Overview of [Materials Engineering Diffraction]

EUROPEAN SPALLATION SOURCE

A.N. Other

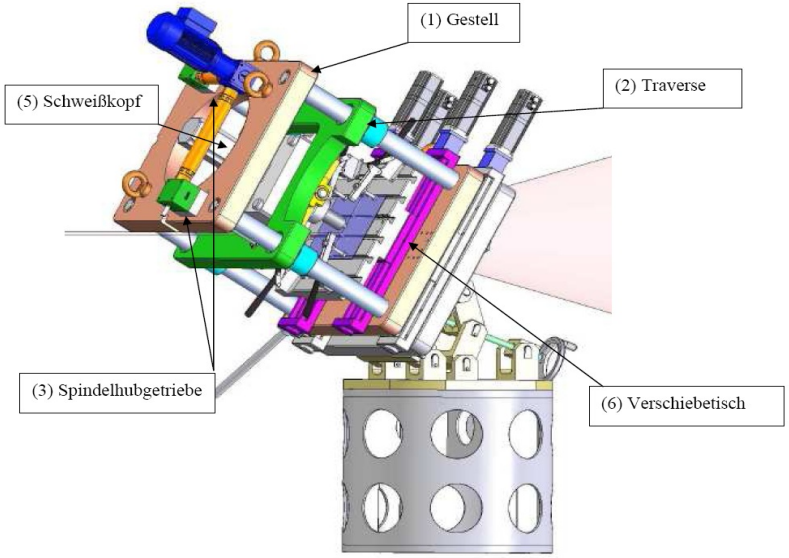
[Instrument Class]

IKON5

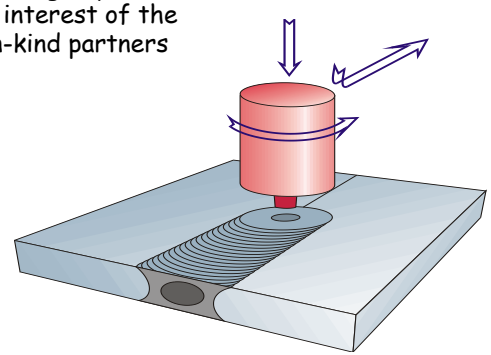
Lund, 2013-09-25 & 26

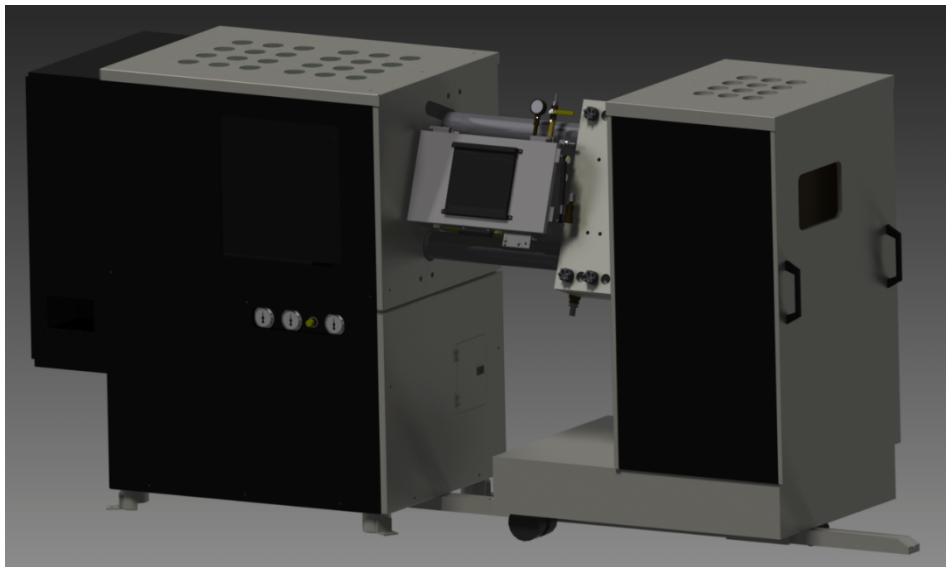
[Materials Engineering Diffraction]

- Science Drivers
  - Stress/Strain
  - Texture
  - In-situ (welding and material processing)
  - Long time studies
- Technical
  - Variable resolution (high to medium)
  - Large sample environment capacity
  - Structured pulse option
  - Variable detector coverage
  - Focusing option
  - Complementary capacities (imaging/SANS)



