Crystallography and Data Management at ChemMatCARS

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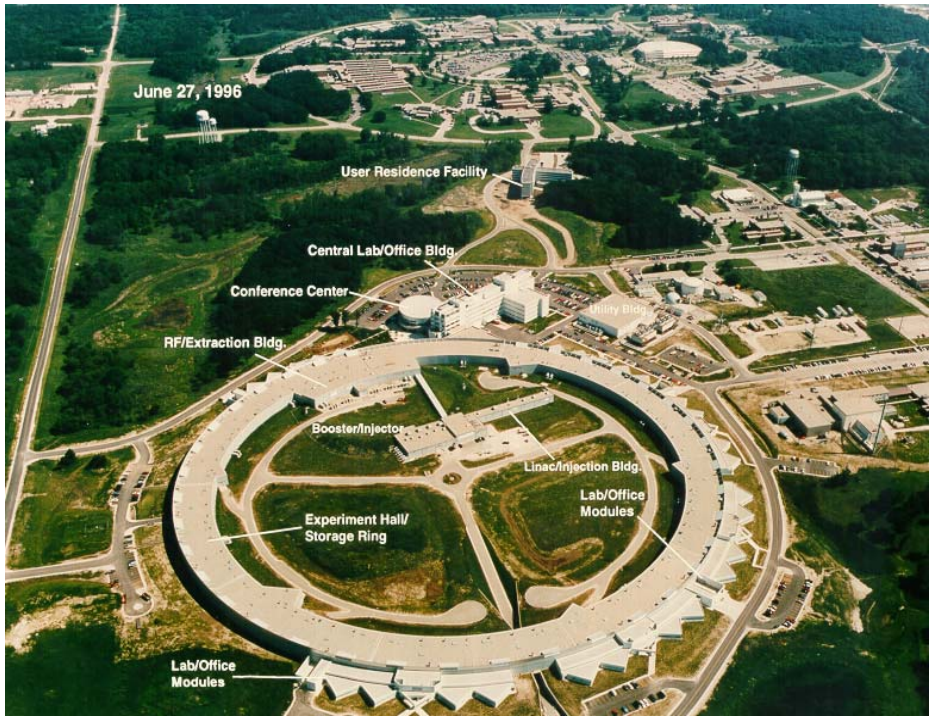
Outline

- Introduction to the APS
- The ChemMatCARS sector
- Crystallography
  - SCrAPS
    - RecipocalNet
    - CIMA and remote presence
  - Micro Crystals
  - Charge Density
  - High pressure
- Data Management

