EUROPEAN SPALLATION SOURCE

Realizing DREAM, a Versatile Powder Diffractometer

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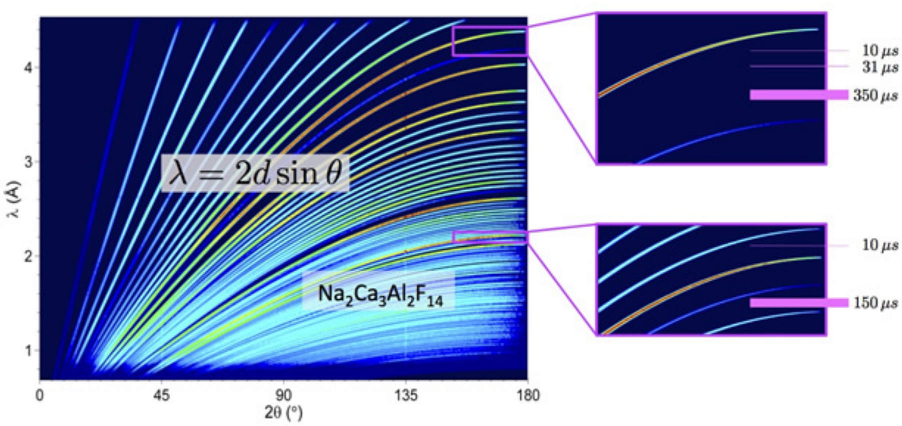
An international collaboration of scientists opens new horizons in powder diffraction and expands the potential for determining the structures of new and more complex materials.

Powder diffraction allows for quick measurement of powder samples, providing structural information on a comprehensive range of crystalline materials. The long-pulse structure of the neutron beam at the European Spallation Source (ESS) offers new opportunities to broaden the scope of powder diffraction research across disciplines and materials, and presents a new challenge for instrument design.

DREAM rises to this challenge. It is a bi-spectral powder diffractometer able to make use of neutrons delivered from both thermal and cold moderators, and to selectively mix them to achieve optimal resolution without sacrificing brightness. This is an important advance made possible by the unique properties of the ESS neutron beam and its innovative moderator designs.



Diffraction diagram of a reference sample in high resolution mode (left). In backscattering, the asymptotic limit is essentially determined by the time resolution, see enlarged regions (right).
-DREAM instrument proposal

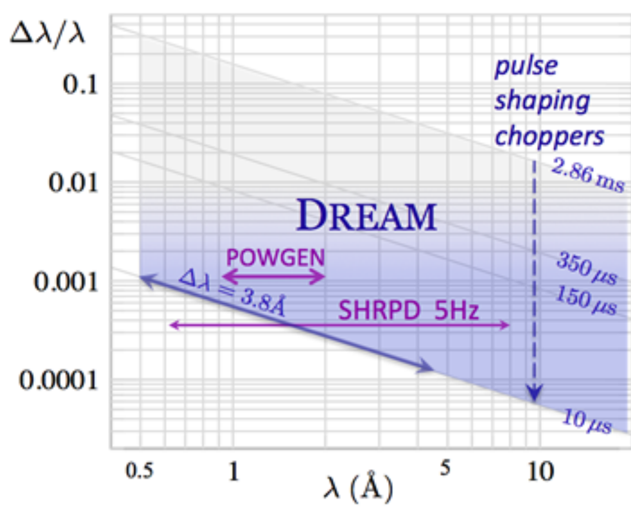
User-Driven Innovation

Proposed by Dr. Werner Schweika, an instrument scientist at ESS and senior scientist at the Jülich Center for Neutron Science (JCNS), DREAM has been developed through contributions from a virtual football team of instrument scientists, engineers, and neutron scientists representing nine institutions across five European nations.

