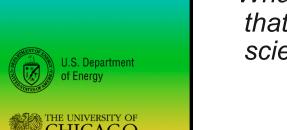


Synchrotron-based Crystallography in 2019



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

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 (>25Å⁻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