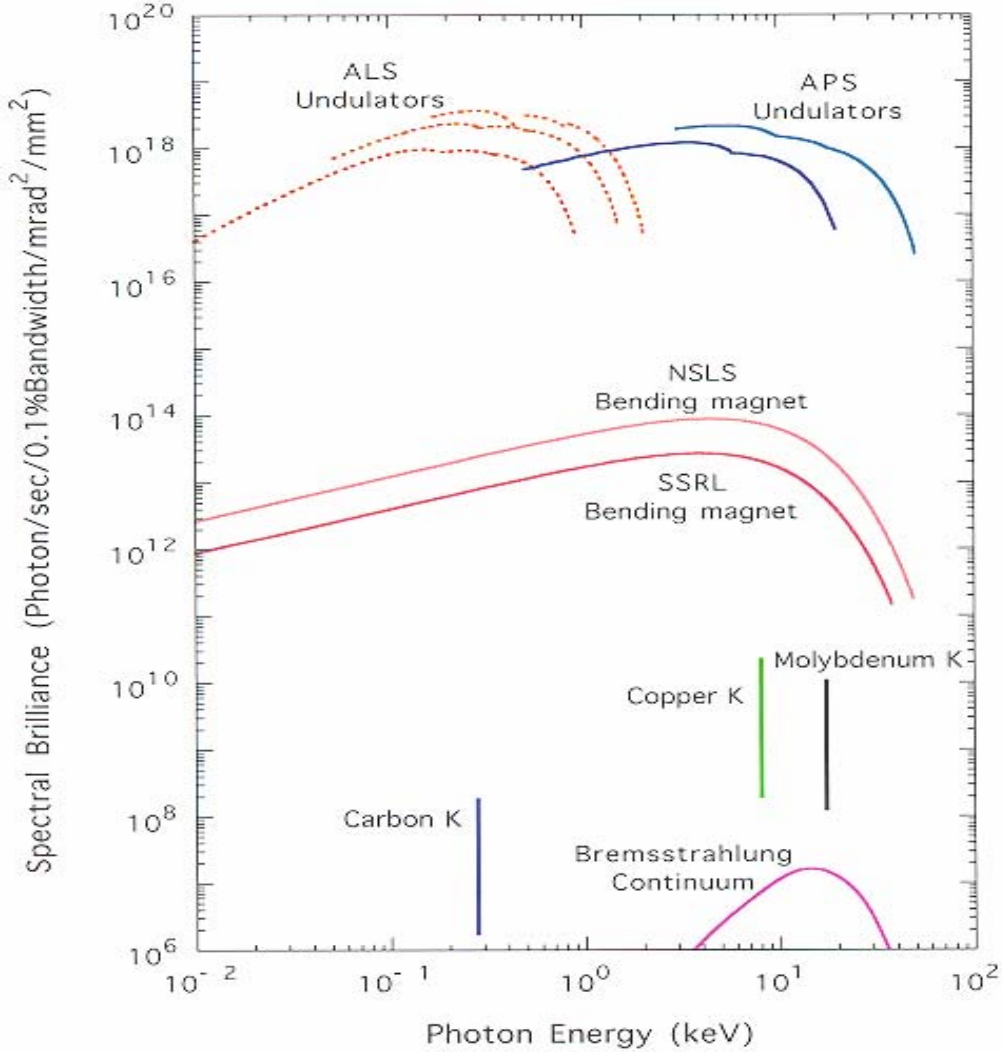
The Advanced Photon Source

The APS is a third-generation synchrotron light source located at Argonne National Laboratory about 40 minutes from downtown Chicago.



Energy: 7GeV
Current: 100 mA
Single bunch current: 5 mA
Circumference: 1104 m
Bunch length: 73 ps
Number of bending magnets: 80
Bend Radius: 39 m
RF: 351.93 MHz
Revolution time: 3.68 msec

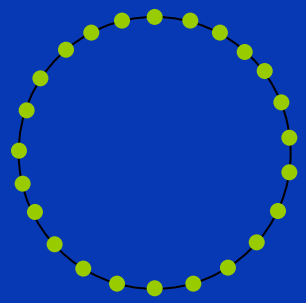
Spectral Brilliance



Fill Pattern

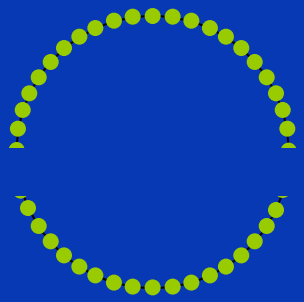
Standard Operation Mode, Top-up User

24 singlets (single bunch) with a maximum current of ~4.25 mA and a spacing of 153 *nanoseconds* between singlets.



Special Operation Mode, non-Top-up User

324 uniformly spaced singlets with a nominal current of 0.31mA, and a spacing of 11.37 *nanoseconds* between singlets.