'Its flexibility is a strong reason why DREAM was chosen as the first powder diffractometer," says Dr. Paul Henry, ESS instrument scientist and coordinator for the Scientific and Technical Advisory Panel (STAP) for powder diffraction. 'Our community is large and varied and the first instrument must address many different needs while also remaining a strong part of a balanced suite of diffractometers once the full instrument complement is available."

Neutrons are classed as thermal or cold based on their kinetic energy. Thermal neutrons, which have the higher kinetic energy, provide more precise information about the positions of atoms in crystalline structures. Cold neutrons help scientists to resolve multi-phase materials, large unit cells, and magnetic structures. ESS will have moderators that produce both types in quantities never seen before.

'Analyzing the user community reveals that users are coming from chemistry, physics and materials science," explains Schweika. '[Research] topics are often related by the specific sensitivity of neutrons to magnetism and light elements, with a trend toward more complex materials. While thermal neutrons are indispensable for powder diffraction, the science case establishes the requirement for a wider neutron spectrum, and to also make use of the optimized high cold flux of ESS."



Flexibility and range of wavelength resolution Δλ/λ versus λ due to pulse shaping from full pulse width 2.86 ms to high resolution 10 μs.
-DREAM instrument proposal

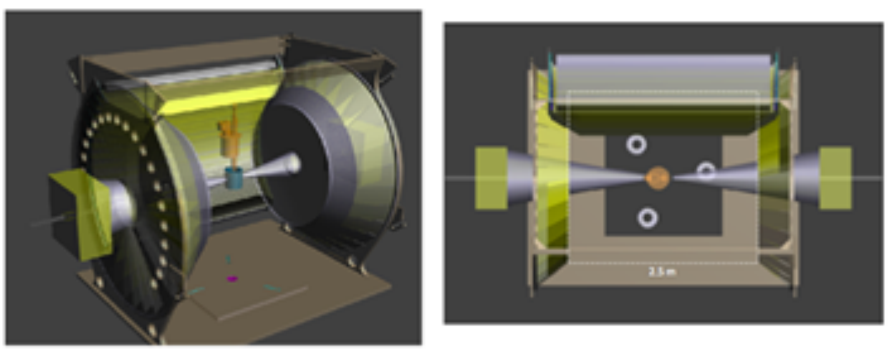
Skepticism Turned to Opportunity

'When I first learned about ESS and the concept of a long pulse source, my main concern was that this seemed incompatible with instruments that rely on a short pulse, such as powder diffractometers," says Dr. Thomas Proffen, Director of Neutron Data Analysis and

Visualization at Oak Ridge National Laboratory, and co-chair of the powder diffraction STAP. 'That concern turned into excitement about the novel designs and ideas turning this 'disadvantage' into opportunity. Discovering the need for higher resolution, for example, during an experiment today will require a new experiment on a different instrument. With DREAM, it will be just a click with the mouse."

DREAM is an acronym for Diffraction Resolved by Energy and Angle Measurements, a reference to the two dimensions that comprise the results of a powder diffraction experiment conducted on the instrument. The original concept came out of investigations by Schweika at JCNS and Dr. Klaus Lieutenant, a VITESS software simulations expert at Helmholtz-Zentrum Berlin (HZB). Further detailed modeling and verification of the DREAM concept by a small core team, including Dr. Nicolo Violini at JCNS, led to a design mature enough for development by a number of additional researchers leading to advancements in both the scientific case and the technological specifications of the instrument.

'DREAM is an example of international collaboration that exemplifies the ESS ideal," says Henry.



The diffractometer (side and top view). The cylindrical detector configuration with 6.2 sr coverage is adapted to the Debye-Scherrer cones around beam axis. The detector is a 3D wire chamber with B-10 film absorbers of high efficiency, homogeneous 2D response with high spatial resolution. Background is reduced by evacuating the primary flight path, a vacuum vessel around the sample and Argon-atmosphere in the scattered flight path. There is convenient sample access from top (standard), side and bottom.
-DREAM instrument proposal

The Chopper and the Detector

The instrument builds on another instrument design that Schweika contributed to, known as POWTEX. Currently under construction at the FRM II reactor in Munich, POWTEX provided the conceptual ideas and some base technologies for DREAM, including that of its innovative pulse-shaping chopper system and the novel boron-10 based Jalousie detector built by Cascade Detector Technologies in Heidelberg. While both designs will be advanced for DREAM, the fact that they are built upon proven technologies means that the inherent risks in the instrument's development are minimized.