In-situ welding experiments
A central interest of the
German in-kind partners





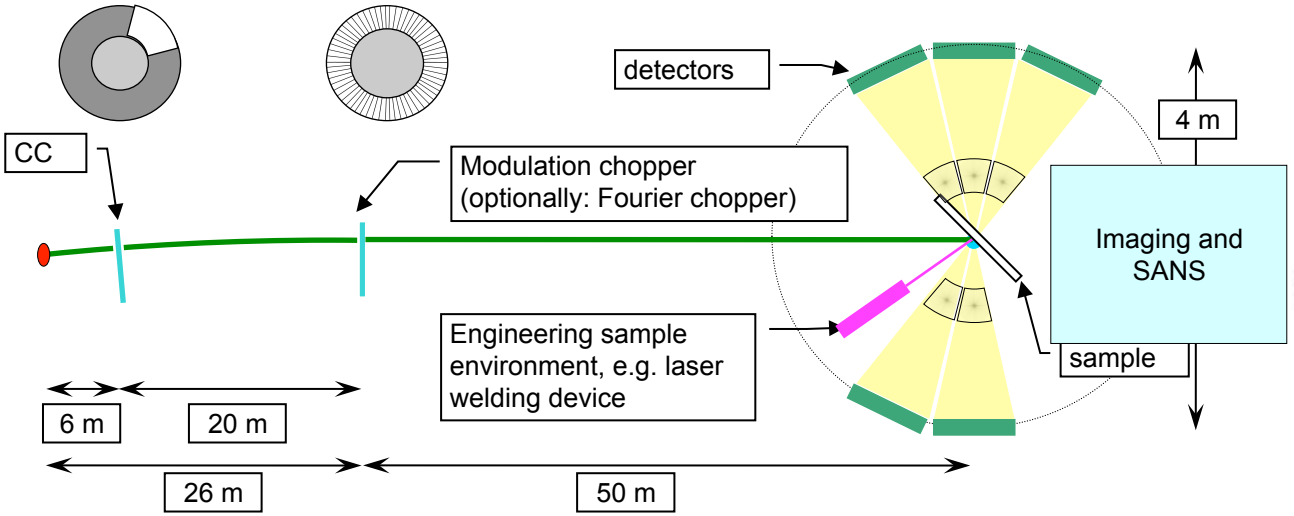
In-situ physical
simulations experiments
with a Gleeble©
a central interest of our
Czech partners

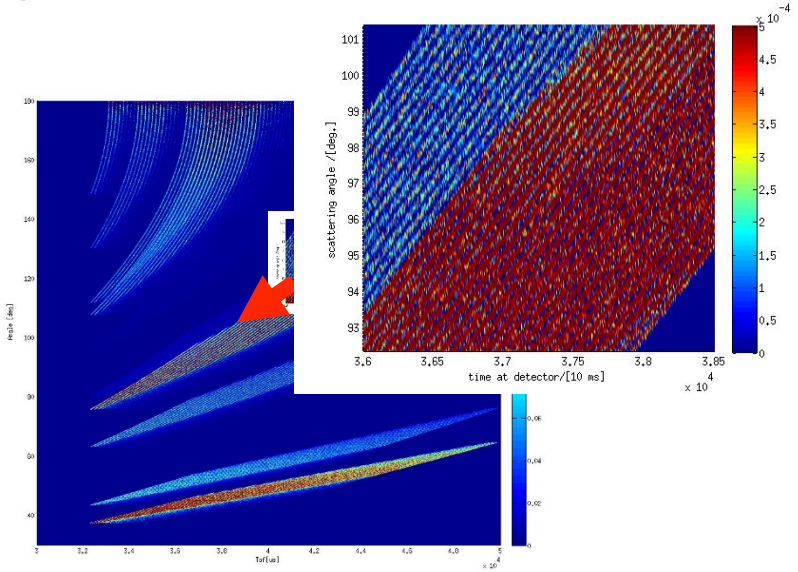
[Materials engineering Diffraction]
Instrument Work Units

