C-SPEC Brings More Light to the Study of Dynamics in Systems

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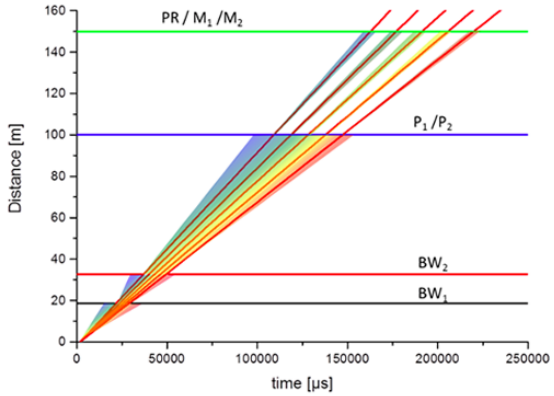
Brighter neutron flux and experienced French-German collaboration brings long-awaited routine to the study of complex molecular and kinetic systems.

The use of neutron scattering research using biological and soft matter materials has long been limited by small sample sizes. Obtainable crystalline samples are suitable for X-ray studies but often too small to produce satisfactory results with neutron sources. This has left key gaps in the knowledge of the structural and dynamical properties of these systems. Producing neutron beams an order of magnitude brighter than the next brightest source, the European Spallation Source (ESS) is inspiring a new generation of instrument designs and technologies that will make these limitations a thing of the past.



Time-distance diagram of C-SPEC. The PR/M-chopper system is used to set the resolution and the operation mode, i.e., to select the number of pulses impinging on the sample.

-C-SPEC instrument proposal

C-SPEC, which stands for Cold Chopper Spectrometer, is a direct geometry, time-of-flight (TOF) spectrometer that will be used to study the structures, dynamics, and functionality of large hierarchical systems, including liquids, colloids, polymers, foams, gels, and granular and biological materials. The wide reach of the instrument's user base also includes investigations into energy materials and magnetism. The C-SPEC concept was developed by Dr. Wiebke Lohstroh, a member of Prof. Winfried Petry's research group at the FRM II neutron source operated by the Technical University of Munich (TUM); and the Laboratoire Léon Brillouin (LLB) research group of Prof. Christiane Alba-Simionesco, director of LLB and chairman of the European Neutron Scattering Association. The instrument will improve

and expand the range of TOF neutron spectroscopy experiments classically limited by a lack of flux.

World-Leading Collaboration

C-SPEC is no incremental step forward. 'C-SPEC will outperform all other spectrometers of its kind in the world, which will lead to new science not accessible today," proclaims Prof. Tobias Unruh, Chair of the Crystallography and Structural Physics Department at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), and Chair of the ESS Scientific and Technical Advisory Panel (STAP) for direct geometry spectroscopy. 'C-SPEC has a clear and well-structured design that will provide efficient, user-friendly, and stable operation, a prerequisite for successful cutting-edge research. C-SPEC will become one of the key pillars for the success of ESS."

The strong collaboration that has arisen between FRM II and LLB is built upon a broad, complementary platform of neutron research. While both institutions are strong in soft matter and biophysics research, LLB additionally focuses on physical chemistry, magnetism, superconductivity, and structural and phase transition studies. FRM II specializes in materials science, structure research, quantum phenomena, nuclear and particle physics, and neutron methods. The result of this partnership is a workhorse spectrometer that will deliver results for both an academic and industrial user base.

Dr. Wiebke Lohstroh, TUM

'Three years ago," explains Lohstroh, 'the German ministry of science asked for ideas and offered funding for innovative instrumentation at ESS. That is when the idea of C-SPEC came up. Conceptual work started at TUM, fueled by our experiences with the cold chopper, direct geometry time-of-flight spectrometer, TOFTOF, at FRM II. Soon we realized that a partnership with LLB would strengthen the project, as LLB was also involved in conceptualizing and building a state-of-the-art spectrometer."

Studies of Life

Spectroscopy research on the steady-state conditions of samples is routine, and a TOF spectrometer is an essential instrument at any neutron source. Limited beam intensity at existing neutron facilities, however, has left research on time-dependent responses along

varied time and length scales in the exploratory stages. 'The unique features of C-SPEC, together with the high brilliance of ESS, will enable *in operando* studies of electrolytes, pump-probe experiments on photosensitive materials, and the investigation of small samples in extreme sample environments," says Lohstroh. 'This will open up [scientific] fields that suffer from flux limitations today."

Among C-SPEC's strengths is that it can be used to study live cells. 'The instrument marries well-known technologies with the possibility to provide a great neutron signal-to-noise at the highest energy resolutions," explains Dr. Pascale Deen, the ESS coordinator for the direct geometry spectroscopy instrument class. 'This is essential to improve our understanding of, for example, biological systems in which the mobility of hydrogen or water is crucial to their function. As such, C-SPEC will play a defining role in understanding life."

