DISCOVER: ORNL's TOTAL SCATTERING DIFFRACTOMETER FOR MATERIALS DISCOVERY

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DISCOVER, an SNS diffractometer for Materials Discovery, is a world-leading instrument concept for BL-8b combining the advantages of high *Q* resolution and wide *Q* range time-of-flight (TOF) neutron scattering with the low and stable background scattering traditionally hallmark to diffuse scattering instruments. DISCOVER will be optimized for studying real materials in their operating environments from day one, and is intended to supply the scientific community with a platform for ground-breaking investigations of the delicate interplay of spin, lattice, and orbital degrees of freedom in disordered crystalline solids and nanostructured materials, as well as kinetic studies of crystalline solids. It will be the world's highest resolution dedicated *total* scattering instrument; the *total* scattering holds the key to determining the crystallographic average structure as well as the local structure, often responsible for the physical properties of complex materials. DISCOVER will provide new opportunities for use in scientific research and industrial development.

COMMUNITY ENGAGEMENT

DISCOVER is the evolution of the previous "RAPID" instrument concept originally proposed at the user workshop "Delivering on the Promise of Powder Diffraction" in June 2013 at Oak Ridge National Laboratory [Huq, 2013]. The change in name reflects its strategic place in the SNS diffraction suite: it will fill a current capability gap between the high flux wide Q diffraction / total scattering instrument NOMAD [Neuefeind, 2012] and the high resolution powder diffraction instrument POWGEN [Huq, 2011]. As such. DISCOVER combines the enormously successful characteristics of the recently closed Neutron Powder Diffractometer (NPDF) [Proffen, 2002] at Los Alamos National Laboratory (which was a world leading PDF diffractometer despite being on a low flux first generation source) with the equally transformational characteristics of the Rapid acquisition PDF (RaPDF) development in the x-ray domain leading to the highly successful 11-ID-B beamline at the Advance Photon Source [Chupas, 2007] and XPD beamline at NSLS-II [Shi, 2013]. The Powder Diffraction Working Group at the Second Target Station (STS) Workshop held in October 2015 named the instrument concept its top priority for the First Target Station (FTS) [Eskildsen, 2015]. Most recently, the inaugural Powder Diffraction Suite Review Committee, meeting in the summer of 2016 to review ORNL's Powder Diffraction programs, concluded as a leading statement in their executive summary, "Our strong recommendation is to construct a rapid acquisition but medium-resolution quiet and stable diffractometer at BL-8 on the FTS as quickly as possible… Such an instrument will restore the US lead in PDF studies of nanostructure, while filling an important gap in our capabilities for in-situ/in-operando studies and should be constructed with all haste."

A workshop is planned for May 2017 to define the science goals, instrument concept, and design requirements for DISCOVER, to review preliminary engineering and neutronics calculations, and to produce a preliminary beamline development proposal for DISCOVER to present to Neutron Science

Directorate management at ORNL. The workshop will additionally serve to initiate the collaborative efforts of an Instrument Advisory Team (IAT), combining an international group of prominent neutron scattering experts with scientists from leading North American Universities and National Laboratories who will guide and ultimately utilize the capabilities of the delivered instrument.

SCIENTIFIC FOCUS

The dedicated total scattering instrument, DISCOVER, will enable the determination of the structure of complex materials and nanomaterials in a relatively short time with high accuracy. A large number of crystalline materials of scientific and technological interest today have internal disorder characterized by aperiodic local displacements of atoms [Billinge and Levin, 2007; Playford et al., 2014; Keen and Goodwin, 2015; Mancini and Malavasi, 2015]. Understanding of the real structure can be achieved only through the combined knowledge of average and local atomic structures. Aperiodic local deviations are best characterized by a real-space approach in which the local atomic structure is described by the atomic pair-distribution function (PDF). This approach, including information from both the Bragg peaks and the diffuse scattering intensities, has related vacancies in high temperature ceramics to both their superionic conductivity and phase stability, nanometer-sized polar domains or nanoregions in relaxor ferroelectrics to their enhanced dielectric and piezoelectric properties [Jeong et al., 2010; Aksel et al., 2013; Keeble et al., 2013; Levin et al., 2014], and vacancy/disorder arrays and other subtle local correlations to the mechanisms of high-Tc superconductivity [Bozin et al., 2000; Park et al., 2011; Caron et al., 2011; Louca et al., 2013; Neilson et al., 2013]. These methods have further proven critical in understanding guest-host interactions [Kim et al., 2009; Chapman et al., 2011], amorphous to crystalline transitions [Hillis et al., 2017; Wang et al., 2017], local spin correlations [Paddison et al., 2014; Frandsen et al., 2016a], and other disordered crystalline materials phenomena [e.g. Page, 2007; Bozin et al., 2010; Shoemaker et al., 2011; Fabini et al., 2016].