Manag. IC1	SANS IC2	Reflectometers IC3	Macromol. Diffraction IC4	Single Crystal Diffraction IC5	Powder Diffraction IC6	Materials Engin. Diffraction IC7	Imaging IC8	Direct Geom. Spectroscopy IC9	Indirect Geom Spectroscopy IC10	Spin-Echo IC11	Fundam. Physics IC12
	Conventional SANS Full DU for fast conv. ext. q-range SANS, SD004DE/ab	Reflectometer for liquid surfaces and soft matter Full DU for wide q and add-ons, SD003DE/a	Macromol. Diffractom. Full DU, potent. farm SD036ESS	Single Crystal Mag. Diffractom. Full DU SD060ESS	Bispectral Powder Diffractometer Full DU, wfm, gen. purp., SD005DE/a	Engineering Diffraction SPEED full DU plus prototyping tests, SD005DE/b	Multi-Purpose High-Res Imaging Full DU in close collab. with CH, dark-field, Bragg edge, polarized SD006DE	Cold Chopper Spectrometer Full DU, high res., RRM and pol. cap., SD001DE/a	Phase Space Transformers Full DU, incl. feasibility studies, focussing, SD007DE/a	High Resolution NSE Full DU, small sample, SD002DE/a	Fund. Physics Full DU Not covered
	Small-sample SANS Full DU SANS, SD004DE/c	Reflectometer for magnetic layers Full DU, focus. pol., SD003DE/b		Single Crystal Mag. Diffractom. Full DU French collaboration	Multi Purp. Extreme Environ.Diffr. Full DU, tests, SD008DE	CEED Full DU, tests, PM, SD033CZ	Larmor Label. Full DU, TOF DF imaging SD056NL	Bispectral Chopper Spectrometer Full DU, RRM pol., SD001DE/b	CAMEA Full DU plus tests and prototyping, SD016DC	Wide Angle NSE Full DU, SD002DE/b	UCN full DU Not covered
	Pol. SANS Full DU, incl. SE devices SD054NL	Vertical focusing reflectometer Full DU, SELENE ,plus prototype tests, design full instrument, SD017DC/a			Hybrid Diffractometer potent. including SANS and imaging Full DU, SD019DC	Hi Flex. Mat. & Engin. Diff. Full DU, Hi flex .res., SPEED, Fourier, POLDI SD059ESS	Multi-Purpose High-Res Imaging Full DU in close collab. GER, phase, fast, high res., SD029CH	Thermal Chopper Spectrometer Full DU, RRM and pol. cap. SD038ESS/a	Backscatt. Spectrometer Full DU, variable 1 to 20 micro eV resolution SD039ESS Danish In-kind	NRSE Resonant NSE, SD007DE/b	
	Compact SANS Full DU, incl. Monochr. mode, SD018DC	Horizontal focusing reflectometer Full DU, SELENE ,plus prototype tests, design full instrument, SD017DC/b			Thermal Powder Diffr. Full DU, variable to high res. SD035ESS		Multi-Purpose High-Res Imaging TOF conceptual design SD040ESS	Cold Chopper Spectrometer Full DU, RRM and pol. cap. SD064ESS	Vibrational Spectrometer Full DU, SD061ESS, Italian collaboration	Focussing optics Full DU, SD007DE/c	
	Broadband SANS Full DU, SD062ESS	Freia Reflectometer Full DU, broad simultaneous q-range, SD034ESS			Pulsed Monochr. Powder Diffr. multi monochromators or chop.; concept. design SD037ESS			Crystal Monochr. Spectrometer Full DU Italian collaboration	Q – TAS Farm Full DU, SD062ESS Not covered		
	VSANS/ GSANS Full DU French collaboration	Spin-Echo label. in Pol. Reflectom. SD055NL			Larmor label. in diffr. (TOFLAR) SD057NL						
Simulation software development, general simulations, supporting GER simulations, VITESS SD015DE											
General simulations, in-house supporting simulations, interface moderator-beam extraction, McStas SD022DK											

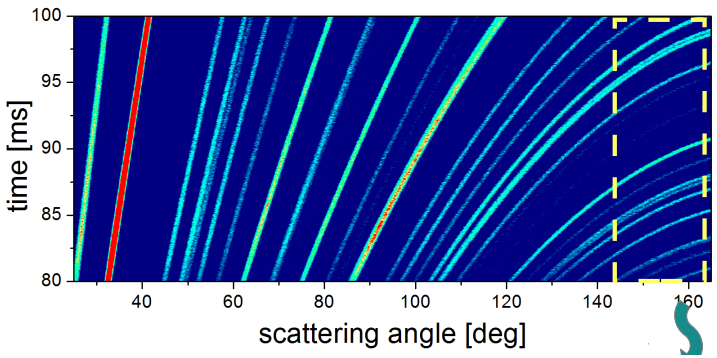
[Materials engineering Diffraction WUs]

