Synchrotron-based Crystallography in 2019

What are the instruments and projects that we want to start in 2012 to do the science of the next decade?

Argonne NATIONAL LABORATORY

... for a brighter future

U.S. Department of Energy

THE UNIVERSITY OF CHICAGO

Office of Science
U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory managed by The University of Chicago

Crystallography is the gold standard in physical characterization

- No other scientific technique provides such detailed information about the composition of matter and the interactions between atoms
- Cornerstone of physical and biological sciences (pivotal for catalysis, condensed matter physics, genomics, inorganic chemistry, mineralogy, materials science, molecular biology…)

- Synchrotrons matter to crystallography & vice-versa
- Majority of state-of-the art problems require synchrotron light
- More than half of synchrotron users/science is associated with crystallographic analysis

The crystallography shopping cart

- Best-in-2019-world instrumental capabilities
  - Macromolecular single crystal diffraction
  - Generalized single-crystal diffraction
  - Powder diffraction crystallography

- Highly engineered beamline optics for ease of use, rapid equilibration and very high stability
  - Routine microfocusing

- Software to allow non-specialists to run beamlines and analyze data

Macromolecular single crystal diffraction

Key growth directions:

- Very large, high performance detectors
  - Large pixel array detection for monochromatic measurements
  - Fast, energy dispersive, PAD for time-resolved Laue measurements

- Beamlines optimized for very small crystals/diffracting domains:
  - Microfocused optics
  - Optics/Source active positioning feedback control systems
  - Improved sample mounting/screening automation

- Making maximal use of “beam ports”
  - As the APS fills all straight sections, multiplexing will be the rule

Generalized single-crystal diffraction

- Beamline optimized for very small crystals/diffracting domains:
  - Microfocused optics
  - Optics/Source active positioning feedback control systems
  - Improved sample mounting/screening automation

- Measurements of crystalline ensembles
  - Microbeam instruments
  - Algorithms for aperture scanning & treating overlapped reflections

- High-energy (40-100 KeV) beamline for extreme environments, resonant scattering and diffuse scattering
  - Highly penetrating
  - High Q (>25$Å^{-1}$) for 3-D PDF studies
  - Resonant scattering for highly absorbing materials

Powder diffraction crystallography

- Single-shot or rapid scan area detection -- Optimized for resolution
  - Beam-sensitive materials
  - Large detector, pixel size to match focusing

- Single-shot medium-resolution detection for *in situ* measurements
  - To be deployed at beamlines specialized for experimental conditions: catalysis, extreme conditions,…
  - Preferred detector technology (strip vs. area) is unclear

- Very high resolution (analyzer-based) -- “super 11-BM”
  - Increase analyzer density to match other facilities throughput

- Ultimate resolution (analyzer-based, ID source) beamline (5-ID-B with 11 -BM detection)
  - BM cannot match ID capabilities
  - Non-focusing
  - For problems where resolution (& flux?) of 11-BM is inadequate

Other needs

- The growth of highly specialized dedicated instruments comes with a loss of general purpose scattering stations
  - Need to keep a small number of reconfigurable, non-dedicated beamlines for trying novel ideas

Software

- Beamline automation and user controls

- Data analysis software
  - Small-Molecule single crystal: needs met by commercial market
  - MX single crystal: considerable development efforts in public sector
  - Crystallite ensemble indexing: in infancy, software is rudimentary
  - Powder diffraction: Software provided by user facilities
    - *Software is aging; learning & use are major bottlenecks*
    - *Efforts for a new generation of software planned via ASISI*