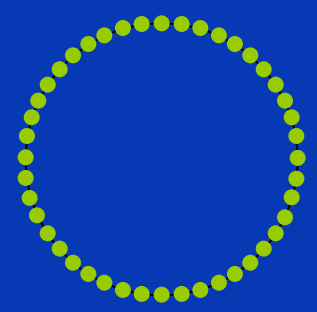
Fill Pattern

Special Operating Mode 1 (SOM1) - Hybrid fill (singlet)

A single bunch containing a maximum of 8 mA isolated from the remaining bunches by symmetrical 1.59 *microseconds* gaps. The remaining current is distributed in 8 groups of 7 consecutive bunches with a maximum current of 12 mA per group and a spacing of 48 *nanoseconds* between groups.

Special Operating Mode 5 (SOM5) - Low emittance fill

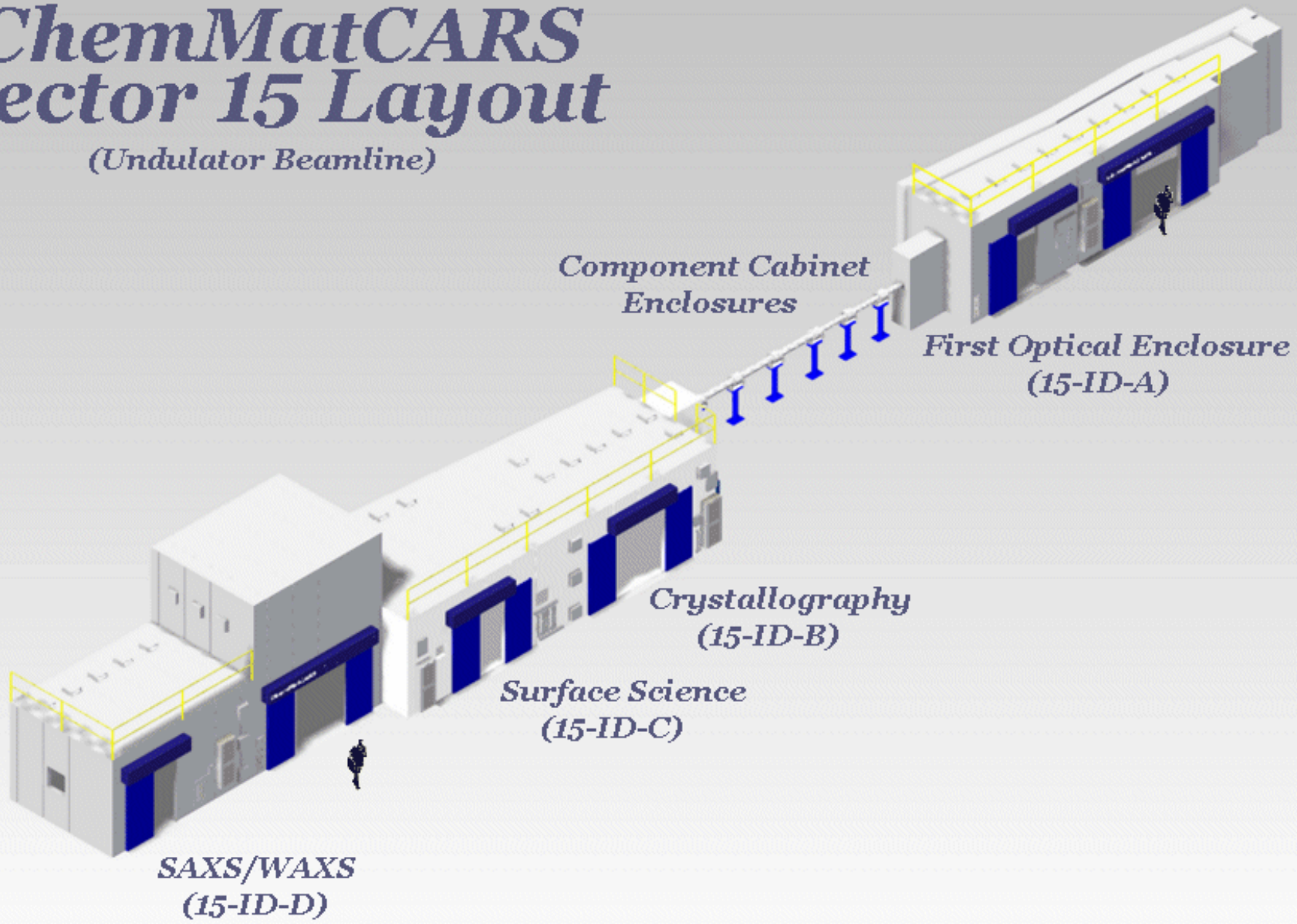
1296 uniformly spaced singlets with a nominal current of 0.08mA, and a spacing of 2.86 *nanoseconds* between singlets.