A large and predominately untapped latent scientific community studying nanomaterials will also make use of DISCOVER [Gilbert et al., 2004; Chupas et al, 2007; Page et al., 2010; Jenson et al., 2012; Wang et al., 2013]. As the highest resolution neutron total scattering instrument in the world, the instrument will provide access to over 200 Å of atom-atom correlations in real space; a regime with emerging relevance to nano- and meso-scale science. The instrument will be applied to the characterization of finite size and shape effects in nanomaterials and the study of the nature and length scales of nanostructured domains in complex disordered materials [Kim et al., 2007; Withers et al., 2008; Liu et al., 2016].

DISCOVER will also be the best instrument in the world for studying short-range magnetic correlations using Magnetic pair distribution function (mPDF) methods on powder samples. mPDF methods are being developed to provide direct access to long-range and short-range magnetic correlations in real space [Keen and McGreevey, 1991; Goodwin et al, 2006; Paddison and Goodwin, 2012; Frandsen et al., 2014; Fransden et al., 2015, Fransden et al, 2016b]. It is anticipated that this method will provide new understanding in fields such as spin order in diluted magnetic semiconductors [Ohno et al., 1998; Zhao et al., 2013], spin-stripe correlations in cuprate superconductors [Tranquada et al., 2006], and spin fluctuations in frustrated magnetic systems [Han et al., 2012].

Finally, the instrument will provide much needed capability for parametric structural studies [Shoemaker et al., 2014] with an excellent balance between measurement time scale and reciprocal space resolution. Indeed, the initial promise of the RAPID instrument concept will also be fulfilled by the DISCOVER instrument. High quality, Rietveld refineable, data sets of crystalline materials will be measureable as a function of temperature, time, or other reaction coordinate [faster time-scales for e.g. in Bugaris et al., 2014; Tamimi and McIntosh, 2014; Whitefield et al., 2016; Taddei et al., 2016].

INSTRUMENT CONCEPT

DISCOVER is an instrument that can be located at beamline 8b at the FTS of SNS. Optimized for medium resolution, wide-Q range, and low and stable background scattering, DISCOVER requires the high wavelength resolution provided by a shallow-poisoned water moderator for increased neutron flux in combination with a moderate incident flight path, wide-angular detector coverage, and primary/secondary collimation for low and stable background scattering. VULCAN (SNS FTS beam line 7) has demonstrated the suitability of the shallow poisoned, 300 K water moderator to produce outstanding powder diffraction measurements providing Δd/d = 0.25% in its high resolution (low beam divergence) mode with detectors at 90 deg 2θ [Wang, 2010]. This moderator produces pulses with FWHM of 10.6 μsec at λ = 1 Å, which should provide better Δd/d at higher scattering angles for an instrument with a total flight path of ~30 m. Assuming geometry matches wavelength contribution, resolution could be as good as $\delta d/d = \sqrt{2}\,\delta\lambda/\lambda = 0.002$. Optimization might result in a slightly shorter or longer instrument; however the instrument must deliver a sufficiently wide wavelength band to cover a broad range of Q-space in a single instrument setting. The site geography allows the instrument to be as long as 32 m. It is envisioned that the secondary flight path will be 2-2.5m. The beam line will be straight to provide uniform illumination across the width of the sample. Position sensitive ^{3}He tubes will be used for detector coverage. Data collection times of ~1hr are anticipated to be sufficient to obtain high quality total scattering data from a 0.5 g sample. Current performance estimates (estimated based on flux, divergence, detector coverage, and moderator gains) are ~30 times higher count rates compared to POWGEN, albeit with reduced resolution. For conventional Rietveld refinable data sets for ample sized samples, collection times will be on the order of mins.

New sample environment concepts will be required within the DISCOVER design criteria to maximize the use of beam time, reducing the time spent controlling parameters such as temperature, pressure, gas flow, etc. and swapping out equipment, and also ensuring high signal-to-noise ratios and stable background scattering. A FERMI chopper option similar to that on the NOVA diffractometer at JPARC and options for beam polarization will also be considered relative to the refined scientific scope of the instrument.

Table 1. Key parameters of DISCOVER

Parameter	**Description**
Moderator	300 K de-coupled H_2O
Sample size	0.5 to 1.0 cm diameter; 1 to 2.5 cm tall
Moderator–sample distance	30 - 32 m
Sample–detector distance	2 - 2.5 m
Wavelength range	0.5 Å ≤ λ≤ 5 Å
Resolution	Δd/d = 0.2%
Detector	0.8 cm diameter ^{3}He linear position-sensitive detector

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