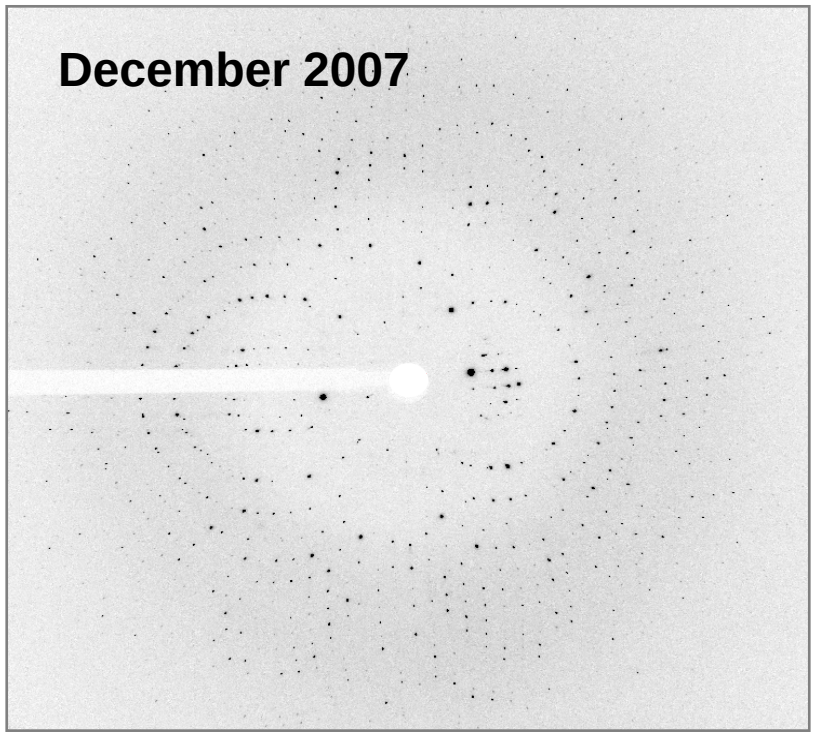
BioCARS 14-ID

A Facility for Time-Resolved Science

Timothy Graber
November 20, 2008



- Single 160ps X-ray pulse (APS hybrid mode)
- ~2×10^{10} photons per 160ps X-ray pulse
- Hemoglobin crystal, HbCO ($35\times100\times200$ μm^3 diffracting volume)

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BioCARS Supported Techniques

- Time-resolved Laue Crystallography
- Time-resolved WAXS
- Monochromatic MAD Capabilities
- All of the above can be performed under Biosafety Level 3 (BSL3) conditions

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New Capabilities at Sector 14

- Doubly focused pink and monochromatic beam with a demagnification of 5:1 vertical and 8:1 horizontal
- Flux density at sample increased by a factor of ~100 (number of pump-probe shots per image reduced from ~80 to ~4)
- Single-bunch isolation in 24-bunch mode increases the available beam time for time-resolved crystallography from 1 to 2 weeks per 12-week run to 9-10 weeks
- New broadly tunable picosecond laser system makes 100 picosecond time resolution possible

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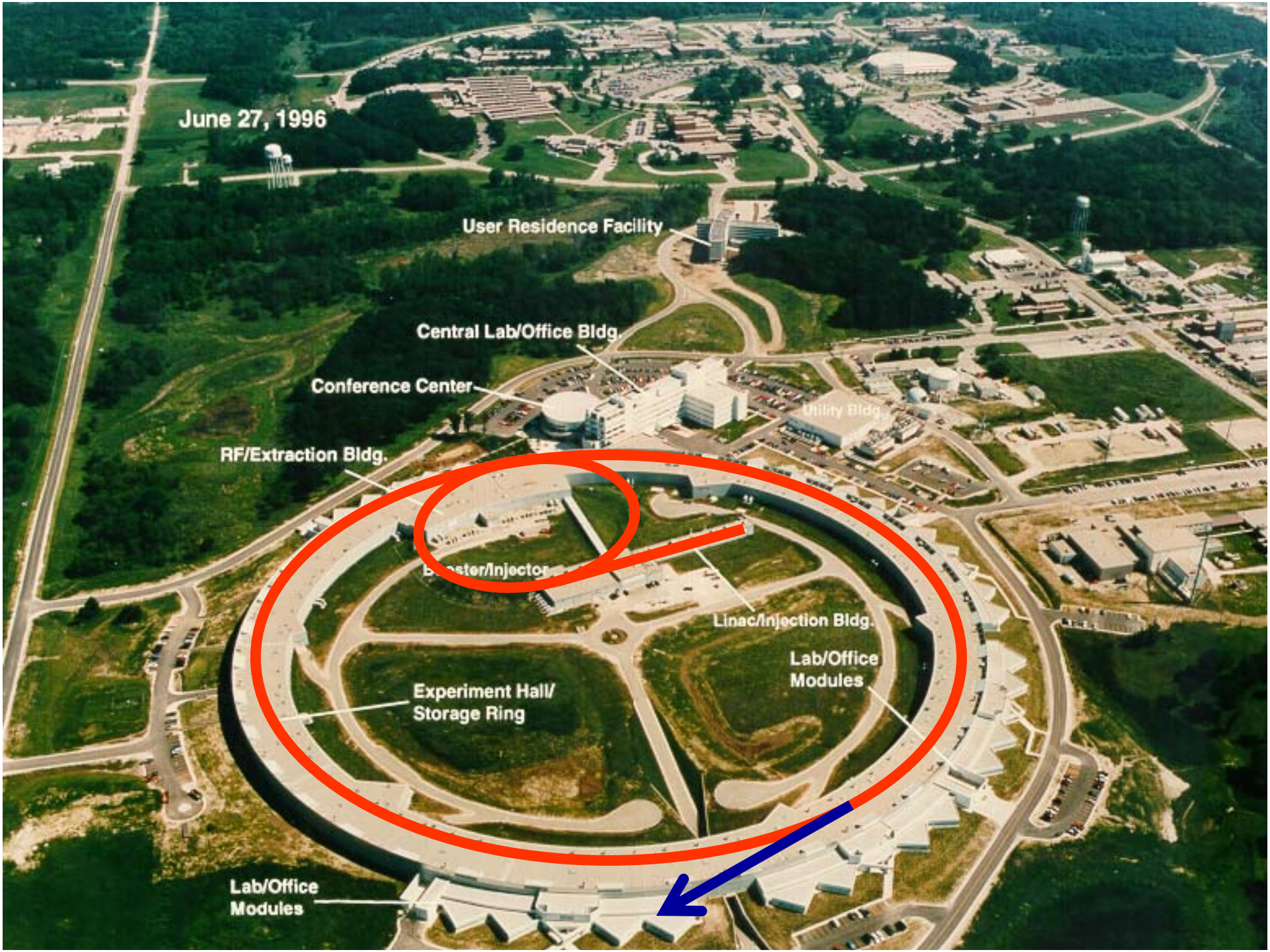
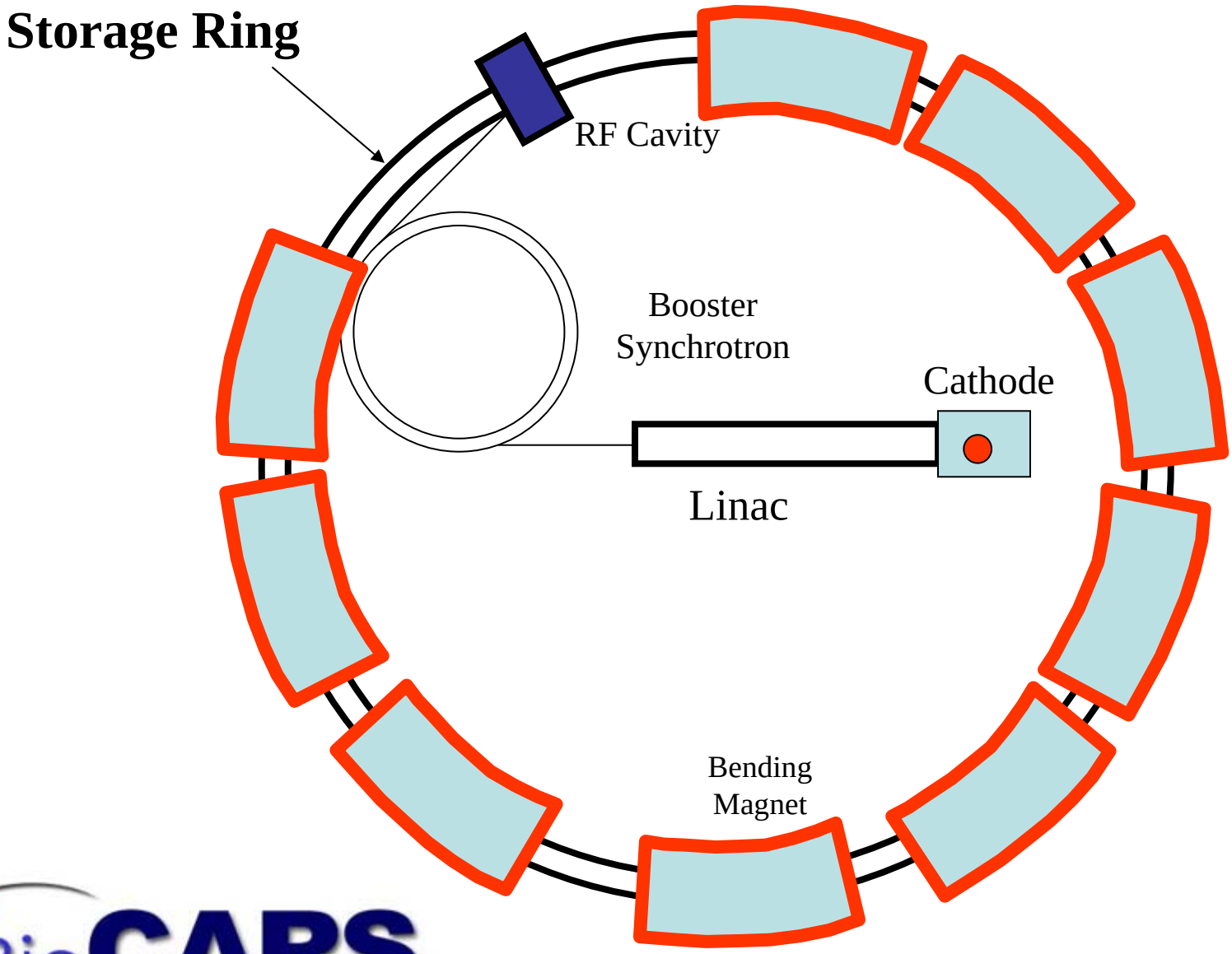