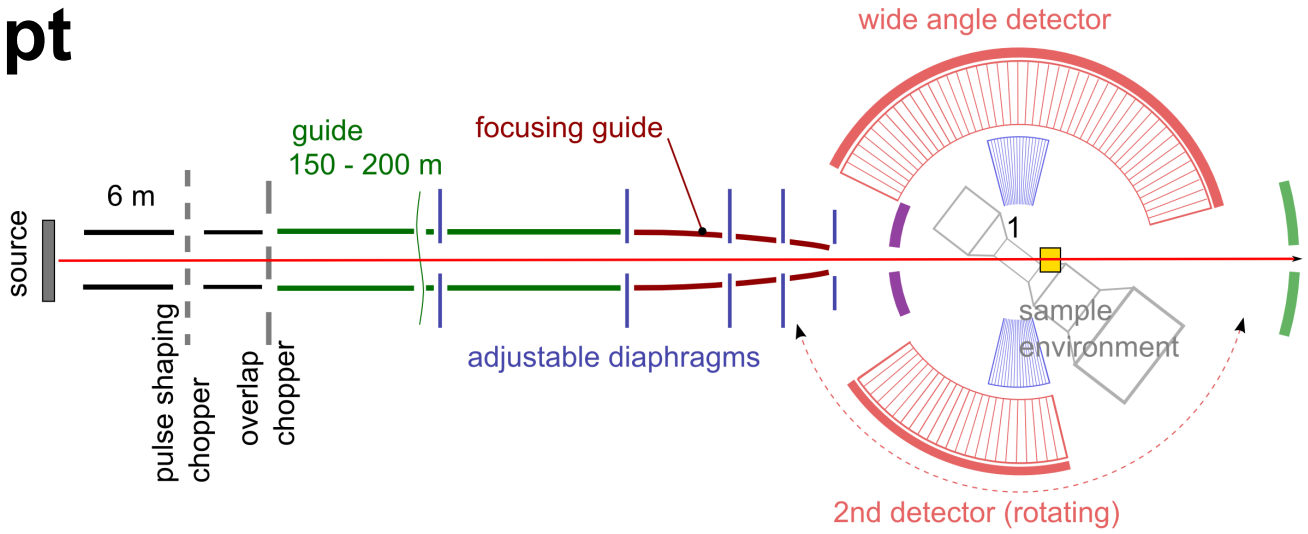
German SPEED concept





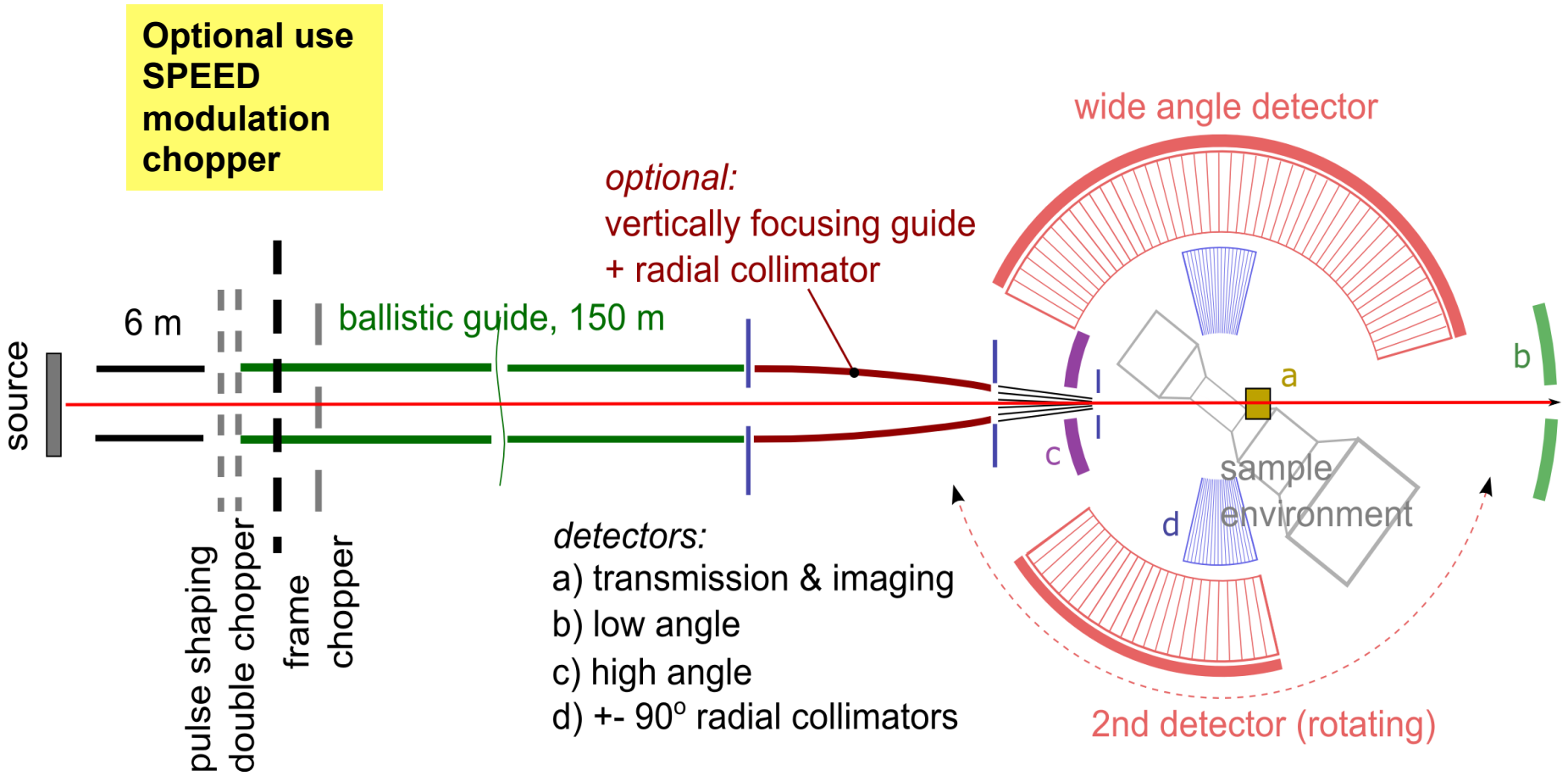
Czech CEED concept





[Materials engineering Diffraction]

A joint DE CZ ESS instrument proposal



Thank you!

