

EUROPEAN SPALLATION SOURCE

Larmor Labelling at ESS: Opportunities and Perspectives

School on Neutron Precession Techniques, 5/7/2017 Erice, Italy

Ken Andersen, Neutron Instruments Division

Contents



- Quick Introduction and Status of ESS
- Instrument Selection
 - TDR reference suite
 - Concept development
 - Proposal rounds
 - 15 instruments chosen out of the 22-instrument suite
- The ESS Spin-Echo Saga
 - WANSE vs HRNSE
 - ESSENSE vs RESPECT
- NSE Add-ons
 - TU-Delft work: TOFLAR, SESANS, SEMSANS, SERGIS
- Future Plans
 - choosing and building instruments 16-22

ESS High-level Description



- Long-pulse spallation source
 - 5 MW, 14 Hz repetition rate, 2.86 ms pulse length
 - peak brightness ~ JPARC at 1 MW
 - time-average brightness ~ ILL at 57 MW
- Next-generation machine
 - Superconducting linac, no compressor ring
 - Rotating W target wheel
 - 3cm-tall butterfly moderators

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 - 22 instruments (15 paid out of construction)
 - 42 beamports: good upgrade possibilities)
- High-level numbers
 - 200 days/year of operation
 - Construction budget: 1843 M€
 - Operating budget: 140 M€/year

Instrument Suite







Tentative Instrument Ramp-up

based on Instrument Construction Working Schedule V3.1, 25/4/2017





Site Layout



Site Photos







Site Photos





Vaals "Experts Meeting" 2010



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-Scale Structures	Radiography & Tomography General-Purpose SANS		Cold Chopper Spectrometer	
	Small-Sample SANS	oectroscopy		
	Combi-SANS Horizontal Reflectometer		Extreme Environments Spectrometer	
Large	Vertical Reflectometer	S	Backscattering Spectrometer	
	Narrow-Bandwidth Tuneable Diffractometer		High-Resolution Spin-Echo	
			Wide-Angle Spin-Echo	
ion	Hybrid Diffractometer		Fundamental & Particle Physics	
fract	Structured Pulse Engineering Diffractometer	Group 1: Paolo Radaelli , Dimitri Argyriou, Robert von Dreele, Takashi Kamiyama, Matt Tucker, Axel Steuwer		
Dif	Extreme Conditions Diffractometer	Gro	Group 2: Bob Cubitt , Albrecht Wiedenmann, Mikhail Zhernenko Frédéric Ott, Jochen Stahn, Joachim Kohlbrecher	
	Single-Crystal Magnetism Diffractometer	Gro	up 3: Toby Perring , Ken Herwig, Arno Hiess, Thomas Keller, Peter Böni, Kenji Nakajima	
	Macromolecular Diffractometer	Gro	up 4: Katia Pappas , Sasha loffe, Oliver Zimmer, Roger Pynn up 5: Dieter Richter , Ken Andersen, Thomas Brückel, Kurt	

Clausen, Feri Mezei

TDR Reference Suite 2013



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Multi-Purpose Imaging General-Purpose SANS

