HighResPD – High Resolution Powder Diffractometer

The High-Resolution Powder Diffractometer (HighResPD) is specified to complement the existing POWGEN and proposed RAPID instruments on FTS. It will provide a high resolution capability to the U.S. science community with a $\Delta d/d$ resolution of 0.035%, matching the world's highest-resolution neutron diffraction instruments at J-PARC and ISIS.

Science Drivers

Neutron powder diffraction has played a key role in the development and understanding of new, complex materials. HighResPD is optimized to provide the highest resolution of any of the neutron powder diffractometers at the ORNL neutron facilities. This diffractometer has a key role in materials discovery and design; by providing the highest precision examination of atomic-sale structure in topics such as:

- Ab-initio structure determination from powder diffraction (SDPD): With improvements in instrumentation, algorithm development and enhanced computing power, great strides have been made in ab-initio structure solution from powder diffraction data. Indexing and determination of space group is the first step in SDPD for which high resolution data is required. The sensitivity of neutrons to light elements can play a crucial role in the determination of the correct space group, and therefore, the correct interpretation of structure-property relationships.
- Addressing complexity and subtlety in functional materials such as zeolitic solids, piezoelectrics, ionic conductors and others that have very large unit cell volumes and/or subtle structural distortions. This structural complexity is often integral to the useful physical properties of these materials. High resolution data is needed both to resolve subtle splitting in peaks or reveal subtle features in diffraction line shapes and to resolve an adequate number of Bragg peaks at high Q, where overlap and loss of information are significant issues for large unit cells.
- Magnetic ordering phenomena and magnetic coupling to other physical properties. Magnetic structures can often be extremely complex, requiring high resolution data to resolve and distinguish long period modulation.[1]

Science Requirements

HighResPD is optimized to provide the highest resolution of the ORNL neutron powder diffraction suite and has the following requirements:

1. The ability to operate at frequencies as low as 5 Hz in order to provide a wavelength bandwidth greater than 6 Å in a single instrument setting.
2. An integrated suite of sample environment equipment that supports a materials chemistry mission of *in situ/in operando* measurements across a wide range of temperature and pressure, electrochemical cells, and gas handling systems.
3. Acquire refinable data from 0.5 gm sample in on order 1 hour.

[1] A typical example is $BiFeO_3$ where the structure consists of unusually long period modulation of 620 ± 20 Å that was only resolved at very high resolution: I. Sosnowska, et al., Physica B 180, 117 (1992)

Technical Description

Optimized for high d-spacing resolution, HighResPD requires the high wavelength resolution provided by a decoupled, poisoned moderator in combination with a long incident flight path. This instrument will be the longest instrument on the SNS site and uses the 10 Hz repetition rate of the STS to give it a sufficiently wide wavelength band to cover a broad range of d-spacing in a single instrument setting. This instrument will view the cold, para-hydrogen 7×7 cm^2 face of the multi-spectral decoupled moderator. This beam line views the moderator at normal incidence in order to minimize flight path differences for neutrons emitted at different locations on the moderator face. The site geography allows the instrument to be as long as 120 m. The moderator is anticipated to provide a moderator pulse width of 6.8 μsec at a neutron wavelength of 1 Å, giving $\Delta\lambda/\lambda$ of $2.2\bullet10^{-4}$ at 120 m, which is sufficient to achieve the desired resolution. The beam line will be straight to provide uniform illumination across the width of the sample. Optimization might result in a slightly shorter instrument at 100 m, providing a bit more bandwidth in a single frame, 4 Å vs 3.3 Å, to cover a broader range in d-spacing at a correspondingly reduced wavelength resolution of $\Delta\lambda/\lambda = 2.6\bullet10^{-4}$. One or possibly two bandwidth choppers will define the incident neutron wavelength band and a T0 chopper will be required. The instrument must preserve the ability to operate effectively at 5 Hz when the broadest wavelength band in a single frame is required. Scaling from current POWGEN experience, 1 hour of data collection time is anticipated to be sufficient to obtain a refinable pattern from a 0.5 g sample.

Key parameters of HiResPD.

Parameter	Description
Moderator	multi-spectral decoupled moderator—cold
Sample size	0.5 to 1.0 cm diameter; 1 to 2.5 cm tall
Moderator–sample distance	120 m
Sample–detector distance	Backscattering and 90°: 2 m Low angle: 3 m
Wavelength range	0.5 Å $\leq \lambda \leq 8$ Å
Resolution	$\Delta d/d = 0.035\%$
Detector	Low-angle: 0.8 cm diameter linear position-sensitive detector, ^{3}He Backscattering and 90°: TBD