http://www.aps.anl.gov/aod/userops/Fill_Pattern.html

ChemMatCARS Sector 15 Layout

(Undulator Beamline)



Crystallography- Instrumental Specifications

Diffractometer Specifications

- **Energy range:** 6 – 32keV (2.0 – 0.38 Å)
- **Maximum beam size:** 500x500µm
- **Minimum beam size:** 100x100µm($3x10^{12}$ ph/s/0.1% bandwidth)
- **Diffractometer Type:** Bruker fixes kappa axis with 2th rotation arm
- **Sphere of confusion:** Currently ~ 20µm radius
- **Software:** Smart (data collection), Saint (data processing)
- **Detector:** Bruker 6000
- **Low Temperature Devices** open flows liquid He and N2

Crystal sample sizes

- Smallest usable – So far - 7 x 7 x 5 µm
- Largest usable – 100 x 100 x 100µm (with heavy beam attenuation!)

Typical collection time

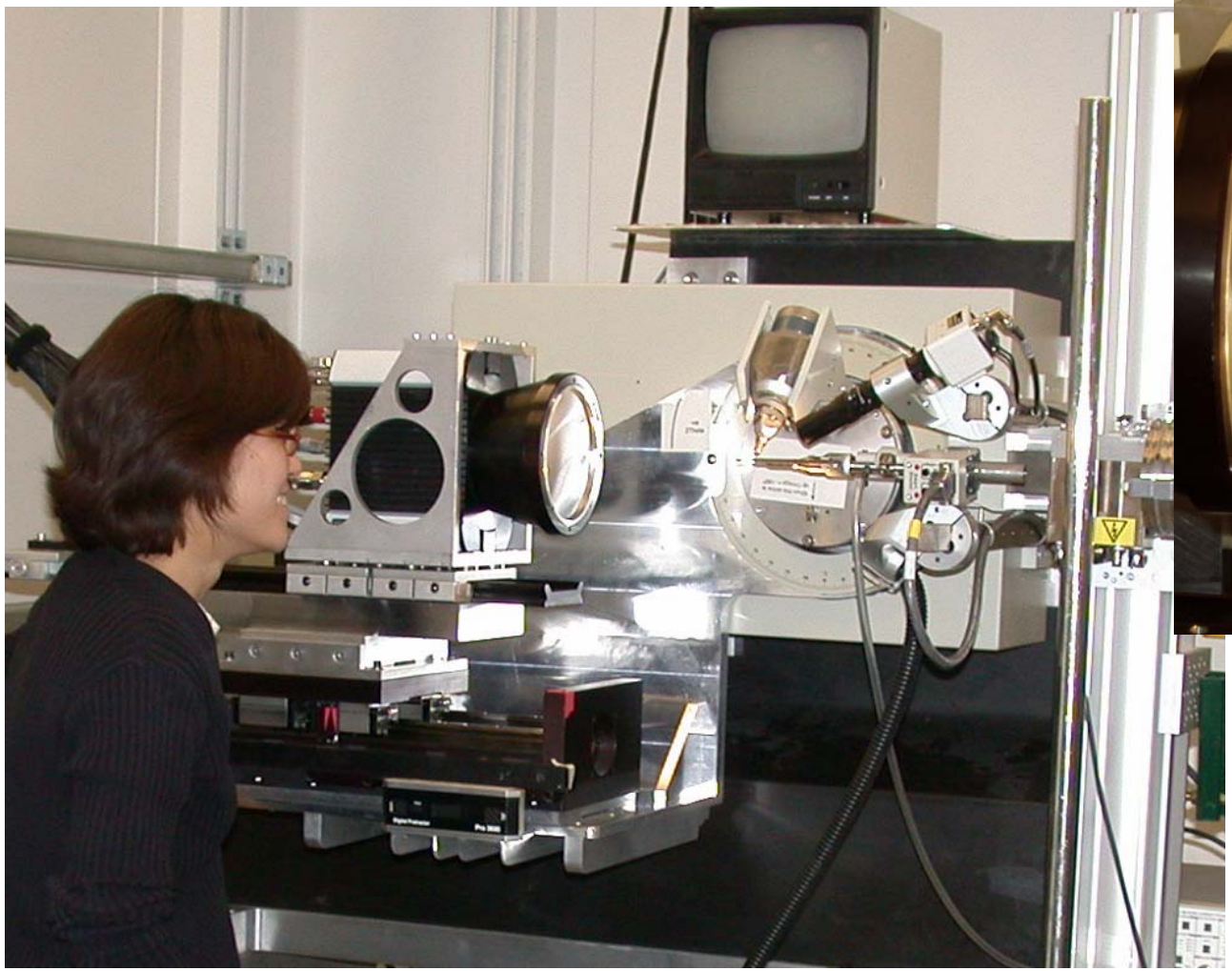
- Two to three hours for complete hemisphere (SCrAPS)

