The workshop will take place in the Guest House Conference Room A.

Friday, Nov. 2, 2018

Morning session

8:00 am	Registration and breakfast	
8:50 am – 9:00 am	Welcome remarks	
9:00 am – 10:00 am	Introduction to lattice dynamics-part 1	John Tse (U. of Saskatchewan)
10:00 am - 10:20 am	Coffee break	
10:20 am - 11:00 am	Introduction to NRIXS	Wolfgang Sturhahn (Caltech)
11:00 am - 12:10 pm	Introduction to PHOENIX	Wolfgang Sturhahn
12:10 pm	Group Photo	
12:20 pm	Lunch	

Afternoon session

1:30 pm – 3:30 pm	PHOENIX	Wolfgang Sturhahn
3:30 pm – 3:45 pm	Coffee break	
3:45 pm – 6:30 pm	PHOENIX	Wolfgang Sturhahn
6:30 pm	Dinner	

Saturday, Nov. 3

Morning session

8:30 am	Breakfast	
9:00 am – 10:00 am	Introduction to lattice dynamics-part 2	John Tse
10:00 am – 10:40 am	Geophysical Applications of NRIXS	Jennifer Jackson (Caltech)
10:40 am – 10:50 am	Coffee break	
10:50 am – 11:30 am	Introduction to Isotope Fractionation	Anat Shahar (CIW)
11:30 am-12:10 pm	Introduction to SciPhon	Nicholas Dauphas (U of Chicago)
12:10 pm	Lunch	

Afternoon session

1:30 pm – 3:50 pm	PHOENIX	Wolfgang Sturhahn
3:50 pm – 4:00 pm	Coffee break	
4:00 pm – 6:30 pm	PHOENIX	Wolfgang Sturhahn
6:30 pm	Dinner	

Sunday, Nov. 4

Morning session

8:30 am	Breakfast	
9:00 am – 9:30 am	Instrumentation and recent development at Sector 3	Jiyong Zhao (ANL)
9:30 am – 10:30 am	PHOENIX	Wolfgang Sturhahn
10:20 am – 10:30 am	Coffee break	
10:30 am – 12:00 pm	PHOENIX	Wolfgang Sturhahn
12:00 pm – 12:20 pm	Open discussion of experimental issues and data analysis	
12:20 pm	Lunch	

Conducting Nuclear Resonant Scattering Experiment at 3ID, APS

Jiyong Zhao

Advance Photon Source,
Argonne National Laboratory

Workshop on Nuclear Resonant Scattering
APS, November 2-4, 2018

Advanced Photon Source

To plan for an experiment of NRS

1. What can be measured?

SMS: hyperfine interactions, magnetic proporties … …

NRIXS: thermal and dynamical properties … …

2. What's available at the beamline

how strong the beam, how small the beam size,
how low/high the temperature or field etc.
what else?

3. How and when to apply the beam time

To plan for an experiment for NRS

1. What can be measured?

   NRIXS: thermal dynamics

   SMS: hyperfine interactions

2. What's available at the beamline

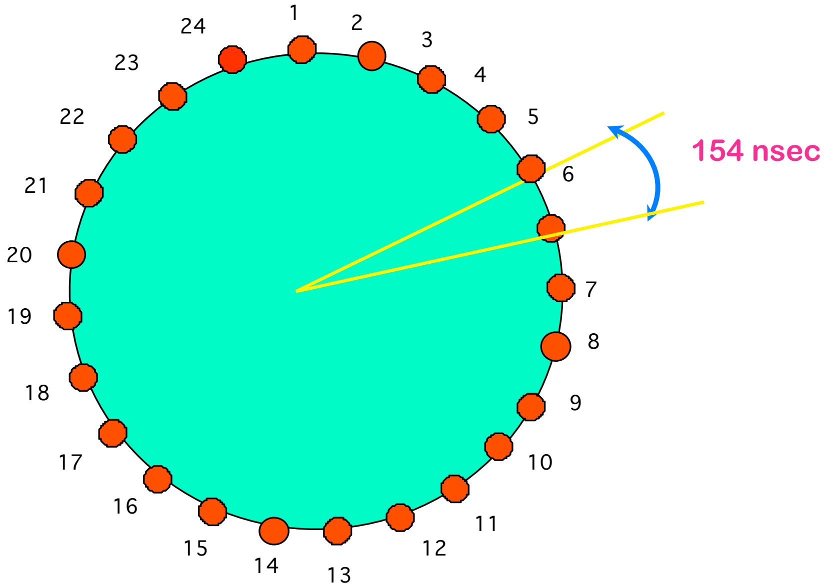
   What are unique features of the SRS?

   How strong the beam?
   Do you need enriched or natural abundant sample?
   What is the beam size,
   What are the existing instruments at the beamline to reach low/high temperatures or fields etc.
   What will happen for the APS-U

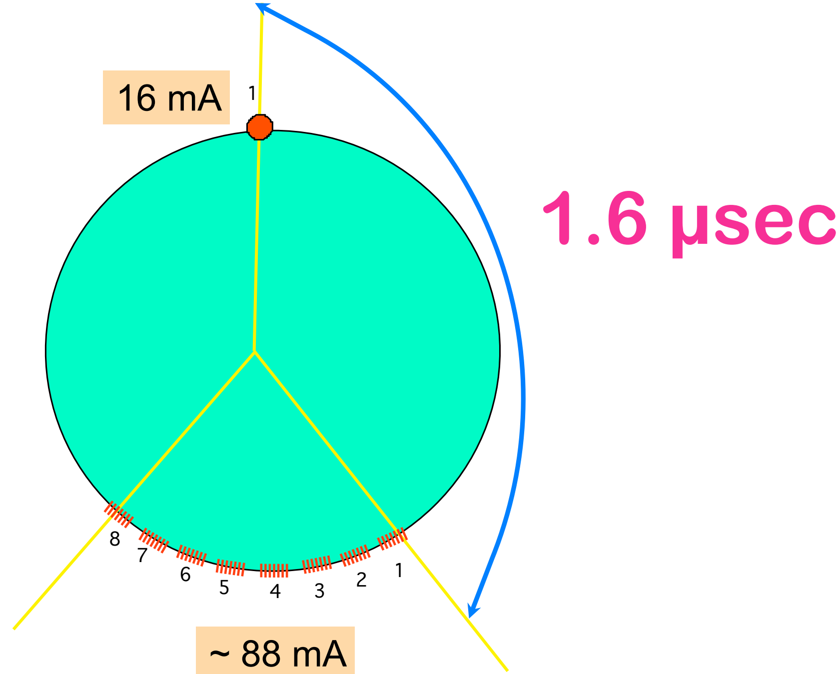
3. How and when to apply the beam time

Nuclear resonance beamlines around the world, 2018

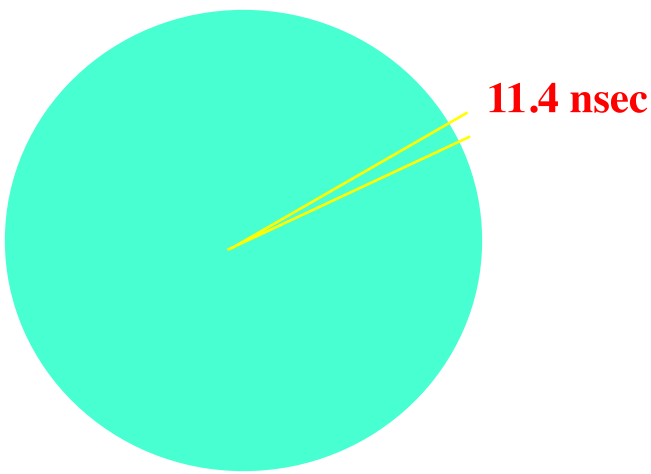
APS storage ring filling pattern



24-bunch mode, 4.25mA/bunch, 65%



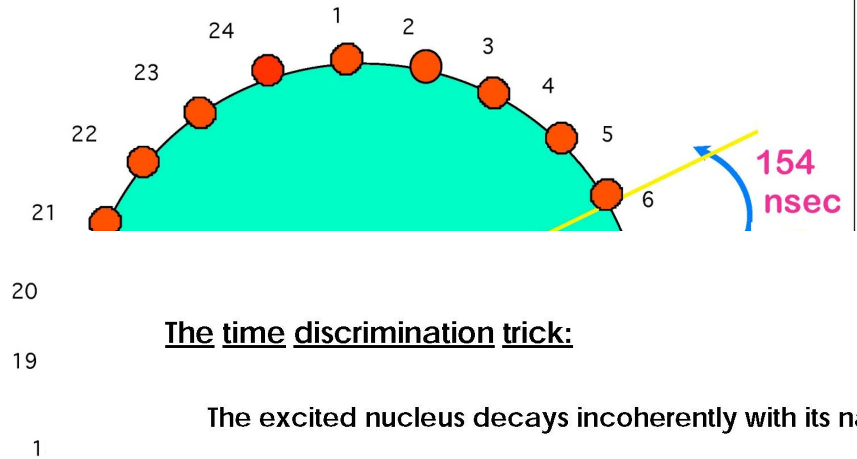
Hybrid mode 1+8X7-bunch, 15%

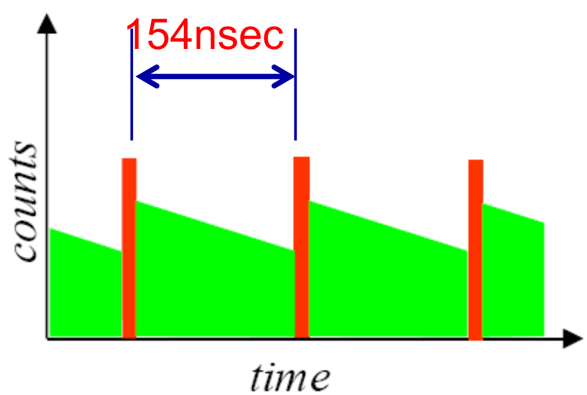


324-bunch mode, 0.3 mA/bunch, 20%

1296 buckets, 2.84 nsec separation

Standard Time structure @ APS





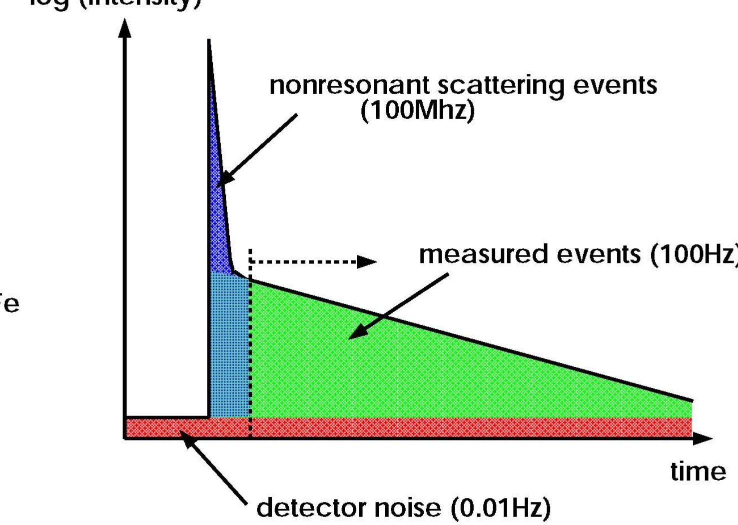
Time gating

The time discrimination trick:

The excited nucleus decays incoherently with its natural life time τ.

