NeSCry – Neutron Single Crystal Diffractometer

The cold-neutron single-crystal diffractometer, NeSCry, optimized for studies of small crystal size (0.01–8 mm^3) will accommodate a diverse range of sample environments to enable ultralow temperatures with or without magnetic fields, high pressure combined with low temperature, and applied electric fields. The main distinction of NeSCry is the ability to study small single-crystals, ≥ 0.2 × 0.2 × 0.2 mm^3, with high-resolution at low-Q and superior flux. Considering the ratio in neutron flux provided by STS with respect to FTS, the optimized optical guide, and significantly improved background, the NeSCry is estimated to gain a factor of over 50 in efficiency compared with the existing single crystal instrument TOPAZ.

Science Drivers

Materials that couple spin, orbital, and lattice degrees of freedom are essential in developing many next-generation technologies. However, many synthesis methods (e.g., flux growth, solvothermal, high pressure, etc.) typically yield small crystal sizes. Neutron diffraction is still the method of choice for elucidating the microscopic magnetic structure of materials and detecting the light atoms in battery or fuel cell materials. Given the increasing complexity of materials (e.g., more elements, low dimensional structures, larger unit cell size, etc.), there is a critical need for neutron diffractometers that have sufficient signal to study much smaller crystals than presently possible. Moreover, at present in the United States, controlled environmental conditions are lacking for single crystal neutron diffraction, which is crucial to detecting emergent phenomena in many areas. In particular, in situ studies of crystal growth and ion exchange will be possible, and this will provide new opportunities to study transition and metastable states of a great variety of materials. NeSCry will address topics including:

- Exotic structure and emergent phenomena generally occur with small structural distortion, spin canting, or long period modulation of the nuclear and spin structures simultaneously due to coupling spin, orbital, electron and lattice degrees of freedom. Their study requires a high Q-resolution and a large Q-range.
- Composite materials that have small lattice misfits are industrially attractive, and in many of these cases, neighboring atoms in the periodic table are also present, necessitating high-Q resolution and neutrons (as opposed to x-rays) (e.g., the phase and microstructure determination of nickel-based superalloys, which are employed in jet engines).
- Energy conversion and storage materials. The large wavelength band provides a great opportunity to study those materials and, more importantly, multiple extreme condition environments are of great importance for in situ studies. Single-crystal diffraction can often reveal the true intrinsic physical behavior of materials, which then can be further optimized using nanostructural engineering.

Science Requirements

NeSCry will be designed to provide optimized signal background ratio versatility as a single crystal diffractometer, with or without polarization capability. The instrument requires:

1. Q range of 0.1 – 30 $Å^{-1}$; Q-resolution 0.2 to 0.4%.
2. Sample sizes as small as 0.2 x 0.2 x 0.2 mm^3, volumes ranging from 0.01 mm^3 to 8 mm^3.
3. An option to use polarized incident neutron beam.
4. Adjustable beam divergence from ± 0.5 – 2 deg.

Technical Description

NeSCry will optimally view the high brightness coupled moderator. NeSCry benefits from the 10 Hz repetition rate giving a large wavelength band per frame, allowing the instrument to be built at 30–50 m from the moderator. This long flight path allows NeSCry to use the broader time pulses of the STS coupled moderators and the significantly higher peak intensity of the neutron pulses, compared with the de-coupled, poisoned moderators typically used on diffraction instruments.

Depending on the choice of instrument length, the instrument will deliver a neutron bandwidth of 7.9–13.2 Å so that the desired Q-range can typically be accessed in a single frame. An elliptical guide system will provide sufficient flexibility to cover a wide range of incident beam divergences. The detector will have high spatial resolution (at least 1 mm x 1 mm) and be located between 0.25 m and 1 m.

Key parameters of NeSCry

Parameter	Description
Moderator	High-peak-brightness coupled moderator, side b
Sample size	as small as 0.2 x 0.2 x 0.2 mm^3
Moderator–sample distance	30–50 m
Sample–detector distance	0.25 to 1 m
λ Range	1.2 Å $\leq \lambda \leq$ 14 Å
Resolution	$\Delta Q/Q$ 0.2-0.4%
Detector	high resolution Anger camera or solid state 2D He-3 detector