June 27, 1996
User Residence Facility
Central Lab/Office Bldg.
Conference Center
Utility Bldg.
RF/Extraction Bldg.
Booster/Injector
Linac/Injection Bldg.
Lab/Office
Modules
Experiment Hall/
Storage Ring
Lab/Office
Modules

Synchrotron Description



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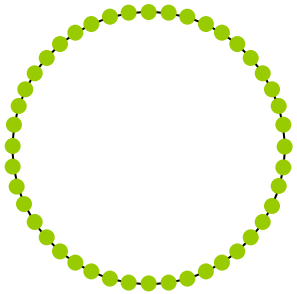
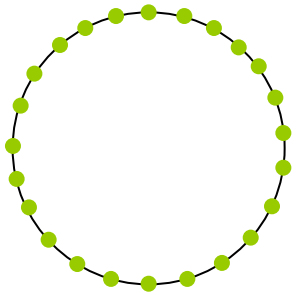
Synchrotron Fill Patterns

Synchrotron period
3.6 microseconds

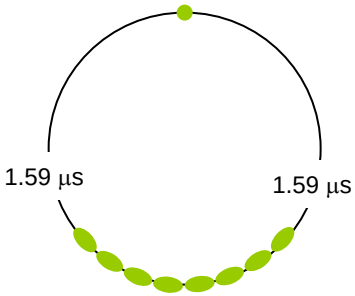
Routine non-Top-up User Operation
Total current is 102 mA. 324 uniformly spaced singlets with a nominal current of 0.31 mA, and a spacing of 11.37 nanoseconds between singlets.
Bunch length (FWHM): 59 ps.



Routine Top-up User Operation (24-bunch Mode)
Total current is 102 mA. 24 singlets (single bunch) with a maximum current of ~4.25 mA and a spacing of 153 nanoseconds between singlets.
Bunch length (FWHM): 94 ps.



Special Operating Mode 1 (SOM1) - Hybrid Fill (singlet)
Total current is 102 mA. A single bunch containing 16 mA isolated from the remaining bunches by symmetrical 1.594 microseconds gaps. The remaining current is distributed in 8 group of 7 consecutive bunches with a maximum of 11 mA per group, a periodicity of 68 ns, and a gap of 51 ns between groups. The total length of the bunch train is 500 ns.
Bunch length (FWHM): Singlet: 153 ps, septuplets: 75 ps .



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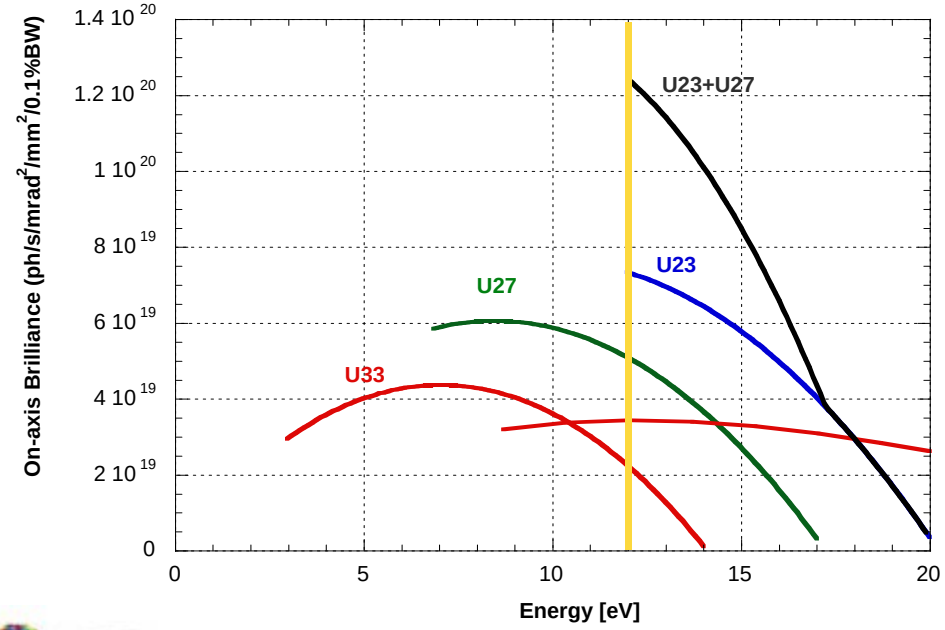
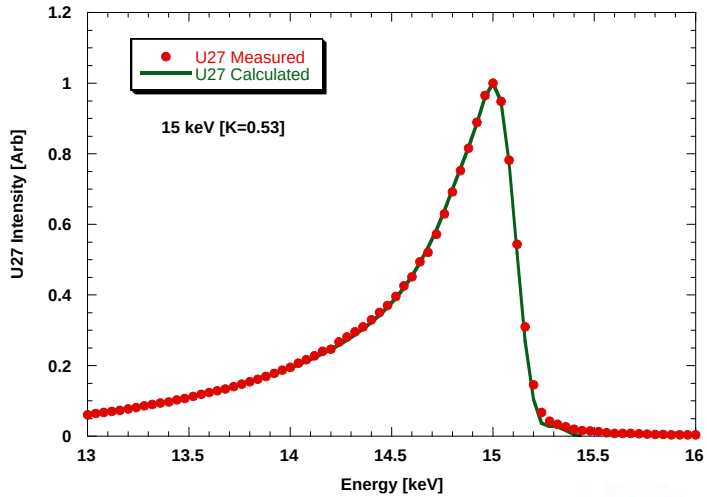
The X-ray Source

