Crystallography and Data Management at ChemMatCARS

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Outline

- Introduction to the APS
- The ChemMatCARS sector
- Crystallography
  - SCrAPS
    - ReciprocalNet
    - 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

![Graph showing spectral brilliance for different sources and photon energies.](Image)
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 0.31 mA, and a spacing of 11.37 nanoseconds between singlets.
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 0.08 mA, and a spacing of 2.86 nanoseconds between singlets.

ChemMatCARS Sector 15 Layout
(Undulator Beamline)

- Component Cabinet Enclosures
- First Optical Enclosure (15-ID-A)
- Crystallography (15-ID-B)
- Surface Science (15-ID-C)
- SAXS/WAXS (15-ID-D)
# Crystallography- Instrumental Specifications

## Diffractometer Specifications

- **Energy range:** 6 – 32keV (2.0 – 0.38 Å)
- **Maximum beam size:** 500x500µm
- **Minimum beam size:** 100x100µm (3x10¹² 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  
[John Bollinger's affiliation is 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.

open flow liquid He
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.