EWALD – Enhanced Wide Angle Laue Diffractometer

EWALD is a single crystal diffractometer optimized for the study of macromolecular single crystal samples typically 0.001 mm^3 in volume with unit cells greater than 100 Å on edge. EWALD will open new frontiers in neutron structural biology by enabling x-ray sized crystals to be used for neutron experiments. EWALD will have a performance gain factor of ~75× compared to MaNDi at the SNS first target station. Manipulation of the nuclear spin of H atoms using dynamic nuclear polarization (DNP) holds the promise of an additional gain in signal to noise greater than 100 for hydrogenous samples.

Science Drivers

Visualizing H atoms in biological materials is one of the biggest remaining challenges in biophysical analysis. While x-ray techniques have unrivaled capacity for high-throughput structure determination, neutron diffraction is uniquely sensitive to H atom positions in crystals of biological materials and can provide a more complete picture of the atomic and electronic structures of bio-macromolecules. This information can be essential in providing predictive understanding and engineering control of key biological processes—for example, in catalysis, ligand binding, and light harvesting—and to guide bioengineering of enzymes and drug design. By significantly reducing required sample sizes, EWALD (especially when coupled with dynamic nuclear polarization (DNP) of hydrogen nuclei) will break through a critical threshold in application of neutrons in biology, opening the door to fundamentally new science:

- Analysis of novel macromolecular structures and rapid structure-activity analysis for the development of inhibitors to human disease targets, engineering enzyme active sites for novel chemistry, and re-engineering enzymes for design properties such as thermal and acid stability for industrial uses.
- Analysis of photochemistry in biology: understanding how hydrogen atoms modulate the site energies and spectral properties of pigment-protein complexes in photosynthetic complexes and the light harvesting machinery that converts light to chemical energy.
- Analysis and refinement of complex active-site electronic structures in metallo-proteins, which are found throughout biology and are used in catalysis, energy capture and conversion, transport and storage, signal-transduction, and genome replication and repair.

Science Requirements

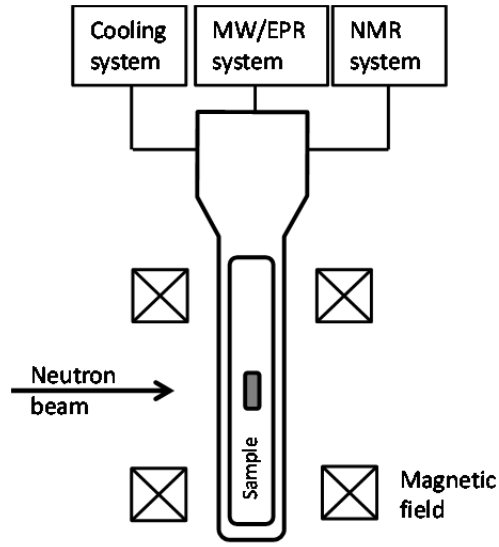
Due to the neutron flux limitations of current neutron sources, neutron macromolecular single crystal diffractometers require samples of at least 0.1 mm^3. EWALD, especially when coupled with DNP, is designed to break this paradigm by the following:

1. The high brightness of the STS coupled moderator provides 50× the neutron flux on sample of MaNDi.
2. Increasing detector coverage by ≈50% relative to MaNDi to approximately 6 steradians
3. The 10 Hz operation of STS allows use of the broader pulse widths and higher flux of a coupled moderator by lengthening the instrument to maintain wavelength resolution and still achieve the desired range in d-spacing.
4. The instrument will be designed to support DNP which will increase the coherent cross-section of hydrogen nearly an order of magnitude (at the expense of polarizing the incident neutron beam[1]) and improving the signal to noise by suppressing hydrogen incoherent scattering.

[1] Polarizing the incident neutron beam will reduce its flux by a factor of two or slightly more.

Technical Requirements

EWALD is a single-crystal diffractometer optimized for macromolecules, with the integrated capability to dynamically polarize the spins of hydrogen atoms in the sample. EWALD will view the 3×3 cm^2 face of the HPCM, face 'b'. At a 90 m moderator–sample distance, EWALD will have the same wavelength resolution as the much shorter MaNDi instrument that views a decoupled, poisoned hydrogen moderator at FTS. At the 10 Hz STS pulse rate, the bandwidth per frame, 4.4 Å, is perfectly matched to the most common MaNDi operating mode. The guide system will be curved to avoid the fast neutrons and gammas produced as the protons strike the neutron production target. At least one and possibly two bandwidth choppers will define the wavelength band incident on the sample. Anger camera neutron detectors will be used to measure the scattered neutrons.



Schematic view of the DNP apparatus and its orientation relative to a polarized neutron beam.

A sample that would currently take 10 days of neutron beamtime to collect on MaNDi could be collected in only six hours on EWALD enabling multiple data sets to be collected within a single day. Data collection on the radically reduced crystal volumes enabled by EWALD (0.001mm^3) would increase data collection times to approximately 5-6 days.

Development of DNP is ongoing at ORNL and at other locations in the world. The schematic illustrates the essential elements of a DNP apparatus that includes a low-T dilution refrigerator, a 2.5–5 T superconducting magnet, and a microwave source (2–4 mm). The requirement to support dynamic nuclear polarization imposes some requirements on instrument design:

- All ferromagnetic materials must be avoided within a radius of at least 2 m from the sample position.
- The sample area must be designed from the outset to support the DNP apparatus that requires specific utilities and room for equipment. (see schematic)
- The detectors must have minimum sensitivity to magnetic fields.

Key parameters of EWALD

Parameter	Description
Moderator	High-peak-brightness coupled moderator, side b
Sample size	1×1 mm^2
Moderator–sample distance	90 m
Sample–detector distance	0.45 m
Wavelength range	2 Å ≤ λ ≤ 8 Å
Resolution	Δd/d = 0.0015
Detector	Anger Camera with 1.2 mm spatial resolution