Undulators U23 and U27

Undulator	U23	U27
Period [mm]	23	27
Energy Range [keV]	11.96-20	6.8-17





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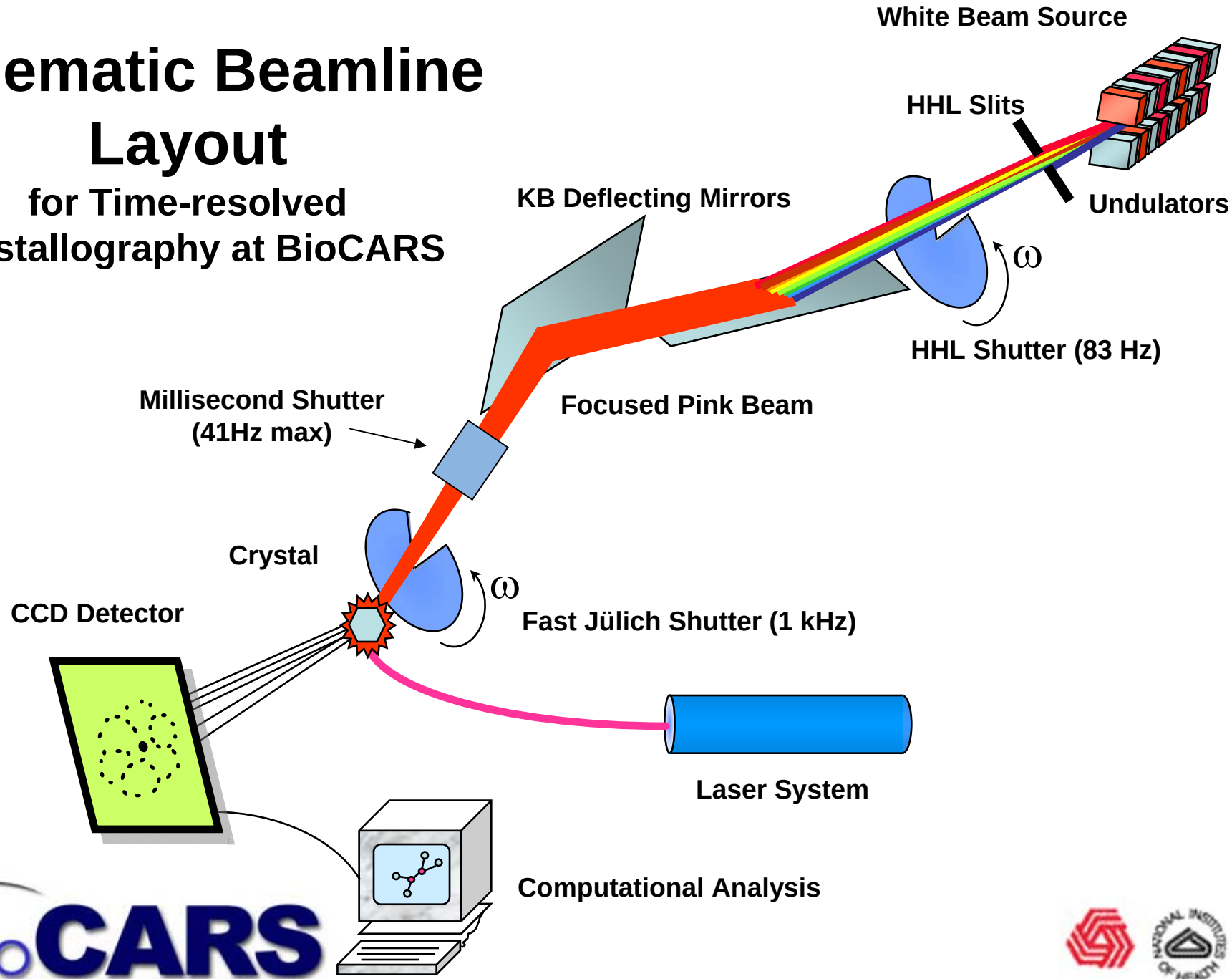
Schematic Beamline Layout

for Time-resolved Crystallography at BioCARS



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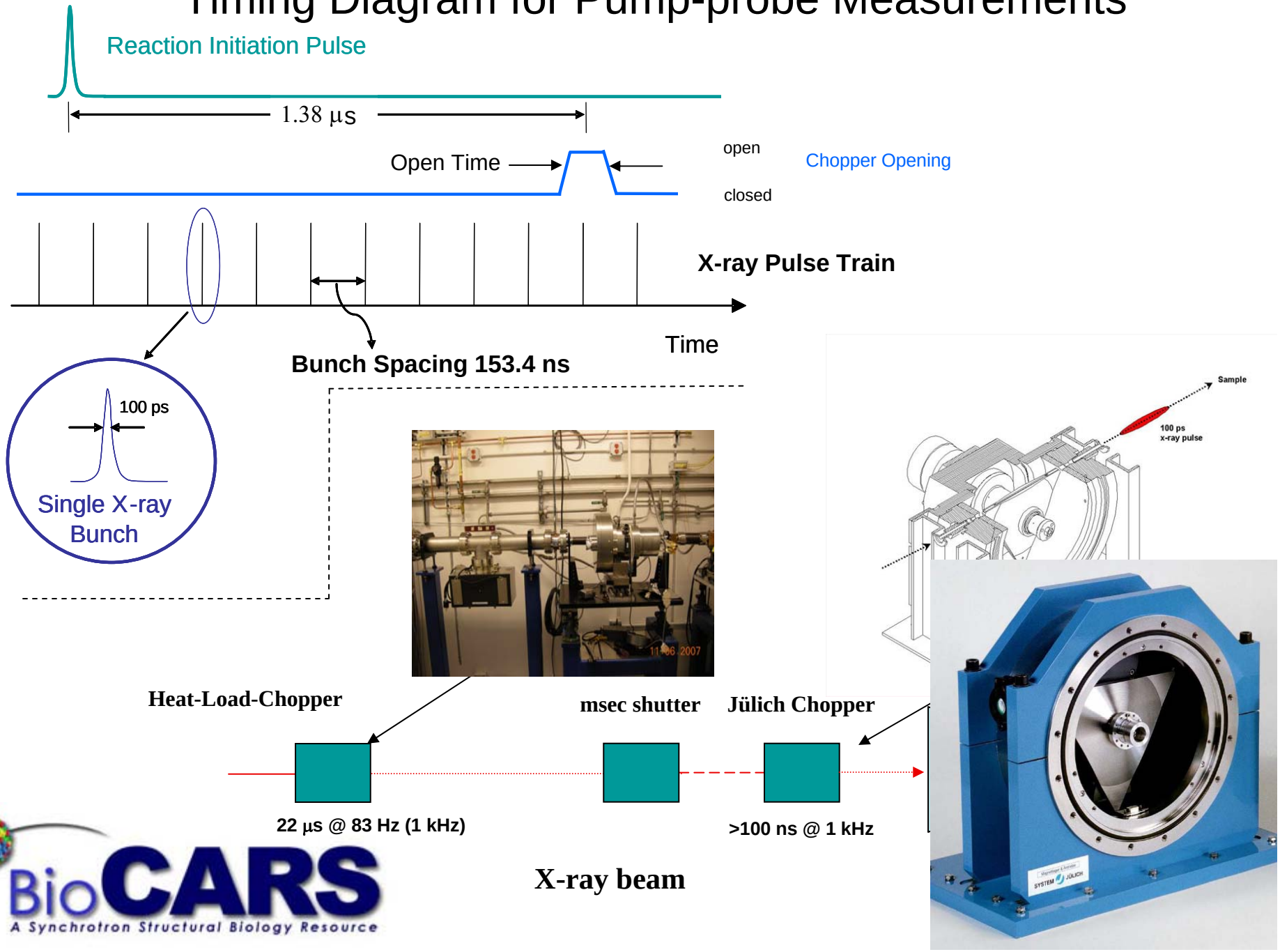
Timing Diagram for Pump-probe Measurements