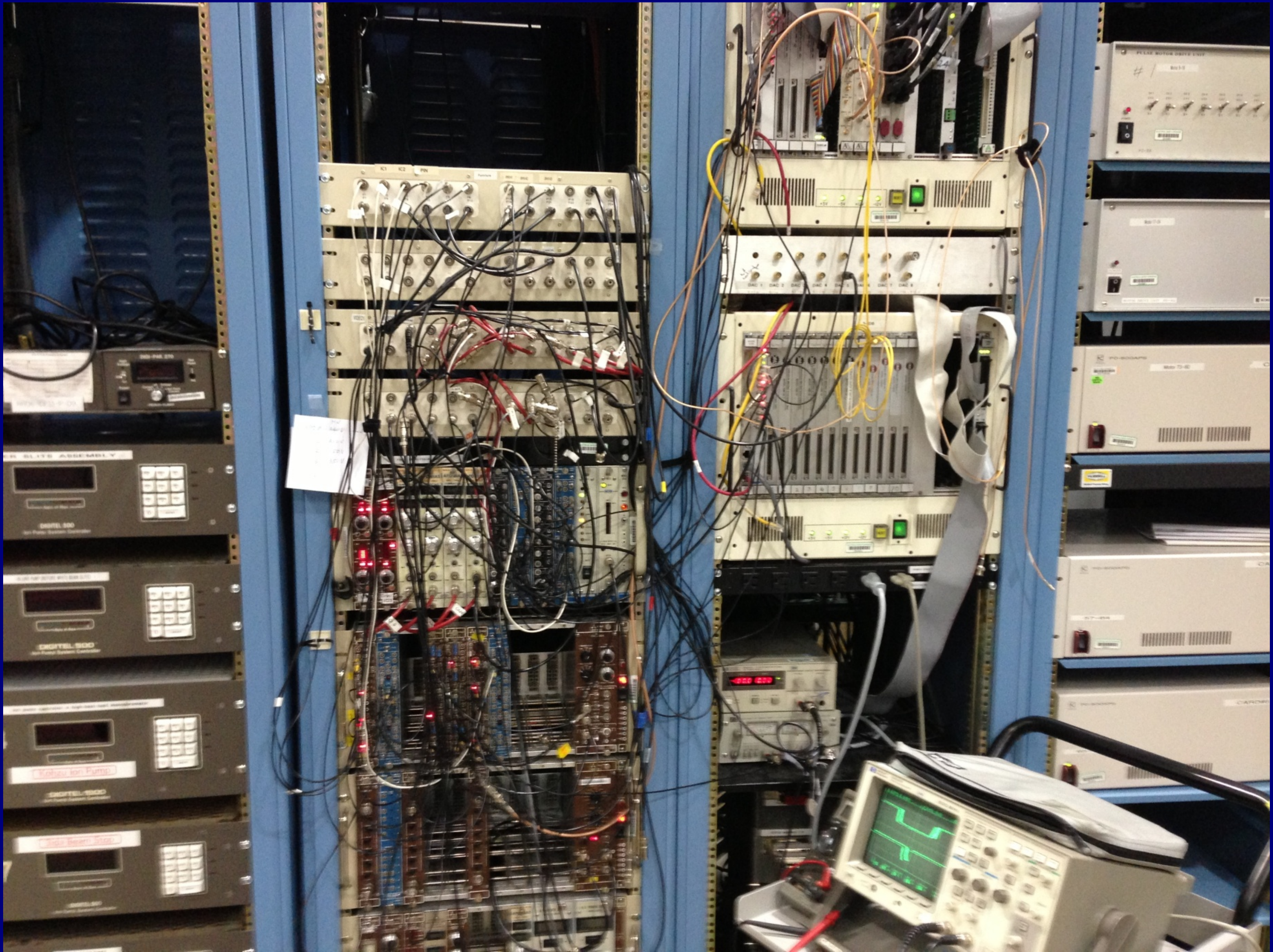
$\tau = \hbar / \Gamma$

141 ns for ^{57}Fe

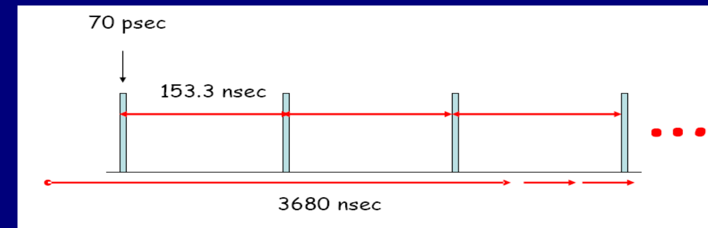


Advanced Photon Source

Timing technique to select NRS delayed signal from a strong electronic scattering background

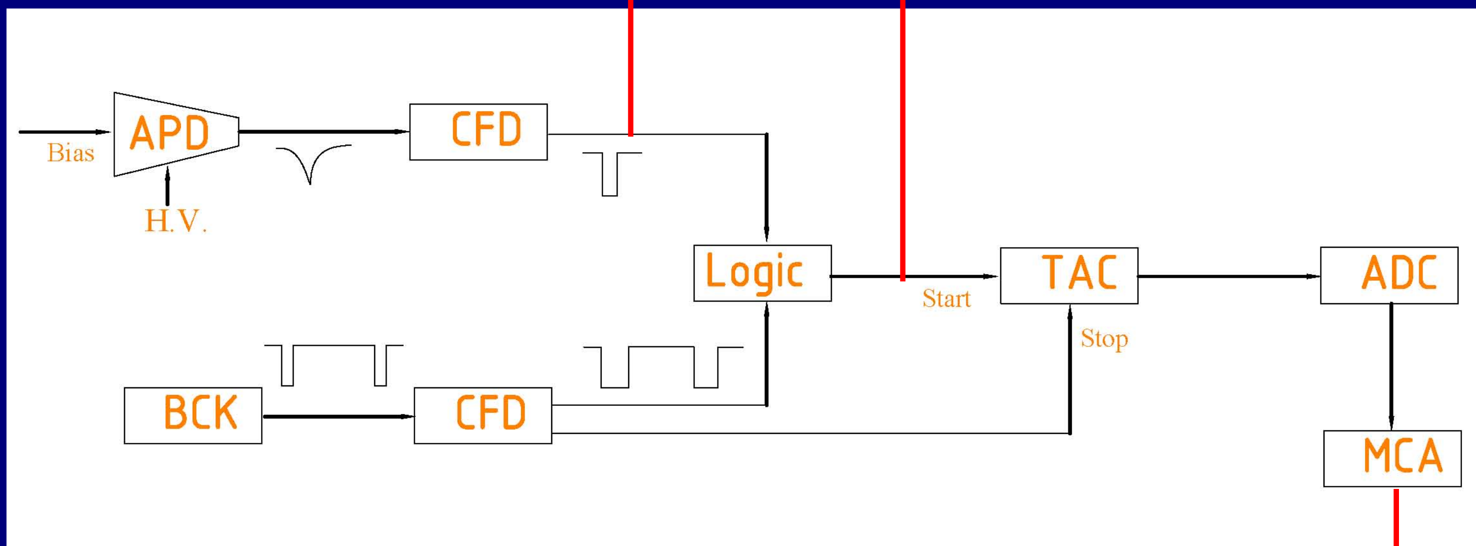


Timing technique

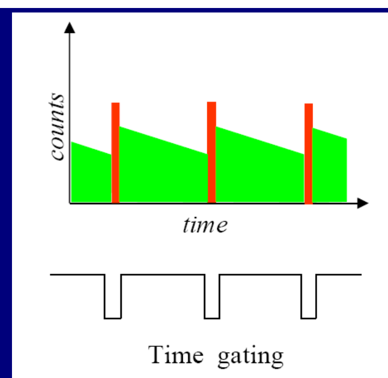


total (prompt)

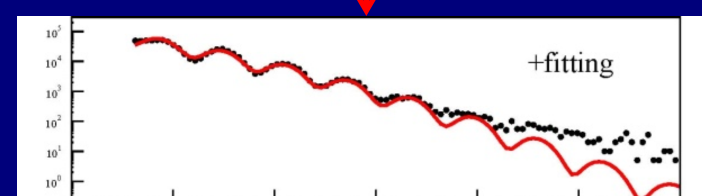
delayed



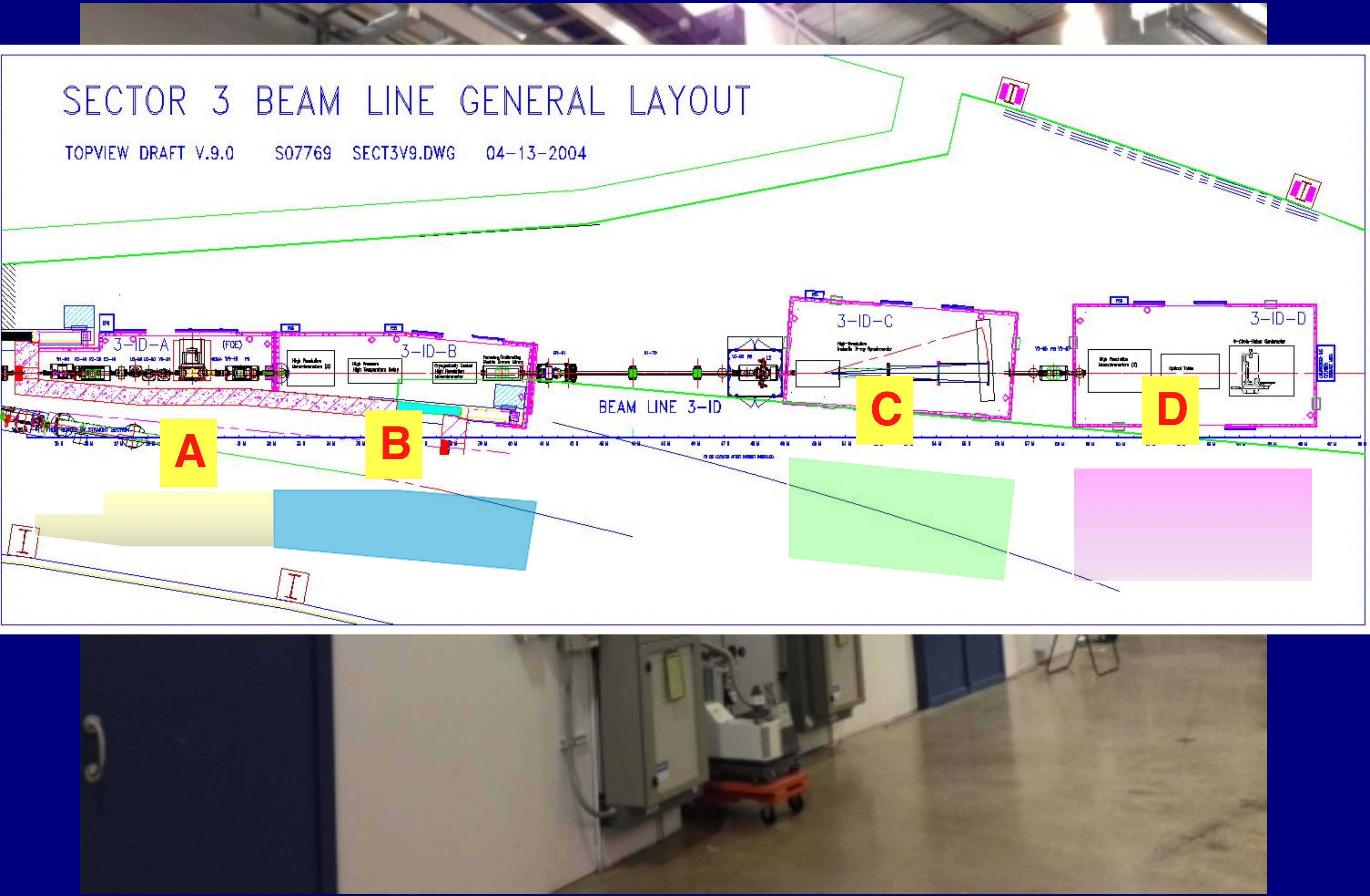
Avalanche photodiode (APD):
100μm Si diode with HV
Efficiency@14keV: 14%
Time resolution: 1ns
Dynamic range: 10^9
Noise: 10^{-2}



Time spectrum



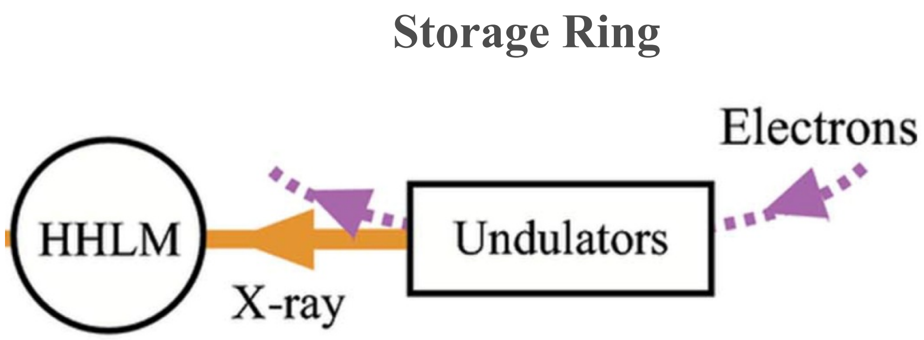
4 stations: **A-B-C-D at 3ID, APS**



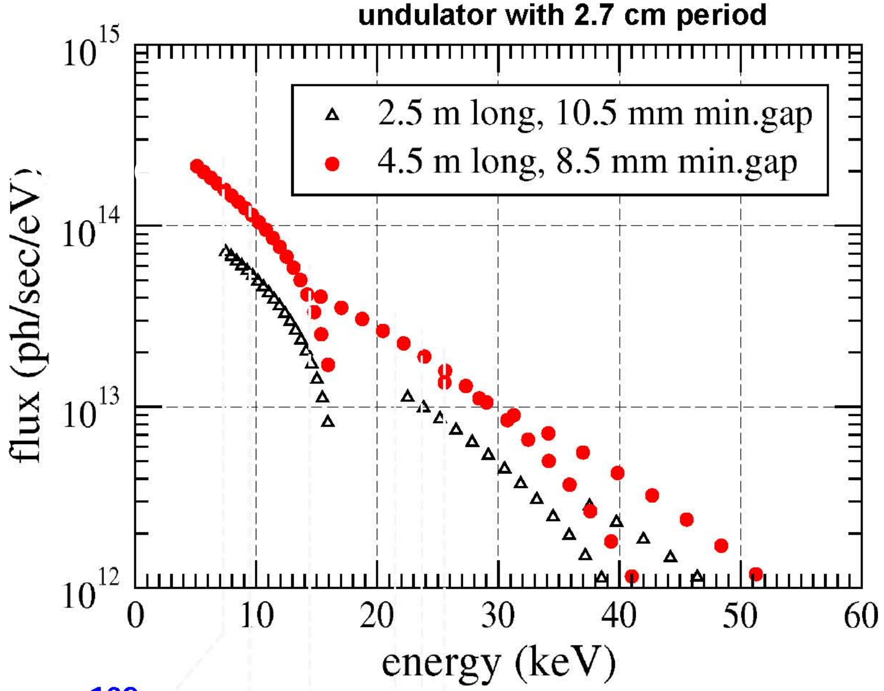
X-ray Source and Instruments for NRS

1. SR Source (undulator)
2. Monochromator (HHLM, HRM)
3. Focusing (KB, toroidal mirror, CRL)
4. Environments (HT, HP, LT,E/M-field)

