Logos for sponsors and organizers

ESS-I

Design and simulations for a long-pulsed spallation source - ESS

Working workshops on ESS LPTS instrumentation

Rencurel, September 2006: 10 instrument experts, 10 simulators

Ven, October 2008: 19 instrument experts, 12 simulators

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Summary

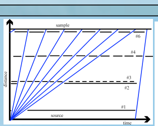
H. Schober et al, NIMA (2008)

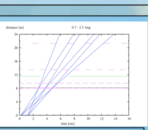
We here briefly list the instruments discussed and (for most instruments) simulated at the workshops in Rencurel (2006) and Ven (2008).

For each instrument, the science case is sketched (KL views, subject to modifications), the discussed instrument length (source-sample) is shown, and the likely effect on the instrument design and performance of having a shorter (1-1.5 ms) pulse or a longer (3-4 ms) pulse is mentioned, under the consition that the integrated flux is constant. The pulse-length discussion is currently a best guess, and subject to modifications. It should eventually be used as an input to the target simulators.

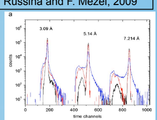
Rencurel was arranged and sponsored by ILL and ESS-I, while Ven was arranged and sponsored by Copenhagen University, DTU, IBM, Lund University and ESS Scandinavia.

Wavelength Multiplication





K. Lieutenant, F. Mezei, M. Russina
M. Russina and F. Mezei, 2009



Basic idea:

- If long time between pulses
- Then produce more pulses at the sample

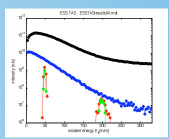
Several cold instruments:

- Use the long source pulse as it comes
- Example: Spectrometer

Most thermal instruments:

- Need to sharpen the source pulse at the source (closest 6 m)
- Example: Diffractometer

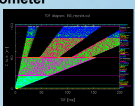
Case 1: Thermal spectrometer challenge

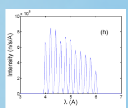


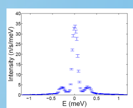
- Which thermal spectrometer will work best on a long pulse?
  - •Multi-analyzer triple-axis ?
  - •Direct chopper time-of-flight (MAPS) ?
  - •Crystal focusing time-of-flight (HYSPEC) ?
- Simulate all 3, under similar conditions
  - •M=3.5 standard curved guide, 40x132 mm^2
  - •dE/E = 2% at sample position
  - •Lengths: Source-sample 50 m, Sample-detector 5 m
  - •Sample 2x2 cm^2
- First comparative result: TAS has 50 x sample flux
- Elliptic guide and wavelength multiplication still to be done

Case 2: Cold chopper spectrometer

- •100 m ballistic guide
- •No pulse shortening
- •Wavelength multiplication
- •100 times IN5 flux
- •Detector counts above 10^7 / sec !
- •Simulations: expected resolution



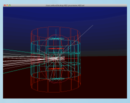




Lefmann, Schober, Mezei, Meas Sci Tech (2008)

Case 3: Diffractometer for small crystals

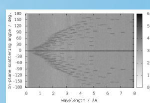
- •Thermal moderator, 0.8-8 Å
- •30 m flight path, elliptic guides
- •Beam spot 3x3 mm^2
- •Beam divergence at sample: 0.5 degrees
- •SNS-type Anger cameras, r = 0.5 m
- •Lattice constants 15-25 Å
- •Exteme environments



- •Virtual experiments performed: C-60 crystal (hkl) < (666)

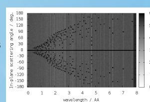
Low resolution:

- Full pulse, 2 ms
- Large flux, 10x TOPAZ
- Peaks separated above 2Å



High resolution:

- Shorten pulse to 0.25ms
- Loose factor 8 flux
- All peaks well separated



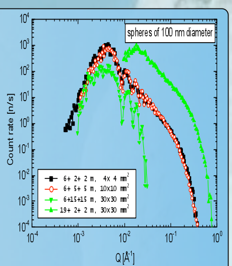
Case 4: New ideas for SANS and reflectometers

General: 5-10% wavelength resolution – 2ms pulse almost too short (!)

a.Short SANS beamline: Workhorse
- large q coverage, high count rate
- Virtual experiment shows feasibility

a.Medium SANS beamline: Bio-SANS
- Optimize for small (bio-) samples
- Idea: beams from different directions
- Has not been simulated in details

c. Reflectometer: liquids instrument
- Large q coverage for real-time studies
- Idea1: beams from 2-4 different directions
- Idea2: multiplex by broad chopper
- Detailed simulations needed



K. Lieutenant, et al

List of long-pulse instruments considered - This is not a draft of the day-one instrument suite. Columns show the estimated source-sample distance, and the effect on the instrument of changing the pulse length (with same time-integrated flux).