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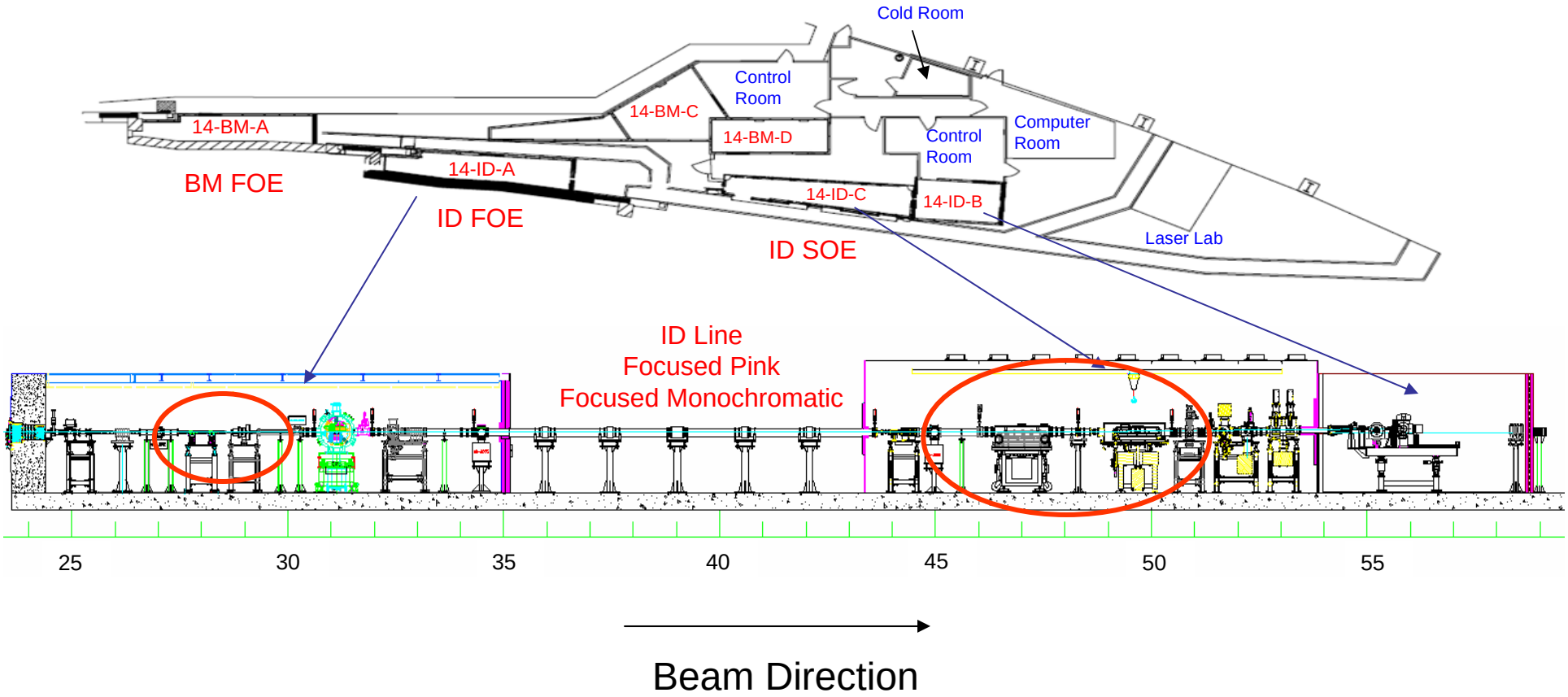
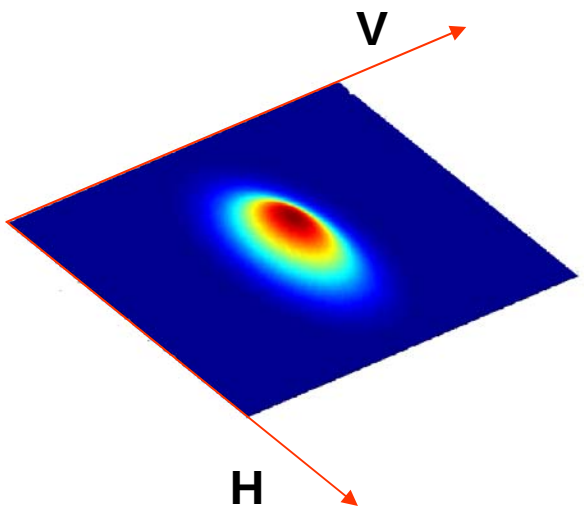
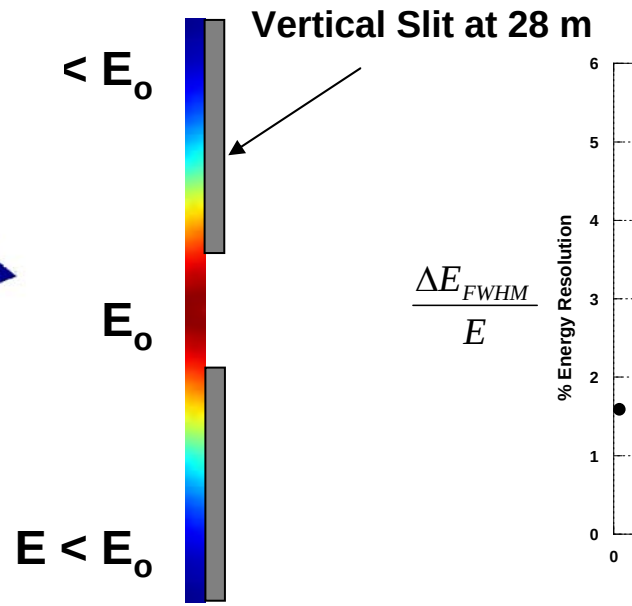
Beamline Layout



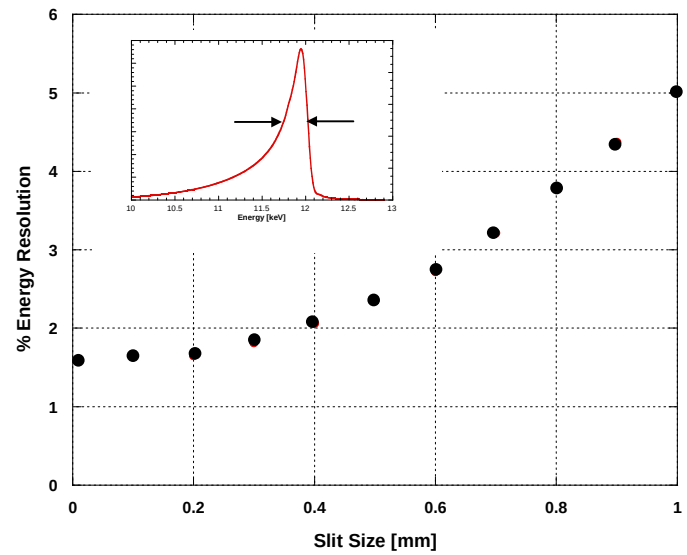
X-ray Bandwidth Control



X-ray beam profile at slits



$$\frac{\Delta E_{FWHM}}{E}$$



- Angle-energy correlation allows some control over bandwidth
- Important for WAXS experiments (improves resolution)