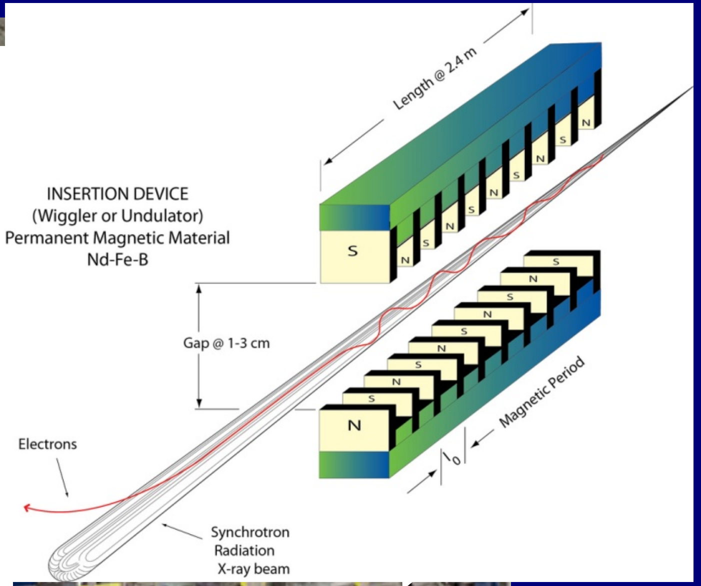
Setup for a synchrotron radiation nuclear resonant scattering experiment



Synchrotron radiation at the Advanced Photon Source:

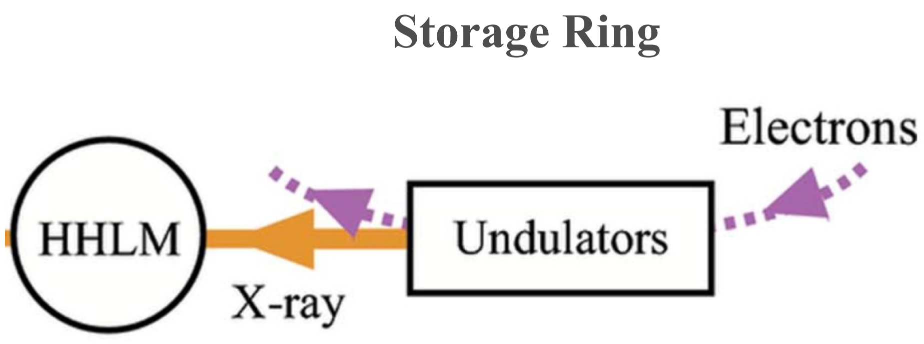


^{169}Tm
^{83}Kr
^{57}Fe
^{119}Sn
^{151}Eu
^{161}Dy

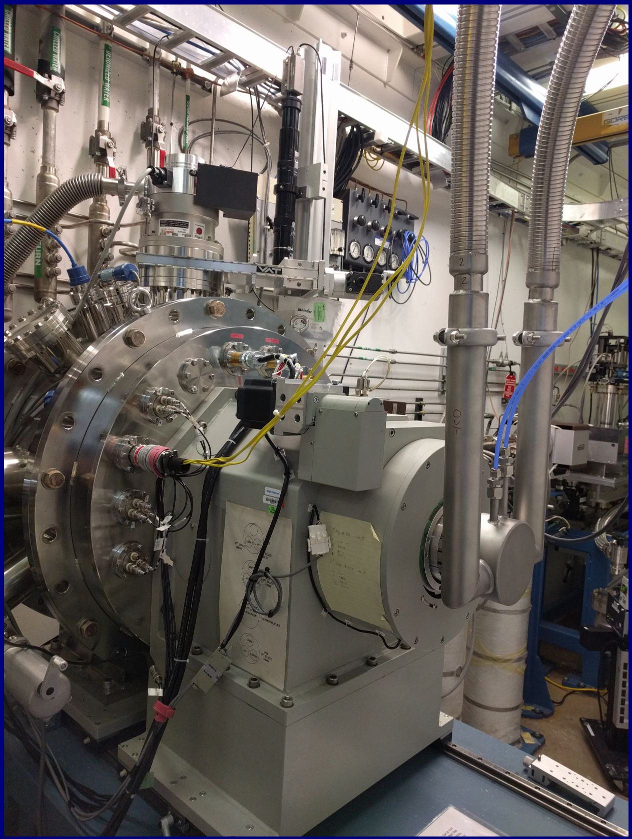


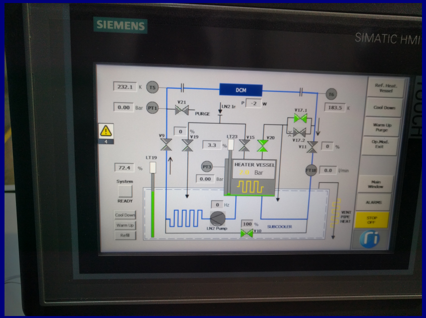
At 3ID, there are two 2.4 m long undulators, with 2.7 cm period

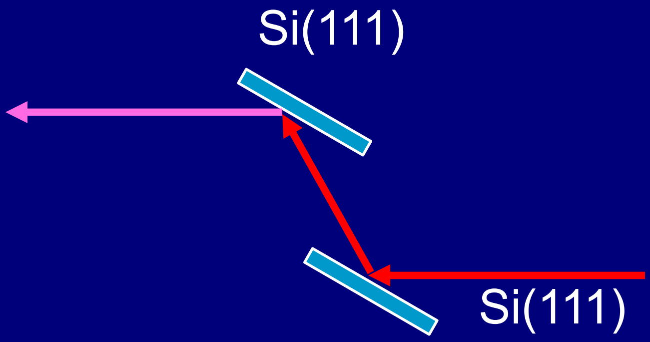
Setup for a synchrotron radiation nuclear resonant scattering experiment