Broadband SANS

Surface Scattering

Horizontal Reflectometer

Vertical Reflectometer

Thermal Powder Diffractometer

Diffraction

Monochromatic Powder Diffractometer

Materials Science Diffractometer

Extreme Conditions Diffractometer

Single-Crystal Magnetism Diffractometer

Macromolecular Diffractometer

Cold Chopper Spectrometer

Cold Crystal-Analyser Spectrometer

Backscattering Spectrometer

High-Resolution Spin-Echo

Wide-Angle Spin-Echo

Fundamental & Particle Physics



TDR Reference Suite 2013



EUROPEAN SPALLATION SOURCE

Diffraction

Multi-Purpose Imaging

General-Purpose SANS

Broadband SANS

Surface Scattering

Horizontal Reflectometer

Vertical Reflectometer

Thermal Powder Diffractometer

Bispectral Powder Diffractometer

Monochromatic Powder Diffractometer

Materials Science Diffractometer

Extreme Conditions Diffractometer

Single-Crystal Magnetism Diffractometer

Macromolecular Diffractometer

	Cold Chopper Spectrometer			
>	Bispectral Chopper Spectrometer			
cob	Thermal Chopper Spectrometer			
stros	Cold Crystal-Analyser Spectrometer			
spec	Vibrational Spectroscopy			
0)	Backscattering Spectrometer			
	High-Resolution Spin-Echo			
	Wide-Angle Spin-Echo			
	Fundamental & Particle Physics			
	Technical Design Report Technical Design Report 2013 TDR European Spallation Squire			

TDR Reference Suite 2013



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Structures Large-Scale

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Monochromatic P Diffractometer **Materials Science** Diffractometer

Extreme Condition Diffractometer

Macromolecular Diffractometer

Multi-Purpose Imaging	🔊 🗞 🖉 🏹
General-Purpose SANS	🕹 🗞 🞸 💈
Broadband SANS	🔊 🗞
Surface Scattering	🔊 🗞 🍐 🞸
Horizontal Reflectometer	🤌 🗞 🍐
Vertical Reflectometer	🧭 🦆 💈 🗞
Thermal Powder Diffractometer	🕹 💈 🥕 👉
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Macromolecular Diffractometer	S

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pede	Vibrational Spectroscopy	💞 🧕 💈
<i>.</i> ,	Backscattering Spectrometer	🔊 🗞 🍐
	High-Resolution Spin-Echo	🔊 🗞 🎍 💈
	Wide-Angle Spin-Echo	🧀 🍪 🎸 💈
	Fundamental & Particle Physics	201
*	life sciences	magnetism & superconductivity
0	soft condensed matter	engineering & geo-sciences
	chemistry of materials	archeology & heritage conservation
/	energy research	fundamental & particle physics

Selected Instruments Now



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Diffractometer \square

MAGIC Magn. Diffr.

NMX Macromol. Diffr.





Instrument Selection Process



- ESS and Partners developed concepts
 - guided by Science Symposia
 - coordinated centrally by ESS
 - concept development as in-kind contributions
- Annual instrument proposal rounds (2012,13,14)
 - peer-review panels (STAPs and SAC)
 - guided by early success strategy
 - accepted instruments built as in-kind contributions

Science Symposia



Neutrons and Food 29 Jan - 1 Feb 2012, Delft

- Organised by the community
- ESS co-funding with some strings attached
 - make recommendations on how ESS can contribute to their field
 - we input into the agenda
 - output: report with specific recommendations for us
- 23 science symposia held during 2011-2015



Instrument Concepts 2010-14



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Diffraction

Conventional SANS	
Small-Sample SANS	
Compact SANS	
Broadband SANS	ess
Liquids Reflectometer	
Magnetism Reflectometer	
Vertical Focusing Reflectometer	8
Horizontal Focusing Reflectometer	
Fast Kinetics Liquids Reflectometer	ess
Macromolecular Diffractometer	ess
Cold Magnetism Single-Crystal Diffractometer	ess
Thermal Magnetism Single-Crystal Diffractometer	Ũ
Bispectral Powder Diffractometer	
Extreme Environments Beamline	
High-Pressure Diffractometer	ess
Hybrid Multiscale Diffractometer	
Thermal Powder Diffractometer	ess
Pulsed Monochromatic Diffractometer	ess
Multiplexing Engineering Diffractometer	
In-Situ Engineering Diffractometer	
High Flexibility Engineering Diffractometer	ess

