# **JCNS Workshop 2011**

# Trends and Perspectives in Neutron Instrumentation:

# From Continuous to Spallation Sources

# 4 - 7 October 2011, Tutzing

**Topics:** 

- Large scale instrumentation
- Inelastic instrumentation
- Neutron diffraction
- Engineering materials diffraction
- Polarization/polarization analysis
- Larmor precession instruments
- Instrument components
- Neutron imaging

# Abstract booklet







#### Dear colleagues,

With new spallation sources taken into operation in the USA and Japan, as well as with the decision to build the long-pulse spallation source in Europe, the centre of gravity in developments of neutron instrumentation is shifted towards the spallation sources.

The aim of this workshop organized by the Jülich Centre for Neutron Science is to discuss this transition from the point of view of the most effective use of the knowledge accumulated during the design/construction of modern instruments at continuous sources. Certainly ideas coming from the use of new instruments at spallation sources, as well as completely new ideas for the spallation source instrumentation are also within the focus of this workshop.

Experts in the neutron scattering instrumentation gather in Tutzing with the aim to discuss the latest advances in neutron instrumentation at the continuous sources and short-pulse spallation sources. The state of the art in some vital components of neutron instruments (choppers, polarizers/analyzers, detectors, etc.) is also covered and necessary developments towards their use for the spallation source instrumentation will be addressed.

Topics include:

- Large scale instrumentation (SANS, reflectometry)
- Inelastic instrumentation (cold/thermal TOF, backscattering)
- Neutron diffraction (powder and single crystal)
- Engineering materials diffraction
- Polarization/polarization analysis
- Larmor precession instruments
- Instrument components (choppers, detectors, etc.)
- Neutron imaging

During the next days about 50 invited and contributed presentations will be given and exciting posters will add additional information in the mentioned topics. We would like to believe that this workshop at a gorgeous site at the Starnberger See will advance the field and we are looking forward to fruitful discussions and to a stimulating exchange of knowledge.

Scientific Organizing Committee

Thomas Brückel Alexander Ioffe Dieter Richter Gernot Heger Michael Monkenbusch Werner Schweika



Tu	esday, 4. October 2011	Der 2011 Wednesday, 5. October 2011		Th	Thursday, 6. October 2011		Friday, 7. October 2011	
08:30		08:30	M. Arai	08:30	F. Mezei			
		09:10	J. Stahn	09:10	T. Unruh	08:50	K. W. Herwig	
		09:30	R. Steitz	09:30	J. Ollivier	09:30	J. Kulda	
		09:50	S. Mattauch	09:50	A. Stampfl	10:10	R. Kampmann	
		10:10	E. Watkins	10:10	J. Voigt	10:30	R. Sadykov	
	Registration	10:30	Coffee break	10:30	Coffee break	11:00	Coffee break	
	-	11:00	V. Haramus	11:00	A. Hiess	11:20	N. Kardjilov, M. Stro	
		11:20	D. Martin Rodriguez	11:20	K. Nemkovskiy	11:40	R. Kampmann	
		11:40	R. Dalgliesh	11:40	J. Kulda	12:00	M. Klein	
		12:00	R. Georgii	12:00	M. Russina	12:20	Closing remarks	
		12:20	Session discussion	12:20	Session discussion	12:30	Lunch	
12:30	Lunch	12:40	Lunch	12:40	Lunch	· · · ·		
13:30	Opening of the workshop	13:30	D. Nekrassov	13:30	F. Demmel			
13:40	K. Andersen	13:50	A. loffe	13:50	B. Frick			
14:20	O. Holderer	14:10	T. Keller	14:10	N. Jalarvo			
14:40	J. Plomp	14:30	T. Oku	14:30	T. Seydel			
15:00	M. Monkenbusch	14:50	C. Zendler	14:50	D. Middendorf			
15:20	W. Häußler	15:10	Session discussion	15:10	Session discussion			
15:40	K. Habicht	15:30	Coffee break	15:30	Coffee break			
16:00	Session discussion	16:00	E. Babcock			-		
16:20	Coffee break	16:20	C. Gösselsberger					
16:50	A. Balagurov	16:40	E. Lelievre-Berna			_		
17:10	M. Blakeley	17:00	M. Strobl	16:45	Walk to the			
17:30	HG. Brokmeier	17:20	Session discussion		Forsthaus "Ilkahöhe			
17:50	A. Gukasov				(about 6km)			
18:10	C. Hoffmann			7 L	(option: bus transfer)	]		
18:30	T. Kamiyama	17:40	Postersession	18:30	Workshop Dinner			
18:50	Session discussion					-		
10.00	Dinner	19.30	Dinner	1				

Status: 2011-09-27

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# **Evangelische Akademie Tutzing**

# Site Map



#### JCNS Workshop 2011 "Trends and Perspectives in Neutron Instrumentation: From Continuous to Spallation Sources October 4-7, 2011, Tutzing

#### Program

#### Tuesday, October 4, 2011

13:30 Opening of the workshop and welcome

#### **Overview Talk**

1 13:40 Ken Andersen, European Spallation Source, Lund, Sweden Long-pulse instruments for the European spallation source

#### **Larmor Precession Instruments**

- 2 14:20 Olaf Holderer, Jülich Centre for Neutron Science, Garching, Germany Depth resolved dynamics studied with NSE under grazing incidence: surface influence on membrane fluctuations 3 14:40 Jeroen Plomp, Delft University of Technology, Delft, The Netherlands Development of DC magnets with a large range in spin-echo encoding angle. 4 15:00 Michael Monkenbusch, Forschungszentrum Jülich, Jülich, Germany The JCNS neutron spin-echo spectrometer SNS-NSE at the Spallation **Neutron Source in Oak Ridge** 5 15:20 Wolfgang Häußler, Forschungsneutronenquelle Heinz Maier-Leibnitz and Physik Department E21, TU München, Garching, Germany **Experiments using NSE, NRSE and MIEZE-I at RESEDA** 6 15:40 Klaus Habicht, Helmholtz Zentrum Berlin, Berlin, Germany Neutron instrumentation paving the way for the future in pulsed sources
  - 16:00 Final discussion larmor precession instruments

#### 16:20 Coffee Break

#### **Neutron Diffraction**

7	16:50	Anatoly M. Balagurov, Frank Laboratory, Dubna, Russia Correlation Fourier technique for high resolution diffractometry at long-pulse neutron sources
8	17:10	Matthew P. Blakeley, Institut Laue Langevin, Grenoble, France LADI-III – A neutron Laue diffractometer for macromolecular crystallography
9	17:30	Heinz-Günter Brokmeier, Clausthal University of Technology, Germany <b>Texture gradients as part of the microstructure</b> – challenge for the ESS

10	17:50	Arsen Gukasov, Leon Brillouin Laboratory, Gif sur Yvette, France Challenges in single crystal neutron diffraction on continuous and spallation sources
11	18:10	Christina Hoffmann, Oak Ridge National Laboratory, Oak Ridge, USA <b>Time-of-flight neutron single crystal diffraction at TOPAZ</b>
12	18:30	Takashi Kamiyama, KEK, Tsukuba, Japan Challenge of the J-PARC neutron powder diffraction
	18:50	Final discussion neutron diffraction
19:00 D	inner	

#### Wednesday, October 5, 2011

#### **Overview Talk**

13	8:30	Masatoshi Arai, J-PARC Center, Tokai Mura, Japan
		An optimization consideration on a pulsed neutron source
		- experiences on J-PARC

#### Large Scale Instrumentation - Reflectometry

14	9:10	Jochen Stahn, Paul Scherrer Institut, Villigen, Switzerland TOF reflectometry at the PSI: from an optical bench set-up to a new instrument concept with a focus on small samples
15	9:30	Roland Steitz, Helmholtz Zentrum Berlin, Berlin, Germany From BioRef to new frontiers – the more to come for soft matter interfaces with next generation instruments
16	9:50	Stefan Mattauch, Jülich Centre for Neutron Science, Garching, Germany From MARIA to a reflectometer at the ESS
17	10:10	Erik Watkins, Institut Laue Langevin, Grenoble, France FIGARO: ILL's horizontal neutron reflectometer

10:30 Coffee Break

#### Large Scale Instrumentation - SANS

18	11:00	Vasyl Haramus, Helmholtz Zentrum Geesthacht, Geesthacht, Germany Variable collimation line for SANS at ESS for high intensity and high resolution
19	11:20	Damian Martin Rodriguez, Forschungszentrum Jülich, Jülich, Germany SANS instrument for small samples at the European Spallation Source
20	11:40	Robert Dalgliesh, ISIS, Didcot, United Kingdom Offspec: SESANS and SERGIS at ISIS
21	12:00	Robert Georgii, Forschungsneutronenquelle Heinz Maier-Leibnitz and Physik Department E21, TU München, Garching, Germany Large scales - long times: Adding time resolution to SANS and reflectometry
	10.00	

12:20 Final discussion large scale instrumentation

#### 12:40 Lunch

#### **Instrument Components I**

22	13:30	Daniil Nekrassov, Helmholtz Zentrum Berlin, Berlin, Germany The VITESS Monte Carlo simulation software
23	13:50	Alexander Ioffe, Jülich Centre for Neutron Science, Garching, Germany <b>Neutron polarization in VITESS</b>
24	14:10	Thomas Keller, Max Planck Institut für Festkörperforschung, Stuttgart, Germany Active monochromators for TAS instruments
25	14:30	Takayuki Oku, JAEA, Tokai, Japan <b>Current status and perspective of neutron optical device developments</b> <b>for neutron scattering experiments at J-PARC</b>
26	14:50	Carolin Zendler, Helmholtz Zentrum Berlin, Berlin, Germany The combination of bi-spectral extraction systems and elliptical guides studied by Monte Carlo simulations
	15:10	Final discussion instrument components I

#### 15:30 Coffee Break

#### **Polarization/Polarization Analysis**

27	16:00	Earl Babcock, Jülich Centre for Neutron Science, Garching, Germany Considerations on tradeoffs between super mirrors and <sup>3</sup> He spin filters for polarization analyzers on wide dynamic Q-range instrumentation
28	16:20	Christoph Gösselsberger, Vienna University of Technology, Vienna, Austria Neutron pulse tailoring by means of a spatial magnetic spin resonator
29	16:40	Eddy Lelievre-Berna, Institut Laue Langevin, Grenoble, France Polarised neutron capabilities: from continuous to pulsed beams
30	17:00	Markus Strobl, Helmholtz Zentrum Berlin, Berlin, Germany and European Spallation Source AB, Lund, Sweden Shared basic concepts for neutron reflectometry and imaging at a long pulse target station
	17:20	Final discussion polarization/polarization analysis
	18:00	Poster Session

#### 19:30 Dinner

#### Thursday, October 6, 2011

#### **Overview Talk**

31 8:30 Ferenc Mezei, European Spallation Source ESS AB, Lund, Sweden Neutron beam generation, extraction and instrumentation at the long pulse source ESS: New opportunities and challenges

#### **Inelastic Instrumentation – Cold/Thermal TOF**

32	9:10	Tobias Unruh, Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany <b>The TOFTOF spectrometer at FRM II and perspectives for a</b> <b>high-resolution chopper spectrometer at ESS</b>
33	9:30	Jaques Ollivier, Institut Laue Langevin, Grenoble, France Time-of-flight spectrometers for single crystal spectroscopy on steady state reactor
34	9:50	Anton P. J. Stampfl, Bragg Institute, Lucas Heights, Australia and The University of Sidney, Sidney, Australia <b>Optics for small-spot neutron spectroscopy: towards neutron</b> <b>spectromicroscopy</b>

35 10:10 Jörg Voigt, Jülich Centre for Neutron Science, Garching, Germany Direct geometry time-of-flight spectrometers for ESS

#### 10:30 Coffee Break

36	11:00	Arno Hiess, Institut Laue Langevin, Grenoble, France and European Spallation Source AB, Lund, Sweden Ideas on inelastic neutron scattering instrumentation for kinetic experiments and when using extreme conditions
37	11:20	Kirill Nemkovski, Jülich Centre for Neutron Science, Garching, Germany <b>TOPAS, the future thermal time-of-flight spectrometer at FRM II</b>
38	11:40	Jiri Kulda, Institut Laue Langevin, Grenoble, France <i>exTAS</i> – <b>next generation crystal spectrometer for small samples and</b> <i>extreme conditions</i>
39	12:00	Margarita Russina, Helmholtz Zentrum Berlin, Berlin, Germany Multiplexing techniques: adjustable short pulses at a long pulse spallation source
	12:20	Final discussion inelastic instrumentation – cold/thermal TOF

#### 12:40 Lunch

#### **Inelastic Instrumentation – Back-Scattering**

40	13:30	Franz Demmel, ISIS, Didcot, UK <b>ToF-Backscattering at ISIS: state of the art and perspectives</b>
41	13:50	Bernhard Frick, Institut Laue Langevin, Grenoble, France The new IN16B at ILL, its BATS option and some thoughts towards backscattering at ESS

