HEIMDAL: A Time-of-Flight Neutron powder Diffractometer for *In-Situ/In-Operandi* Materials Science Studies at the European Spallation Source

Laboratory for Neutron Scattering and Imaging

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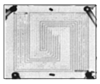
HEIMDAL- Concept

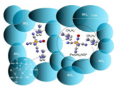
The hybrid instrument HEIMDAL (named after a god in the Norse mythology) is combining thermal (TPD) and cold (CPD) neutron diffraction, SANS and neutron imaging in one instrument as requested by many in-situ experiments where sample change for example with time. Chemical reactions, technical materials in operations, materials showing phase separations, where single shot measurements on different instrument would yield information on a different status of the material, will be investigated on different length scales from 0.01nm up to 1000nm.

New Science on HEIMDAL

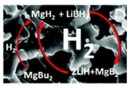
Developing new materials is of paramount importance to combat future energy demands, and environmental damage. Improvements in material performances are reached for example by the incorporation of advanced ceramics and polymers into heterogeneous systems. Their performances usually depend on the interplay between properties defined by the atomic, nano/mesoscopic and microscopic structure. ***In-situ* and *in-operandi*** investigations will be in the focus of such investigations.



Picture: Lehman *et al.*/PSI



Cervellino/Schaniel *et al.*, PSI/Nancy

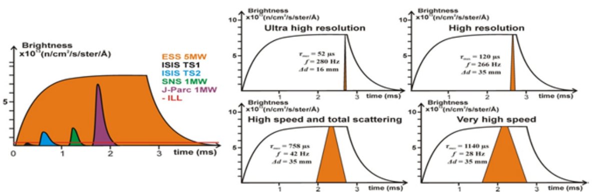


Nielsen *et al.*

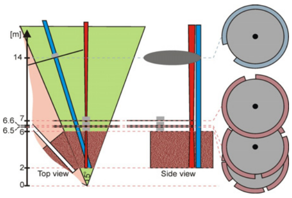
Energy storage:
Li-ion batteries, hydrogen storage materials
Efficient energy use: solid oxygen fuel cells (SOFC)
Composite, scaffold or matrix embedded systems
Most new materials will be composite materials where a host is embedding the active compound
Phase transitions and nucleation Extra-stimuli investigations
Materials with magnetic properties:
Ferroelectric materials, e.g.

Layout

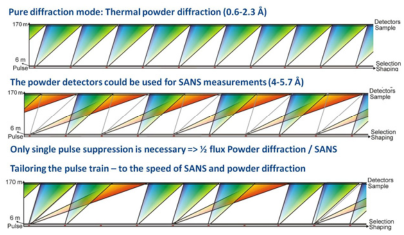
HEIMDAL is meeting this demand by combining an optimized neutron powder diffractometer with a variable resolution and a narrow band SANS machine. A thermal double-elliptic guide for NPD and a simple cold guide for the SANS, converging at the sample position, allow an optimized neutron optics for both parts of the instrument. The guides exit from the same beam port. An imaging camera will allow to select the sample volume to be investigated.



Adapting the pulse length: high-resolution vs. high-speed
The ESS pulse is 2.86ms. HEIMDAL uses the advantage for NPD !

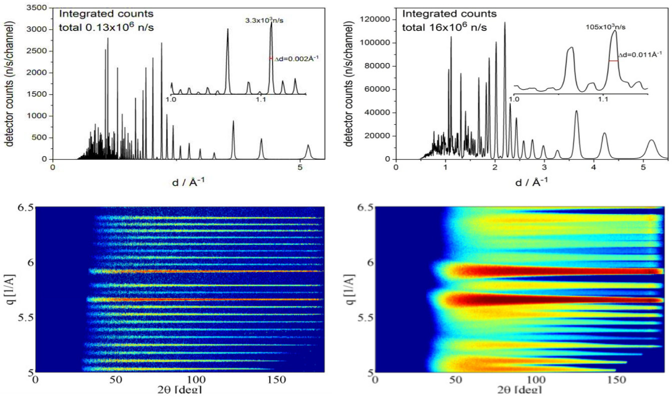


Chopper systems for cold (blue) and thermal (red) guide



"Mixing" the spectra from the two guides with no frame overlap.

HEIMDAL Performance



HEIMDAL in the high resolution mode (left) and the high intensity mode (right). In the top diagrams, the 2D-data (q versus scattering value Θ) are summed up to "normal" 1D powder diffraction pattern.

Instrument		Type	Δd/d@ 2Q=90⁰	Δλ (Å)	λ_{mean} (Å)	q_{range} ($Å^{-1}$)	Detector Type	D_{area} (sr)	flux ($n/s/cm^2$)	G_{eff}
GEM	ISIS	TOF	**0.50%**	3.5	1.8	0.04-100	Sc	3.9	2e6	**1**
New Polaris	ISIS	TOF	0.50%	5.5	2.9	0.7-125	Sc	5.67	~1e7	**~7**
Nomad	SNS	TOF	0.60%	3.0	1.6	0.5-125	^3He	4	~1e8	**~71**
PowGen	SNS	TOF	0.50%	2	1.1	3-120	Sc	4.4	~2.5e7	**~14**
I-materia	JPARC	TOF	0.50%	6	3.3	0.007-70	^3He	4	~1e8	**~86**
Nova	JPARC	TOF	0.50%	7	3.6	0.4-100	^3He	5	~4e8	**~385**
D20	ILL	CW	1.6%	-	1.3	0.2-8	^3He	0.27	~1e8	**~2**
Powtex	FMR2	TOF	0.60%	1.4	1.6	0.4-13	^{10}B	6.2	~1e7	**~7**
Wombat	OPAL	CW	1.0%	-	2.4	0.4-4	^3He	0.59	~1.3e8	**~8**
HEIMDAL (high res.)	**ESS**	**TOF**	**0.17%**	**1.7**	**1.5**	**0.6-21**	**Sc**	**2.25**	**~3.8e6**	**~3**
HEIMDAL (Med res.)	**ESS**	**TOF**	**0.60%**	**1.7**	**1.5**	**0.6-21**	**Sc**	**2.25**	**~6.2e8**	**~150**
HEIMDAL (high flux)	**ESS**	**TOF**	**1.0%**	**1.7**	**1.5**	**0.6-21**	**Sc**	**2.25**	**~2.0e9**	**~290**

In the high resolution mode, HEIMDAL outperforms GEM by a factor of 9 at the same resolution of Δd/d=0.5%.

Conclusions

- ✓ HEIMDAL will be a state-of-the-art neutron TOF powder diffractometer at ESS with a G_{eff} of 3 to 290 in the international comparison
- ✓ HEIMDAL extends the length scale of the NPD significantly by the integrated SANS option
- ✓ HEIMDAL will match the future needs for in-situ/in-operandi studies to develop new materials
- ✓ HEIMDAL will attract a new user community

This work has been supported by the Swiss State Secretariat for Education, Research and Innovation, the Danish Government, the universities of Copenhagen and Aarhus, Denmark, as well as Paul Scherrer Institut, Villigen PSI, Switzerland.