Z	Cold Chopper Spectrometer	
	Bispectral Chopper Spectrometer	
	Thermal Chopper Spectrometer	
Ö.	Broadband Chopper Spectrometer	ess
OSC	Crystal Monochromator Spectrometer	
	Crystal-Analyser Spectrometer	
Ő	Backscattering Spectrometer	
<u>N</u>	Vibrational Spectrometer	
	High-Resolution Spin-Echo	
	Wide-Angle Spin-Echo	
	Longitudinal Resonance Spin-Echo	
	Fast Kinetics Imaging	
ag	High-Resolution Imaging	
Ξ	Multi-Purpose Imaging	ess
	Fundamental Physics Beamline	ess
	Ultra-Cold Neutron Facility	ess
È	Chip Irradiation Facility	
	Neutron-AntiNeutron Oscillations	

39 instrument concepts studied + 8 add-ons

Managing Instrument Concept Development

- Arrange into 11 Instrument Classes
 - SANS, Reflectometry, Macromolecular Diffraction, Single-Crystal Diffraction, Powder Diffraction, Engineering Diffraction, Imaging, Direct-Geometry Spectroscopy, Indirect-Geometry Spectroscopy, Spin-Echo, Fundamental Physics
- Recruit Instrument Scientists to manage Concept Development
 - Instrument Class Coordinators
- Set up an advisory panel for each Instrument Class:
 - Scientific and Technical Advisory Panel (STAP)
- Persuade/Cajole/Push/Manipulate teams into collaborating and adapting
 - Instrument Class Coordinators and STAPs
 - Twice-Yearly In-Kind Collaboration (IKON) Meetings
- Deliverable for each Instrument Concept Development: Instrument Proposal
 - science case, instrument description & performance, technical risks
- Annual Reviews of Instrument Proposals
 - 2012: 4 proposals
 - 2013: 16 proposals
 - 2014: 11 proposals
- Peer Reviews by STAPs and Scientific Advisory Committee (SAC)

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Instrument Concepts 2010-14



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Instrument Concepts 2010-14



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Large-Scale Structures

Diffraction

Conventional SANS		proposal 2013 🗸		
Small Sample SANS				
Compact SANS	pro	oposal 2012&13 🗡		
Broadband SANS		proposal 2012 🗸		es
Liquids Reflectometer		proposal 2013 🗡		
Magnetism Reflectometer	pro	oposal 2013&14 X		
Vertical Focusing Reflector	met	proposal 2013 🗸		
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Fast Kinetics Liquids Refle	cton	proposal 2013 🗸		ess
Macromolecular Diffracto	met	proposal 2012 🗸		ess
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Pulsed Monochromatic Di	ffra	proposal 2014 🗡		ess
Multiplexing Engineering	liffr	actometer		
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bG	Fast Kinetics Imaging				
agi	High-Resolution Imaging	proposal 2012			
Ë	Multi-Purpose Imaging				
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Selected Instruments Now



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Diffractometer \square

MAGIC Magn. Diffr.

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- TDR: 2 NSE instruments: high-resolution (IN15) and wide-angle (SPAN)
- 2014 proposal round
 - ESSENSE (FZJ) not supported by SAC: unclear if high-resolution or wide-angle should be first
 - NSE science workshop: high-resolution NSE is priority

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- 2015 competing proposals
 - ESSENSE (FZJ) conventional high-resolution

				Fully-compensated superconducting
Wavelength range	3 – 25 Å	Max. field integral	> 1.5 T.m	coils with magnetic shielding
Bandwidth	8 Å	τ-range	1ps-1µs	Very low field-integral inhomogeneity



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 - RESPECT (TUM) longitudinal neutron resonant spin-echo (LNRSE) not endorsed by STAP
 - SAC advice: postpone decision until LNRSE is more mature
- Technical issues to address
 - ESSENSE: resistive or superconducting (IN15 and J-NSE upgrades)
 - RESPECT: longer Fourier times (RESEDA), focusing guide with LNRSE, study field correction
- Project decision
 - Go ahead with the other 15 instruments
 - NSE not included in instrument suite yet