42	14:10	Niina Jalarvo, JCNS-SNS, Oak Ridge, USA BASIS backscattering spectrometer at SNS
43	14:30	Thilo Seydel, Institut Laue Langevin, Grenoble, France Perspectives and science examples using the backscattering technique
44	14:50	H. Dieter Middendorf, University of Oxford, Oxford, United Kingdom Biomolecular dynamics with neutrons: Instrumental aspects of the widening scope and likely impact of experiments on functionally important systems
	15:10	Final discussion inelastic instrumentation back-scattering

#### 15:30 Coffee Break

#### 18:30 Workshop Dinner at the Forsthaus "Ilkahöhe"

#### Friday, October 7, 2011

#### **Overview Talk**

45	8:50	Kenneth. W. Herwig, Oak Ridge National Laboratory, USA Neutron scattering instrumentation at the ORNL spallation neutron source: some lessons learned
46	9:30	Jiri Kulda, Institut Laue Langevin, Grenoble, France Neutron instrumentation at a continuous source: the ILL Millenium programme and beyond

#### **Engineering Materials Diffraction**

47	10:10	Reinhard Kampmann, Helmholtz Zentrum Geesthacht, Germany Perspectives for materials investigations at the structured pulse engineering diffractometer (SPEED)
48	10:30	Ravil A. Sadykov, Institute for Nuclear Research, Moscow and HPPI, Troits, Russia <b>The first experiments on high pressure neutron diffractometer</b> <b>"Hercules"</b>

#### 10:50 Coffee Break

#### **Neutron Imaging**

49	11:20	Nikolay Kardjilov, Helmholtz Zentrum Berlin, Germany,
		and ESS-AB, Lund, Sweden
		Prospects of neutron imaging and imaging instrumentation at a long
		pulse source

#### **Instrument Components II**

50	11:40	Reinhard Kampmann, Helmholtz Zentrum Geesthacht, Geesthacht und
		DENEX – Detektoren für Neutronen, Lüneburg, Germany
		Development of novel neutron detectors with thin conversion layers
51	12:00	Martin Klein, CDT* GmbH, Heidelberg, Germany The <sup>10</sup> B based Jalousie neutron detector – our alternative for for <sup>3</sup> He filled PSD counter tubes
	12:20	Closing remarks, end of the workshop

#### 12:30 Lunch

#### **Poster presentations**

Aurel Radulescu, Jülich Centre for Neutron Science KWS-2 – the high intensity/wide-Q SANS diffractometer for biology and soft-matter systems at FRM II

Marcus Trapp, University of Heidelberg Neutron spin echo encoded scattering at BioRef – a new approach to studying complex interfaces

Vitaly Pipich, Jülich Centre for Neutron Science Very small angle neutron scattering diffractometer with focusing mirror: from continuous to spallation sources

Andreas Houben, RWTH Aachen POWTEX – high intensity neutron time-of-flight diffractometer at FRM II

Tobias E. Schrader, Jülich Centre for Neutron Science Design considerations for the instrument BioDiff and some implications for a similar instrument at a spallation source

Ravil Sadykov, Institute for Nuclear Research, Troitsk High pressure diffractometer "Hercules" on a spallation source of IN06 (INR RAS)

Nadir Aliouane, Paul Scherrer Institute Development concepts of Trics: the neutron single crystal diffractometer at the SINQ

Henrich Frielinghaus, Jülich Centre for Neutron Science Structure of microemulsions confined near planar surfaces

Thomas Krist, Helmholtz-Zentrum Berlin Neutron optics from Helmholtz-Zentrum Berlin

Michaela Zamponi, Jülich Centre for Neutron Science The Jülich neutron spin echo spectrometer J-NSE at the FRM II

Nikolas Arend, Jülich Centre for Neutron Science Current technical status and performance of the spin-echo spectrometer SNS-NSE at the spallation neutron source in Oak Ridge

Thomas Krist, Helmholtz-Zentrum Berlin The neutron guide upgrade project at HZB

Andrew Cole, The University of Sheffield Fast neutron scintillation detectors using wavelength shifting lightguides

John McMillan, The University of Sheffield High-efficiency large area neutron scintillation detectors as replacements for helium-3 proportional tubes John McMillan, The University of Sheffield The Sheffield pulsed neutron facility

Julius Schneider, Ludwig-Maximilians-Universität München Pseudostatistic TOF-chopper system for separation of elastic and inelastic neutron scattering with continuous variation of energy resolution

Paul Henry, European Spallation Source ESS AB Powder diffraction instrumentation at the ESS

Roland Steitz, Helmholtz-Zentrum Berlin Design of a generic neutron reflectometer adapted to a long pulse spallation neutron source

Earl Babcock and Zahir Salhi, Jülich Centre for Neutron Science Design study of magnetic environments for XYZ polarization analysis using <sup>3</sup>He for the Diffuse Neutron Scattering spectrometer DNS

Earl Babcock, Jülich Centre for Neutron Science Status of instrumentation using polarized <sup>3</sup>He neutron spin filters at the JCNS

Philipp Schmakat, Physik-Department E21, Technische Universität München and Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Garching Neutron depolarisation imaging JCNS Workshop 2011

### **Trends and Perspectives in Neutron Instrumentation:**

### **From Continuous to Spallation Sources**

#### Abstracts

Status: September 27, 2011

#### Depth resolved dynamics studied with NSE under grazing incidence: surface influence on membrane fluctuations

**Olaf Holderer<sup>1</sup>**, Michael Kerscher<sup>2</sup>, Michael Monkenbusch<sup>2</sup>, Henrich Frielinghaus<sup>1</sup>, Dieter Richter<sup>1,2</sup>

 <sup>1</sup>Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, 85747 Garching, Germany
 <sup>2</sup>Jülich Centre for Neutron Science & Institute for Complex Systems, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Microemulsions near planar hydrophilic surfaces are ordered lamellar, while the bulk structure is bicontinuous. This has been proven with grazing incidence small angle neutron scattering measurements (GISANS), neutron reflectometry, and computer simulations [1]. The GISANS studies have been extended in the present work to neutron spin echo experiments under grazing incidence (GINSES – Grazing Incidence Neutron Spin Echo Spectroscopy). By varying the incident angle and the overall contrast of the liquid against the solid, the penetration depth of the evanescent wave has been tuned between  $\sim 40 - 100$  nm. The dynamics of the surfactant membrane of the microemulsion could be studied with this setup as a function of the distance to the hard wall. It was found that the characteristic relaxation time of the membrane undulations decreases close to the hard surface. This effect is interpreted as a modified dispersion relation of the undulation spectrum of the membrane due to the confining wall. The depth resolved dynamic measurements on the nanosecond scale are the first of its kind.

[1] M. Kerscher et al., Phys. Rev. E 83 030401(R) (2001).

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October 4, 2011, 14:40h

#### Development of DC magnets with a large range in spin-echo encoding angle.

Jeroen PLOMP<sup>1</sup>, Steven JARGO<sup>2</sup>, Robert Dalgliesh<sup>2</sup>

<sup>1</sup>Faculty of Applied Sciences, Delft University of Technology, Mekelweg 15, 2629 JB Delft, The Netherlands

<sup>2</sup>ISIS, Harwell Science and Innovation Campus, Science and Technology Facilities Council, Didcot OX11 0QX, UK

Using DC magnets with parallelogram shaped pole shoe in combination with RF flippers have been used for spin-echo small angle encoding for years. It has also been shown that the magnetic angle produced by such a configuration is usually different compared to the physical angle of the magnet with the beam. We will demonstrate that the line integral measurements of such a magnet will give the same result as calibration measurements using neutrons and a grating. Even detailed simulations of the magnetic field of such a magnet in OPRA have resulted in the same answer. Therefore we have use OPRA to design a new shaped magnet that can be set within an unprecedented large range of encoding angles, from 90° to 25°. The predictions by these computer simulations of the encoding angle and resolution have been confirmed with a scaled simplified prototype.

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# The JCNS neutron spin-echo spectrometer SNS-NSE at the Spallation Neutron Source in Oak Ridge

Michael OHL<sup>1</sup>, Nikolas AREND<sup>1</sup>, Changwoo DO<sup>1</sup>, Tadeusz KOZIELEWSKI<sup>1</sup>, **Michael MONKENBUSCH<sup>2</sup>**, Melissa SHARP<sup>3</sup>, Dieter RICHTER<sup>4</sup>

<sup>1</sup>Jülich Centre for Neutron Science, Outstation at the SNS, Oak Ridge, USA

<sup>2</sup> JCNS-1, Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, 52425 Jülich

<sup>3</sup> European Spallation Source AB (ESS), JCNS Outstation at the SNS, Oak Ridge, USA

<sup>4</sup> ICS-1 & JCNS-1, Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, 52425 Jülich

The new instrument NSE@SNS is a high resolution neutron spin-echo spectrometer located at beamline 15 (could coupled  $H_2$  moderator) of the SNS. Currently it is the only spin-echo spectrometer at a pulsed spallation source. It has two superconducting main solenoids, which are stray field compensated such that the instrument can be operated in a double walled magnetic shielding. The latter is integrated in the radiation shield. The neutrons are polarized by a solid state bender realizing also a  $3.5^{\circ}$  kink in the beam direction such that direct sight is avoided. A system of 4 disk choppers is used to select the wavelength frame and to adopt its width according to the chosen distance from the moderator (detector distance 18m..27m). Auxiliary coils and flippers enable a special mode for very short Fourier times (ps). The field integral correction in the standard mode is performed by 3 sets of correctors ("Pythagoras coils") in each arm. Detection is performed by a  $30x30cm^2$  area detector behind a supermirror analyzer.

First results and operation experience will be reported.

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October 4, 2011, 15:20h

#### Experiments using NSE, NRSE and MIEZE-I at RESEDA

**Wolfgang HÄUßLER**<sup>1,2</sup>, Peter BÖNI<sup>2</sup>, Alexander TISCHENDORF<sup>1,2</sup>

<sup>1</sup>Forschungsneutronenquelle Heinz Maier-Leibnitz II, Lichtenbergstr.1, 85747 Garching,Germany <sup>2</sup>Technische Universität München, Physik Department (E21), James-Franck-Str. 1, 85748 Garching, Germany

The cold neutron spectrometer RESEDA is located in the guide hall of the FRM II (Munich). Using both, the Neutron Spin Echo (NSE) technique and its variant, the Neutron Resonance Spin Echo (NRSE) technique, several studies on magnetic fluctuations in ferro- and helimagnetic compounds and the diffusion of water and hydrogen in porous samples have been performed.

In NRSE as in NSE, the beam polarization is the measured quantity yielding information on the slow dynamics of the sample. Depolarization of the neutron beam by the sample makes NRSE and NSE experiments very challenging. In studies on spin-incoherently scattering samples, i.e. hydrogen containing materials, the theoretical limit for the polarization of the scattered beam is 1/3. In practice, even this value is hardly reached. Moreover, also experiments on magnetic systems, which influence the beam polarization, are difficult or even not feasible at all.

The MIEZE-I technique overcomes these drawbacks of the NSE and NRSE techniques. In this variant of NRSE, all the spin manipulations are performed before the sample in the first spectrometer arm. Thus in MIEZE-I, the depolarization of the neutron beam due to the sample or sample environment does not affect the quality of the measured intermediate scattering function leading to an immediate efficiency gain of a factor of 10 for incoherently scattering samples when compared with NSE or NRSE.

We report on the installation of the MIEZE-I option at the NRSE spectrometer RESEDA focusing on new coil and detector concepts. We present results of first MIEZE measurements comparing them with conventional NRSE data. Finally, we provide an outlook on a new spectrometer concept including NSE, NRSE and MIEZE options.

#### Neutron instrumentation paving the way for the future in pulsed sources

Klaus HABICHT<sup>1</sup>, Markos SKOULATOS<sup>1</sup>, Felix GROITL<sup>1</sup>, Markus STROBL<sup>1</sup>, Muhammer BULAT<sup>1</sup>, Klaus LIEUTENANT<sup>1</sup>, Thomas WILPERT<sup>1</sup>

#### <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

A substantial part of the upgrade program aimed at enhancing the instrument capabilities at the BER II neutron source at the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) is the upgrade of the cold-neutron triple-axis spectrometer FLEX [1]. We report on the current status and recent progress in delivering the new primary spectrometer of FLEX. Important features are the extension of the range of incident neutron energies into the thermal range and the strengthened performance for polarized neutron work. As Larmor labeling is seen as one of the key techniques in the development of novel neutron instrumentation, latest advances in neutron resonance spin echo (NRSE) spectroscopy, where FLEX continues to act as a development platform, will be discussed [2]. The planned upgrade of the secondary spectrometer with a flat-cone option relates the TAS technique hitherto optimally implemented at continuous sources to indirect TOF spectrometers with their high potential at spallation neutron sources.

In the second part of the talk a brief overview is given on several instrumentation and simulation activities which are currently ongoing in the framework of HZB's contribution to the ESS Design-Update phase. A multi-purpose beamline which hosts a flexible chopper cascade is currently under construction. The key feature is a chopper mimicking the ESS source pulse characteristics in pulse length and frequency. This dedicated test beamline is provided for real tests of prototype hardware, new instrument concepts and methodological developments. The HZB detector group contributes with their expertise in MSGC detectors based on <sup>157</sup>Gd/CsI-converters and focuses on high performance readout electronics. The Monte Carlo simulations group tackles a variety of simulation tasks ranging from spectroscopy, neutron spin echo and Larmor instrumentation, diffraction to in-depth studies for a liquid reflectometer and extreme environment instrument optimizations.