SCrAPS - Participating Crystallographers

John Bollinger	formerly Indiana University
Christopher L. Cahill	George Washington University, Washington D.C.
Michael Carducci	formerly University of Arizona
Graciela Diaz De Delgado	Università de Los Andes, Merida, Venezuela
Phil Fanwick	Purdue University
James C. Fettinger	University of California, Davis
Stephen Geib	University of Pittsburgh
Urs Geiser	ANL, Chemistry
Judith Gallucci	Ohio State University
Ilia Guzei	University of Wisconsin
John C. Huffman	Indiana University
Kianosh Huffman	Indiana University
Jeanette Krause-Bauer	University of Cincinnati
Xaing Ouyang	Texas A&M University
Maren Pink	Indiana University
Nigam Rath	University of Missouri
Charlotte Stern	Northwestern University
Dale Swenson	University of Iowa
Fook Tham	University of California, Riverside
Don Ward	formerly Michigan State University
Victor G. Young Jr.	University of Minnesota

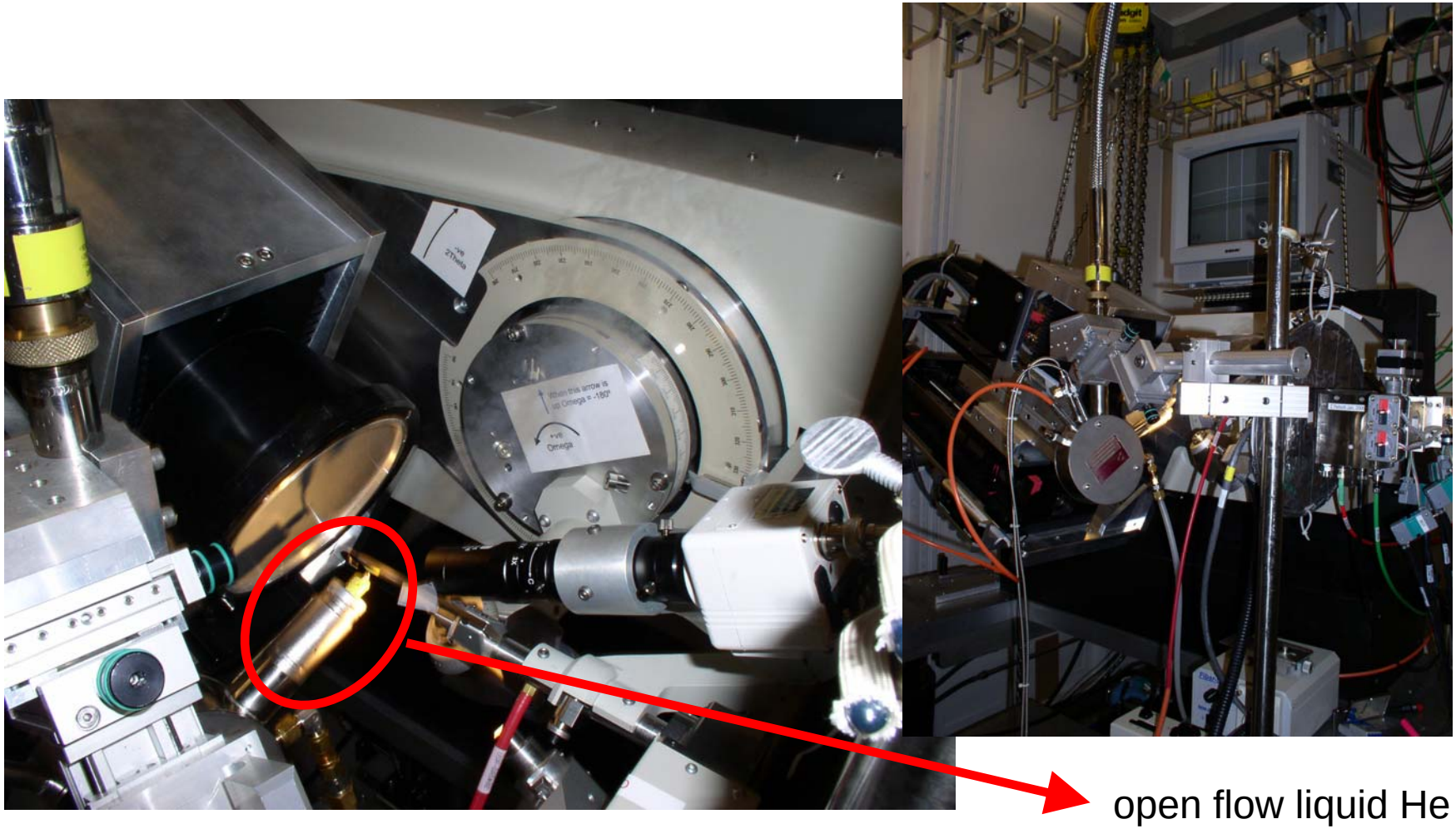
SCrAPS

User/Sample Coordination : Yu-Sheng Chen (CARS)
and Maren Pink (IU)