‘What is special about ESS is its long pulse,” explains Schweika. ‘The pulse shaping that is necessary is a great opportunity for high flexibility adapted to the user's needs. We cannot do this at short-pulse sources without wasting immediately an order of magnitude or more in flux. The proposed chopper system will provide a novel flexibility to this new concept.”

Dr. Graeme Blake, assistant professor at Rijksuniversiteit Groningen in the Netherlands, and a contributing scientist for DREAM, explains it this way: ‘[DREAM's ability to] tailor the pulse shape will give an ideally symmetric peak shape, which will allow more precise refinement of both crystal and magnetic structures.”

Shaping the beam entering the instrument is one key to DREAM's efficiency, and its particular manner of capturing and analyzing the neutron scattering pattern after diffraction is the second. The use of a large cylindrical, volumetric, boron-10 based detector, with new approaches to data analysis by 2D Rietveld refinement, is something the team borrowed from POWTEX. The novel detector provides an alternative to the standard helium-3 technology, the availability of which has been called into question.

‘Now with the new detector capabilities, we would not like to step back to old technologies even if helium-3 became available again,” says Schweika. ‘It supports better resolution, improves the signal to background ratio, and its large angle of detection is a gain, beyond the use of powder diffraction, for single crystal studies.”

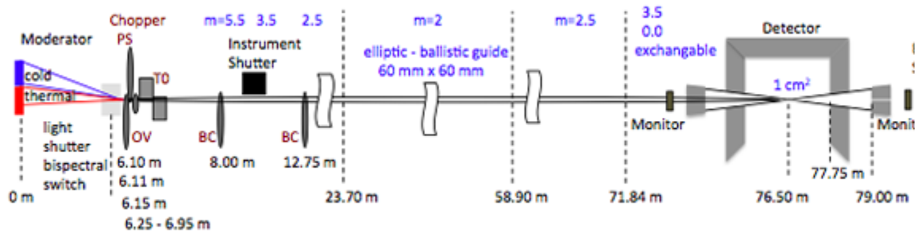
Moreover, adds Blake, ‘[Enabling] the novel 2D Rietveld data analysis as a function of wavelength and diffraction angle will fully exploit the intensity available at ESS.”

A New Benchmark for Science and Society

Using advanced VITESS simulations performed by Lieutenant's group at HZB, the proposal team was able to demonstrate precisely in what ways and by what degree DREAM, coupled to ESS, would improve on the world-leading powder diffractometers in service at ISIS in the UK (WISH), the Institut Laue-Langevin in Grenoble (D20), and the Spallation Neutron Source in Oak Ridge, Tennessee (POWGEN).

Some powder diffraction experiments require either high resolution or high beam intensity, others a large detector coverage area for fast data collection, and many will make use of special sample environments to control conditions like temperature and pressure. Taking control of each of these variables using DREAM, scientists can answer new questions about the atomic and magnetic structure of materials.

Society has much to gain. Matter in our world, the stuff of both life and the inanimate world, is largely explored through crystal diffraction. We are only 100 years out from the discovery of x-ray diffraction by Max von Laue, and there is much work still to be done, particularly with neutrons. Recent powder diffraction studies have enabled the design of more efficient and environmentally friendly electrical components such as capacitors, ultrasonic transducers, gas igniters, and sensors. They may also pave the way for enhanced optical devices, memory devices, and solar cells, and improve industrial molecular processes like chemical synthesis, separation, and catalysis.



Schematic layout of the DREAM diffractometer.

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