**SPHIINXS – Spherical Indirect Inelastic Xtal Spectrometer**

SPHIINXS is a high resolution, broadband indirect geometry spectrometer designed to study small samples. The SPHIINXS concept moves beyond the first target station VISION spectrometer by increasing the analyzer area coverage and retaining Q-resolution.

## Science Drivers

Neutron vibrational spectroscopy (NVS) provides insight into molecular structure, chemical bonding, and intermolecular interactions. It is analogous to more common IR and Raman spectroscopies used by chemists but has several well-known advantages including: high sensitivity to hydrogen via its large incoherent cross section; no selection rules; isotopic sensitivity; high penetrating power enabling use of complex sample environments; and quantitative comparison of spectra to theory for both position and intensity. NVS addresses a number of topics in materials chemistry including catalysis, adsorption, storage, separation, and bonding and non-bonding interactions; as well as providing unique insight into the local environments in materials from biochemistry, geochemistry, and condensed and soft matter science. Even with the breakthrough performance of the VISION spectrometer, a next generation spectrometer is needed that will:

- Be optimized for studying small or weakly scattering samples. This will enable studies of new materials produced through synthesis techniques that can only produce small sample quantities. Smaller samples will also enable use of more complex and extreme sample environments including high pressure.
- Provide both Q and energy resolution by preserving both azimuthal and elevation angle information. Current spectrometers integrate over momentum transfer, averaging out vibrational directional information. Q-resolution will facilitate study of single-crystal samples. Applications include investigation of highly anisotropic local potentials and thermoelectrics where preferential directions can be explored with application of applied electric field.
- Enable rapid data collection for time-resolved, kinetics measurements on time scales of 10s of seconds. One application is monitoring temperature and environmental condition induced decomposition.

## Science Requirements

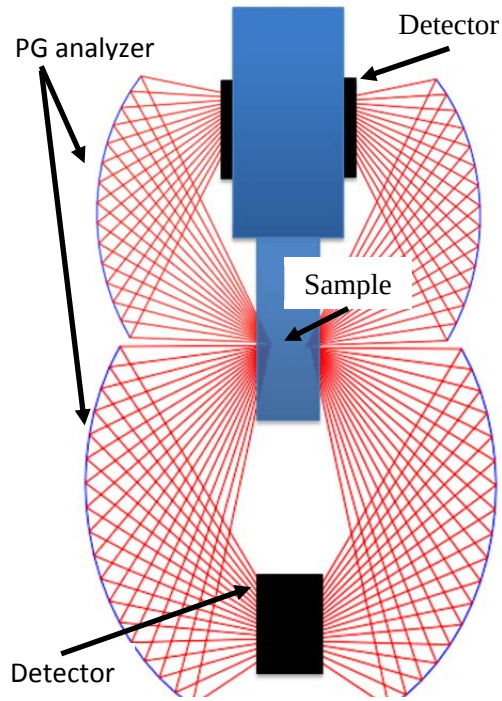
SPHIINXS will address these challenges by providing:

1. A focusing optics system that effectively illuminates a sample area as small as 1 x 1 $cm^2$; 15x smaller than typically used today.
2. Large dynamic range of energy transfer from -1.5 meV to 1000 meV
3. Energy resolution: 1% $\Delta\omega/\omega$; ~35 μeV (FWHM) at elastic line
4. Integrated suite of sample environment equipment that provides control of sample temperature, pressure, gas flow and others. Multiple assemblies must exist that permit measurements on one sample while others are being processed out of neutron beam (e.g. while waiting for chemical reactions to progress).

Technical Description

SPHIINXS requires a low-repetition rate, taking advantage of the 10 Hz frequency of STS to simultaneously cover a large range of energy transfers while maintaining good resolution at the elastic line. SPHIINXS will increase the solid angle covered by the analyzer crystals beyond VISION by extending the analyzer array in two-theta very much like the geometry employed on more traditional backscattering spectrometers such as BaSiS (see the illustration of a vertical slice through the sample position in the figure).

This instrument will nominally view 7 x 7 $cm^2$ water face of the multispectral decoupled moderator. As envisioned, SPHIINXS will use pyrolytic graphite analyzers and requires use of a high-order filter. The analyzers will cover ~10 sr of solid angle, 2.5 x the coverage on VISION. At 40 m from the moderator, SPHIINXS can use neutron wavelengths as long as 9.9 Å in the first frame. SPHIINXS will have at least one T0 chopper (two if warranted) to eliminate the prompt pulse and bandwidth choppers to provide sharp definition of the wavelength band incident on the sample.




Vertical slice of the analyzer and detector(black) geometry proposed for SPHIINXS. Red lines indicate paths of scattered and analyzed neutrons.

**Key parameters of SPHIINXS**

| Parameter | Description |
|---|---|
| Moderator | 7 x 7 $cm^2$ water face of the multi-spectral decoupled moderator |
| Sample size | $1\times1$ $cm^2$ |
| Moderator–sample distance | 40 m |
| Wavelength range | $0.4$ Å $\leq \lambda \leq 9.9$ Å |
| Q-range | $0.06$ $Å^{-1} \leq Q \leq 0.6$ $Å^{-1}$ (elastic) |
| Resolution | 35 μeV (FWHM) at the elastic peak |
| Detector | linear position-sensitive $^3$He |