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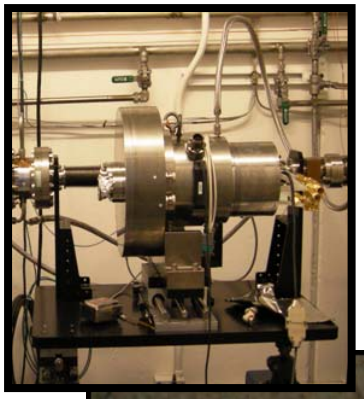
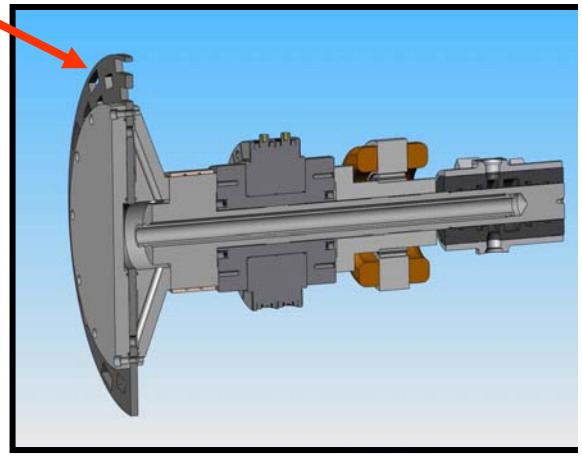
White-beam Chopper



- **Air Bearing**
- **Water Cooled**
- **Vacuum Isolated**
- **Reduces downstream heat load**

Slot Width [mm]	Open Time [us]
48	789 (6.5%)
24	386 (3.3%)
12	189 (1.6 %)
6	92 (0.8%)
3	45 (0.4 %)
1.5	22 (0.2 %)

- Nominal frequency 4980 rpm
- 83 Hz or 1kHz operation
- Temperature rise 16°C



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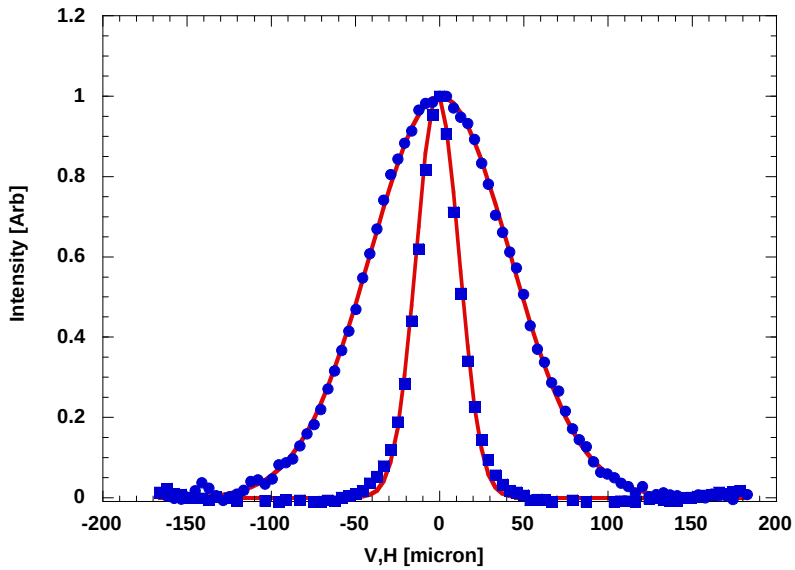
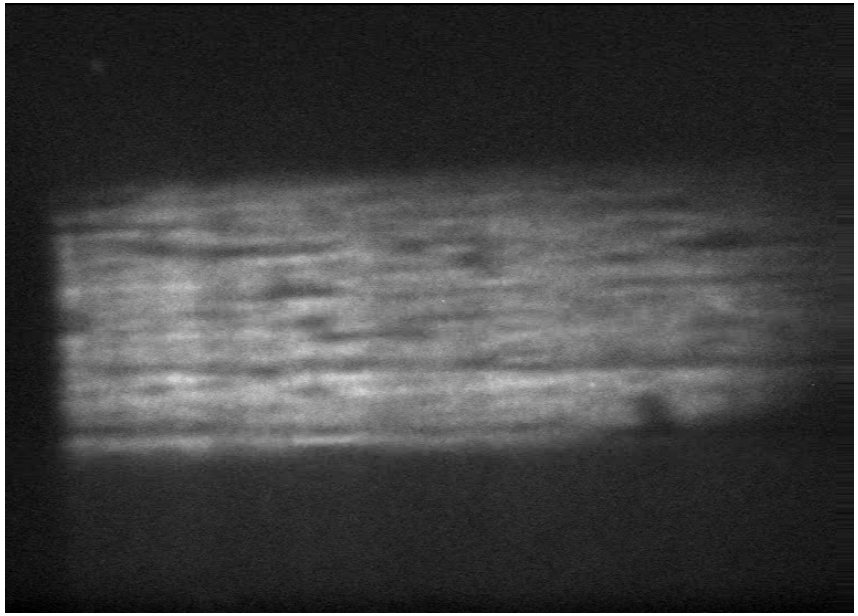
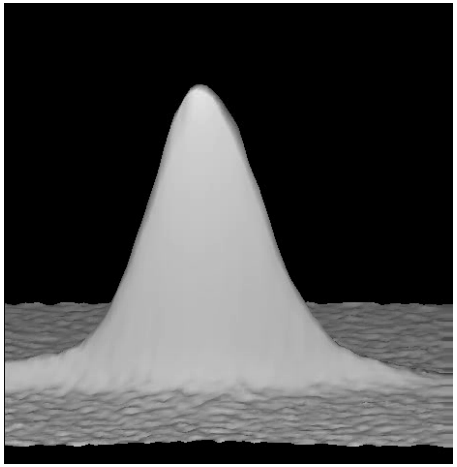
Mirror Performance







Horizontal Beam Size: 95μm FWHM

Vertical Beam Size: ~20μm FWHM

- 50% of total flux measured through a 65μm x 40 μm slit
- Theoretical value for a 2D Gaussian with this slit size is 51%

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Theoretical and Measured Beamline Parameters at 12 KeV

Parameter	Theoretical	Measured
White beam power U27 (K=0.92, measured at exit window)	150 W	142 W
White beam power U23 (K=1.16, measured at exit window)	329 W	329 W
Total power focused pink beam (U23+U27 measured at sample)	125 W	103 W
Number of photons in a single bunch in 24 bunch mode.	1.0×10^{10} γ	8.4×10^{9} γ
Number of photons in a single bunch in hybrid mode.	3.9×10^{10} γ	3.2×10^{10} γ
Pink beam mirror reflectivity	76.4%	74.3%
Monochromatic flux with U27 (both mirrors 2.5 mrad)	5.5×10^{13} γ/sec	2.8×10^{13} γ/sec
Monochromatic Flux with U23 (both mirrors 2.5 mrad)	8.1×10^{13} γ/sec	4.3×10^{13} γ/sec
Monochromatic mirror reflectivity (Rh Stripe)	95%	93%
Horizontal focus size	~82.2 μm	~95 μm
Vertical focus size	~38.3 μm	~20 μm