▪ 3ID-A: High heat-load monochromator

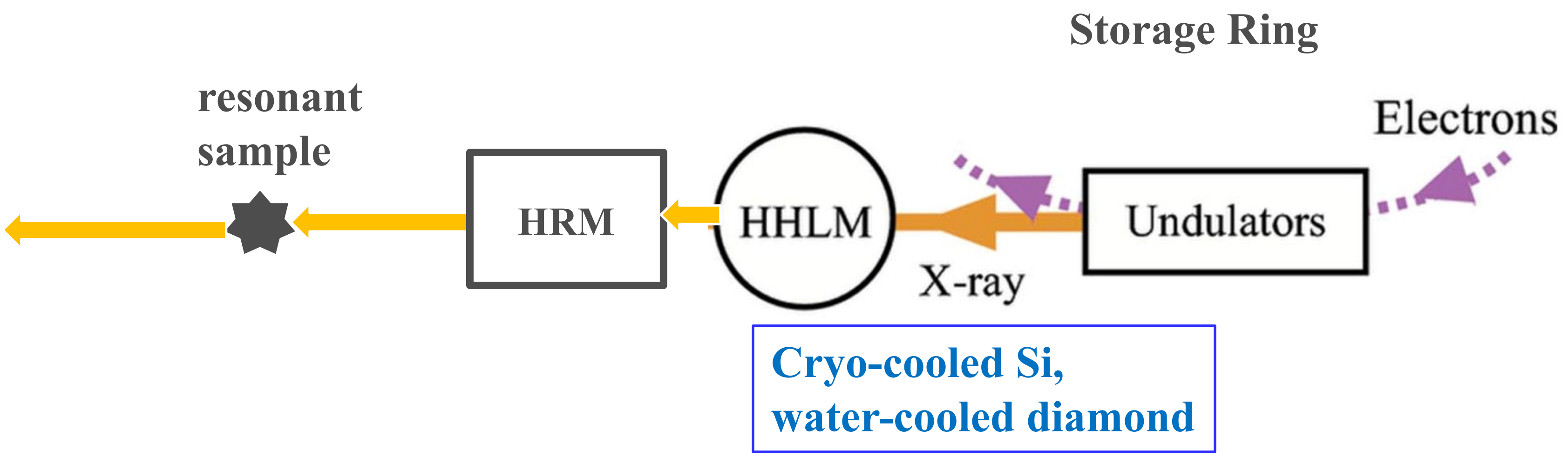


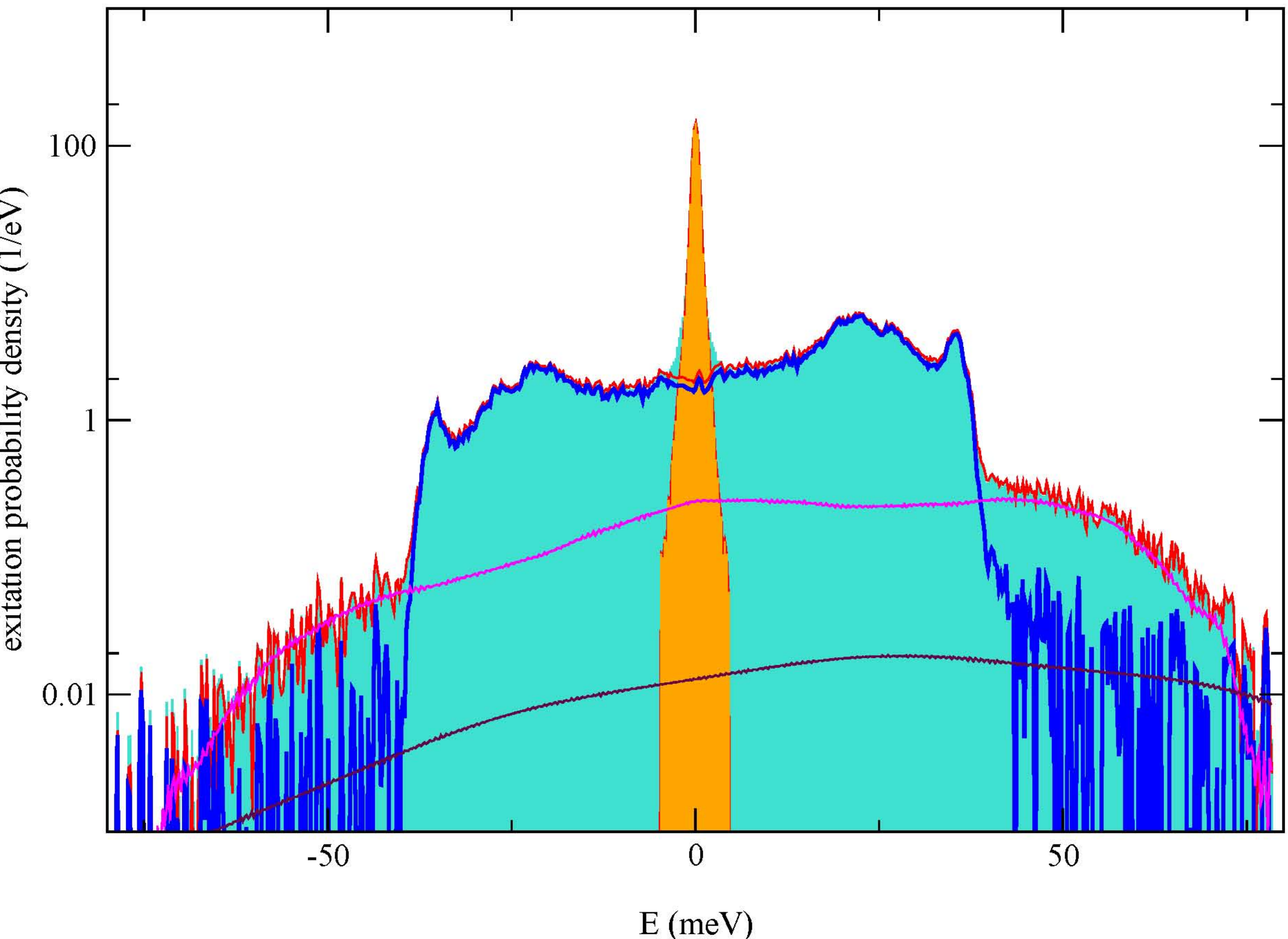




Kohzu high-heat-load monochromator consists of two cryogenic cooled silicon

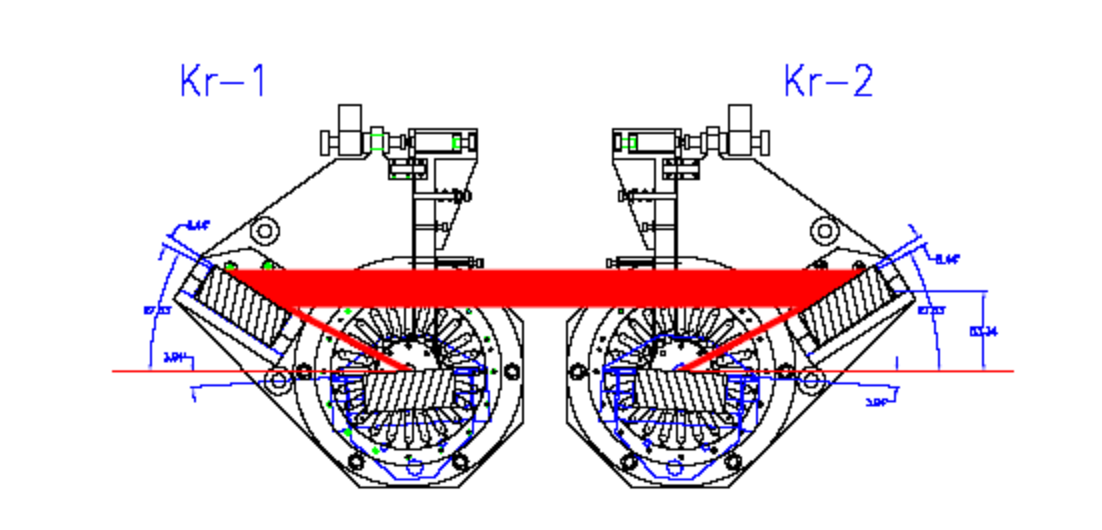
Setup for a synchrotron radiation nuclear resonant scattering experiment

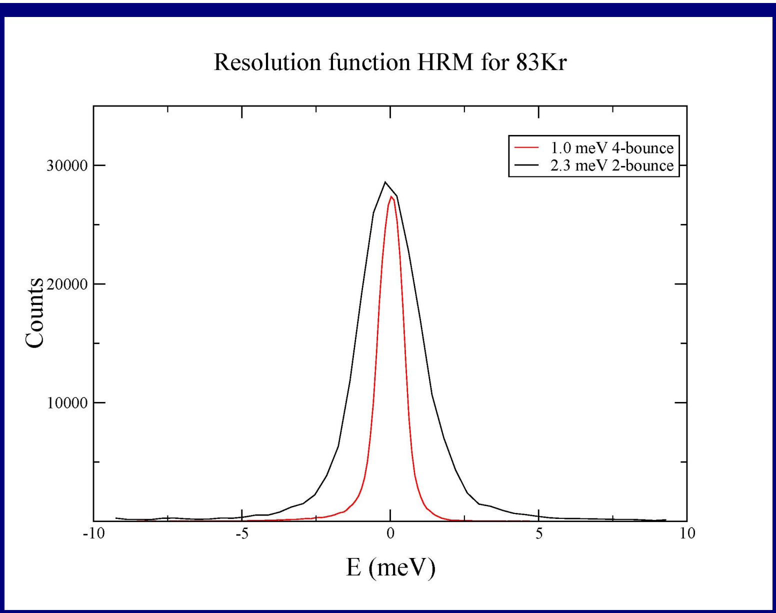




100
1
0.01
-50
0
50
E (meV)
exitation probability density (1/eV)

High-energy resolution monochromator (HRM)

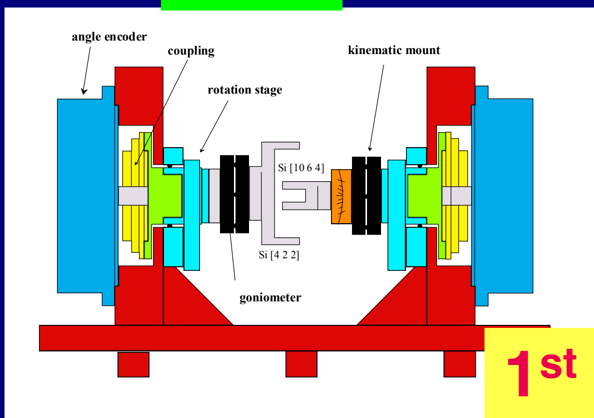




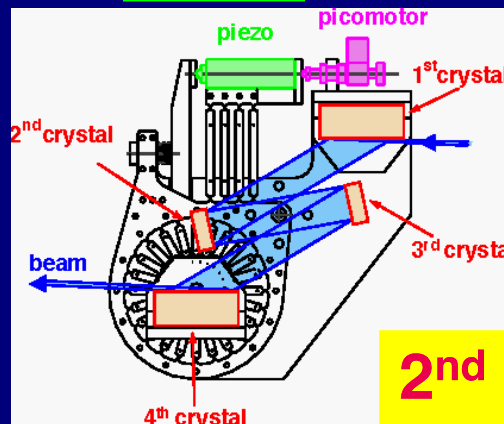
3ID-B: High energy-resolution monochromator and focusing optics

Generations of high-resolution monochromators

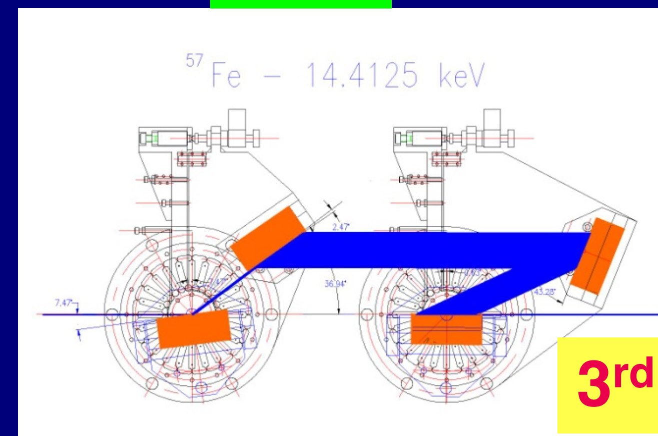
1992

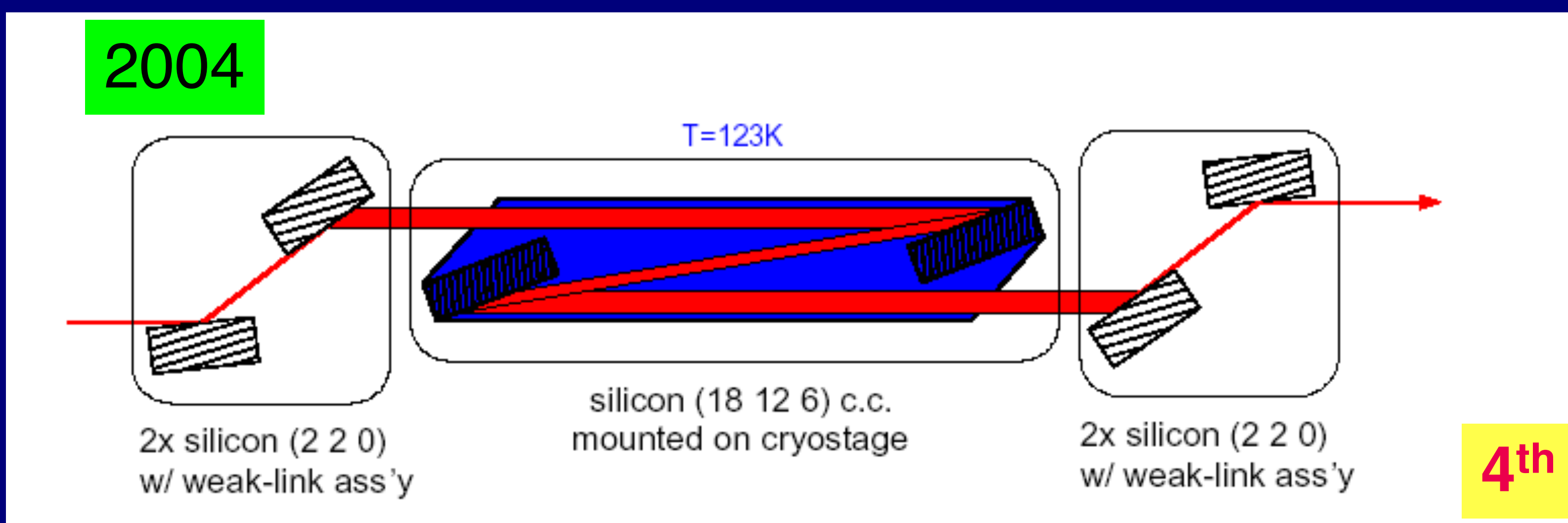


1999



2002





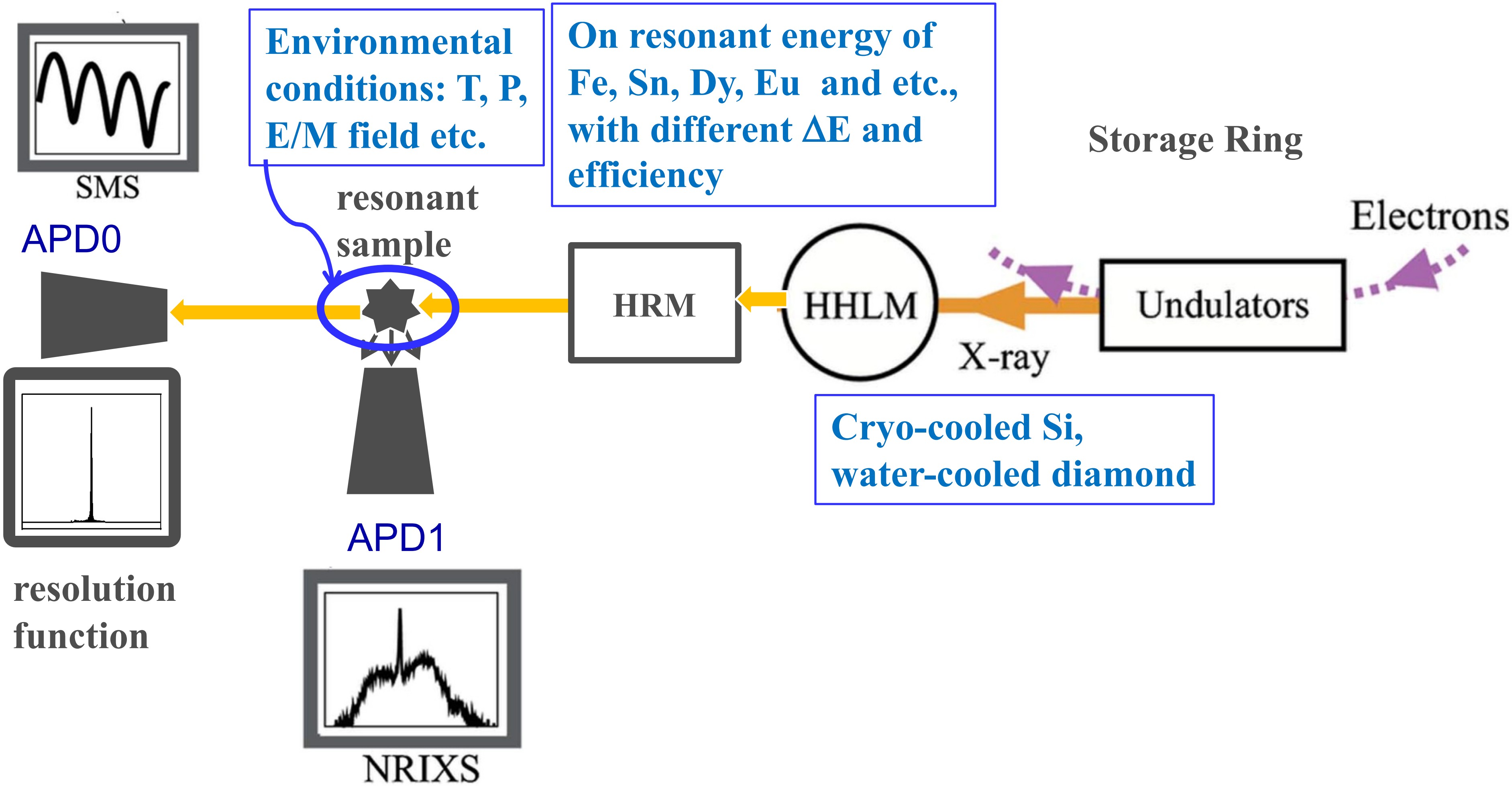
HRM at Sector 3

^{57}Fe,	14.4 keV,	HRM: 1/0.8/2.3/5 meV
^{151}Eu,	21.541 keV,	HRM: 0.8 meV
^{119}Sn,	23.880 keV,	HRM: 0.85/0.14 meV
^{161}Dy,	25.651 keV,	HRM: 0.5 meV
^{83}Kr,	9.404 keV,	HRM: 2.3/1.0 meV