EUROPEAN SPALLATION SOURCE

A.N. Other

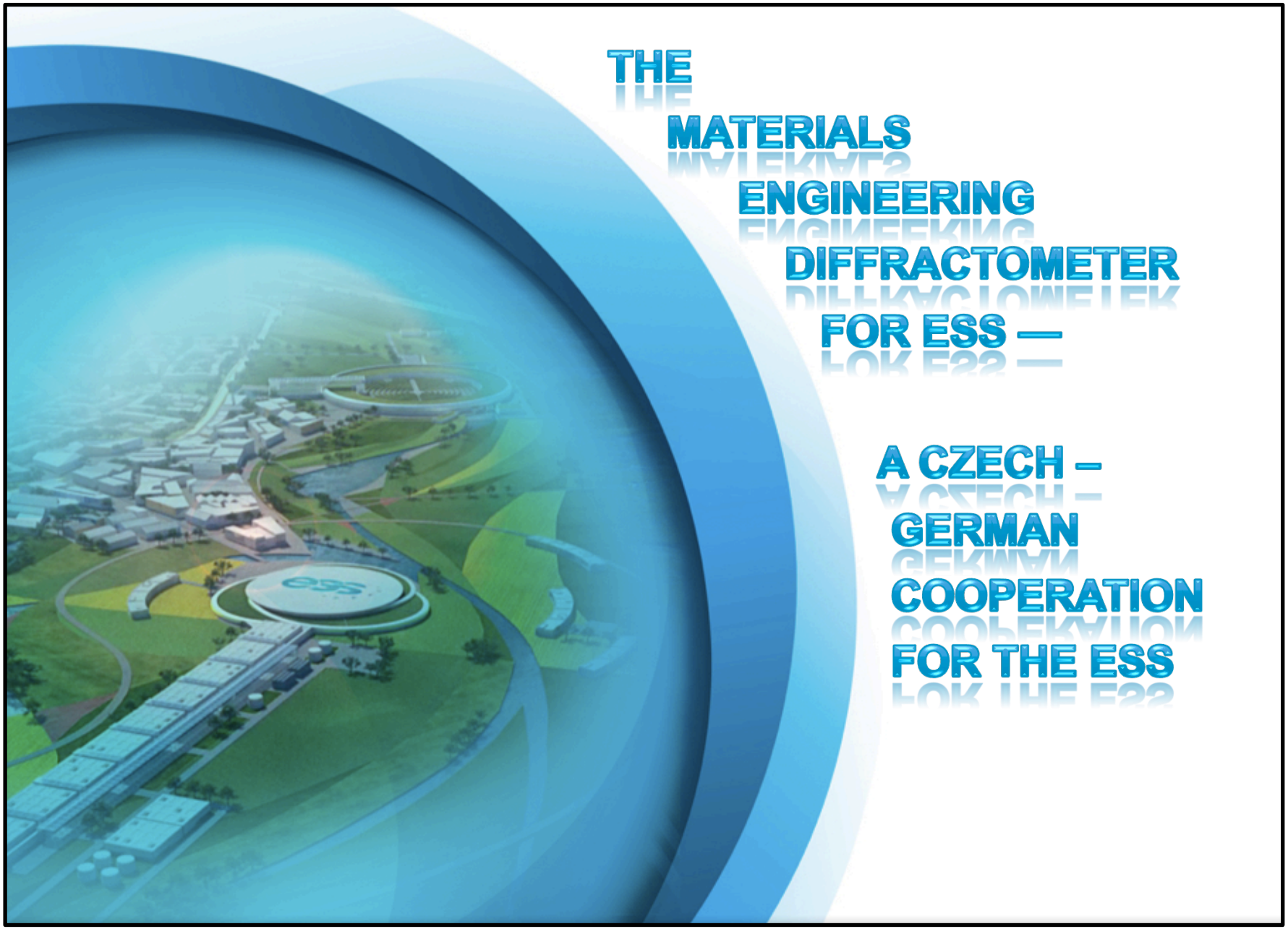
[Instrument Class]

The Materials Engineering Diffractometer for ESS

— *Part I: Scientific drivers* —

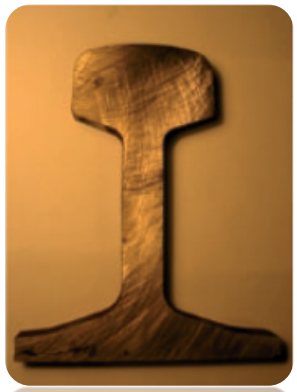
J. Šaroun[1], P. Šittner[2], J. Pilch[1], P. Lukáš[1], P. Beran[1],
L. Kadeřávek[1], J. Navrátil[1], P. Mikula[1], V. Ryukhtin[1], P. Strunz[1]
P. Staron[3], R. Kampmann[3], J. Fenske[3], M. Rouijaa[3], G. Nowak[3],
H.-G. Brokmeier[3], M. Müller[3], A. Schreyer[3]
M. Strobl[4]

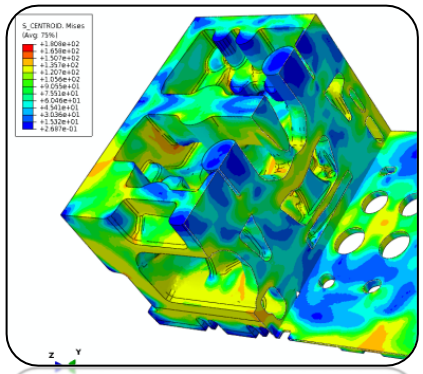