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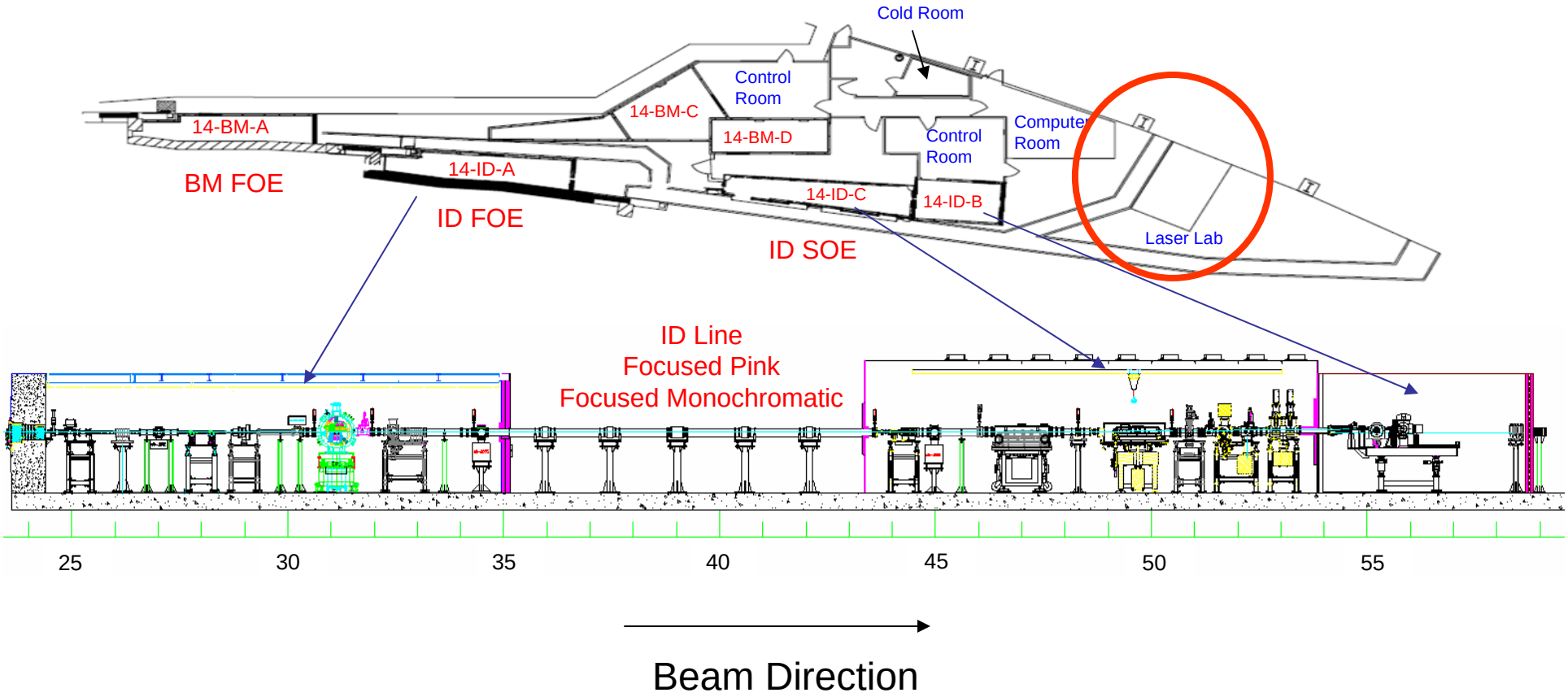
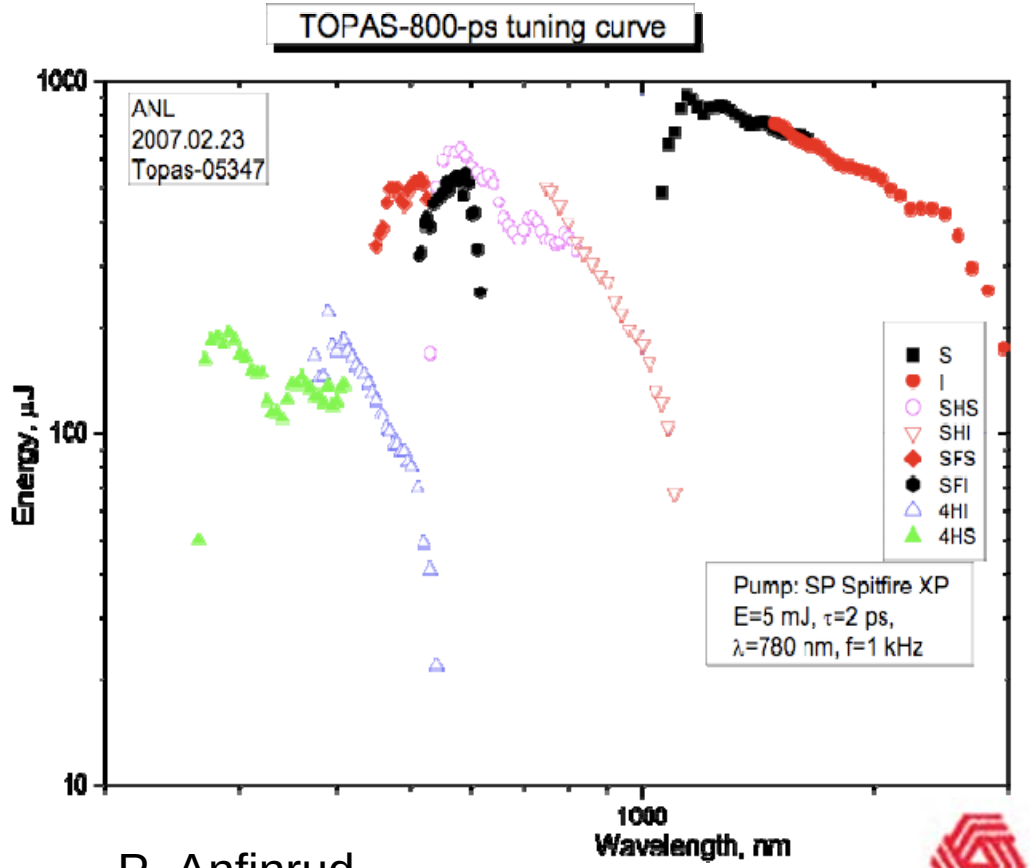
Beamline Layout



Picosecond Laser System Specifications

Laser	Wavelength	Pulse Width	Max Rep Rate	Energy/Power
Millennia	532 nm	CW	CW	5W
Tsunami	780 nm	100 fs	70 MHz	850mW
Empower	527 nm	300 ns	1kHz	15mJ/15W
Spitfire	780 nm	1.2 ps	1kHz	4.8mJ/4.8W
Topas	See Plot	1.2 ps	1kHz	See Plot