[1] M. Skoulatos, K. Habicht, NIM A, 647, 100 (2011).
[2] F. Groitl, K. Kiefer, K. Habicht, Physica B, 406, 2342 (2011).

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# Correlation Fourier technique for high-resolution diffractometry at long-pulse neutron sources

#### Anatoly M. BALAGUROV<sup>1</sup>, Valery A. KUDRYASHOV<sup>2</sup>

<sup>1</sup>Frank Laboratory of Neutron Physics, JINR, Dubna, Russia <sup>2</sup>Petersburg Nuclear Physics Institute, Gatchina, Russia

The reverse time-of-flight Fourier (RTOF) technique [1] is very promising for obtaining a very high resolution at a short flight path and at any type of neutron source. Recently it has been developed to a high degree of perfection at a long-pulse neutron source, the IBR-2 reactor in Dubna [2]. The HRFD and FSD Fourier diffractometers constructed at the IBR-2 proved to be competitive in various applications, especially in precise structural studies and residual stress measurements in bulk samples. Also, there is good reason to believe that the use of a fast Fourier chopper would be the best compromise between the highest  $\Delta d/d$  resolution today and intensity. In particular, the HRFD *d*-spacing resolution depends on the maximum frequency of intensity modulation and may amount to the value of  $\Delta d/d \approx 0.001$  in a wide  $d_{hkl}$  range (0.7 - 5 Å) for the flight path between the Fourier chopper and sample position as short as 20 m.

The pressing problem that has been revealed during the operation of HRFD and FSD instruments is a complicated shape of diffraction lines, which could be asymmetric and usually have small negative depths on one or both sides of the diffraction peak.

In the present paper, after a short introduction of the RTOF technique, a possible solution of this problem is discussed, which is based on the potentialities of modern pickup units and electronics. In addition, a new concept of the HRFD detector is suggested making it possible to considerably increase the detector solid angle. Finally, the idea of improving HRFD resolution to  $\Delta d/d \approx 0.0003$ , which is close to the level obtained at synchrotron diffractometers, is described.

[1] P. Hiismaki, H. Poyry, A. Tiitta, J. Appl. Cryst., 21, 349 (1988).[2] A.M. Balagurov, Neutron News, 16, 8 (2005).

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#### LADI-III - A neutron Laue diffractometer for macromolecular crystallography

#### Matthew P. BLAKELEY<sup>1</sup>

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The <u>Laue diffractometer LADI-III</u> is used for single-crystal neutron studies of biological macromolecules (proteins, nucleic acids) at high resolution (2.5 - 1.5 Å), providing unique information complementary to that derived from macromolecular X-ray studies. By locating the positions of the protons and deuterons, the protonation states of key amino-acid residues, substrates, or inhibitors can be determined, along with the positions and orientations of individual water molecules, providing details that can often be crucial towards understanding the macromolecule's specific function and behaviour.

LADI-III uses a large cylindrical area detector composed of neutron-sensitive image-plates (Gd<sub>2</sub>O<sub>3</sub> doped BaF(Br.I):Eu<sup>2+</sup>), which completely surround the sample (greater than  $2\pi$  steradian coverage) and allows large numbers of Bragg reflections to be recorded simultaneously. A Ni/Ti multilayer filter is used to select a narrow wavelength band-pass of neutrons ( $\lambda_{range} \approx 3-4$  Å,  $\delta\lambda/\lambda \approx 25\%$ ) such that data are collected using quasi-Laue methods, increasing the flux on the sample relative to monochromatic data collection while reducing background scattering and reflection overlap compared to the use of the full white beam. LADI-III is therefore able to rapidly collect diffraction data (~1–14 days) from macromolecular systems covering a wide range of complexity (unit-cells from ~50,000–1,500,000 Å<sup>3</sup>). Moreover, LADI-III is well suited to harness the advantages that perdeuteration (*i.e.* all H replaced by D) offers for data collection (*e.g.* vastly reduced background, increased signal) so that relatively small crystal volumes of ~0.1–0.2 mm<sup>3</sup> can be used. Data are generally collected at room temperature but can also be collected at temperatures down to ~15K, opening the way for new areas of science such as neutron studies of freeze-trapped intermediates of enzymatic reactions.

Operational since mid-2007, LADI-III is an upgraded replacement of the LADI-I instrument, as part of the ILL Millennium Programme. In the first phase of the upgrade (from 2007–2010) LADI-III was installed at the end of cold neutron guide H142. Enhancements to the design of LADI-III, including an improved read-out system and a larger cylindrical neutron image-plate detector (400mm in diameter with a height of 450mm), provided a ~3-fold gain in detective quantum efficiency (DQE) relative to LADI-I (DQE<sub>LADI-III</sub>  $\approx$  46% *cf*. DQE<sub>LADI-I</sub>  $\approx$  16%). The second phase of the LADI-III upgrade is currently underway and involves the relocation of LADI-III to a higher flux end-position, installed on a new super-mirror guide (H14) whose characteristics are tailored to the needs of the instrument. Scheduled to start commissioning in its new position in late October 2011, LADI-III is expected to provide yet further reductions in data collection times and sample volume requirements, and increase the limits on unit-cell volumes that can be studied.

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October 4, 2011, 17:30h

# Texture gradients as part of the microstructure -challenge for the ESS-

#### **Heinz-Günter BROKMEIER**

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The classical definition of microstructure given by Bruno Sander in then 1920<sup>th</sup> includes everything which is related to the arrangement of grains inside a geological sample or body. Consequently, crystallographic texture later-on transferred to metallic materials was considered as part of the microstructure. Because of limitations of suitable experimental methods different part of the microstructure are treated and discussed separately. Recent developments of the last 15 years, on instrumental side as well as on a combined data analysis, offer the investigation of the orientation stereology as described by Bunge and Schwarzer [1]. Orientation stereology is going back to the original definition and combines texture gradient descriptions with grain size and phase distribution as well as misorientation angles between neighbouring grains. Orientation stereology by Bunge and Schwarzer was focused on electron back scattering diffraction (EBSD). Meanwhile, neutron and photon investigation go similar ways combining different information's of the microstructure together.

One way is to use micro-Laue methods to determine single grain orientations which can be a quite favourable technique for time of flight. High penetration, high flux and sufficient local resolution allow in many technical products non-destructive investigations of large samples.

A second way is the combined investigation of intensity pole figures (texture), peak broadening pole figures (defect) and peak shift pole figures (residual stresses). The investigation of texture component related evaluations of time dependant deformation-, recovery- and recrystallization processes have great potential for alloy and process developments in all key technologies.

Texture gradients are important for materials where on one hand anisotropic flow during direct processing of semi-finished and final products occurs and on the other hand where existing anisotropic materials properties favour or limit an application. Present studies focus on acentric tubes and pipes. Sample manipulation using the Stress-Spec robot overcomes the size limits of Eulerian cradle based instruments [2].

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#### Challenges in single crystal neutron diffraction on continuous and spallation sources

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Neutron single-crystal diffraction is the tool of choice to determine the accurate positions of hydrogen atoms in solids and the arrangements of magnetic moments. Since neutron fluxes are typically low compared to those available at synchrotron X-ray facilities, there has been a major effort to maximize the exploitation of the available scattering data. Much emphasis has been placed in particular on the provision of large area detector systems. At present the best performing single crystal diffractometers are located on the continuous sources.

The D19 diffractometer at the ILL which has been equipped with a 120° x 32° multiwire proportional counter since 2007 provides very high data quality for crystallographic work in structural chemistry, physics and the biosciences. Another slightly less precise single-crystal diffraction method is the Laue method where the crystal is illuminated by a broad spectrum of wavelengths, and a large area of neutron-sensitive image plates (VIVALDI at the ILL, KOALA at ANSTO) is used to measure the diffraction spots. Recently a CCD-based Laue diffractometer, CYCLOPS at the ILL, has been constructed which should provide a unique possibility for real-time exploration of reciprocal space and rapid data collection through phase transitions due to its fast readout system. Finally the Very Intense Polarized neutron diffractometer (VIP) at the LLB which combines a large area detector and a hot polarized neutron beam shows an unprecedented efficiency in the measurement of spin densities.

However, the supremacy of the reactor instruments in the domain is threatened by the appearance of the new generation diffractometers on spallation sources like WISH on TS2 at ISIS, TOPAZ at SNS, which in turn will be challenged later by the construction of the long pulse ESS. In this talk a review of neutron diffractometers with area detectors, the receipts of the data reduction and trends of their development will be given.

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October 4, 2011, 18:10h

#### Time-of-flight neutron single crystal diffraction at TOPAZ

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The TOPAZ diffractometer at the Spallation Neutron Source at the Oak Ridge National Laboratory was designed to map large areas of reciprocal space simultaneously using a 3 Å bandwidth spanning a wide wavelength range of 0.5 to 9 Å. Large area detector coverage and a highly efficient guide system contribute to a high flux on sample.

Neutron diffraction data collection time is limited and high efficiency of hardware and software is desirable. The ability of tailoring experiment time and setup to each sample is greatly beneficial to data quality and completeness. Good experiment planning requires not only preparing a suitable sample and adequately aligned beam line hardware but also a software suite that allows optimizing the measurement time and providing efficient data reduction. A sophisticated suite of data planning, data collection and data reduction software specifically developed for TOPAZ provides corrected data for inorganic, organic, large molecule, and thin film single crystal samples.

This contribution will show examples and applications of the first experiments conducted at TOPAZ.

This research is supported by UT Battelle, LLC under Contract DE-AC05-00OR22725 for the U.S. Dept. Energy, Office of Science.

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October 4, 2011, 18:30h

#### **Challenge of the J-PARC neutron powder diffraction**

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Before starting the NPD (Neutron Powder Diffraction) project at J-PARC, we thought we would like to 1) explore the science regions not possible with existing NPD, plunge into 2) real time studies (and *in situ* studies), 3) high throughput measurements (analytical use of NPD), and design 4) dedicated NPD's. 1) is only possible with the highest resolution NPD without sacrificing intensity. 2) is most important now and still room to be developed. 3) is important for materials scientists and we are always trying to attract researchers in industries. 4) includes NPD for engineering diffraction, high pressure, magnetism, chemical reaction, charge/discharge reaction *etc.* Before the end of FY2011, we will have 1) SuperHRPD, 2) NOVA, 3) iMATERIA, 4) Takumi (engineering), PLANET (pressure), SPICA (battery). Our footsteps paused due to the earthquake, but we will restart to shape the future of NPD for materials science.

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October 5, 2011, 8:30h

#### An optimization consideration on a pulsed neutron source - experiences on J-PARC -

#### Masatoshi ARAI

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In order to realize a good performance of an instrument in a pulsed neutron source, it is indispensable to have a thought on "total optimization as a whole".

Especially this philosophy is important for a short pulsed neutron source. Not only a design of instrument itself, but also power of accelerator, of course, proton pulse width, repetition rate, moderator material, moderator temperature, structure of moderator etc. are free parameters for optimization. Those components are directly connected each other and give a resulting performance.

Neutron facility is an interdisciplinary facility and can provide research opportunities for many scientific fields. Hence, it is impossible to identify which instrument has the first priority and we may find a confliction in desired parameters. With this circumstance, finally we need to find a total optimization as a whole and make a decision for a design of instruments and facility with a great compromise. In my talk I will report our experiences on building/designing J-PARC, as an example.

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# TOF reflectometry at the PSI: from an optical bench set-up to a new instrument concept with a focus on small samples

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The neutron reflectometer *Amor* is special in the way that it is built on an optical bench and equipped with choppers. This allows for various operation modes (monochromatic, TOF, polarized, liquid surfaces, etc.) and for rather exotic set-ups. E.g. energy analysis concepts [1] or converging beam optics [2] could be tested.

Recently a 2 m long elliptic reflector was used to focus the divergent beam in the scattering plane to the sample (*Selene* set-up). [3] This way the measurement time for specular reflectometry could be reduced by almost one order of magnitude in TOF mode. First tests using a ml monochromator revealed shortcomings in the reflector geometry, but they showed that a wavelength-angle encoding is possible and should lead to the same gain factor as the TOF operation mode.

A future combination of the Selene concept with an in-plane focusing will lead to an effective flux gain for small samples (*i.e.* of the mm<sup>2</sup> range) of 2 orders of magnitude. The draw-back of this approach is that off-specular reflectivity and incoherent scattering lead to an increased background so that the  $q_z$  range and the dynamic are limited. On the other hand, samples of this size are not accessible at all without focusing or multiplexing.

Based on the experience obtained with *Selene*, a design study for a full instrument is developed, which can be optimized for TOF-mode or white beam operation. This instrument can be seen as a conventional (energy or angle dispersive) set-up with a focusing guide allowing for the convergent beam geometry if appropriate.