[1]Nuclear Physics Institute, ASCR; [2]Institute of Physics, ASCR;
[3]Institute of Materials Research, Helmholtz-Zentrum Geesthacht;
[4]ESS

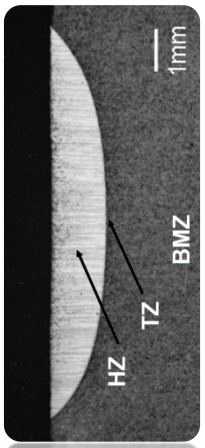

THE
MATERIALS
ENGINEERING
DIFFRACTOMETER
FOR ESS —
A CZECH –
GERMAN
COOPERATION
FOR THE ESS

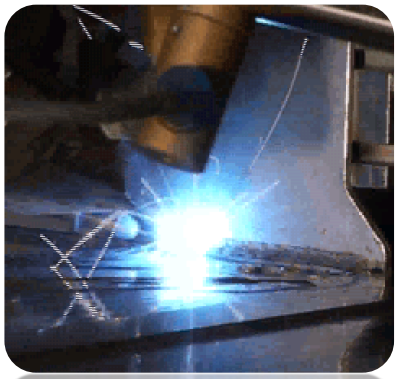
high flux

thick specimens	many points	high spatial resolution	many samples	high time resolution
real products	3D strain maps	gradients, surface	process optimization	*in situ* experiments