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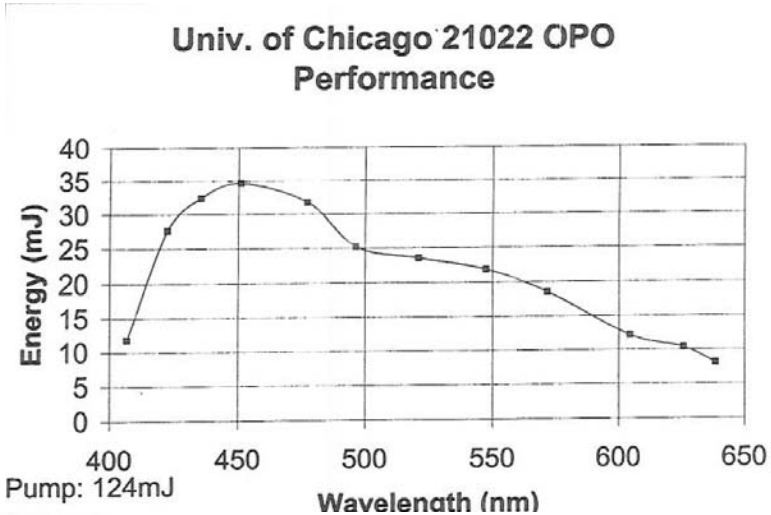
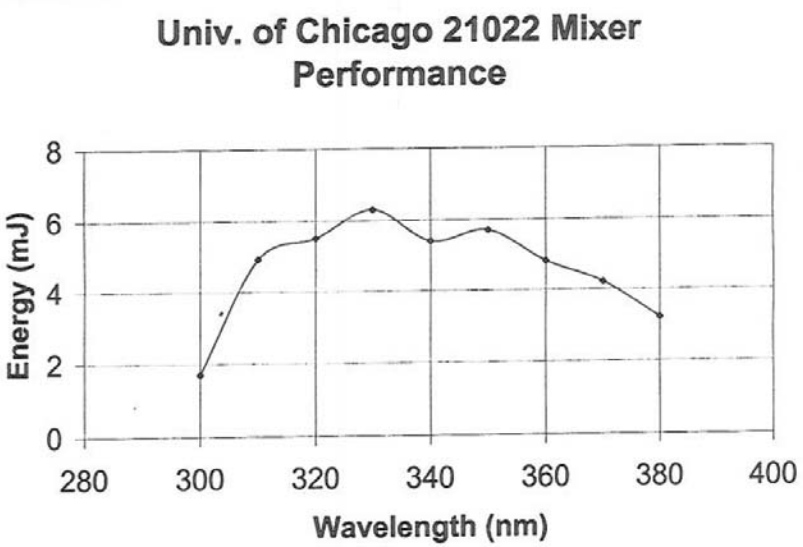
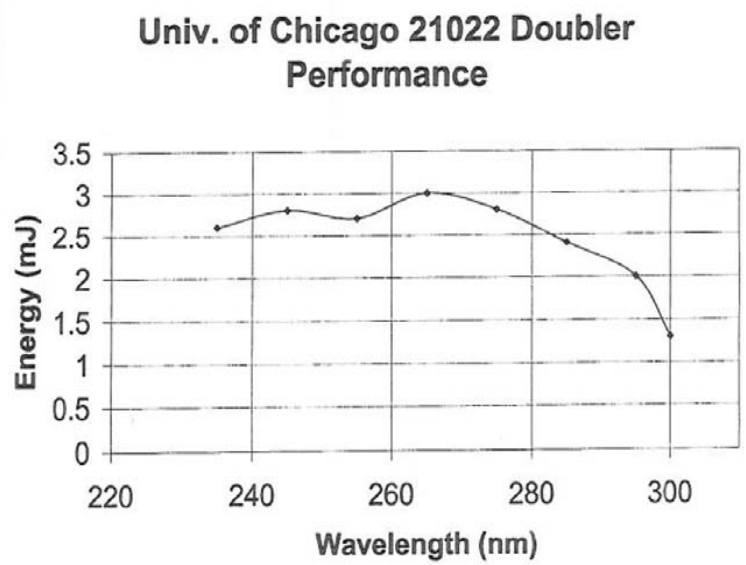
Fiber Coupled OPOTEK Laser



Pulse Width
6 nsec

Rep Rate
10Hz





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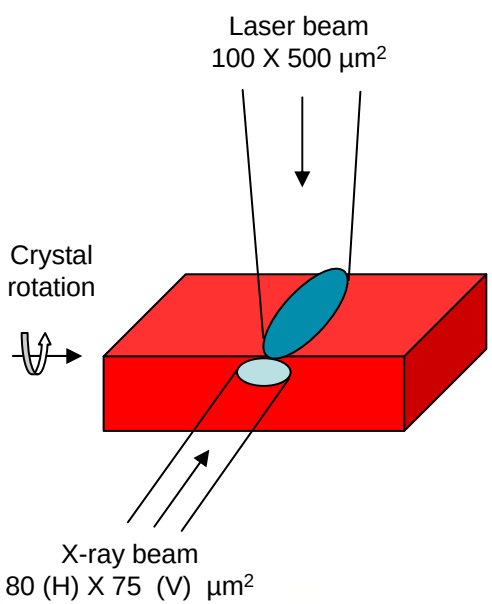
X-ray-beam Overlap with Laser Space and Time

- X-ray 1 Å
  ~100ps pulse duration
  ~80 (H) X 75 (V) μm^2 beam size
- Laser 480nm
  ~35ps pulse duration
  ~140µJ, 100 X 500 μm^2 beam size

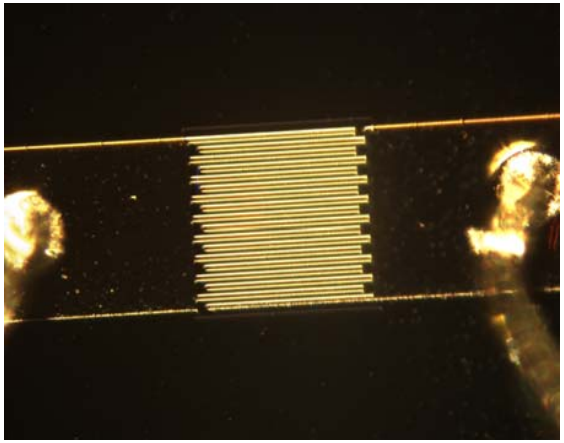
Crystal and X-ray/laser beam geometry.

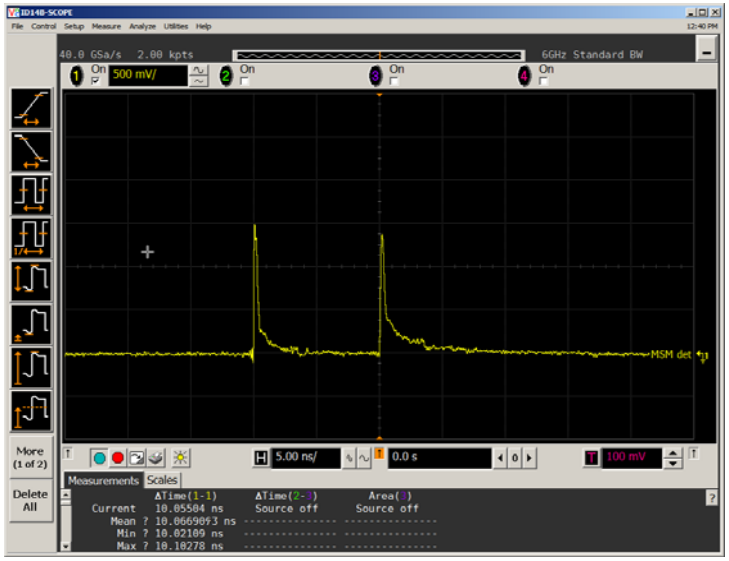


Metal-Semiconductor-Metal

632 µm

476 µm





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Future Directions

Irreversible Reactions

- Difficulty: It requires diffraction patterns from many crystals (of differing quality) to get the necessary number of pump-probe time points
- Solution: Fast time-slicing pixel array detector used in conjunction with a logarithmic x-ray chopper allows a single reaction-initiation pump pulse to be followed by many probe pulses