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October 5, 2011, 9:30h

# From BioRef to new frontiers - the more to come for soft matter interfaces with next generation instruments

# Markus STROBL<sup>1</sup>, Marcus TRAPP<sup>2</sup>, Martin KREUZER<sup>1,2</sup>, Daniil NEKRASSOV<sup>1</sup>, Klaus LIEUTENANT<sup>1</sup>, **Roland STEITZ**<sup>1</sup>

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BioRef is a versatile novel time-of-flight neutron reflectometer featuring a sample environment for in situ infrared spectroscopy at the reactor neutron source BER II of the Helmholtz Zentrum Berlin für Materialien und Energie (HZB). Due to flexible resolution modes and variable addressable wavelength bands that allow for focusing onto a selected scattering vector range, BioRef enables a broad range of surface and interface investigations and even kinetic studies with subsecond time resolution. The instrumental settings can be tailored to the specific requirements of a wide range of applications. [1, 2]

Based on the flexibility of BioRef we will further present a design study of a next generation instrument operated at a long pulse spallation neutron source and dedicated to soft matter systems addressing in particular free liquid surfaces.

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- [2] M. Strobl, R. Steitz, M. Kreuzer, M. Rose, H. Herrlich, F. Mezei, M. Grunze and R. Dahint, Review of Scientific Instruments 82 (5), 055101-055109 (2011).

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October 5, 9:50h

#### From MARIA to a reflectometer at the ESS

**Stefan MATTAUCH<sup>1</sup>**, Ulrich.RÜCKER<sup>2</sup>, Denis KOROLKOV<sup>1</sup>, Earl BABCOCK<sup>1</sup>, Alexander IOFFE<sup>1</sup> and Thomas BRÜCKEL<sup>2</sup>

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The JCNS has installed the new, high-intensity reflectometer MARIA in the neutron guide hall of the FRM II reactor in Garching. This instrument uses a velocity selector for the monochromatization of the neutron beam, an elliptically focussing guide to increase the flux at the sample position and a double-reflecting supermirror polarizer to polarize the entire cross-section of the beam delivered by the neutron guide.

Unique features of MARIA include (i) vertical focussing with an elliptic guide from 170 mm down to 10 mm at the sample position, (ii) reflectometer and GISANS mode, (iii) polarization analysis over a large 2d position sensitive detector as standard, (iv) adjustable wavelength spread from 10 to 1 % by a combination of velocity selector and chopper, (v) flexible sample table using a Hexapod for magnetic field and low temperature sample environment and (vi) in-situ sample preparation facilities. Together with a 400 x 400 mm<sup>2</sup> position sensitive detector and a time-stable <sup>3</sup>He polarization analyzer based on in-situ Spin-Exchange Optical Pumping (SEOP), the instrument is dedicated to investigate specular reflectivity and off-specular scattering from magnetic layered structures down to the monolayer regime. In addition the GISANS option can be used to investigate lateral correlations in the nm range. This option is integrated into the reflectometer's collimation, so it can be chosen during the measurement without any realignment.

MARIA is a state of the art reflectometer at a constant flux reactor. It gives you the opportunity to investigate easily reflectivity curves in a dynamic range of up to 7-8 orders of magnitude, off-specular scattering, GISANS and even simple SANS measurement. We will discuss the differences and the corresponding parts in the concepts for a time of flight reflectometer at the ESS which has to get the world class instrument.

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#### FIGARO: ILL's horizontal neutron reflectometer

#### Erik WATKINS<sup>1</sup>, Richard CAMPBELL<sup>1</sup>, Robert CUBITT<sup>1</sup>

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The Fluid Interfaces Grazing Angles ReflectOmeter (FIGARO) is a horizontal neutron reflectometer at Institut Laue-Langevin, Grenoble, France. The instrument is a versatile timeof-flight reflectometer suitable for a range of studies in soft condensed matter, chemistry, physics and biology at interfaces. Principal instrument features include a choice of six chopper pairs to balance resolution and flux, deflector mirrors that direct the incident beam upwards or downwards towards the reflecting surface (enabling the study of air/liquid and buried liquid/liquid interfaces) and a 2D detector to record off-specular scattering. The flexibility afforded by this design allows the optimization of flux, minimization of data acquisition times, and the ability to perform fast kinetic studies of thin films.

Launched as a user instrument in April of 2009, FIGARO has now seen two years of service to the neutron science user community. Here, we describe the features of the instrument and its sample environments, and outline some of the scientific highlights to date. Additionally, we discuss progress made in using prisms to encode the neutron wavelength thus allowing a neutron reflectometer on a continuous source to use the full mean flux. With the use of a CCD detector the resolution is satisfactory with considerable flux gains over the conventional TOF technique. Work is continuing to make this an option on either FIGARO or the D17 reflectometer at ILL.

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October 5, 2011, 11:00h

#### Variable collimation line for SANS at ESS for high intensity and high resolution

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We propose a fast change between different options for the collimation line for a conventional SANS instrument at the ESS. A very modular design of the collimation line, which serves for the investigations from fast kinetic in the time scale of milliseconds to samples of less than millimeter size, is a concept with large potential. A SANS instrument with a flexible 4-path collimation line comprised of fast changeable collimators-neutron guides system for kinetic studies of normal large sample, focusing lenses on detector for very small Q, focusing lenses on sample for very small samples and elliptical neutron guides is currently under discussion. We present numerical calculations for a SANS beamline with a 10 m fast changeable collimators/neutron guides with respect to intensity gain (~ 100 times) and discuss the impact on measurement time and the possible studied objects, which are currently out of range and can be studied with such a system.

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October 5, 2011, 11:20h

#### SANS instrument for small samples at the European Spallation Source

#### **Damian MARTIN RODRIGUEZ<sup>1</sup>**, Henrich FRIELINGHAUS<sup>2</sup>

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The European Spallation Source is going to be the most powerful neutron source in the world and pretends to satisfy the needs of the European scientific community. Due to the difficulty of obtaining biological samples with the required size for a conventional SANS experiment, the design of an instrument fully dedicated to small samples is one of the main needs for the user community.

In this report we study the different possibilities of such an instrument. One of the most obvious solutions is to scale the instrument, and make all the components smaller. Monte Carlo (MC) simulations show that such a miniaturisation of the instrument is possible at almost no loss in flux and keeping a similar minimum momentum transfer (Q). However, reducing the pixel size in the detector array is not possible at the moment, and therefore the miniaturisation would worsen the Q resolution. For this reason we determine the size of the pixel in order to keep the Q resolution as in the conventional case.

On the other hand, we also explore the use of elliptical guides for a high resolution SANS [1] as a possible concept to use for experiments on small samples.

[1] D. Martin Rodriguez, S. Kennedy and P. Bentley, J. Appl. Cryst, 44, in press.

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#### **Offspec: SESANS and SERGIS at ISIS**

#### **Robert DALGLIESH**

STFC, ISIS, Didcot, United Kingdom

The continuing commissioning and running of a user program on the OffSpec spin-echo instrument at ISIS has enabled further study of future prospects for the Spin-Echo Small Angle Neutron Scattering (SESANS) and Spin-Echo Resolved Grazing Incidence Scattering (SERGIS) techniques. Recent work has highlighted the care with which experiments must be designed to enable spin-echo scattering to be observed. The advantages and disadvantages of using time-of-flight and the current OffSpec RF flipper design will be discussed. Finally the current design and plans for the new Larmor spin-echo instrument, which is now under construction on the ISIS Second Target station, will be reviewed.

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October 5, 2011, 12:00h

#### Large scales - long times: Adding time resolution to SANS and reflectometry

**Robert GEORGII<sup>1,2</sup>**, Georg BRANDL<sup>1,2</sup>, Wolfgang HÄUSSLER<sup>1,2</sup> and Peter BÖNI<sup>2</sup>

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The Neutron Spin Echo (NSE) variant MIEZE (Modulation of IntEnsity by Zero Effort), where all beam manipulations are performed before the sample position, offers the possibility to perform low background SANS and reflectometry measurements in strong magnetic fields and depolarizing samples. However, MIEZE is sensitive to differences  $\Delta L$  in the length of neutron flight path through the instrument and the sample. We will discuss the major influence of  $\Delta L$  on contrast reduction of MIEZE measurements and its minimization.

Finally we will present a design case for enhancing a small-angle neutron scattering (SANS) instrument at the planned European Spallation Source (ESS) in Lund, Sweden, using a combination of MIEZE and other TOF options, such as TISANE offering time windows from ns to minutes. The proposed instrument would allow obtaining an excellent energy- and Q-resolution using present day technology to  $\mu$ s for 0.01 Å<sup>-1</sup>, even in magnetic fields, depolarizing samples as they occur in soft matter and magnetism while keeping the instrumental effort and costs low.

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October 5, 2011, 13:30h

#### The VITESS Monte Carlo simulation software

# Klaus LIEUTENANT<sup>1</sup>, Michael FROMME<sup>1</sup>, Sergey MANOSHIN<sup>2,3</sup>, Andreas HOUBEN<sup>3</sup>, **Daniil NEKRASSOV**<sup>1</sup>, Carolin ZENDLER<sup>1</sup>

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VITESS software is a widely used simulation tool for neutron scattering experiments. The program incorporates a large number of instrument components, in particular components used for instruments working with polarized neutrons. It provides the users the opportunity to optimize existing instruments on both reactor and spallation neutron sources and to plan and study the performance of future instruments, e.g., at the European Spallation Source ESS, which is supposed to be in operation in 2019. To optimize the applicability of VITESS software for the current ESS development phase, more ressources have been recently put into the development and improvement of VITESS at the Helmholtz Zentrum Berlin.

In this talk, the concept of VITESS, its current features and various ESS applications of the VITESS package will be presented. In particular, guides of different shapes, lengths and properties have been simulated, optimized and their performance compared. The influence of guide waviness has been studied systematically. Finally, it has been checked whether bispectral extraction systems can be combined with elliptical guides.

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October 5, 2011, 13:50h

#### **Neutron polarization in VITESS**

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As neutron simulations packages are used for analysis of the expected performance for practically all new built neutron instruments, possibilities for simulations with polarized neutrons have been relatively underdeveloped.

During last years we developed a new approach for the representation of time-dependent magnetic fields (both in magnitude and direction) for the VITESS simulation package. This allowed us to simulate the neutron spin dynamics in practically all polarized neutron devices (RF neutron flipper, adiabatic gradient RF flipper, the Drabkin resonator, etc.). In this presentation the above-mentioned VITESS instrument components (modules) we will be presented and the simulated performance of a number of polarized neutron scattering instruments (NRSE, MIEZE, SESANS, etc.) will be demonstrated. Recently, we expanded the possibilities of simulations towards the use of external (measured or simulated) magnetic field maps.

Thus, we practically completed the polarized neutron suite of the VITESS that seems sufficient for the simulation of performance of any existing polarized neutron scattering instrument. Future work will be concentrated on developments of dedicated sample modules (kernels) to allow for virtual experiments with VITESS.

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October 5, 2011, 14:10h

#### Active monochromators for TAS instruments

### **Thomas KELLER<sup>1</sup>** and Klaus HABICHT<sup>2</sup>

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Is there any hope for the 'notorious DC instruments', a classification introduced by Reinhard Scherm, to reach reasonable performance at a pulsed source? Probably the most typical representative of this DC class is a triple-axis spectrometer combined with spin-echo, such as the TRISP spectrometer at the FRM II. It allows for high resolution spectroscopy of elementary excitations and for high resolution diffraction (Larmor diffaction). As stringent tuning requirements to specific  $(q, \Omega)$  points impede the use of a variable ki, one interesting alternative are active monochromators compressing broad wavelength bands into one single wavelength. We will discuss the feasibility of such devices.

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October 5, 2011, 14:30h

### Current status and perspective of neutron optical device developments for neutron scattering experiments at J-PARC

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Material and Life science experimental facility (MLF) of J-PARC center have started user program in which experiments using pulsed neutron beam are available from December 2008. The source power of the pulsed spallation neutron source JSNS is gradually increasing and now reached 120 KW, where its final goal is 1MW. With increasing the neutron source power, the number of user programs is also increasing. In this situation, a 5-years project, which aims at higher efficient utilization of neutrons in neutron scattering research, have started since 2008 in Japan. 6 Japanese institutes join this project, and neutron optical devices including <sup>3</sup>He spin filters, neutron imaging device and neutron scattering method are being developed. In this paper, we report the current status of optical devices development and application and future perspective in Japan.

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October 5, 2011, 14:50h

#### The combination of bi-spectral extraction systems and elliptical guides studied by Monte Carlo simulations

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During the last years, elliptical guide shapes have been chosen for more and more neutron scattering instruments, because this shape yields the highest intensity and a clean divergence distribution at the sample. Gains are expected to be especially large at the ESS because of the expected great instrument length - typically 150 m.

On the other hand, bi-spectral extraction system are very appealing. By reflecting long wavelength neutrons on a mirror that is transparent to short wavelength neutrons, they allow to nearly obtain the maximum of thermal and cold moderator spectrum. After the experimental proof at HZB that bi-spectral extraction system work, this is also foreseen for the ESS in two different types. Many instrument groups are interested to use it.

The crucial question how these two approaches can be combined is investigated in this study using the Monte Carlo simulation package VITESS. Four different geometries are simulated and their performance compared for a typical ESS instruments, thus allowing estimations of the expected gains or losses.