Nuclear data for Mössbauer isotopes

Isotope	Energy E(keV)	Life time $t_{1/2}$(ns)	Energy width Γ(neV)	Natural abundance(%)	Internal conv. coefficient α	Cross section σ_0(cm^2 10^{-18})	Recoil energy E_R (meV)	Type
^{181}Ta	6.22	6800	0.067	99.99	46	1.6	0.116	E1
^{169}Tm	8.41	3.9	1.17	100	268	0.31	0.24	M1
^{83}Kr	9.40	147	3.1	11.5	19.9	1.1	0.56	M1
^{73}Ge	13.26	$4\ 10^3$	0.11	7.8	1000	0.0076	1.29	E2
^{57}Fe	14.41	97.8	4.7	2.15	8.21	2.57	1.95	M1
^{151}Eu	21.53	9.7	0.47	47.9	28.6	0.23	1.66	M1
^{149}Sm	22.49	7.1	0.641	13.9	50	0.0711	1.82	M1
^{119}Sn	23.88	17.7	0.257	8.6	5.12	1.40	2.58	M1
^{161}Dy	25.65	28.1	0.162	19.0	2.9	0.95	2.2	E1
^{40}K	29.56	4.26	1.07	0.012	6.6	1.6	11.6	M1

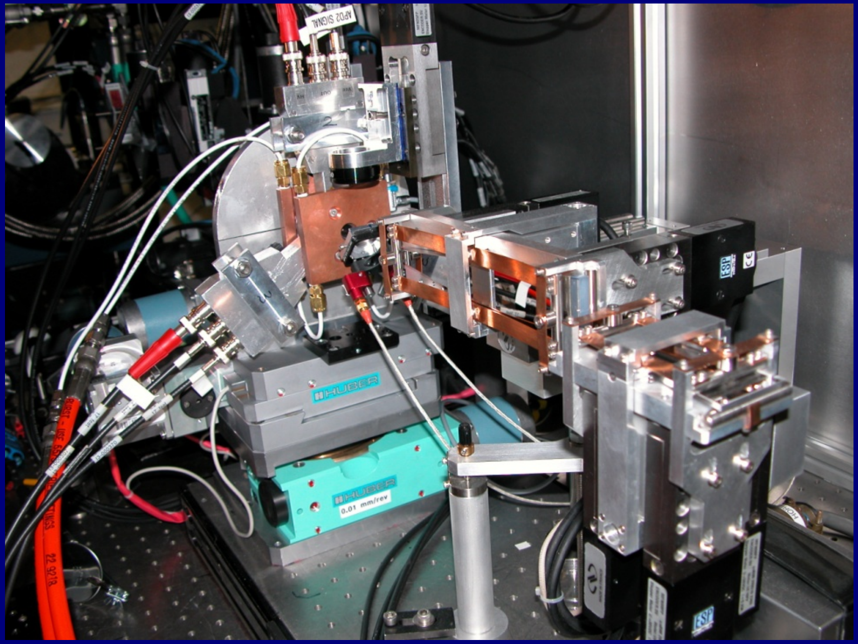
Setup for a synchrotron radiation nuclear resonant scattering experiment



Unique capability at 3ID for NRS

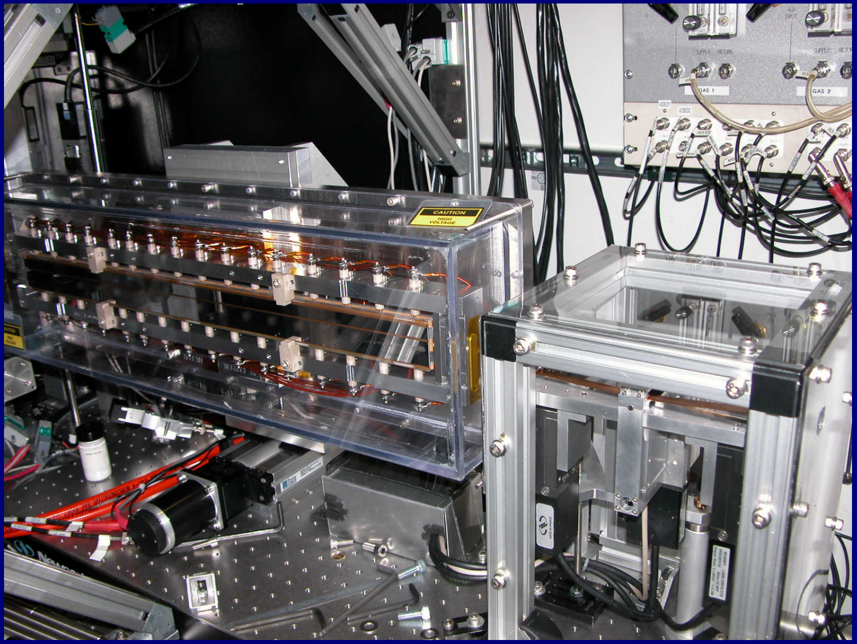
Beam focusing at 3ID-B

K-B focusing mirror



Beam size: 6 μm x 7 μm

Acceptance: 0.4mm x 0.6 mm



Beam size: 18 μm x 12 μm

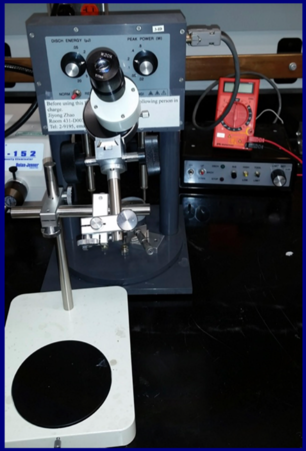
Acceptance: 0.4mm x 1.8 mm

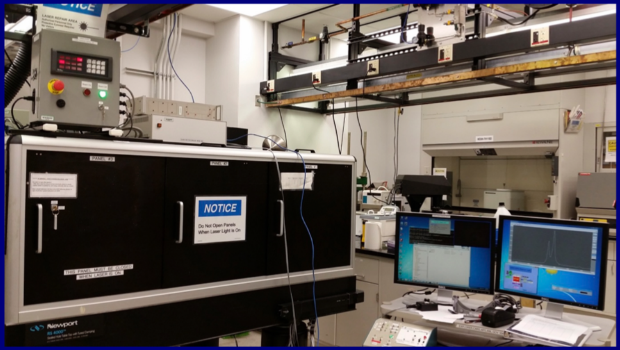
Sample environment for NRS at 3ID

- Low temperature, flow cryostat
- High pressure and high temperature
- High pressure and low temperature

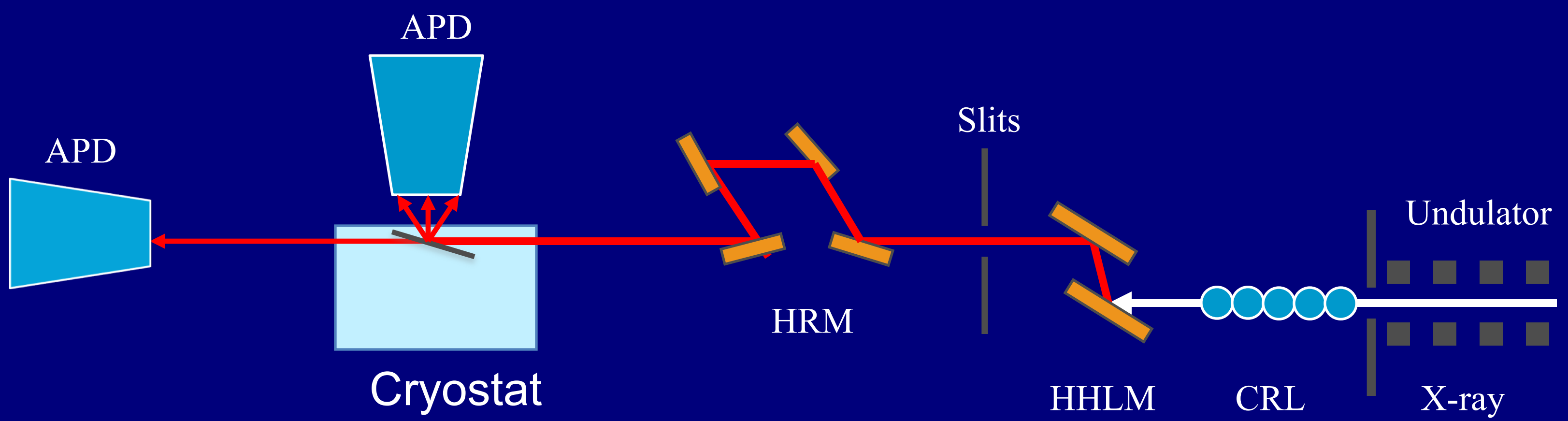
Sector 3-ID offline high pressure instruments

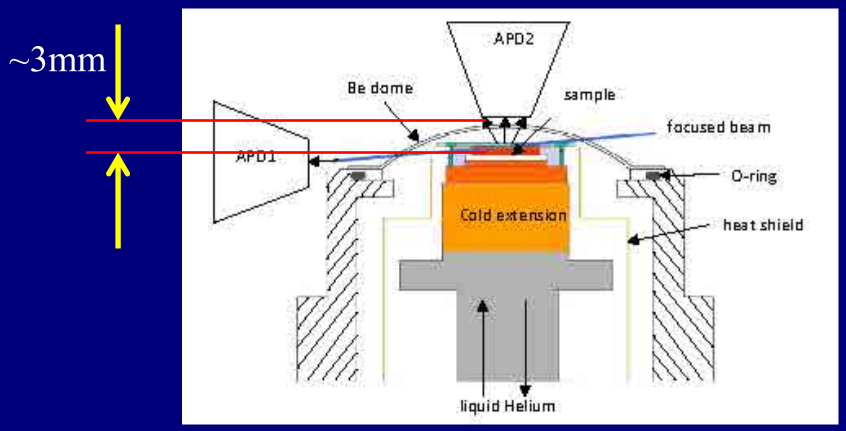
- Started the HP experiment at Sector 3 in 2000. Developed many on-line and off-line capabilities of HP at HT/LT/HF and etc.
- ~**50%** beamtime allocated for high pressure experiments,
- **20** independent user groups in the past year,
- **37** publications in the past 5 years.
- Currently there are
  - DACs:
    - panoramic DACs of various designs
    - symmetric DACs
    - nonmagnetic mini-DACs
    - gas loading gearboxes/adapters for special DACs
  - EDM for non-Be gasket drilling
  - microscopes
  - Ruby/Raman system
  - glovebox with built-in microscope for high pressure sample loading
  - Mössbauer lab capable of taking high pressure data in DAC

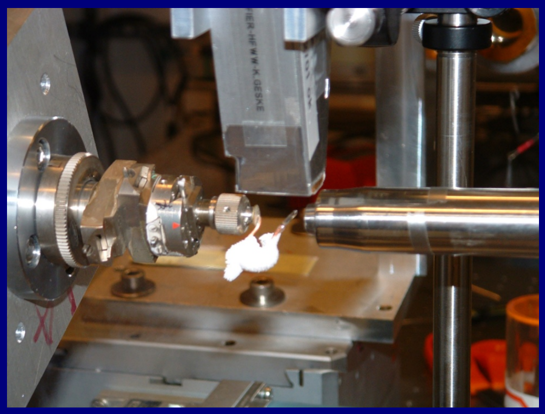




Experimental Setup for Nuclear Resonant Inelastic X-ray Scattering under low temperature