Neutron Spin-Echo



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36

Neutron Spin-Echo at ESS in 2015



- Strongly flux-limited technique
 - rather specialised community
- ESS instrument may be transformative for wider user community
- Technical uncertainties
 - ESSENSE: resistive or superconducting coils?
 - RESPECT: very immature technique
- Two-year programme
 - demonstrate promise of longitudinal resonant spin-echo
 - can neutron guides be used within "precession" region?
 - can conventional and LNRSE techniques be combined?
- August 2015: FZJ and TUM decide to collaborate on CONSENS
 - ESS welcomes collaboration and emphasises resolving technical issues
- November 2015: CONSENS kick-off meeting
 - work plan agreed on for answering technical issues
 - hybrid instrument being developed
 - plan to end work in 2017
 - agreement to invite STAP advice in 2016
 - ESS needs to be able to make a well-informed decision on the best HR-NSE instrument

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Spin-Echo STAP Meeting (Garching)



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Friday 16/9/2016

9:00	Welcome & ESS Update Ken Andersen
9:30	NSE History and Meeting Scope Melissa Sharp
10:00	Presentation of CONSENS design
13:00	Presentation of CONSENS results
15:00	Closed Session
16:00	Feedback

STAP members

Georg Ehlers

Stéphane Longeville

Thomas Keller

(Hitoshi Endo)

Peter Falus

Jason Gardner

ESS team

Ken Andersen

Melissa Sharp

ESSENSE team

Michael Monkenbusch

Stefano Pasini

Teddy Kozielewski

RESPECT team

Christian Pfleiderer

Peter Böni

Instrument Status

- CONSENS
 - highest possible resolution for both soft and hard condensed matter
 - combines standard NSE and LRNSE
 - MIEZE option allows high magnetic fields at sample



Instrument Status



- Coil upgrades: IN15 & J-NSE
 - field profiles
 - correction elements
- RESEDA upgrades
 - L-MIEZE demonstrated: 5 orders of magnitude in t_{NSE}
 - demonstration of straight guide
- Optimisation of CONSENS primary spectrometer
 - adaptation to new moderator geometry
 - improved polarisation
 - chopper system



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NSE STAP Findings & Recommendations

- Hybrid CONSENS instrument is not viable
 - well-optimised ESSENSE
 - highly compromised RESPECT add-on
- Great progress made in LNRSE development
- Stop development of hybrid instrument
- Update and improve ESSENSE
 - study SNS-NSE limitations and apply lessons
 - profit from IN15 and J-NSE upgrades: evaluate NC vs SC coils
- Continue work on RESEDA to improve RESPECT
 - demonstrate longer Fourier times
 - compatibility with focusing optics
 - need for and performance of field correction elements
- Produce updated proposals in 2017/18
 - timing to be determined by proposal rounds for instruments 16-22

NSE Add-Ons



- Only full instrument concepts considered so far
 - 8 add-on options were also considered
- TU-Delft considered several NSE add-ons in 2011-15
 - SANS: accessing lower Q via SESANS and SEMSANS
 - Reflectometer: measuring in-plane structures via SERGIS
 - Imaging: dark-field imaging using SEMSANS
 - Diffractometer: accessing inelastic information using TOFLAR

Larmor labelling techniques

- TOFLAR labelling of wavelength
- SESANS
 SERGIS labelling of scattering angle
 SEMSANS



Larmor labelling techniques

• TOFLAR labelling of wavelength



Intensity at detector: $I(B) = \int i(B, \lambda) d\lambda$ is the Fourier transform of the spectrum





TOFLAR applied in neutron diffraction



Bragg peaks: elastic-coherent

Background:

- Elastic-coherent (static disorder)
- Elastic-incoherent
- Inelastic-coherent
- Inelastic-incoherent

can be determined by means of TOFLAR add-on (modulator, < 2m, in primary beam)

Test measurements at SNS and ISIS are not yet decisive^{1,2}, will be continued

¹Kusmin *et al.*, EPJ Web of Conferences **83** (2015) 03009 ²Kusmin *et al.*, ISIS experimental report RB1620260