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## Considerations on tradeoffs between super mirrors and <sup>3</sup>He spin filters for polarization analyzers on wide dynamic Q-range instrumentation

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Polarization analysis will be used prominently on modern neutron scattering instrumentation designed to measure wide dynamic Q-ranges. These instruments will often use large area detectors and potentially multiple neutron wavelength bands. This will place high demands on the method used for the polarization analysis. Two methods, super mirrors (SM) and <sup>3</sup>He neutron spin filters (<sup>3</sup>He NSF), are often considered as solutions to perform the required task. Both these methods have made ever increasing advancements with respect to performance, leading to wider applications. With <sup>3</sup>He NSF for example; the cells can be polarized in situ leading to steady analyzing powers and higher time averaged performance, <sup>3</sup>He polarizations have increased dramatically leading to higher efficiency and transmission bandwidth, the ability to flip <sup>3</sup>He polarization means neutron flippers after the sample are not needed, and the entire polarization system can be characterized in-situ in terms of absolute analyzing and polarizing power and flipper efficiency over wavelength. SMs have higher m-values leading to better bandwidth, open areas have increased, and polarization and transmission characteristics have improved with new device designs. However the fundamental underlying properties of SM and <sup>3</sup>He NSF based systems remain, giving the two very different properties with respect to the neutron performance. These intrinsic properties should be considered carefully when one is choosing the "ideal" polarization analysis system for the best possible final instrument. These factors should be the starting point before other harder to quantify factors such as but not limited to, manpower costs, overheads, and manufacturing and development lead-times are considered. We will discuss these basic differences and how they effect neutron performance and desired moderator specifications, presenting simulations and information from existing devices as support.

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#### Neutron pulse tailoring by means of a spatial magnetic spin resonator

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Spatial magnetic spin resonance (SSR), first proposed by Drabkin et al. [1], allows for velocity-selective spin flipping of a polarised neutron beam. It has found a series of applications, for instance as a neutron monochromator with variable output wavelength at fixed take-off angle [2-4], as an electronically tunable energy analyser in inverted geometry neutron time-of-flight spectrometers [5], or as neutron time-of-flight focusing device [6]. This technique exploits the fact that upon passage of polarised neutrons through a spatially alternating transverse static magnetic field each neutron in its rest frame experiences its own frequency according to its velocity and the spatial period of the alternating field. If this frequency equals the Larmor frequency - determined by the strength of an orthogonally oriented static field - a resonant spin flip will take place. This effect can be used to single out a specific wavelength from an initially polychromatic polarised neutron beam. We have developed a novel design of such a resonator, consisting of a sequence of separate modules which fulfils the specifications required for fast chopping of the beam intensity. On the basis of this design concept we have realised a first prototype resonator which we have installed at a polarised neutron beamline at the 250 kW TRIGA reactor of the Vienna University of Technology. First test experiments showed up a very promising performance of this prototype, but we still see a series of possibilities for further improvements [7]. Very likely our novel pulsed spin resonator could be quite useful for polarised neutron beamlines at the ESS, because it would allow for fast chopping of the (planned) 2 ms ESS source pulses into shorter wavelength-selected sub-pulses. It will be of clear advantage that the time structure of these sub-pulses will be almost arbitrarily adjustable in the microsecond regime by purely electronic means.

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October 5, 2011, 16:40h

#### Polarised neutron capabilities: from continuous to pulsed beams

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Indispensable information can be obtained from polarised neutron scattering experiments: magnetic ordering and excitations in single- and poly-crystalline samples, liquids, thin films and nano-particles; creation and dynamics of vortices in superconductors; dynamics of polymers and micro-emulsions; distribution of magnetic fields in bulk samples, etc. Polarised neutron techniques also contribute a lot in the area of fundamental neutron physics.

Unfortunately, not so much work has been performed with pulsed polarised neutrons [1-4] and most of the polarised neutron capabilities developed for many years at continuous neutron sources cannot be transferred directly to pulsed spallation sources. Indeed, most of the polarised neutron techniques presently available cover a limited wavelength band or are limited to monochromatic beams. New instrument concepts, polarisation devices and components must therefore be developed.

We shall discuss some of the difficulties encountered with wide-band beams, in particular wide-angle polarisation analysis and polarimetry [5-7]. We shall also consider the global shortage in <sup>3</sup>He, the effects of high intensity neutron flux on spin filters and evaluate alternative techniques [8-10].

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### Shared basic concepts for neutron reflectometry and imaging at a long pulse target station

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On a first glance neutron reflectometry (NR) and neutron imaging (NI) do not have much in common. However, taking into account novel imaging methods that utilize neutron scattering and neutron scattering approaches, namely Bragg edge imaging [1], dark-field contrast imaging [2] and polarized neutron imaging [3], (all of which are most promising to profit from pulsed neutron sources [4,5],) similar requirements can be found concerning a variety of wavelength resolutions over a significant wavelength band range, which are needed for an ever efficient application of both NR and NI. This might result in a similar solution for the chopper systems of the corresponding instruments at a long pulse neutron source like ESS and will also have influence on the guide systems. Additionally, there is an analogy in the approaches to resolve grazing incidence scattering at neutron reflectometers through spin echo encoding [6] and small angle scattering in NI by dark field imaging [2]. These novel approaches of spin echo modulation small angle neutron scattering will be introduced and discussed with respect to both techniques at a long pulse source as well.

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#### Neutron beam generation, extraction and instrumentation at the long pulse source ESS: New opportunities and challenges

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The design of the target station at the 5 MW is aimed at meeting a number of new challenges compared to established state of the art. These include time average proton beam power and energy per pulse on the target enhanced by, respectively, 5 and 20 times compared to previous spallation sources; the use of most efficient and experimentally proven moderator technologies and the goal to extract an unprecedented number of beam lines at one target station. From the point of view of instrumentation long pulses offer a level novel flexibility for pulsed spallation sources by the capability of delivering both largely enhanced number of neutrons per pulse and the highest peak flux achieved by now in pulses of variable length from a few  $\mu$ s to a few ms, in order to meet the individual needs of a broad variety of experiments. Efficient use of these new opportunities requires a careful matching of features of the target station to the instrumental requirements, including the choice and accommodation of chopper system, beam extraction neutron guides, minimizing the fast neutron background, utilization of the floor space available around the beam-lines. The talk will also include a review the progress of the collaborative design effort on ESS target station and beam extraction.

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October 6, 2011, 9:10h

# The TOFTOF spectrometer at FRM II and perspectives for a high-resolution chopper spectrometer at ESS

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The cold neutron time-of-flight spectrometer TOFTOF is a direct geometry multi chopper instrument. It is the combination of highest resolution, perfect symmetric resolution function, high intensity, huge flexibility, and exceptionally low background that makes this instrument to one of the best neutron spectrometers of its kind worldwide [1]. This is demonstrated by more than 50 original contributions in well known international journals since 2008.

The instrument was continuously upgraded and refurnished since its commissioning and the begin of normal user operation in 2005. In this talk the status of the instrument and the experience during the first five years of user operation will be presented including the latest upgrades during the long shutdown (2011) of the reactor of the FRM II. The detector array was extended to roughly 1000 detectors now and the electronics could be improved which should lead to a further reduction of the already perfectly low background. New ideas and first developments for the upgrade of the neutron guides will shortly be addressed.

Finally some comments on perspectives of high-resolution chopper spectrometers on long pulsed spallation neutron sources like the ESS will be given focusing on the needs in the area of soft matter research.

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#### Time-of-flight spectrometers for single crystal spectroscopy on steady state reactor

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Widely used for single crystal spectroscopy on spallation sources where the three-axes spectrometers (TAS) are less relevant, time-of-flight spectrometers (TOF) were, up to recently, mostly constrained to powder and amorphous materials on steady state reactors. The advent of large surface of positions sensitive detectors (PSD) on recent TOF, thanks to the development of this technology, has given a regain of interest to single crystal spectroscopy with these reactor-based instruments.

IN5 at the ILL is a typical case of TOF where the possibilities offered by the PSD have been fully exploited by the neutron community [1-3]. Despite that IN5 serves a wide user base as a general-purpose instrument, a successful opening to the single crystal community has now become effective with the  $30m^2$  ( $0.6\pi$  Sr) almost perfectly seamless PSD complementing its rather high count-rate at sample.

In this contribution we propose to present the lessons learned while showing some typical examples of single crystal studies gathered along the past three years of operation.

Among the performed experiments, one can find studies on collective excitations in a frustrated magnet, magnetism in iron-based pnictide superconductors for example. High quality measurements of spin-waves on IN5 and the complete modeling of the data obtained in a chiral multiferroic were essential to elucidate the exchange interactions responsible of the ferrochiral order in the compound [4]. Studies on single crystals of molecular nanomagnets, are opening way for direct observation of spin correlations of these complex systems [5].

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#### **Optics for small-spot neutron spectroscopy: towards neutron spectromicroscopy**

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Spectroscopy is a flux-limited technique. On the sample downstream-side much has been achieved to maximise throughput. Low energy cutoff-off filter spectrometers are "grunt" instruments that collect as much solid angle as possible to achieve high-throughput. We are currently building such a high-throughput spectrometer at OPAL in Australia to measure vibrational density of states on powder samples [1]. Such "grunt" instruments suffer from a number of rather crippling limitations due to the humorously enormous size of the sample required to collect all available flux coming from the source. Such a situation has been tolerated but is in need of rectification.

In most cases there is little sample to work with or one wishes to measure many samples, in their hundreds over a reasonable period of time, or one wishes to measure on samples that have spatial chemical variation. Small spot neutron spectroscopy conducted on continuous sources are now possible that ultimately will lead to the analysis of micron-sized samples and fundamentally different spectrometer designs.

Clearly, small is good and must be strived for. Our analysis using a variety of optical elements upstream from the sample, lobster-eye focusing guides, axisymmetric mirrors, compound refractive lenses, and Fresnel zone plates clearly show the advantages of reducing the analysis spot size as flux densities may be increased by one to two orders of magnitude. Discussion is given on new measurements achievable given such flux densities as well as improved instrument designs that take advantage of the small spot-size. An ultimate goal is to achieve spatial and temporal resolution both at continuous and pulsed neutron sources.

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October 6, 2011, 10:10h

#### Direct geometry time-of-flight spectrometers for ESS

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Direct geometry time of flight spectrometers benefit especially from the pulsed spallation sources. It has been shown that in particular instruments using cold neutrons profit strongly from the long pulse at ESS [1,2].

Reviewing recent publications from world class TOF spectrometers shows that often one uses high energy and low energy neutrons for comprehensive studies of the dispersion in novel functional materials. As an example, the excitation spectrum in high temperature superconductors extends well above 200 meV, while interesting features of the spectrum require good resolution and therefore lower energies.

We discuss the implications for a spectrometer at a long pulse spallation source using a wide wavelength range, extending to the thermal and epithermal region.

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### Ideas on inelastic neutron scattering instrumentation for kinetic experiments and when using extreme conditions

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Even on the most advanced neutron sources with well-optimized instruments the incident neutron flux often determines the feasibility of an experiment. Flux limitations become an almost invincible obstacle when the sample or the sample environment imposes additional time constraints prohibiting long (continuous) count rates. This is the case when studying kinetics (such as non-equilibrium transient states present during chemical reactions or phase transitions) or using extreme conditions (such as pulsed magnetic fields). Building on pioneering experimental work [1] but using a superfluid helium based ultracold neutron (UCN) source and storage [2] combined with a (crystal- or accelerator-based) phase space transformer PST [3], we here present an original possibility to produce single strong monochromatic polarized neutron pulses with a very low repetition rate. Using pyrolytic graphite for the PST leads to monochromatic pulses with a wavelength lbd ~ 3.3 Å and a pulse length t pulse ~ 500µs compatible with standard TOF detection. The so-produced pulses would be about 100x stronger than neutron pulses currently available for time-of-flight (TOF) instruments. We compare this idea with other instrument concepts for continuous and pulsed sources, considering the low repetition rate ( $f \sim 0.01$ Hz) is well matched for kinetic experiments or when using pulsed magnetic fields. Nevertheless, based on currently developed UCN equipment the proposed technique does not overcome the reduced average flux resulting from the low repetition rate imposed by either the sample or the sample environment, which nowadays require stroboscopic methods [4] or static magnetic fields [5], respectively. On a medium term perspectives we might expect further improvements on the UCN production and storage. Inscribed in a changing neutron research landscape such a PulsedKicker instrument will provide a new tool for the study of kinetics and make the use of pulsed fields viable, complementing static (superconducting, conventional or hybrid) magnet facilities.

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October 6, 2011, 11:20h

#### TOPAS, the future thermal time-of-flight spectrometer at FRM II

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TOPAS is a new thermal time-of-flight spectrometer that is being built by JCNS at the research reactor FRM II.

The instrument is dedicated to study of spin, lattice and molecular dynamics in novel materials in the energy range up to 150 meV. A special emphasis is put on the mapping of dispersive excitations in the Q-space and neutron polarization analysis.

