel per pulse

Frame rate: 120 Hz, although not highest priority

jbh@slac.stanford.edu
Jerry Hastings

XPCS: Detector Specifications Cont'd

Detector #2: 12 - 24 keV (monochromatic)

Angular resolution: 2.3 microradians

Sample to detector: 5 m (depends on hutch)

Pixel size/spatial resolution: 12 microns

Area: ~100 modules of ~10^6 pixels; small dead space between modules in one dimension

DQE: >0.5

Typical signal rate: average 0.01 count per pixel per pulse

Noise: Need to discriminate pixels with one photon, two photons, and more photons. Error rate in determining double hits less than a few percent.

Pre-processing: Algorithm to locate photon positions

Max signal rate: ~100 photons per pixel per pulse

Frame rate: 120 Hz, although not highest priority

jbh@slac.stanford.edu
Jerry Hastings

Detector Specifications Cont'd

Detector #3: Streak Camera

Time resolution: 200 fs

DQE: can be small (direct beam diagnostics)

Detector #4: Soft X-ray Area Detector

(requirements discussed below)

jbh@slac.stanford.edu
Jerry Hastings

Derived Specifications (1)

'General' Specifications for imaging and pump-probe diffraction

Pixel size	100 micron (point spread function)
Working Distance	variable, 20-200 mm
dimension	512 x 512 minimum
Expected signal rate per pixel (maximum)	few x 10^3
Noise level required	<< 1 photon
Photon energy range	0.8-8.0 keV
Needed DQE	0.8 at 8 keV
Environment (Vacuum or air)	both vacuum and atmosphere
Frame rate	120 hz

jbh@slac.stanford.edu
Jerry Hastings

Derived Specifications (2)

'General' Specifications for nanoscale imaging

Pixel size	15-25 microns
Working Distance	5 meters
dimension	400 sq. cm, 1×10^8 pixels, reconfigurable (modular)
Expected signal rate per pixel (maximum)	10
Noise level required	<<1 photon
Photon energy range	6 - 24 keV
Needed DQE	> 0.5
Environment (Vacuum or air)	air
Frame rate	120 hz

jbh@slac.stanford.edu
Jerry Hastings