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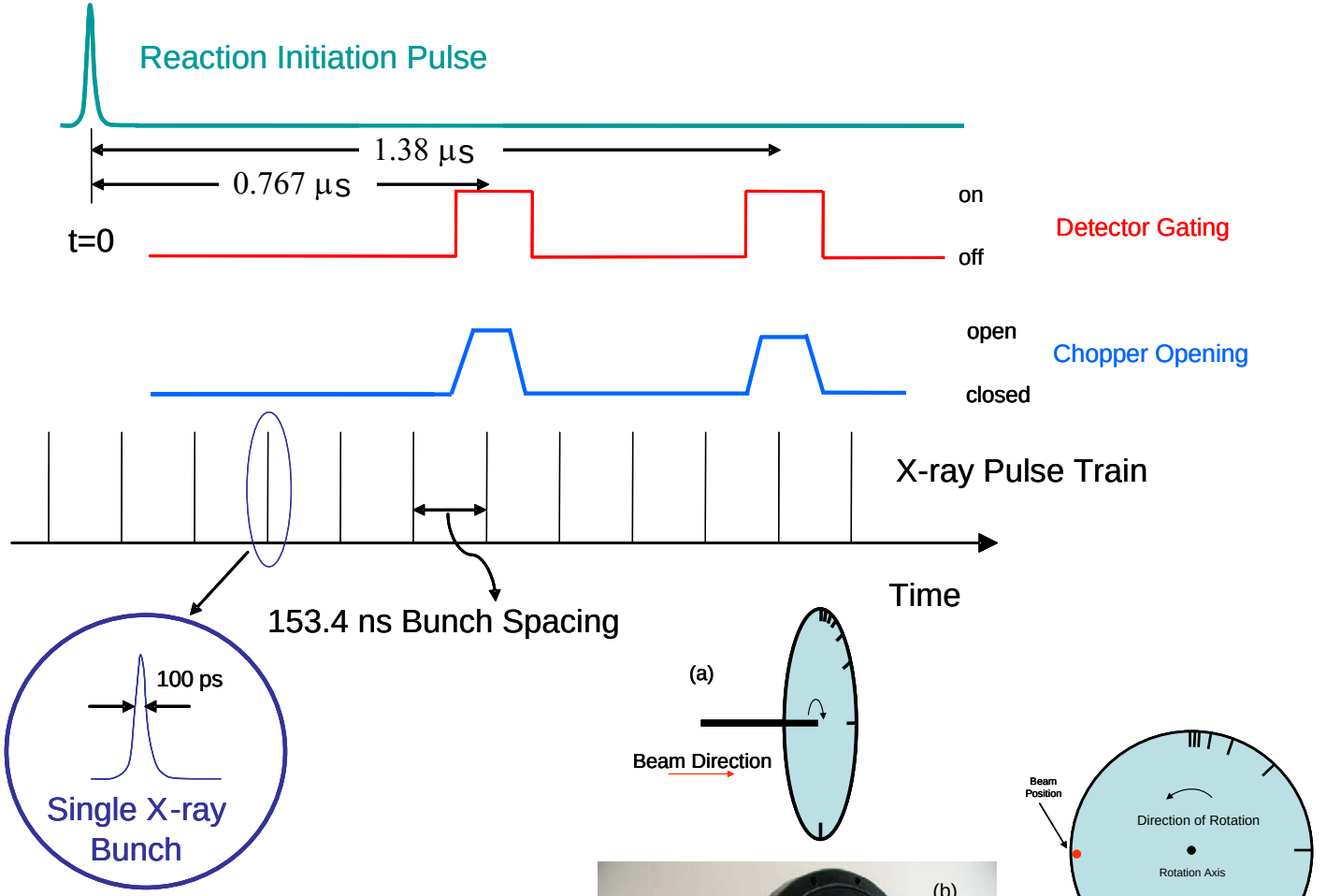
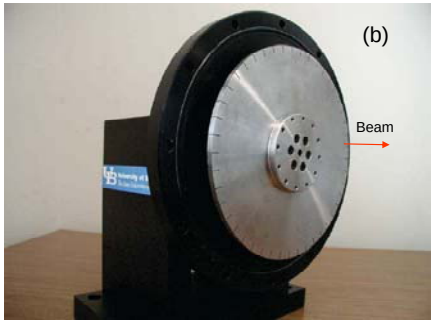
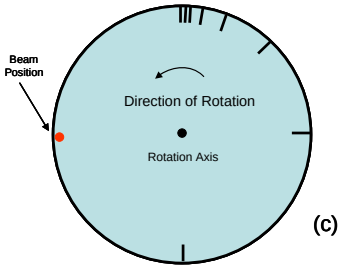
Timing diagram for detector-chopper x-ray pulse gating







Irreversible Reaction Wheel

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CCD and Pixel Array Detectors

?

- CCD detectors relatively slow and in general must be read out between exposures.
- Two types of pixel array detectors demonstrated - counting and integrating.
- Best for our purposes an integrating PAD with on-board storage for each pixel.

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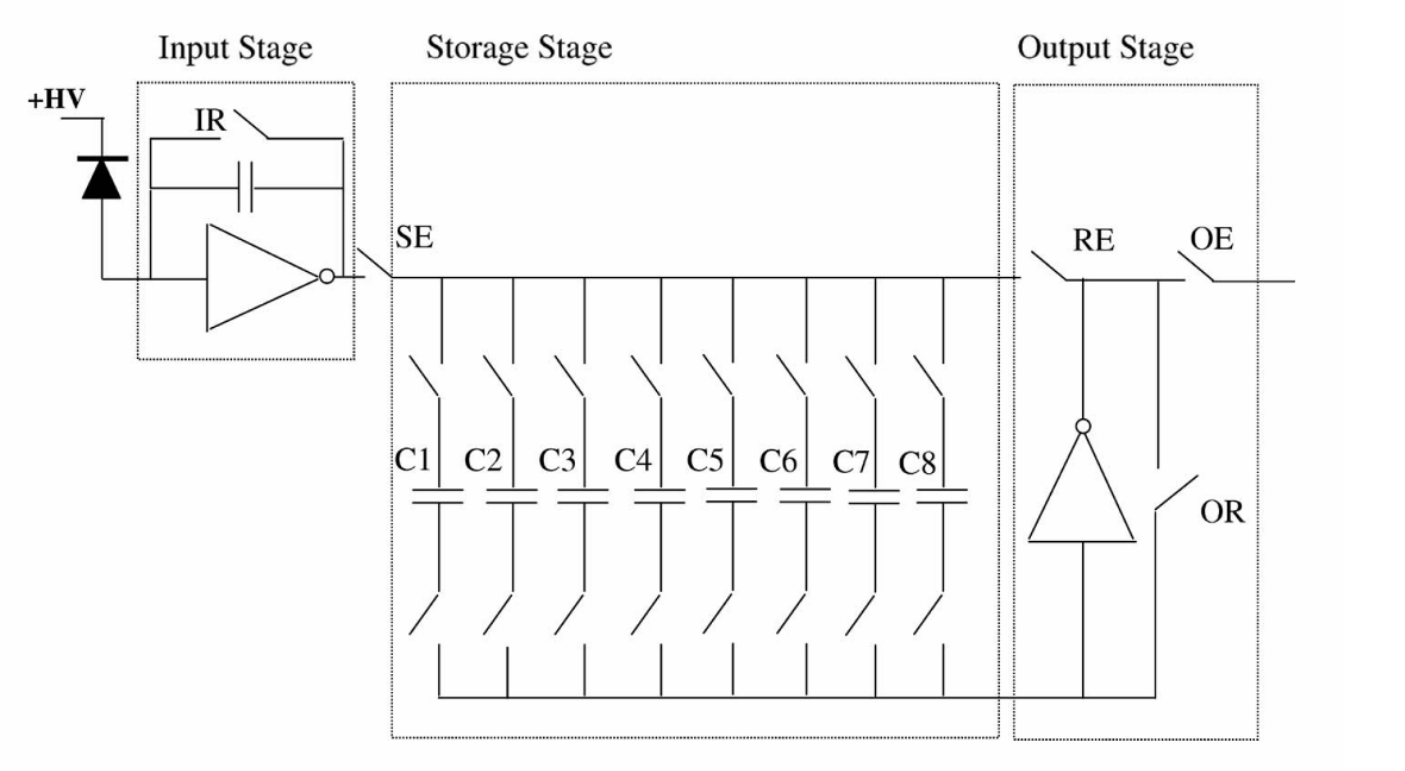
On-board storage for each pixel

Gruner's group at Cornell University is developing an analog-integrating PAD or APAD



- Allows multiple frames to be taken in quick succession
- The detector must be capable of measuring very high instantaneous count rates
- Typical count rate ~5000 photons per ~100 ps X-ray pulse per pixel, equivalent to 50 THz/pixel.

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