The concept of the spectrometer is based on the combination of high intensity with reasonably good energy and momentum resolution, achieved using an elliptic focusing neutron guide, a cascade of Fermi-choppers with high repetition rate (up to 600 Hz) and a compact secondary spectrometer with large-solid-angle position-sensitive detector. The polarization analysis will be realized by means of spin polarized <sup>3</sup>He neutron spin filter cells.

In this talk we report on the current status of the instrument development and construction.

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#### *exTAS* – next generation crystal spectrometer for small samples and extreme conditions

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The currently used implementations of horizontally and vertically focusing optics in threeaxis spectrometers (TAS), both in their classical and multiplexed variants, permit efficient studies of excitations in sub-cm<sup>3</sup>-sized single crystals. With the *exTAS* [1] project we wish to stimulate a further paradigm shift into the domain of mm<sup>3</sup>-sized samples. This is particularly important for applications in emerging fields, where precious time is often lost before crystal growth technologies adapted to the new materials can be found. Moreover the complementary bulk characterization data also refer to much smaller samples of better homogeneity.

As the present state of the art of neutron optics pushes the efficiency of neutron transport, focusing and detection close to its absolute limits, further progress in absence of neutron sources offering significantly higher brilliance in terms of average flux is only possible by further improving the signal-to-noise ratio. The way to achieve a significant progress in this direction is to adapt and optimize the volume and shape of the spectrometer resolution element both in real space and in the Q,  $\omega$  phase space to the particular experiment needs and, possibly, to implement a time structure of the incident beam to eliminate the high-order contamination of the incident beam and to reduce the general background.

In order to achieve these goals *exTAS* combines highly focused mm-sized focal spots with a spectrometer layout downscaled to a tabletop size to provide high flexibility in optimizing acceptance angles and to achieve sub-millimeter positioning accuracy. Moreover, its monochromatic focusing geometry with a mm-sized source size will permit to employ the variation of the monochromator/analyzer thickness to tune the energy resolution and to match narrow non-dispersive excitation branches (e.g. gaps in spin systems) in the Q,  $\omega$  space.

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#### Multiplexing techniques: adjustable short pulses at a long pulse spallation source

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The main challenge in the instrument design at the future European Spallation Source is how to take full advantage of the high neutron peak flux and at the same time to take control over the pulse parameters to best suit the instruments and individual experiments. Novel multiplexing techniques, such as Repetition Rate Multiplication and Wavelength Frame Multiplication allow us to create instead of one long pulse a number of mini-pulses with variable frequencies and pulse lengths but with the same peak flux as original pulse. The underlying principle of multiplexing techniques is to use a set of monochromatic wavelengths or a set of wavelength bands coming from the same source pulse by means of mechanical chopper system. In this case the instrumental parameters, such as wavelength resolution, wavelength band, repetition rate are not any more determined by the source pulse parameters, but can be flexibly defined by the chopper frequency, speed and chopper pulse.

The design of chopper systems for realization of multiplexing methods is different from those at a reactor. Similarly to the reactor based instruments the main requirement for multiplexing chopper system is to assure that a neutron detected at any given time can only come from a single pulse shaping chopper pulse. However, multiplexing entails specific conditions leading to "quantized" chopper configurations in terms of the choice of the chopper positions  $L_i$  and chopper frequencies  $f_i$  relative to the source and source frequency f, respectively.

The results of first experimental implementation of Repetition Rate Multiplication (RRM) and Wavelength Frame Multiplication (WFM) methods deliver full proof-of-principle of these key techniques for long pulse spallation sources. They demonstrate multiply enhanced data collection rates and individual tuning of the pulse length and/or pulse repetition rate largely independently of the actual source pulse parameters. For implementation we used reactor based instruments, the TOF spectrometer NEAT at HZB, Berlin and the TOF diffractometer at BNC, Budapest, operating in non-standard modes. The pulsed source in these studies has been emulated either by a disc chopper rotating with 10-40 Hz or defined by the chopper system as a virtual pulsed source operating around 10 Hz. Application of the RRM method allowed us to simultaneously collect up to six inelastic spectra with different incoming wavelengths. Using WFM several incoming wavelength bands could be joined together for gap free coverage of about 9Å bandwidth in TOF powder diffraction with chopper shaped pulses. The experimental data in both cases can be treated in conventional manner. Probing the sample with multiple wavelengths or multiple wavelength bands, however, can offer enhanced quality of information by broader dynamic range.

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#### **ToF-Backscattering at ISIS: state of the art and perspectives**

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The time of flight backscattering instruments IRIS and OSIRIS have and are still serving well the user community with access to high energy resolution for quasielastic and inelastic investigations. The main difference to classical backscattering instruments at continuous sources is the enlarged dynamic range, paid by a decline in energy resolution.

To extend the dynamic window at ISIS by an order of magnitude a novel high-resolution backscattering spectrometer, FIRES, was proposed. As a novelty for this type of instrument, short pulses will be generated with a fast chopper [1].

Recent successes on the present spectrometers IRIS and OSIRIS will be presented and the performance of the future FIRES will be discussed, assessing also the potential for a FIRES type instrument at a long pulse source.

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### The new IN16B at ILL, its BATS option and some thoughts towards backscattering at ESS

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We report on the status of the backscattering instrument IN16B at the Institut Laue-Langevin and its expected performance. The instrument is optimised for a Phase Space Transformation (PST) configuration using Si(111) backscattering crystals. In this mode we expect IN16B to perform best. Other crystal options foreseen are Si(311) and GaAs(002), which may be installed in a second phase. A new ballistic neutron guide, a compact PST and a secondary vacuum chamber with tall analysers as well as flexibility towards later options are the main characteristics of the new IN16B. Thus it is foreseen that IN16B can operate at the side position of the guide but it could also be operated as an inverted Time-Of-Flight backscattering instrument (BATS) by installing a chopper system upstream of the instrument. We review this option which would enable new experiments at ILL by closing todays gap between backscattering and TOF. We compare the BATS performance with respect to spallation source backscattering and IN5. Furthermore we discuss some ideas for spallation source backscattering at ESS.

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October 6, 2011, 14:10h

#### **BASIS** backscattering spectrometer at SNS

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The spallation source near-backscattering spectrometer BASIS, at the spallation neutron source SNS, Oak Ridge National Laboratory, USA, has been in operation since 2007. It is in many aspects similar to some existing TOF-backscattering spectrometers, but employs some new features that allow very good resolution to dynamic range ratio. In this presentation the energy resolution contributions, the layout, the performance and the current status of BASIS will be described. A few examples will be given to illustrate new experimental possibilities.

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#### Perspectives and science examples using the backscattering technique

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The future backscattering spectrometer IN16B at the ILL will comprise a Phase Space Transformer (PST) as an essential neutron optical component.

The PST had originally been proposed for the application in spallation source instruments [1]. Recent progress in developing a numerical and analytical framework to model the PST [2] will be explained in detail with view at possible applications for ESS instruments. Subsequently, the importance of the backscattering technique in a large dynamic range will be illustrated by recent experiments relevant for biologically inspired colloid physics [3]. This could contribute to the science case for a new spallation source backscattering instrument.

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#### Biomolecular dynamics with neutrons: Instrumental aspects of the widening scope and likely impact of experiments on functionally important systems

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Energy-resolving neutron scattering techniques have been applied to a remarkably wide and diverse range of biomolecular systems since the 1970s. Despite this long history, quasielastic and inelastic neutron scattering are still regarded as niche techniques by biophysicists engaged in studying time-dependent processes. With the commissioning of third-generation sources and spectrometers, we are currently at the threshold of a major expansion in neutron facilities which holds great promise in particular for studies of the functional dynamics of biomolecules and their building blocks. There are, broadly, two avenues along which future work can develop: one class of projects aiming to study "more of the same, but much better", and one taking advantage of the rich opportunities for expanding the scope of biodynamics experiments with significantly improved or entirely novel instrumentation. The latter category will be paramount for exploring the dynamics of ternary systems requiring selectively deuterated samples, ideally in parallel with diffraction projects.

This contribution focuses on instrumental aspects in areas where (i) pilot experiments or limited initial work have already been done but could not be followed up due to flux and access constraints, and where (ii) the large and rapidly expanding body of theoretical studies (mainly MD simulations) provide the motivation and interpretational basis for more ambitious experiments. The spectral region considered here covers 5-6 decades including the important transition region from diffusive to vibrational processes, corresponding to time scales from ~100 ns to around 0.1 ps. Advanced spin-echo, backscattering, and time-of-flight spectrometers can be expected to furnish the high-quality data sets needed for the analysis of difference dynamic structure factors  $\Delta S(Q, \omega)$  and intermediate scattering functions  $\Delta F(Q, \tau)$  characterising functionally relevant interactions in the physiological temperature range that is of direct interest to molecular biologists. This entails a significant shift away from the past emphasis on more physics-oriented experiments which were primarily concerned with understanding glass-like transitions, mode-coupling processes, and proton mobilities in anhydrous or minimally hydrated biomolecules at cryogenic temperatures.

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October 7, 2011, 8:50h

#### Neutron scattering instrumentation at the ORNL spallation neutron source: some lessons learned

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Building a major new neutron scattering facility is a wonderful challenge and a time of great accomplishment and excitement. These efforts result in very visible, tangible, and quantifiable outcomes as buildings, the technical equipment associated with the source, and the neutron scattering instrumentation are built and installed. There are sponsor expectations that must be fulfilled during the construction phase that center on timely delivery and installation of facility equipment and capabilities within the allocated budget and it is easy to focus entirely on this goal. However, many activities that can be initiated during the construction phase that will speed instrument commissioning and ease the transition to an operational facility that is delivering impactful science. This talk will review the experience gained at the Oak Ridge National Laboratory's Spallation Neutron Source and discuss some lessons learned.

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October 7, 2011, 9:30h

#### Neutron instrumentation at a continuous source: the ILL Millenium programme and beyond

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Since the commissioning at the beginning of 1970's the ILL high flux reactor has been the worldwide most intense neutron source. The subsequent tremendous progress in the sensitivity and productivity of the neutron scattering experiments has been exclusively achieved by the improvement and optimization of the instruments and computing techniques. The latest phase of this evolution, the Millenium programme, carried out since 2000 and going on till the years 2014/2015, resulted in a global increase of the detection efficiency of the ILL instrument suite by a factor of 20. As a result, confirmed by the recent review, the user community considers the overwhelming part of the ILL instrument suite as representing the present state of the art and matching users' expectations.

In many areas, ranging from the design optimization techniques to the component manufacturing technologies, neutron instrumentation has been pushed close to its absolute limits. The "hardware" progress has been accompanied by development and implementation of new software for instrument control, data acquisition and visualization. Significant efforts have been invested into creation of infrastructures for off-line sample preparation and characterization as well as for computer simulation of scattering response in spectroscopic experiments. Although the impact of these additional facilities is difficult to quantify in general, it is clear that without their decisive role the purely instrumental developments in the domains molecular spectroscopy or of soft-matter physics would never have brought the full effect.

In this presentation we shall review the most recent achievements, putting emphasis on instruments and instrumentation developments, which have importance for the broad community and which have potential impact also for the newly constructed pulsed sources like the ESS.

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#### Perspectives for Materials Investigations at the Structured Pulse Engineering Diffractometer (SPEED)

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One important goal of modern engineering investigations is to improve our understanding of materials behaviour and failure on a microstructural basis. Various experimental investigations are performed to achieve this goal comprising measurements of stresses and textures. Those characterizations need neutron measurements if well defined gauge volumes located deep in the bulk of materials are to be analyzed. Complementary investigations are performed with X-rays to characterize surface structures or to investigate lightweight structures with hard X-rays. Neutron investigations should allow for three-dimensional maps of stresses and textures within engineering components or in-situ studies of fatigue behaviour or stresses in rotating machinery. Those measurements are, however, extremely time consuming and can thus not be performed to the required extent at modern instruments such as SALSA at ILL or STRESS-SPEC at FRM II. New perspectives for engineering applications will be offered by new instruments at MW spallation sources such as VULCAN at SNS.

Against this background the Helmholtz-Zentrum Geesthacht proposes to build a novel structured pulse engineering diffractometer (SPEED) at the European Spallation Source (ESS) in Lund/Sweden. The instrument will be based on a novel ToF-design distinguished by a modulation chopper positioned at a distance of ~ 25 m from the source. This chopper will be located ~ 50 m from the sample and allows setting the wavelength resolution almost independently of the wavelength in a broad range from about 0.15% to 2%. Despite the high resolution the chopper system in total has a transmission of about 30% of the 2 ms long source pulses for a broad and selectable wavelength range - the transmission of the chopper system is almost only reduced by the need of the pulse modulation. SPEED thus will make full use of the high flux of the long pulse spallation source for high resolution diffractometry. The design of SPEED is introduced and its performance based on numerical simulations for texture and stress measurements is outlined. The development of SPEED is performed as an in-kind contribution to the ESS instrumentation, it is part of the German support to the ESS Pre-Construction Phase and Design Update.