Two-Mode Chopper and Exchangeable Guides

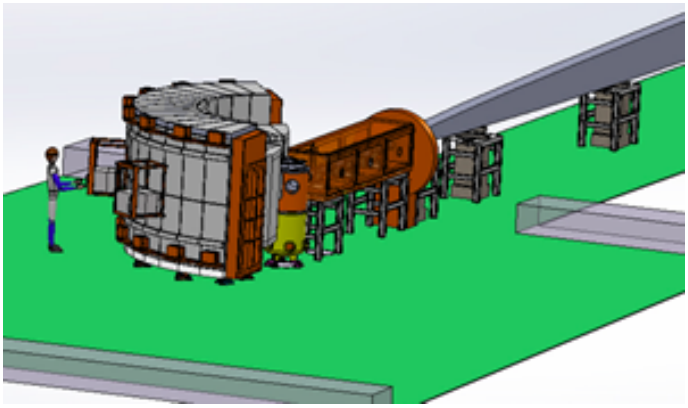
Neutron spectroscopy measures the atomic and magnetic motions, or random movement, of atoms. Studying such dynamics is necessary to learn the inherent physics of phase changes in materials and to identify basic characteristics such as diffusion coefficients, thermal conductivity, specific heat, and dielectric properties. With C-SPEC and other direct geometry spectrometers, a neutron pulse hits a sample and the neutrons are scattered. Researchers then measure the time-of-flight, that is, the time it takes for outgoing neutrons to travel a known distance before registering on the detector.

C-SPEC's chopper system controls the incoming energy of the neutrons delivered to the sample, and therefore the energy resolution, with options for a single-pulse or multi-energy mode. This represents a novel adaptation to the ESS neutron beam's long-pulse structure that enables more efficient experiments by providing data along different time and length scales simultaneously. The system includes seven choppers, whose multiple parameters work together to control bandwidth, pulse shape, pulse number, wavelength, and energy resolution.

'The instrument is designed for optimum use of the long pulse," explains Lohstroh. 'It will utilize the innovative concept of multi-energy mode while maintaining the possibility for single-pulse mode. [One] would normally use a shorter pulse, working with the traditional pulse structure. The time structure of the source at ESS, like for many of the other research groups…it's an adventure for all of us."

The spectrometer will also be outfitted with an exchangeable neutron beam guide section that adjusts to different user needs. One guide configuration will accommodate experiments in single-crystal spectroscopy by providing a homogenous distribution of neutrons on the crystal, while the other is optimized for small samples and situations where access to the sample is restricted on account of a controlled sample environment. This second guide delivers a high flux, focused beam necessary for pump-probe and externally driven experiments.

'C-SPEC will cover a wide area in the range of high-energy resolutions, which is a particular strength of neutron scattering," adds Unruh. 'Thus C-SPEC will perform extremely well for quasielastic neutron scattering studies covering a wide time range, from sub-picosecond to about one nanosecond, in which atomic and molecular motions can be studied. This is for instance important for understanding the molecular motions in liquids, biological membranes, polymers, proteins, and many other systems."



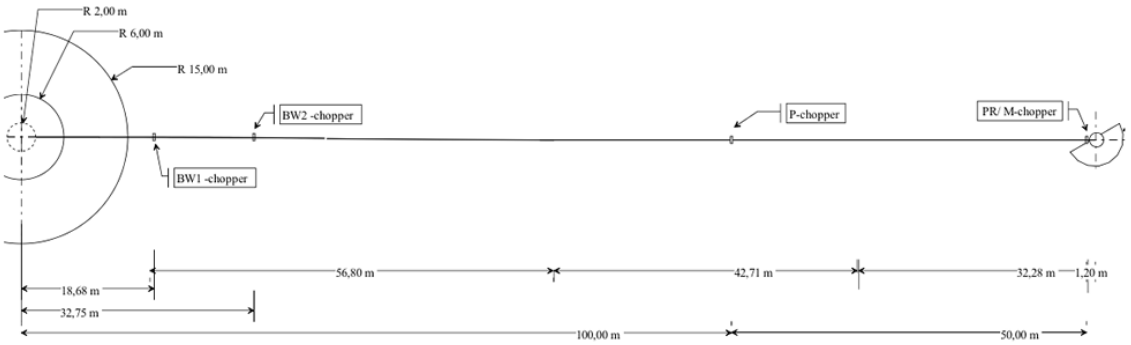
Artist's impression of the instrument.
-C-SPEC instrument proposal

Novel Research in Geoscience, Magnetism, and Energy
Aside from its long-awaited contributions to soft matter and life science studies, C-SPEC is expected to contribute to some other noteworthy advances. Geoscience research into the diffusion of water under extreme pressure holds considerable promise for expanding our knowledge of the hydrogenated systems of Earth's mantle and extraterrestrial environments such as outer planets, moons, and comets.

In the field of magnetism, spectroscopy experiments on highly frustrated magnets, spin ices, and spin liquids can reveal the secrets to better computer data storage and RAM, and can contribute to our understanding of the elusive mechanisms of high-temperature superconductors.

C-SPEC, like most of the instruments to be built at ESS, will also contribute to the development of energy materials at the farthest reaches of innovation. It is an especially powerful tool for probing the electrolyte properties in applications such as lithium batteries and fuel cells. In combination with nuclear magnetic resonance (NMR) technology, the C-SPEC innovations can improve our comprehension of the dynamics of protons in polymer electrolyte-based lithium batteries.

So-called pump-probe experiments, with laser excitation, can enhance our surprisingly limited knowledge of photosynthesis. Through time-resolved measurement, using synchronized neutron and photon pulses, information can be gathered about the light harvesting and internal dynamics of pigment-protein complexes.



Schematic layout of the instrument. The P-chopper is located at 100 m just after the monolith and the PR/M-chopper system is positioned at 150 m from the source. The position of the BW1 / BW2 choppers is generic. At 18.16 m from the source an s- shaped bender brings the guide out of the line of sight. The sample will be positioned at 151.4 m, and the secondary spectrometer consists of a 4 m flight path.

-C-SPEC instrument proposal

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