Larmor labelling techniques

SESANS
 SERGIS labelling of scattering angle



- precession field before and after sample
- spin-echo polarisation as a function of wavelength and magnetic field yields structural correlation function in real space
- coding direction / structural information : *y*-direction
- length scale: 30 nm 10 μ m



Larmor labelling techniques

• SEMSANS labelling of scattering angle



- alternative for SESANS³
- all spin-manipulation components before sample (magnetic samples possible)
- for right combination α_1 , α_2 , B_1 , B_2 , L_1 , L_2 : intensity modulation on detector
- with sample: decrease of modulation amplitude \rightarrow structural information
- length scale: 30 nm 10 μ m

³Bouwman *et al.*, Physica B 404 (2009) 2585

SANS with SEMSANS add-on at LOKI ⁴



- replace beam stop by SEMSANS detector
- simultaneous SANS/SEMSANS: scale probed: $1 \text{ nm} 10 \mu \text{m}$

⁴Kusmin *et al.,* NIM A. **856** (2017) 119





length scale (nm)

TUDelft

Conclusions from one decade of research

- Spin-echo signal (SERGIS) in specular intensity only measurable in very special cases (highly-scattering sample, e.g. from gratings⁵)
- SERGIS has to be determined in off-specular intensity
- This means that in-plane structures > 10 μ m should be present
- SERGIS is sensitive for structures ~ 10 500 nm
- Science case: samples with large range of length scales of in-plane structures





Example: dewetted block-copolymer P(dS-b-pMS)⁶



⁶P. Muller-Buschbaum, J. Phys.-Cond. Matter **17** (2005) S363-S386

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Example: dewetted block-copolymer P(dS-b-pMS)

SERGIS with monochromatic reflectometer (ADAM, ILL)⁷



SERGIS signal was determined in off-specular intensity (ROI), i.e. very weak signal

⁷A. Vorobiev *et al.,* J. Phys. Chem. B **115** (2011) 5754



Example: dewetted block-copolymer P(dS-b-pMS)

SERGIS with TOF reflectometer (Offspec, ISIS)⁸



⁸A. A. van Well *et al.*, ESS-report (2014)



Conclusion:

- With monochromatic setup all neutron intensity cab be focussed on narrow area in Q-space, while in TOF setup intensity is spread over large Q-area (compare 3-axis - TOF)⁹
- That is why the ILL SERGIS on weak-scattering samples is more successful as compared to the ISIS experiments
- Since the average neutron flux of ESS is comparable to ILL flux, the SERGIS signal at ESS will sufficient
- Moreover, a large Q-range will be probed simultaneously, with at least the same quality as the ILL results (see figure: total plot, TOF, versus white line, mono)
- Science case: large range of length scales should be present
- Possible inplementation in FREIA





⁹S.R. Parnell *et al.*, ICANS (2017)

Tentative Instrument Ramp-up



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based on Instrument Construction Working Schedule V3.1, 25/4/2017



Instrument Concepts for Evaluation



- Update Existing Instrument Proposals
 - VOR Broadband Chopper Spectrometer (already endorsed by SAC)
 - ESSENSE & RESPECT High-Resolution NSE
 - ANNI Fundamental Physics
 - ESPRESSO High-Pressure Diffraction
 - SLEIPNIR Bio-SANS
 - HOD Crystal-Monochromator Diffractometer with Polarisation Analysis for Hydrogenous Systems
- Develop New Instrument Proposals
 - Surface Scattering
 - Alternative High-Resolution NSE
 - Wide-Angle NSE
 - Very Fast Crystal-Analyser Spectrometer (as proposed by Rob Bewley at ECNS 2015)
 - Ultra-Cold Neutrons (based on Expression of Interest from 2015 proposal round)

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Diffractometer \square

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Possible Instruments for Round 1 (2019)?



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Possible Instruments for Round 1 (2019)?



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Round 2 (2021): Space for exciting new ideas Open call with competitive process



Tentative Instrument Ramp-up

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Thank You!