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October 7, 2011, 10:30h

#### The first experiments on high pressure neutron diffractometer "Hercules"

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We report on the neutron diffractometer Hercules designed for the measurements under high pressure. This instrument includes a sealed safe with a press inside which yields more than 200 t of force. Hercules has a set of diffraction modules, a few inelastic neutron scattering modules are planned. The instrument is well-suited for the measurements at pressures up to 100 kbar with a sample size of about 1 cm<sup>3</sup>. Hercules allows to measure in situ the process of hydrogenation at high pressures and in a wide temperature range, getting a record pressure for samples up to 1 cm<sup>3</sup>, enables the simultaneous measurements of structure and dynamics of materials.

The neutron concentrator was installed to increase the neutron flux incident on the sample under pressure. The concentrator is based on the neutron supermirrors designed to focus the neutron beam on the sample. This devise allows to increase the flux at the sample position by a factor of ~ 2 for the neutrons with the wavelength  $\lambda$ > 2.5 Å. In addition to it a set of three neutron collimators was installed in the beamline of Hercules.

The first experiments on Hercules have been performed in November 2010. The detector block used in the measurements was based on one sector with three helium neutron counters. The neutron spectrum of the direct beam was measured. We measured the neutron diffraction patterns of a few test samples: steel, TiZr (zero matrix), black diamond (synthetic diamond powder).

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#### October 7, 2011, 11:20h

#### Prospects of neutron imaging and imaging instrumentation at a long pulse source

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Beside the powerful tool of conventional attenuation contrast imaging with a broad thermal or cold energy spectrum a number of novel imaging methods exploiting a monochromatic beam or energy resolved approaches have become available within the last decade. These developments have the potential and do extend the range of applications of neutron imaging significantly. Modern short pulse spallation neutron sources are advantageous as compared to continuous sources especially for methods requiring relatively high wavelength resolution, which are those utilizing Bragg scattering for imaging contrast and providing spatially resolved information about crystalline structures present in a sample. The planned long pulse target station of the ESS on the other hand provides the potential to serve most to date available neutron imaging contrast methods with an outstanding efficiency [1,2] including (i) conventional attenuation contrast, (ii) energy resolved attenuation contrast imaging exploiting Bragg scattering [2,3], (iii) phase contrast imaging addressing the refractive index distribution of the sample, (iv) polarized neutron imaging with the aim to investigate magnetic structures, fields and phenomena [4] as well as (v) dark-field contrast imaging with the potential to investigate (magnetic) microstructures beyond real space resolution [5,6]. The potential of wavelength resolved application of the latter methods, i.e. polarized neutron imaging, phase and dark-field contrast imaging but also Bragg edge imaging has been outlined [2,3]. The state-of-the-art as well as directions of progress will be presented and discussed together with the design of an efficient future instrument with such a range of flexibility.

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#### Development of novel neutron detectors with thin conversion layers

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The Helmholtz-Zentrum Geesthacht (HZG, formerly GKSS Research Centre) operates neutron beamlines at the research reactor FRM II in Germany and is engaged in designing new ones at high flux reactors and the new European spallation source ESS. For those instruments thermal and cold detectors covering a large part of the spatial angle are needed. Due to the current shortage of <sup>3</sup>He HZG has started a development of neutron detectors with thin boron conversion layers to be used for high and low resolution diffraction, reflectometry and SANS as well as for inelastic instruments. The new detectors are required to meet the high performance of current <sup>3</sup>He-detectors, this includes especially high neutron and low Gamma sensitivity as well as high local and global count rates. Detectors with high spatial resolution (about 1 mm to 2 mm) shall allow for covering medium sized areas (up to 1 m<sup>2</sup>) whereas detectors with low resolution (about 10 mm to 20 mm) are designed to cover large areas (some 10 m<sup>2</sup>). The development is performed as an in-kind contribution to the ESS instrumentation, it is part of the German support to the ESS Pre-Construction Phase and Design Update. The status of both the coating techniques and detector concepts are introduced.

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#### The <sup>10</sup>B based Jalousie neutron detector – our alternative for <sup>3</sup>He filled PSD counter tubes

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Jalousie is a new detector in its prototyping phase, developed to serve as alternative for classical <sup>3</sup>He position sensitive detector tubes (PSD). It is thus thought to resolve today's <sup>3</sup>He availability crisis for neutron scattering instruments. The neutron converting material is <sup>10</sup>Boron and replaces <sup>3</sup>He. The comparatively small overall detection efficiency of an individual layer is enhanced by tilting the layer towards the incoming neutron path, thus increasing the effective absorption depth. Additionally, eight such boron layers are arranged along any neutron path to further enhance the overall detection efficiency. A Jalousie detector system comprises many lamella shaped individual modules, where each makes up an enclosed multi wire proportional chamber with two anode planes and one cathode plane that carry the converter layers. Several such lamellae, when stacked and tilted with respect to the neutron paths, may be arranged to cover square meter sized planes, or alternatively a cylindrical surface to enclose a scattering sample. The design described is under development and currently in a prototyping stage for POWTEX at FRM II, where an overall area of 9 sqm will be covered. Spatial resolution 5 mm (FWHM) as well as time of flight resolution 3-10µs (FWHM) may be altered through design parameters. The POWTEX lamella length was chosen to be 1,6m and includes a concentric orientation of the readout channels towards the scattering center. The detector concept and first measurement results of the first two prototypes will be presented.

\* CDT under contract with RWTH Aachen (POWTEX) and in cooperation with the Physikalisches Institut Heidelberg (BMBF funded).

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### **Posters**

## KWS-2 – the high intensity / wide-Q SANS diffractometer for biology and soft-matter systems at FRM II

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The KWS-2 classical pinhole SANS diffractometer is dedicated to the investigation of mesoscopic structures and structural changes due to rapid kinetic processes in soft condensed matter, chemistry and biology systems. The combination of high neutron flux supplied by the cold neutron source of FRM II, newly designed neutron guide system, the new collimation system allowing for a larger experimental flexibility and the new "fast" detection electronics with a dead-time constant of 0.64  $\Box$ s enabling counting rates as high as 0.6MHz supports the high-intensity operation mode. This opens opportunities to study fast kinetics within the millisecond range. The high neutron flux, comparable with that at the world leading SANS instruments, allows for an optimal use of the high-resolution mode: neutron optics elements (aspherical MgF<sub>2</sub> lenses) in combination with a small entrance aperture and an additional high resolution detector (0.45x0.45 mm<sup>2</sup> space resolution) enable smallest Q vectors in the range of  $10^{-4}$  Å<sup>-1</sup>. The chromatic aberrations and gravitational effects are avoided by the use of short neutron wavelength with low spread (around 2%) as obtained by using a double-disc chopper (max. 200Hz) in concert with the velocity selector. The wide Q-range covered by combining the high resolution and classical pinhole operation modes enables structural investigations over a length scale from 1nm up to 1µm. The instrument performance will be presented.

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## Neutron spin echo encoded scattering at BioRef - a new approach to studying complex interfaces

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We will present a design study on second wave BioRef set up for the investigation of laterally structured interfaces. [1] After successful installation and commissioning of the instrument for specular and offspecular neutron reflectivity investigations BioRef is now furnished with an add-on facility for spin echo resolved grazing incidence scattering (SERGIS) [2] for the investigation of laterally structured interfaces on the mesoscopic scale. A first layout of the set-up with its components adapted to the requirements of a TOF-instrument is presented and potential limitations are discussed.

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#### Very small angle neutron scattering diffractometer with focusing mirror: from continuous to spallation sources

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KWS-3 is the world only very small angle neutron scattering instrument running on the focusing mirror principle. It allows performing scattering experiments with a wave vector transfer resolution between  $3 \times 10^{-5}$  and  $3 \times 10^{-2}$  Å<sup>-1</sup>, bridging a gap between Bonse-Hart and pinhole cameras. The principle of this instrument is a one-to-one image of an entrance aperture onto a 2D position-sensitive detector by neutron reflection from a double-focusing toroidal mirror. The instrument has considerable intensity advantages over conventional pinhole-SANS and Double Crystal Diffractometers and perfectly bridges the "Q-gap" between U-SANS and very small angle scattering (V-SANS). In this presentation we will discuss possibility to use a V-SANS instrument like KWS-3 in time-of-flight mode at a spallation source.

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#### POWTEX – High-intensity neutron time-of-flight diffractometer at FRM II

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In order to provide the chemistry and geo-science communities with a very powerful tool for rapid neutron-data acquisition, the new time-of-flight diffractometer POWTEX will be installed at the FRM II reactor in Munich. The instrument is being designed and built by the RWTH Aachen University and the Forschungszentrum Jülich. The University of Göttingen will provide sample environments for geo-science applications. Both projects are funded by the German Federal Ministry of Education and Research (BMBF). Once finished, POWTEX will be part of the JCNS instrumentation pool.

POWTEX is an abbreviation for POWder and TEXture. The instrument will fulfill the needs of the solid-state chemistry, the geo- and partly the materials science communities with regard to powder and texture diffraction. We expect to outperform comparable monochromator instruments by one order of magnitude in intensity (>  $10^7 \text{ n/cm}^2\text{s}$ ) for samples of less than a cubic centimeter. This extraordinary performance will be achieved by combining several new concepts. These are, namely, the double-elliptic neutron-guide with an octagonal cross section, the four-unit disk-chopper system, including the pulse double-chopper and the access of full Debye-Scherrer cones by a huge solid angle ( $\approx 10 \text{ sr}$ ). The high intensity will allow us, to perform in situ powder diffraction experiments on chemical reactions and to characterize phase transitions as a function of *T*, *p* and *B*<sub>0</sub> (or others) by parametric studies in comparatively short measurement times. Geo- and materials sciences applications at this instrument are mainly related to texture measurements on series of natural samples, in situ deformation and recrystallization/annealing experiments and simultaneous stress/texture measurements.

While POWTEX is under construction at the very moment, we expect to conduct the first measurements in the year 2012. The current project status and conceptual evolutions, including new concepts in instrument simulations and the status of our <sup>3</sup>He-free detector prototypes, are shown in our contribution.

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## Design considerations for the instrument BioDiff and some implications for a similar instrument at a spallation source

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The new instrument BioDiff –now approaching first test with neutrons—has been built at the FRM II as a joint project between the Jülich Centre for Neutron Science and the Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II). Its main scientific purpose is the investigation of hydrogen positions in crystals of biological macromolecules. This implies that the unit cells encountered will be rather large of with typical lattice parameters of the order of 100 Å.

The concept of the instrument is to use a monochromatic neutron beam of a  $\Delta\lambda/\lambda$  between 2 and 3 %. Monochromatization and beam extraction is achieved using the Bragg reflection off a pyrolytic graphite crystal in the white neutron beam of the NL 1 in the neutron guide hall of the FRM II. To remove the higher order wavelength contaminations a velocity selector is employed. Additionally, the beam divergence can be adjusted with slits in order to optimize the compromise between intensity and good separation of Bragg-reflexes. The wavelength of the incident neutrons can be chosen between 2.4 and 5.6 Å. This allows adjusting the wavelength to the size of the unit cell of the molecular crystal and to the resolution needs which are desired for the respective scientific question.

This concept will be compared to a quasi Laue diffractometer using an order of magnitude larger wavelength band than the BioDiff. Furthermore, implications for a similar instrument at a spallation source are discussed. Here, a time resolving detector is needed to distinguish between the incident neutron wavelengths by their arrival time with respect to the neutron pulses supplied by a spallation source.

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#### Development concepts of Trics: the neutron single crystal diffractometer at the SINQ

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With the development of the synchrotron facility and laboratory X-ray single crystal diffractometer, the aim of neutron single crystal diffraction (NSCD) is nowadays focused toward solving complex magnetism (unpolarized and polarized neutron scattering) in classical and challenging sample environment (high magnetic field, pressure, He3 dilution temperature) other than structural crystal determination. This later is still attractive since only neutron scattering can determine the position of light weight element i.e. H, Be, Li.

These targets fix the instrumentation requirement for the development of NSC 4circles diffractometer like low background (improvement of neutron filter and use of PG analyzer), non-magnetic environment around the sample (High magnetic field), large momentum transfer (thermal neutron and large scattering angle) for limited geometry (Horizontal and vertical scattering with cryomagnet) and structural determination, polarized thermal neutron beam for complex and quantum magnetism. All these aspects will be considered for the development concepts of TriCs, the thermal NSC diffractometer at the SINQ facility (LNS, Paul Scherrer Institut).

In this work, infinitesimal calculations have been used for magnetic field force calculation indicating that by increasing the sample to monochromatic distance of 25cm with changing the secondary instrument to non-magnetic ones, 15T are reachable vs. 5T nowadays. Bench mark experiment using instrument beam time development have been performed to determine the beam characteristics for the present two vertically focused monochromators (Ge311 d=1.7058 Å and PG002 d= 3.3540 Å, take off angle of 40°) and focusing functioning. These results have been compared with Monte Carlo ray tracing simulations (Vitess and Mcstas). Simulations show that the focusing system worked as expected. Additional Vitess and Mctas simulation were performed to determine the optimized polarizing bender geometry for polarization efficiently of our beam at the present sample and new sample position for  $\lambda = 1.20$  Å. Additional simulations for flux and background gains perspective of a new monochromator (Cu111) have been investigated.