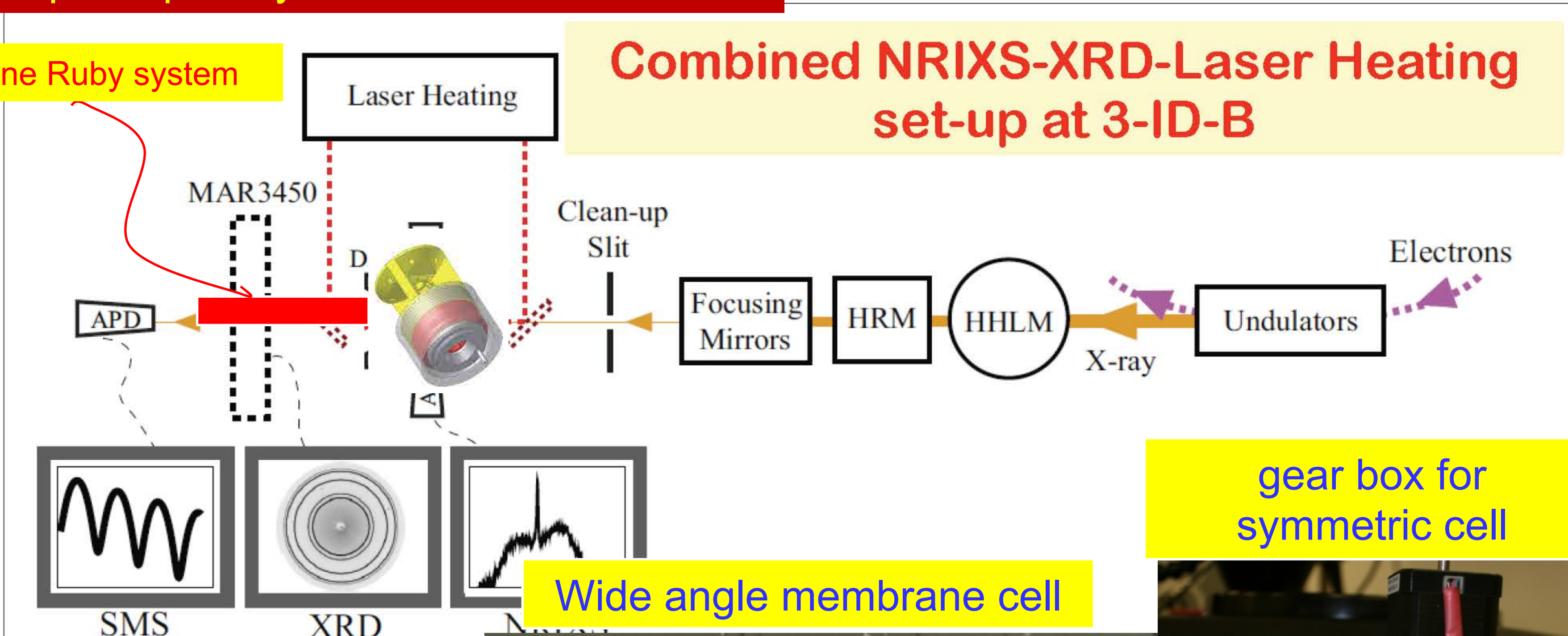






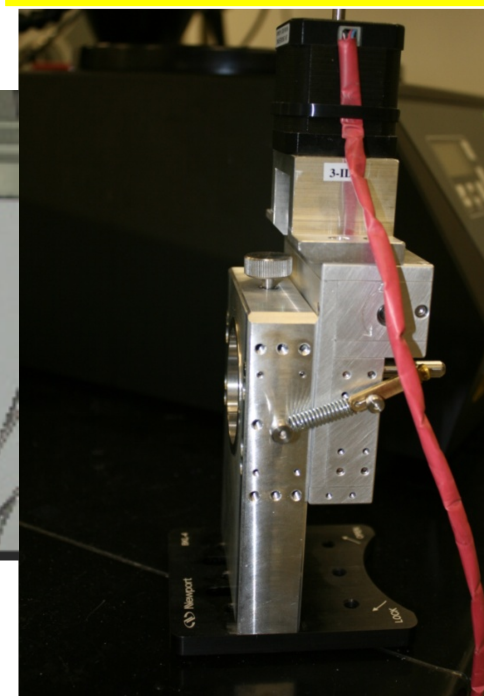
Unique capability at 3ID: HP/HT for NRS

On-line Ruby system



gear box for symmetric cell

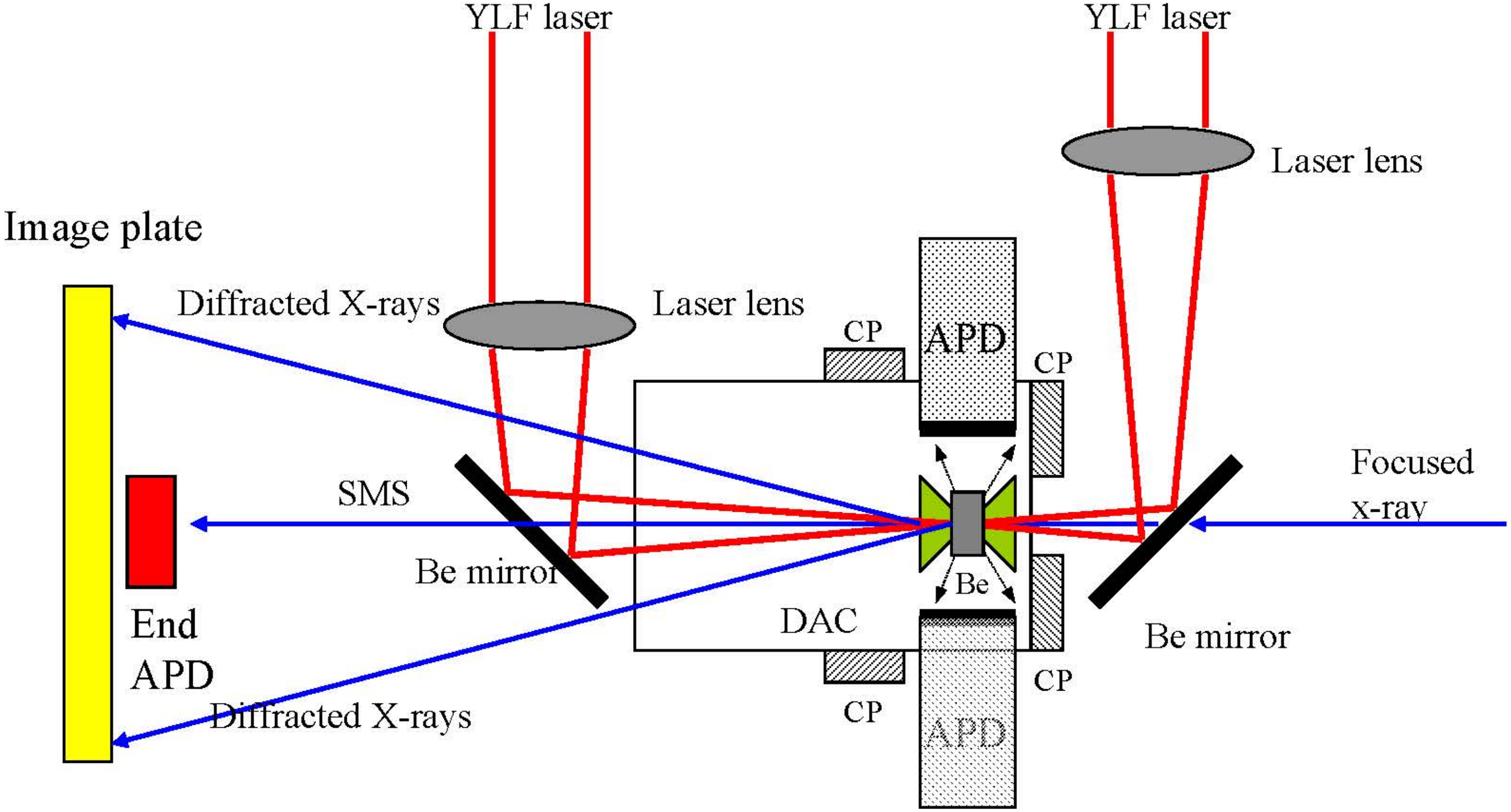
Wide angle membrane cell

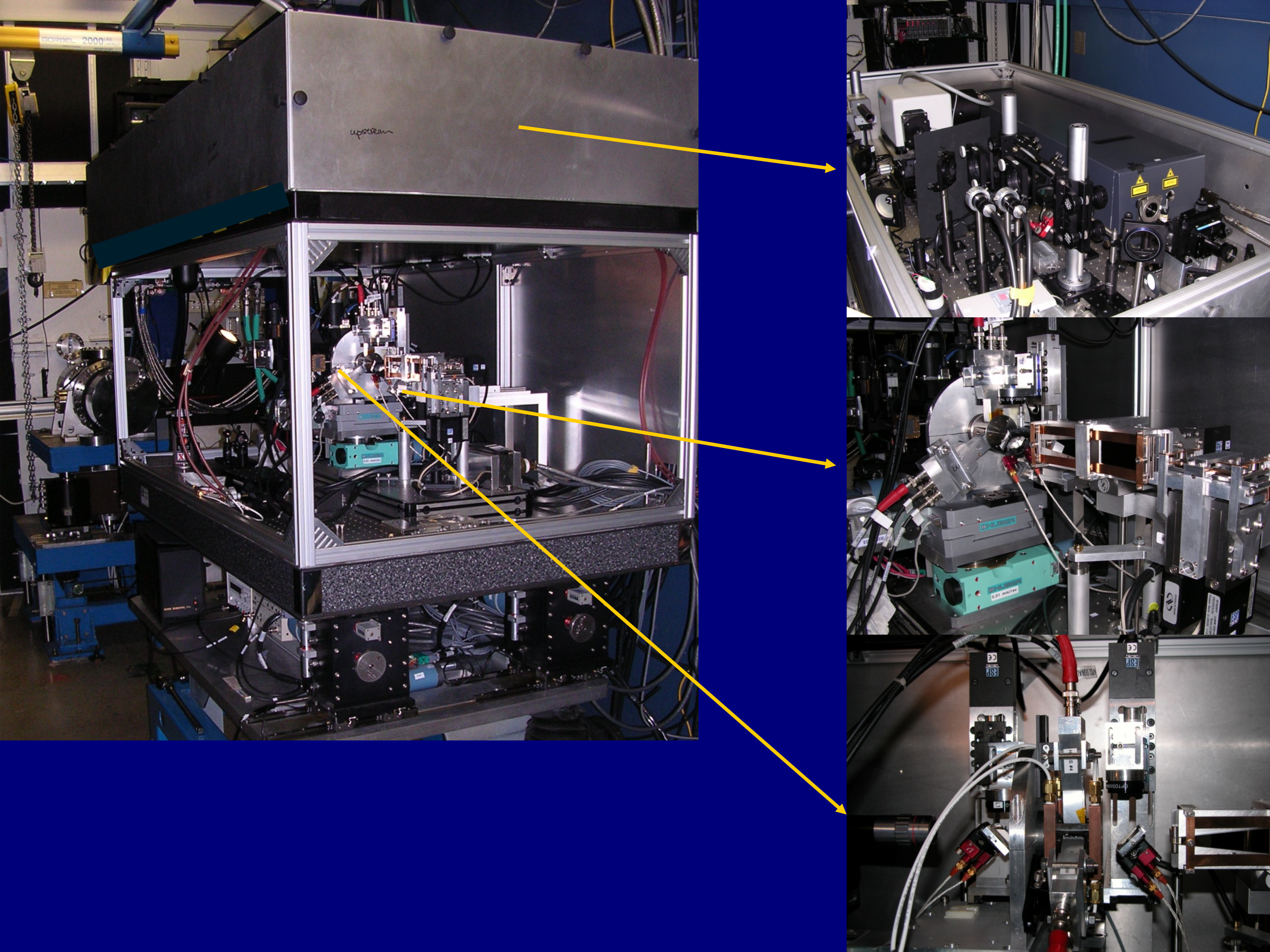


Glove box for DAC loading,
H_2O: 1 ppm, O_2: 20 ppm

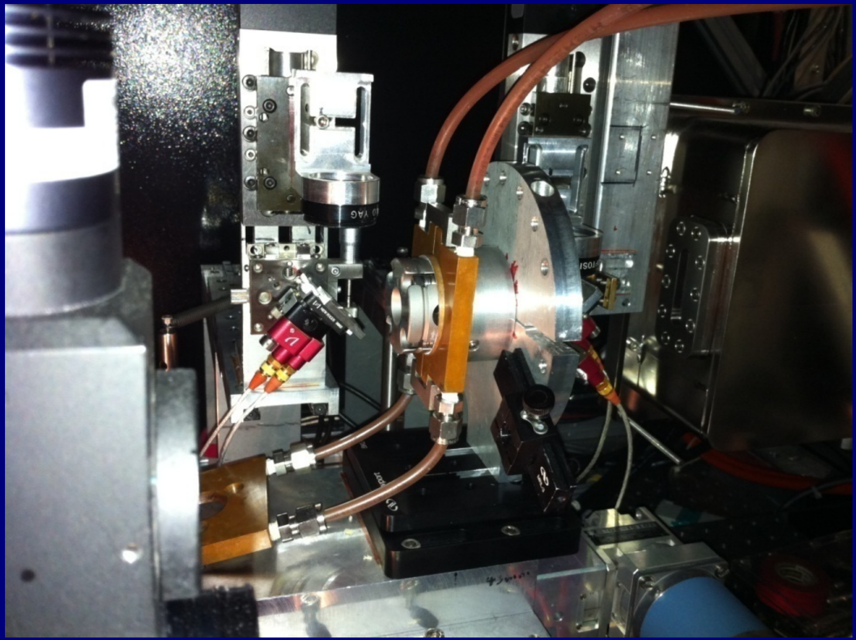
NRIXS-SMS and diffraction

In situ **X-ray diffraction, NRIXS, and SMS studies in a LHDAC provide structural (density), magnetic, elastic, vibrational, and thermodynamic information of the sample. This is also a powerful tool to detect melting.**