List of instruments simulated – full pulse

Instrument (Full pulse)	Purpose	Year	Guide length	Shorter pulse	Longer pulse
Cold chopper Spectrometer, repetition rate multiplication	Dynamics in-materials, e.g. bio- and magnetism	2006	100 m	Same guide length, Better resolution OR Shorter guide, Higher intensity	Cut pulse, Lower intensity OR Longer guide, Lower intensity
Triple-axis spectrometer	Excitations in single crystals	2006 2008	30 m- 50 m	No effect	No effect
Off-backscatter. Spectrometer (around 10 μeV)	Diffusion, molecular rotation, slow dynamics,	2009	200m – 300 m	Same guide length, Better resolution OR Shorter guide, Larger E-range	Cut pulse, Lower intenisty OR Longer guide, Smaller E-range
Hybrid thermal spectrometer	Excitations in single crystals	2008	50 m	No effect	Slight intensity loss
SANS, small sample	Biological structures	2008	40 m	No effect (better resolution)	No effect
SANS, workhorse	Macromolecular and biological structures	2008	20 m	No effect (better resolution)	No effect
Spin-echo SANS	Micrometer-size structures	2006	40 m	No effect (better resolution)	No effect
Spin-echo spectrometer	Very slow dynamics	2006	40 m	No effect (better resolution)	Longer guide, smaller wavelength band
Inverted geom. thermal spectrometer	Excitations in single crystals	2006	100 m	Better resolution	Worse resolution
Liquids reflectometer	Surface layers, biophysics	2008	40 m	No effect (better resolution)	Longer guide, smaller wavelength band
Single crystal diffractometer, low resolution (full pulse), OR medium res. (shape pulse)	Small crystals, Extreme environments, dynamic studies	2008	30 m	Low-res. mode: better resolution same flux Medium-res. mode: same resolution, more flux	Both modes: Longer instrument Same resolution Less flux

List of instruments simulated - shaped pulse

Instrument (Shaped pulse)	Purpose	Year	Guide length	Shorter pulse	Longer pulse
Backscattering spectrometer (below 1 micro eV)	Diffusion, molecular rotation, slow motion	2006	180 m	Higher intensity, same resolution	Lower intensity, same resolution
Thermal chopper spectrometer Repetition rate multiplication	Magnetic excitations, Lattice dynamics	2008	80 m	Higher intensity, Fewer repetitions, Slight advantage	Lower intensity, More repetitions, Slight disadvantage
Single crystal diffractometer, large flux, Repetition rate multiplication	Protein crystallography	2006	70 m	Higher intensity, smaller wavelength band, advantage (<1 μs huge advantage)	Lower intensity, Unchanged wavelength band, disadvantage
"Hard surface" reflectometer	Multilayers, nanotechn.	2008	40 m – 80 m	Higher intensity, same resolution	Lower intensity, same resolution
"Cold" powder diffractometer	Crystal structure, magnetism	2005 2008	200m	Higher intensity, same resolution	Lower intensity, same resolution
Disordered materials diffractometer		2008	NOT on ESS long pulse		

Outome

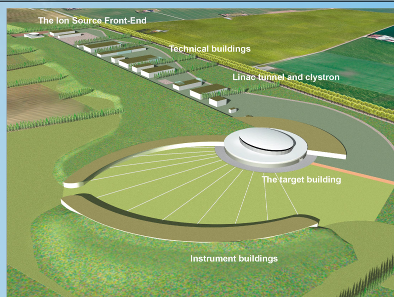
- •Close contact between simulators and instrument experts
- •Involvement of many partners
- •Open home page www.essworkshop.org
- • Knowledge disseminated in journal articles

ESS

5 MW spallation source with extremely high flux and pulses of 2 ms.

Important to determine:

- •Optimal pulse length for the full suite
- •Optimal guide length for each instrument
- •Which instruments are worth building



Conclusions

- We have initiated a process to define the ESS instruments
- Many new ideas have emerged
- The overall is promising: ESS will be leading in most fields
- In general, much more simulation is needed:
  - •Guide optimizations
  - •Consideration of alternatives, e.g. pulse length
  - •Virtual experiments
- For a fast convergence, coordinated efforts are needed
- The collaboration of all facilities has been and will continue to be essential
- Plans of continuous work by a scientific team are required
- More workshops will be organized - Another 'Engelberg' meeting will take place