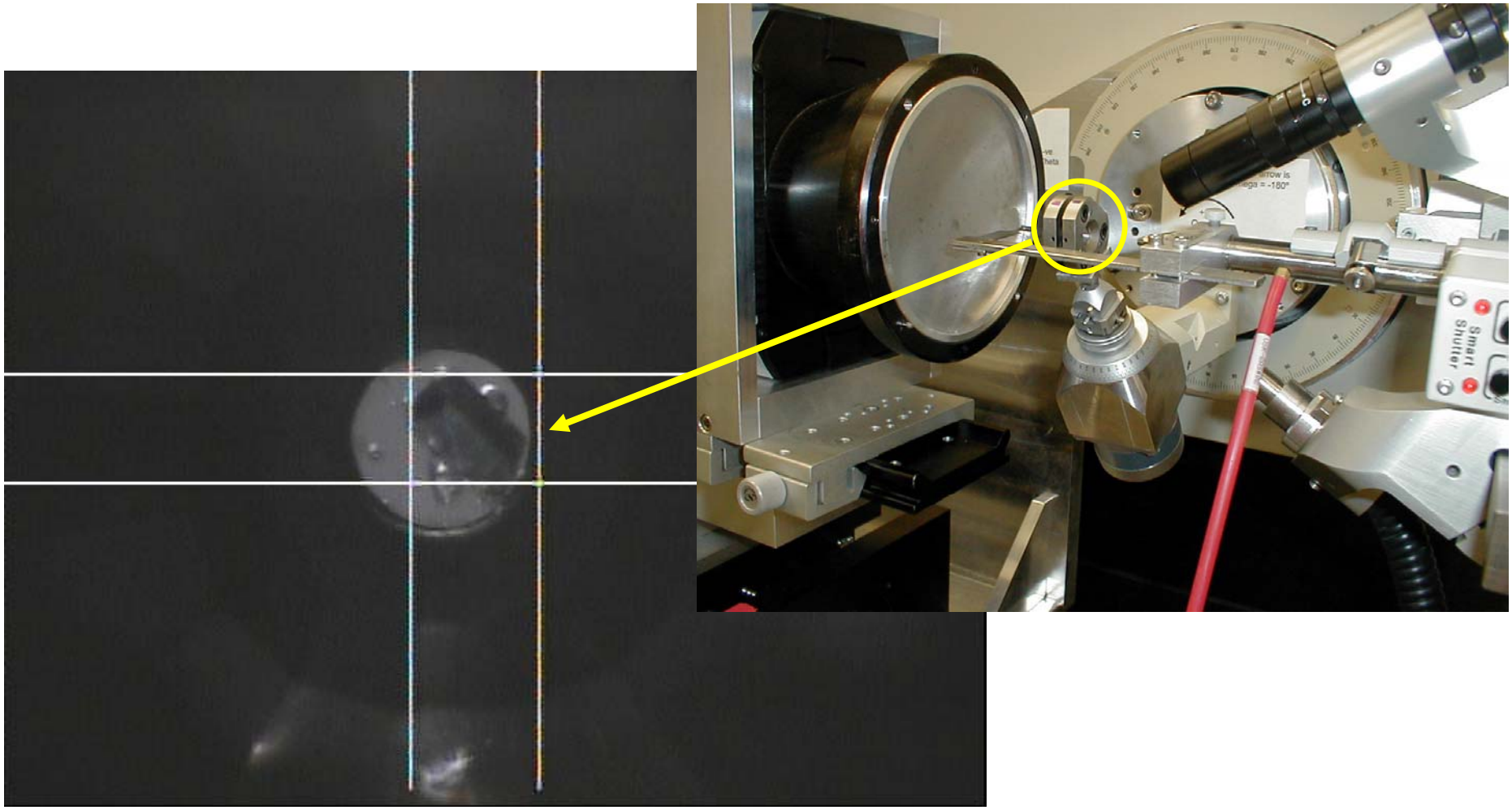
High Resolution Charge Density

Collaborator: Bo B. Iversen, University of Aarhus, Denmark.



High Pressure (ongoing)

- Collaborator: Simon Parsons, University of Edinburgh, Great Britain



Data Management

- **SCrAPS / Micro-crystallography**
  - Raw data are managed by CIMA in collaboration with Indiana University and remain on CARS servers for up to 6 months
  - Derived data are stored using RecipnetNet

- **Charge Density / High Pressure and others**
  - Raw and derived data are managed by the user
  - ChemMatCARS stores the data for up to 6 months

Crystallography at ChemMatCARS
Future Directions

- **New Faster Readout CCD Detector**

- **Remote crystallography**
  - CIMA and web-based protocols developed jointly between IUMSC and ChemMatCARS. This will allow crystallographers at remote locations to participate in the experiment**.**

- **ReciprocalNet at ChemMatCARS**
  - ChemMatCARS is a ReciprocalNet site, all users are encouraged to document and track the experiment and post results after the experiment is completed.