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### Structure of microemulsions confined near planar surfaces

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Bicontinuous microemulsions near planar hydrophilic surfaces were studied by reflectometry, grazing incidence small angle neutron scattering (GISANS), and computer simulations. While reflectometry probes the laterally averaged structure in the normal direction, the GISANS experiment reveals the full structural information. Reflectometry proved that a lamellar order decays to the volume, which agrees well with the computer simulations. GISANS experiments identified even better the lamellar and bicontinuous structures with 2d-scattering patterns. We varied the scattering depth by different incident angles and different contrasts between the solid and the overall microemulsion. For the intensity ratio of the bicontinuous structure normalized by the lamellar scattering we obtained an increasing behaviour which is nearly linear for scattering depths between 400 and 1000Å. The linear behaviour points to a zero at a scattering depth of 400Å which we could address to the beginning of the isotropic structure. The computer simulations were evaluated similarly and confirmed this way of interpretation. The computer simulations found a perforated lamellar structure directly behind the ideal lamellar order. On the one hand it explains the way of a decaying order into the volume – on the other hand it is the first isotropic-like structure behind the perfect lamellae, because the perforations have the same structural sizes than the bulk microemulsion. So far only computer simulations identified the perforated lamellar structure.

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### Neutron optics from Helmholtz-Zentrum Berlin

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In the last years a variety of new neutron optical devices have been developed at HZB. These are mainly solid state elements where the neutrons are transported in thin silicon wafers with coated walls.

We show results of solid state polarising benders, solid state collimators with absorbing and with reflecting walls and a solid state radial bender for the polarisation analysis of neutrons over an angular range of 3.8 deg. A newly developed solid state device consists of a solid state polarising bender used in transmission together with a collimator. This allows to polarize or analyze neutrons without deflecting them from their original direction.

Two-dimensional polarisation analysers for an angular range of 5 degrees in both directions are presented.

A polarizing cavity in a guide with a cross section of 60mm x 100mm was built which polarizes neutrons with wavelengths above 0.25nm.

In all polarizing devices polarisations around 95% were realised.

With a focusing solid state lens which can transport the full divergence of a neutron guide a focus with a FWHM of 2.4mm was reached and an intensity increase of 5.6 compared to the intensity there without the lens.

The work was partly supported by the EU initiative NMI3 under contract no. RII3-CT-203-505925.

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### The Jülich neutron spin echo spectrometer J-NSE at the FRMII

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Neutron Spin Echo (NSE) spectroscopy is due to its high energy resolution a well-suited method for studying slow dynamic processes on mesoscopic length scales. Typical applications include (but are not limited to) the dynamics in polymers, glasses or complex liquids. The upgrade and relocation of the instrument to FRMII already resulted in a significant increase of the accessible dynamic range [1, 2]. The spectrometer is there positioned at the end of a neutron guide, giving access to a broad band of incident wavelengths between 5-18Å. Ongoing improvements, as e.g. the correction coils, now also allow to measure low intensity problems like biological samples or grazing incidence NSE. Some selected examples from experiments from different fields, as e.g. microemulsions or polymers in confinement will be presented.

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# Current technical status and performance of the spin-echo spectrometer SNS-NSE at the spallation neutron source in Oak Ridge

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The new instrument SNS-NSE is a high resolution neutron spin-echo spectrometer located at beamline 15 (cold coupled  $H_2$  moderator) of the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory. Currently it is the only spin-echo spectrometer at a pulsed spallation source.

The poster will describe the instrumental layout and current status of the technical implementation. We will discuss future upgrades and improvements, with respect to both instrument components and control software. Furthermore, the current performance of SNS-NSE is demonstrated using latest benchmark measurements.

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### The neutron guide upgrade project at HZB

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The Helmholtz-Zentrum Berlin (former Hahn-Meitner-Institute) exchanges its cold source since October 2010. At the same time most of the neutron guide system in neutron guide hall 1 is rebuilt.

The state-of-the-art neutron guide system was designed using advanced neutron optics in order to fully exploit the new cold source and to reduce the beam losses during transport.

The system comprises the complete guide system from the extraction part to the instruments.

The change of the guide system offers the unique chance to relocate some of the instruments and bring them to optimal positions. Especially the cold triple axis instrument FLEX will profit from an end position and the cold time-of flight instrument NEAT will have an extended flight path ending in a new building. In this process an additional guide is created which will be used as a test beam line for the ESS upgrade project.

Since the guide cross section will be doubled and the coating will be changed from 58Ni to supermirrors with m=3 the gamma radiation will increase by a factor of 20. Based on MCNP calculations a shielding system was designed close to the neutron guides to ensure that present radiation levels are kept or even reduced.

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### Fast neutron scintillation detectors using wavelength shifting lightguides

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The design and construction of fast neutron detectors is described. These detectors are based on scintillation in composites of zinc sulfide and acrylic resin following the design of Hornyak [1]. In the original design the thickness of detector and hence the efficiency is limited by the opacity of the composite. By reading the light out via wavelength shifting lightguides to the photomultiplier, a number of layers may be utilized giving increased efficiency. Neutron discrimination is achieved using specially developed pulse counting circuits. Measurements of efficiencies and gamma rejection are presented. A variant of this design in which zinc oxide scintillator is used is also presented. This variant has a rapid time response and is intended to measure the time structure of neutron pulses.

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# High-efficiency large-area neutron scintillation detectors as replacements for helium-3 proportional tubes

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The design and construction of prototype large-area neutron detectors is described. These detectors are based on scintillation in a mixture of zinc sulfide and boron nitride. The light from the scintillation is read out via wavelength shifting lightguides to photomultipliers. Neutron discrimination is achieved using specially developed pulse counting circuits. Measurements of efficiencies and gamma rejection are presented. These detectors require no isotopically enriched or exotic compounds, being constructed from easily available materials and should provide and attractive alternative to helium-3 proportional tubes.

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### The Sheffield pulsed neutron facility

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A new facility for the investigation of pulsed neutron activation analysis has been constructed at the University of Sheffield. This is intended to provide a testbed for air cargo screening applications. 14MeV neutrons are produced by a pulsed linear inertial electrostatic confinement (IEC) device. This note gives the characteristics and capabilities of this device. Collimation and shielding Monte Carlo studies for the facility are presented and the data acquisition and monitoring systems are described.

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# Pseudostatistic TOF-chopper system for separation of elastic and inelastic neutron scattering with continuous variation of energy resolution

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Simple single pulse white beam TOF-instruments have the disadvantage of measuring a superposition of elastically and inelastically scattered neutron spectra.

By adding an asychronous pseudostatistical chopper close to the sample, Pellionisz [1] proposed a method to simultaneously measure the pure (integral) inelastic spectrum. Thus, by forming the difference, the pure elastic spectrum is available also.

Important applications would be elastic diffuse (off-Bragg) disorder scattering as well as fast registration of integral inelastic scattering maps (thermal diffuse scattering etc.) in reciprocal space. A TOF-system of this type was realized and tested by Schneider [2].

Here, a new variant of this method is proposed by using it in back-scattering mode, where neutrons pass the same statistical chopper twice, namely before and after being scattered by the sample. By increasing the distance between the sample and the statistical chopper, it's virtual opening time can be reduced and thus also the energy resolution of the system. Especially on pulsed neutron sources this simple device could be a cheap and fast method to map elastic and integral inelastic neutron scattering in reciprocal space.

Replacing the single pulse entrance chopper by a pseudostatistical chopper, Pellionisz [3] proposed an advanced version of this system, that offers a substantial increase of luminosity (duty cycle) for continuous neutron sources.

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[2] Schneider J., PhD-thesis, Technical University of Munich, 1975.

[3] Pellionisz P., Atomkernenergie 17 (1971) 277.

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# Design of a generic neutron reflectometer adapted to a long pulse spallation neutron source

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We will present first results of a design study on a virtual generic neutron reflectometer adapted to the time structure of a long pulse neutron spallation source (LPSS). Based on analytical considerations a reflectometer with horizontal sample position and wavelength frame multiplication (WFM) [1] is considered the most flexible set-up for a Day-1 instrument at LPSS. The length of that instrument is 50+6 m, enabling easy adaptation of resolution  $\Delta\lambda\lambda$  from 1% to 10%. Focussing of the incident beam is on a sample size of 1 x 1 cm<sup>2</sup> with potential beam deflection in both downward and upward direction.

The generic reflectometer is to be benchmarked against a reference instrument of 150+6 m length without WFM and a high intensity short instrument of 28 to 36 m without WFM and fixed resolution. The latter two instruments will also be designed and set-up for neutron optical simulation via VITESS [2].

Polarization and polarization analysis as well as focussing and GISANS options are designed as additional modules to be implemented separately in the virtual generic instrument layout.

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# Design study of magnetic environments for XYZ polarization analysis using <sup>3</sup>He for the Diffuse Neutron Scattering spectrometer DNS

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Polarization analysis, PA, of polarized neutrons is a powerful tool for separation of nuclear spin-incoherent background, analysis of complex magnetic structures and the study of magnetic excitations. Several wide angle spectrometers with polarization analysis exist or are under construction in which PA is used. The PA can be performed in a variety of ways depending on the instrument's parameters. The Diffuse Scattering Spectrometer, DNS (JCNS @ FRM II), can currently perform XYZ polarization analysis with supper mirror analyzers, but with performance limited by the analyzer height and integration over the height of the detectors. Installation of a new longer, height-position sensitive detector bank gives a unique opportunity to prototype and test a polarized <sup>3</sup>He XYZ analysis system which could utilize the full height and position resolution of these new detectors. We present an initial design study with finite element magnetic field (FEM) calculations of possible XYZ field configurations suitable for polarized <sup>3</sup>He and adapted to the DNS instrument geometry. Two clear options exist, a magnetized mu-metal geometry, similar to ref [1], or a resistive coil set similar to ref [2], however in our proposed designs, certain key differences exist which build on the experiences from prior devices.

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### Status of instrumentation using polarized <sup>3</sup>He neutron spin filters at the JCNS

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Polarization analysis will be an integral component for much of the instrumentation and thus science at the JCNS. Several instruments will require polarization analysis over very large area detectors, broad wavelength and/or divergence range, and some at high neutron energy. Instruments planning to implement polarization analysis with NSF at the JCNS include the reflectometer MARIA, the small-angle scattering diffractometer KWS1 and the spectrometers DNS and TOPAS (wide angle inelastic scattering). Each of these applications will place a specific demand on the polarization analysis instrumentation. Whenever it is possible to polarize the <sup>3</sup>He in-situ, there will be certain advantages over off-beam polarization methods. One advantage is to make a system that is low maintenance in routine operation and would not require a large amount of training or man-hours to operate from day to day, further in-situ polarization is the only way to obtain the true maximum neutron performance of a given NSF. The recent observations of <sup>3</sup>He polarizations well in excess of 80% in neutron spin filter cells provide new performance benchmarks and allow one to perform effective polarization analysis over ever wider neutron wavelength bandwidths. Additionally, if each application has its own dedicated <sup>3</sup>He polarizer, it provides decoupling of resources. Moreover, the possibility to maintain higher time averaged polarizations will also ensure the maximum data quality and shortest measurement times. At the JCNS there are two initial applications where in-situ polarization will be developed. The first is MARIA, a reflectometer for studying magnetic systems, the second is small angle scattering (SANS), further down the road PA systems for wide angle spectrometers DNS and TOPAS are also under development which are foreseen to use a local filling approach. We will describe the status of these projects, and the prospects in terms of neutron performance that can currently be obtained.

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## Powder diffraction instrumentation at the ESS

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### Neutron depolarisation imaging

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At the neutron imaging beam line ANTARES at FRM II, Munich, we have recently developed the Neutron Depolarisation Imaging (NDI) technique. This method, which is a combination of neutron radiography and polarisation analysis allows mapping of variations of magnetic properties over a sample on a length scale of ~300  $\mu$ m, which may, for instance, result from variations of the chemical composition of the sample [1-4]. We have tested the performance of different polarisers and analysers, e.g. a polarising periscope, standard benders and <sup>3</sup>He spin filter cells. A closed cycle cryostat including a <sup>3</sup>He/<sup>4</sup>He dilution insert has enabled us to reach temperatures as low as 75 mK. The technique makes use of the neutron spin depolarisation after transmission of a polarised beam through a series of ferromagnetic domains or clusters. Measurements on the metallurgically inhomogenous, itinerant ferromagnets Pd<sub>1-x</sub>Ni<sub>x</sub> and Nb<sub>1-y</sub>Fe<sub>2+y</sub> as well as on the Kondo lattice system

 $CePd_{1-x}Rh_x$  have been performed to demonstrate the potential of the NDI technique. Additional magnetic fields applied at the sample position allow the identification of spin glass behaviour in  $CePd_{1-x}Rh_x$  at low temperatures. NDI can also be used to determine frequency dependent, field dependent and temperature dependent properties of magnetic materials being, for example, exposed to time dependent fields. In our contribution we will discuss the experimental technique as well as its applications to ferromagnetic and superconducting materials that undergo quantum phase transitions. Furthermore, we will discuss developments and adaptions necessary to apply Neutron Depolarisation Imaging at pulsed spallation sources.

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