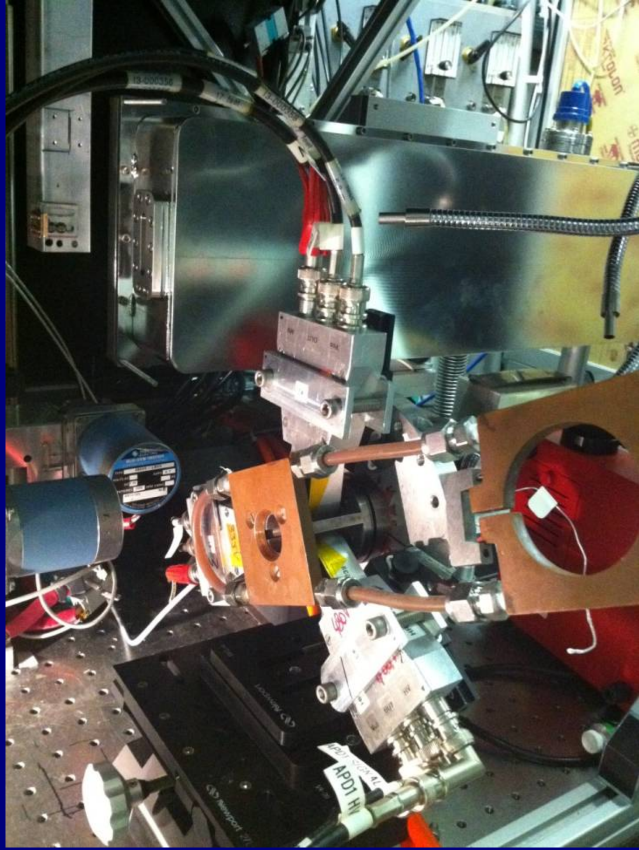

GORBEL 2000
upstream
0.01 mm/rev

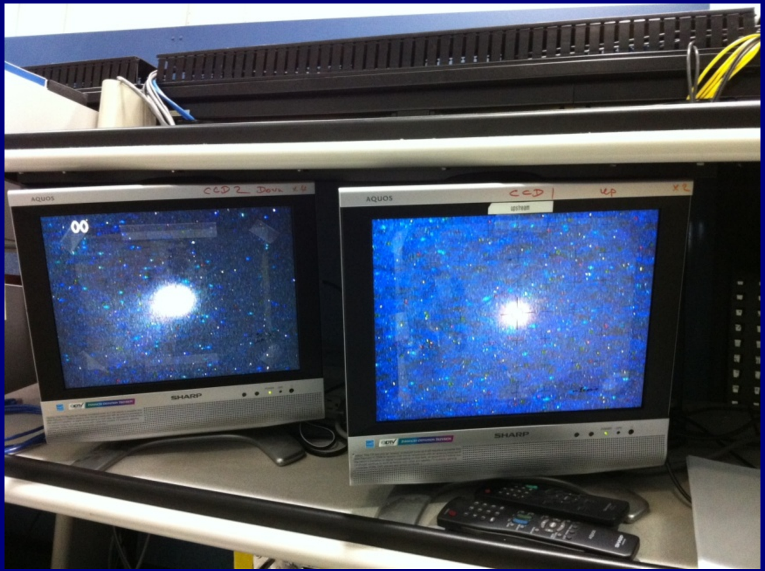
NRS at HPHT setup



NRIXS ->

<- SMS



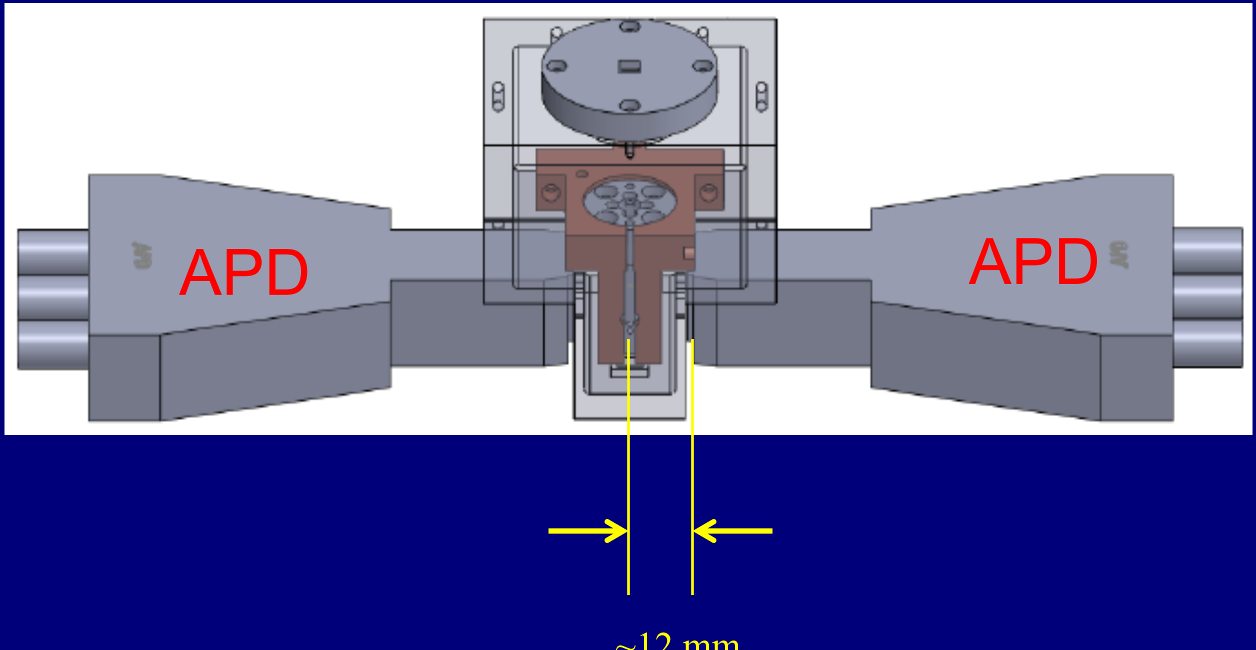


<- Hotspot

Example sample loading->

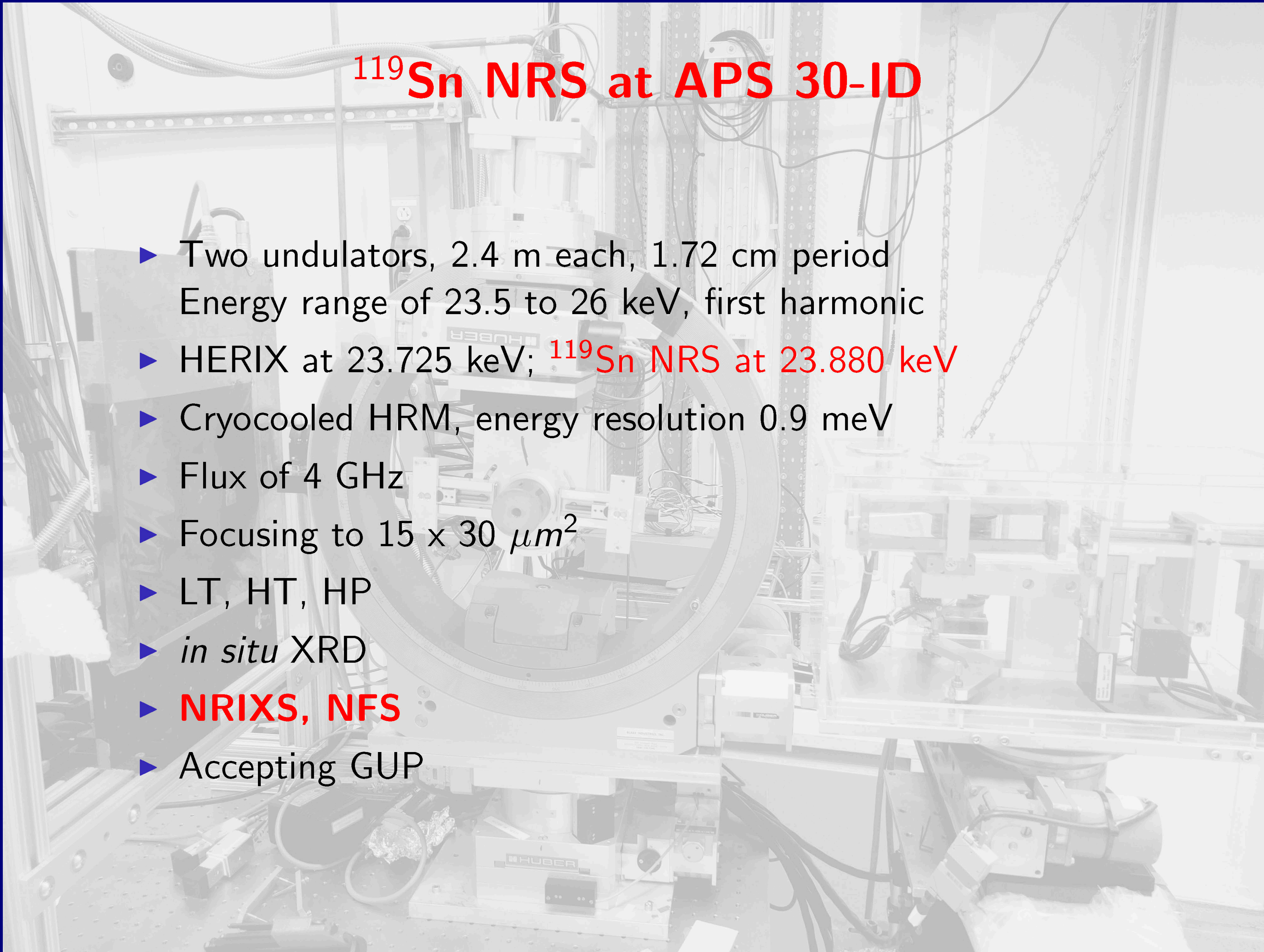
NRIXS at High-P Low-T

Design of a miniature panoramic diamond anvil cell (DAC) .



Active user programs at 3ID, APS with the following unique capabilities

1. A low temperature (4K) and high magnetic field (9T) and high pressure system for NFS. (since 2007)
2. A laser heated diamond anvil cell system (since 2002)
3. An In-situ diffraction system (since 2008)
4. An on-line Ruby system (since 2011)
5. Dynamic pressure adjusting system (gear box and gas-driven membrane cell). (since 2011)
6. Low temperature (9K) and high pressure (Mbar) system for NRIXS.

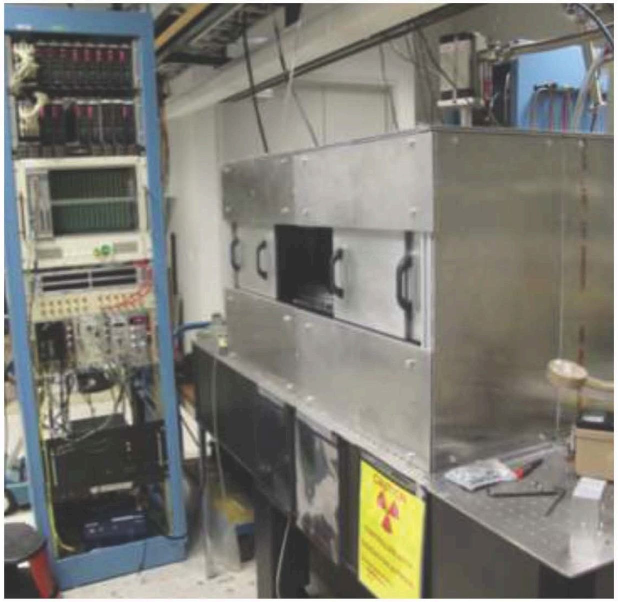


^{119}Sn NRS at APS 30-ID

- Two undulators, 2.4 m each, 1.72 cm period
  Energy range of 23.5 to 26 keV, first harmonic
- HERIX at 23.725 keV; ^{119}Sn NRS at 23.880 keV
- Cryocooled HRM, energy resolution 0.9 meV
- Flux of 4 GHz
- Focusing to 15 x 30 μm^2
- LT, HT, HP
- *in situ* XRD
- **NRIXS, NFS**
- Accepting GUP

Mössbauer Spectroscopy Laboratory of 3-ID beamline

Room Temperature/high pressure set-up

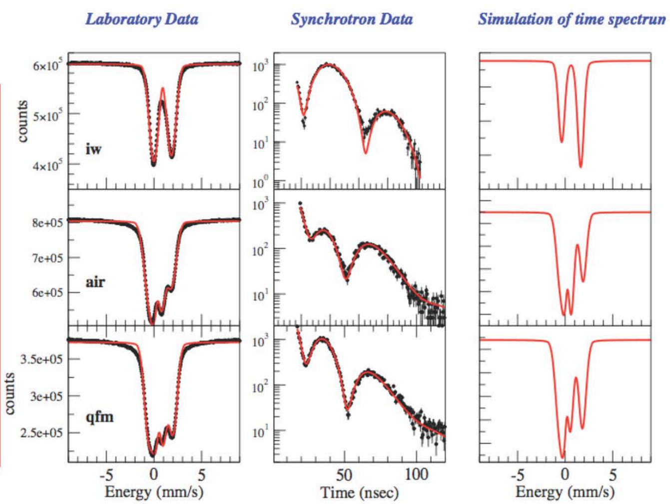


Low temperature (4.2 K) set-up

Current users:

Arizona State U.
Argonne Chemical Sciences
Univ. of Chicago
University of Illinois, Urbana
Yale University
Michigan State University
University of Wisconsin
University of Connecticut
Carnegie Institute
University of Lyon
Caltech
Princeton U.
MIT
Carnegie Mellon University
Yale U.
Michigan State U.
Northwestern U.

