BWAVES – Broad-range Wide Angle Velocity Selector

BWAVES, a small beam size, broadband inverted geometry spectrometer optimized for biological and soft-matter samples that utilizes a novel wide-angle velocity selection device, WAVES[1], instead of traditional crystal analyzers, for the final energy selection of scattered neutrons. BWAVES alone will cover 5 orders of magnitude in energy transfer, from several μeV to several hundred meV, making it a one-stop instrument for vibrational spectroscopy of biomolecules. The combination of MBARS and BWAVES will cover more than 6 orders of magnitude in relaxation time. In the quasielastic regime, these two spectrometers will provide access to the same lower-Q range (particularly relevant to soft matter and biology systems) because of identical choice of the scattering angle coverage and the final wavelength of 20 Å.

Science Drivers

Inelastic neutron scattering (INS) is indispensable for studying the microscopic dynamics of complex biological and soft matter systems because of a combination of: one, high sensitivity to hydrogen and hydrogen/deuterium selectivity, unmatched by other probes except NMR; two, high energy resolution, far exceeding that attainable in synchrotron x-ray inelastic scattering experiments; and three, sensitivity to the geometry of motions via Q-dependence, which NMR and dielectric spectroscopy do not possess.

However, there are barriers limiting the use of INS for studying biomolecules, including the relatively large incident beam size, which requires large samples, and the limited dynamic range of current neutron spectrometers. The challenge is exacerbated by the complex microscopic dynamics exhibited by soft matter systems, and even more so by proteins, because of the simultaneous presence of vibrational and relaxational processes. This calls for continuous, rather than piecemeal, coverage of energy transfer in a single experiment. Such continuous coverage is provided by inverse geometry spectrometers like VISION, which, however, lack the energy resolution to simultaneously study the quasielastic signal originating from relaxations in soft matter. BWAVES will address a wide range of topics including:

- Biomolecules in real-life biological solvents. Neutron scattering studies to date have been commonly performed on powder samples with limited hydration. Study of real-life biomolecules solvated in aqueous, biologically active media requires an instrument with BaSiS-like resolution but a much broader dynamic range.
- Microscopic dynamics in complex liquid electrolytes. The research focus for better liquid electrolytes has recently shifted to complex systems such as room-temperature ionic liquids (RTILs). The performance of RTILs in applications is tied to the microscopic dynamics of their cations and anions, which can be quite complex. In the practically important liquid state, the low-energy modes overlap with the quasielastic signal because of both the center-of-mass and side group ion relaxation dynamics, requiring an instrument which can simultaneously measure both quasielastic and inelastic scattering.

Science Requirements

BWAVES is designed to address these challenges by providing:

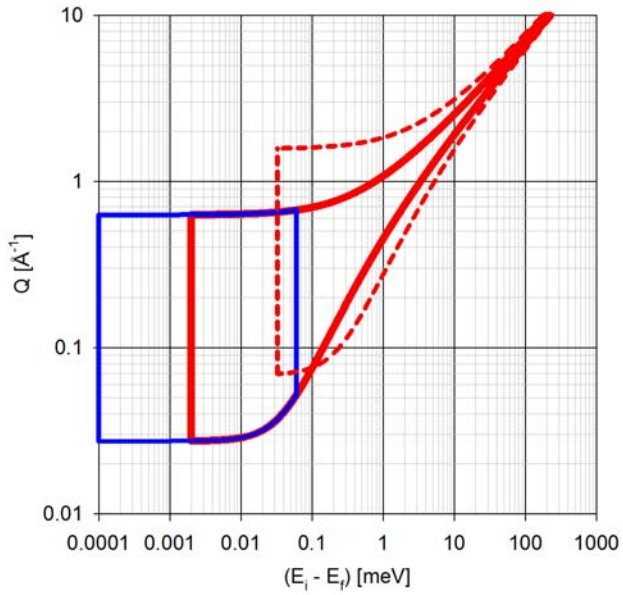
1. Energy resolution: ≤ 3 μeV (FWHM) at the elastic line
2. Large dynamic range of energy transfer up to 500 meV
3. Q-range: $0.06\ Å^{-1} \leq Q \leq 0.6\ Å^{-1}$ (in the quasielastic range)
4. Sample size: $0.5 \times 0.5\ cm^2$

[1] E. Mamontov, Nucl. Instrum. Meth. A, 759, 83–91 (2014).

Technical Description

BWAVES requires a low-repetition rate; therefore, it is ideally matched to the 10 Hz repetition rate of STS. This concept relies on development of the WAVES device. Unlike its use on MBARS as an order filter with final energy selected by analyzer crystals, WAVES selects, with high precision, the final energy on BWAVES.

This instrument will view the 3×3 cm^2 face of the coupled, cold para-hydrogen moderator which provides sufficient timing resolution (moderator pulse width) to support the energy resolution desired for BWAVES. In order to cover the maximum dynamic range of energy transfers in a single STS pulse, the instrument requires a short primary flight path of approximately 16 m. BWAVES will have at least one T0 chopper (two if warranted) to eliminate the prompt pulse and two bandwidth choppers to provide sharp definition of the wavelength band incident on the sample. Vertical divergence is likely limited to ±0.5° by the WAVES device, but much broader horizontal divergence could be used. The final flight path can be relatively short so large detector coverage can be readily achieved. The momentum and energy space spanned by MBARS and BWAVES is shown in the figure to the right. The table below lists key parameters of BWAVES.



Blue shows the phase space covered by MBARS and solid and dashed red that by BWAVES when operating WAVES at a final neutron wavelength of 20 and 8 Å respectively.

Key parameters of BWAVES

Parameter	Description
Moderator	3 x 3 cm^2 high brightness coupled moderator
Sample size	5×5 mm^2
Moderator–sample distance	16 m
Sample–analyzer distance	0.75 m
Wavelength range	0.4 Å ≤ λ ≤ 23 Å
Q-range	0.06 $Å^{-1}$ ≤ Q ≤ 0.6 $Å^{-1}$ (elastic)
Resolution	3 μeV (FWHM) at the elastic peak
Detector	linear position-sensitive ^{3}He