XTREME-X – Extreme Environment Multi-Energy Spectrometer with Xtal Analyzers

EXTREME-X is an indirect geometry time-of-flight spectrometer optimized for measuring inelastic neutron scattering (INS) in a horizontal scattering geometry. The choice of horizontal geometry is a necessary consequence of the geometrical restrictions that appear when performing neutron scattering experiments under extreme conditions such as high-pressure or with certain magnetic field designs. The basic concept is to maximize count rates for neutron scattering in the horizontal plane with quasi-continuous analyzer angular coverage of the scattered neutrons. High efficiency will be obtained using banks of concentric analyzers placed behind one other. Each bank analyzes a different scattered neutron energy, which is the indirect geometry spectrometer equivalent of repetition rate multiplication for direct geometry spectrometers.

Science Drivers

Synthesis of innovative materials to address our growing energy needs is a key objective in materials sciences. Exploiting extreme environments, notably high temperature and high pressure, has tremendous potential for the synthesis of novel materials with unique, highly useful properties. For example, pressure-induced band-gap engineering may enable the formation of future photovoltaic or superconductive applications from cheap, abundant elements like silicon. Equally, desirable mechanical properties can be engineered such as the immensely increased mechanical strength possessed by diamond and boron-nitride (both high pressure synthesized) or the unprecedented strength-to-weight ratio exhibited by diamond nanothreads recently synthesized at ORNL.[1] The use of specialized, innovative sample environments, radical reduction of background and considerable increase in neutron flux proposed for XTREME-X will ensure that ORNL maintains its status as a world-leader in high pressure inelastic neutron scattering.

INS under high applied pressures or high magnetic fields are routinely used to explore quantum critical behavior and novel phases of matter found in high temperature superconductors, heavy fermion compounds, complex magnetic materials, or other correlated electron systems. Studies at extreme sample conditions such as high magnetic field or ultra-high pressure either necessitate use of small samples or often provide a limited view of the sample from detector locations. Use of the highest vertical magnetic fields limit the view to as small as a few degrees vertically, emphasizing the need to maximize data collection efficiency in the scattering plane. High-pressure is perhaps the cleanest tuning parameter to explore quantum critical phenomena but, of necessity is limited to small sample volumes and limited angular access to scattered neutrons. The efficiency of EXTREME-X in collecting data in the scattering plane will facilitate these studies.

Science Requirements

1. A focusing optics system that effectively illuminates a sample area of 1 x 1 mm^2 to 1 x 1 cm^2.
2. Large dynamic range of energy transfer from -2.4 meV to 500 meV
3. Energy resolution: 1.5% $\Delta\omega/\omega$; ~80 μeV (FWHM) at elastic line
4. Integrated suite of sample environment equipment that provides extreme sample conditions in high pressure, low temperature, and high magnetic field).
5. Polarization analysis is required to separate magnetic and nuclear scattering.

[1] T. C. Fitzgibbons, M. Guthrie, E.-s. Xu, V. H. Crespi et al., Nature Materials, doi:10.1038/nmat4088.

Technical Description

This instrumental concept for XTREME-X is based on the design of the CAMEA[2] spectrometer (now BIFROST[3]) proposed at the European Spallation Source (ESS). CAMEA is an indirect geometry spectrometer that uses multiple sets of analyzers (one after the other) to select a number of discrete final neutron energies at each sample scattering angle (two-theta). Identical banks of analyzers surround the sample in a semi-continuous fashion. CAMEA was originally envisaged for a long pulse source, but we believe that the CAMEA concept, with some modifications, is significantly better suited for a short pulse source like STS. XTREME-X can be built at a source with a low repetition rate, such as 10 Hz STS. With a frame 100 ms long, it can be positioned at 50 m from the moderator with a direct view of the moderator and still have no frame overlap so that the energy transfer range available is from -2.4 meV to >500 meV and includes the elastic line. The use of solid parahydrogen as a band-pass filter for the neutrons in the secondary spectrometer will remove the higher orders from the spectra. Unlike the CAMEA concept for the ESS, our implementation will provide access to the whole energy transfer range at constant resolution in terms of $\Delta E/E$~1.5%.

This instrument will nominally view 7 x 7 cm^2 water face of the multispectral decoupled moderator. At 50 m from the moderator, XTREME-X can use neutron wavelengths as long as 8.2 Å in the first frame. XTREME-X 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.

Key parameters of EXTREME-X

Parameter	Description
Moderator	7 x 7 cm^2 water face of the multi-spectral decoupled moderator
Beam size	1×1 mm^2 to 1×1 cm^2
Moderator–sample distance	50 m
Wavelength range	0.4 Å $\leq \lambda \leq 8.2$ Å
Q-range	0.06 $Å^{-1} \leq Q \leq 0.6$ $Å^{-1}$ (elastic)
Resolution	80 μeV (FWHM) at the elastic peak; $\Delta E/E$ ~1.5%
Detector	linear position-sensitive ^3He

[2] P.G. Freeman, et al., EPJ Web of Conferences 83, 03005 (2015)

[3] https://europeanspallationsource.se/article/bifrost-prismatic-approach-neutron-spectroscopy