Basalt glass samples

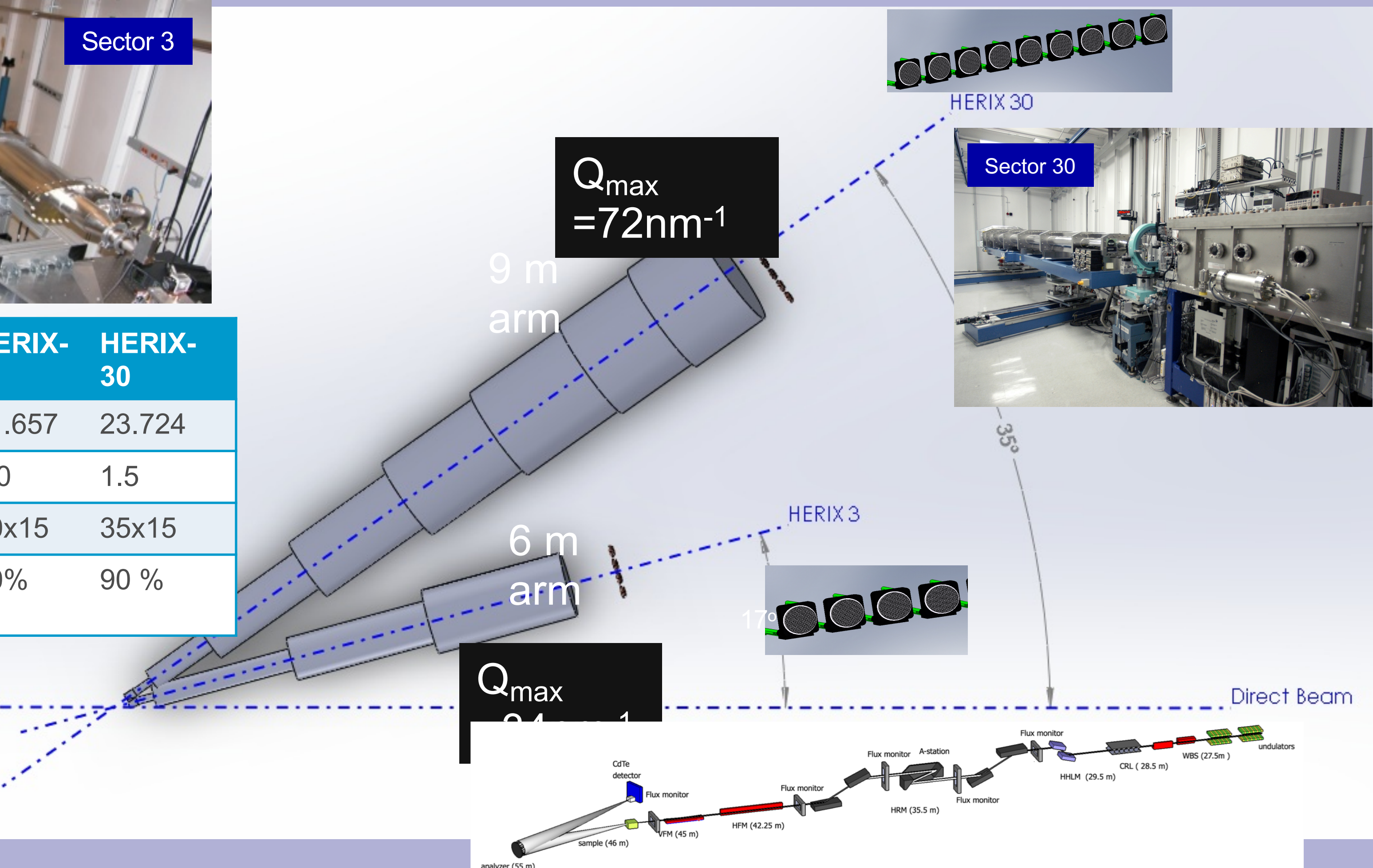


Available radioactive sources:

^{57}Co for iron,
^{119m}Sn for tin,
^{151}SmO2 for europium, and
^{121m}Sn for antimony

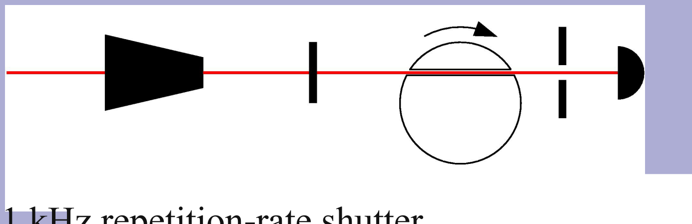
The HERIX spectrometers @ the APS

	HERIX-3	HERIX-30
Energy (keV)	21.657	23.724
ΔE (meV)	2.0	1.5
Beam size (μm^2)	20x15	35x15
Beamtime available	20%	90 %



Synchrotron Mössbauer Spectroscopy with a high-speed shutter

- Demonstration setup

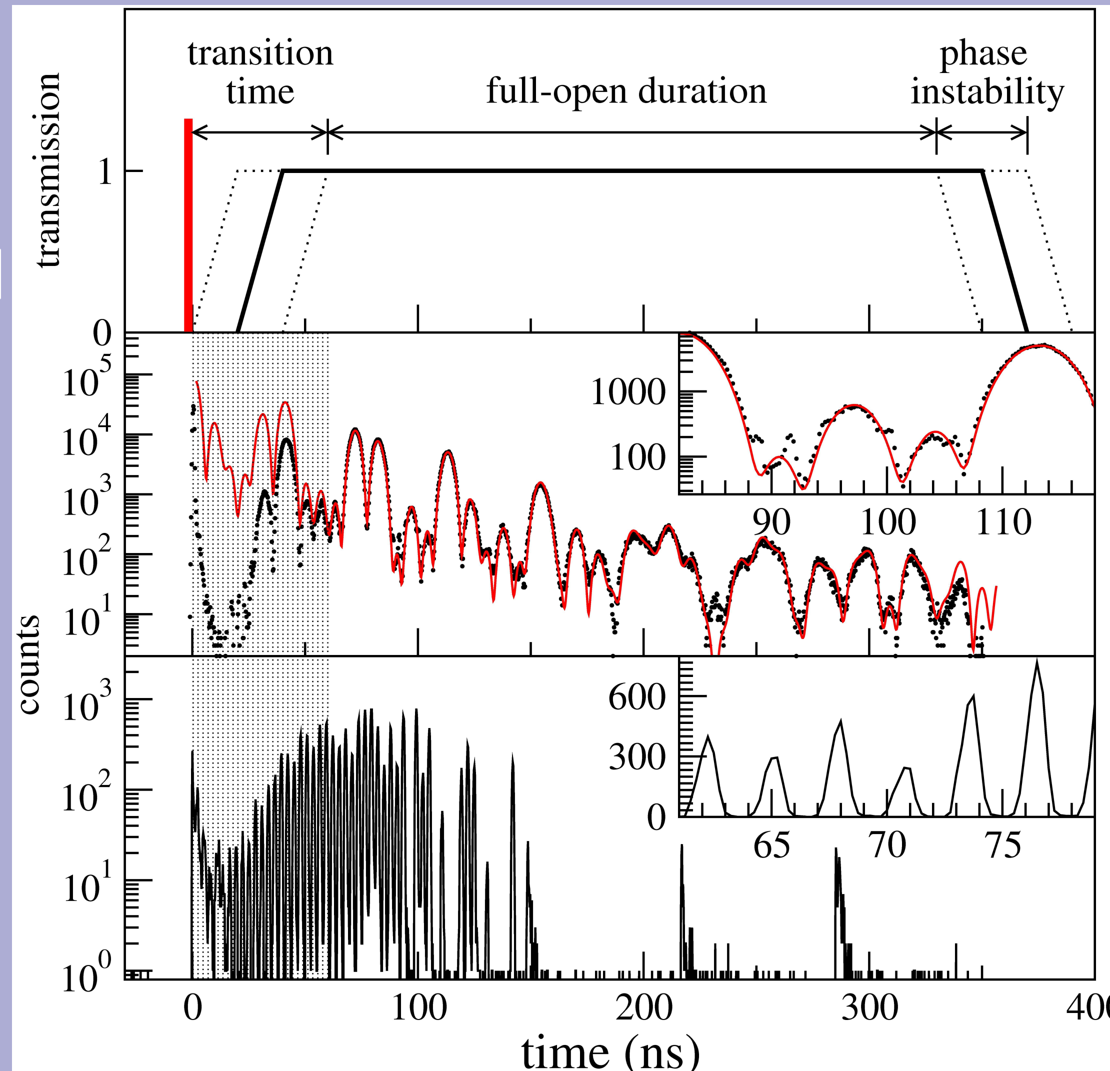


- 1 kHz repetition-rate shutter

- Closed shutter – detector shielded from enormous electronic charge scattering (10^{13-14} ph/s)

- Opens quickly (10^{-8} s) to allow detection of nuclear resonant scattering (10^2 ph/s demonstrated, but improved shutter with higher rep. rate will allow 10^5 ph/s)

- Open shutter – allows detection of nuclear resonant scattering with 100% transmission, but also opens the door for unwanted spurious bunches emanating from the storage ring (10^{0-2} ph/s)



Toellner, et al., JSR (2011) **18**, 183-188.

© Data taken at 14-ID of APS (BioCARS)

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APS-U by the Numbers

	APS-U Timing Mode	APS-U Brightness Mode	APS Now	Units
Beam Energy	6	6	7	GeV
Beam Current	200	200	100	mA
Number of Bunches	48	324	24	
Emittance	32	42	3100	pm-rad
Emittance Ratio	1.0	0.1	0.013	
Horizontal Beam Size (rms)	12.6	14.5	274	µm
Horizontal Divergence (rms)	2.5	2.9	11.3	µrad
Vertical Beam Size (rms)	7.7	2.8	10.8	µm
Vertical Divergence (rms)	4.1	1.5	3.7	µrad
Brightness - 20 keV	154	325	0.6	10^{20} ph/sec/0.1%BW/mm^2/mrad^2
Pinhole Flux - 20 keV	186	217	20.1	10^{13} ph/sec/0.1%BW/in 0.5x0.5 mm^2
Coherent Flux - 20 keV	148	312	0.6	10^{11} ph/sec/0.1%BW
Single-Bunch Brightness - 20 keV	321	100	2.6	10^{18} ph/sec/0.1%BW/mm^2/mrad^2

3ID @ APS-U

- Opportunities:
  - smaller focused beam size
  - 2 x beam current
  - More stable and better resolution HRM
  - Reconfigure C and D station
- Challenges:
  - Time window is smaller, from 154 ns to 77 ns

To use the facility at 3ID, APS

- Nine months of running, in three periods
  - T1-period, Feb~Apr;
  - T2-period, Jun~Aug;
  - T3-period, Oct-Dec.

- Two type of proposals
  - GUP (General User Proposal)
    - effective for two years
  - PUP (Partner User Proposal):
    - Jointly developing new capability for the beamline, with guaranteed beam time each run

To become a user at 3ID

- Plan ahead
- Talk to the beamline scientists
  - (Sample preparation, expectation, instruments …)
- Apply through either
  - GUP (General User Proposal) or
  - PUP (Partner User Proposal)

Deadline: 2019-1, Oct-26-2018

2019-2, Mar-1-2019

2019-3, Jul-5-2019

Thank you for your attention

and

See you at the beamline!