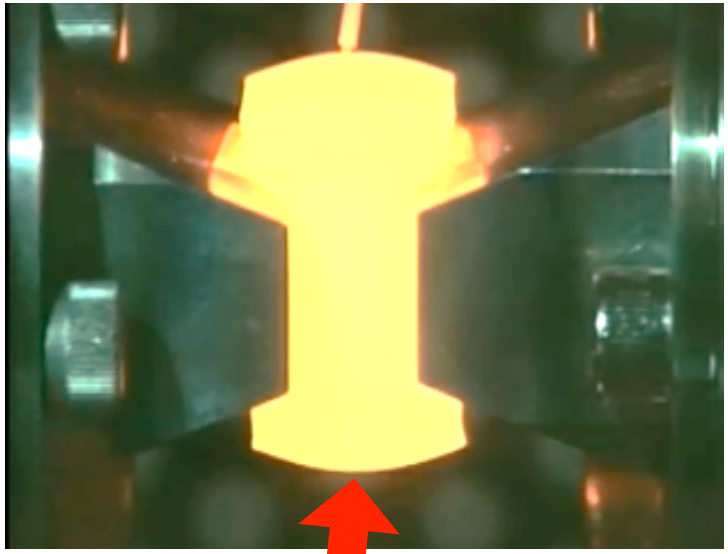


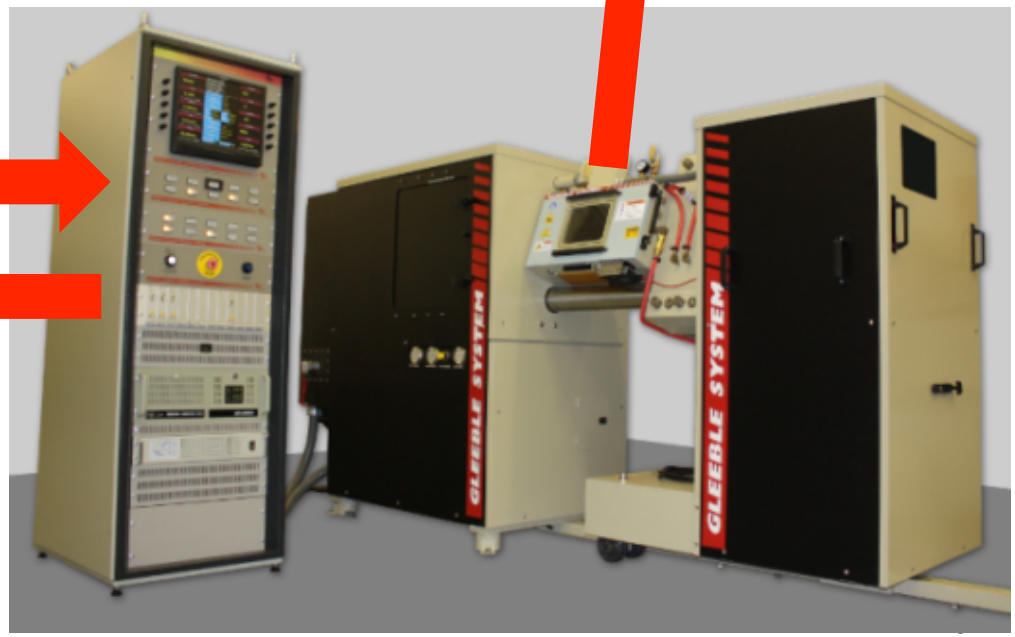
residual stress	texture analysis	*in situ* studies	thermomech simulation	long-term experiments

New *in situ* experiments

Gleeble, a thermo-mechanical simulator:

- fast heating and deformation
- study microstructure during **real industrial processes**
- does not yet exist at a neutron instrument,
  first worldwide at the Brazilian synchrotron

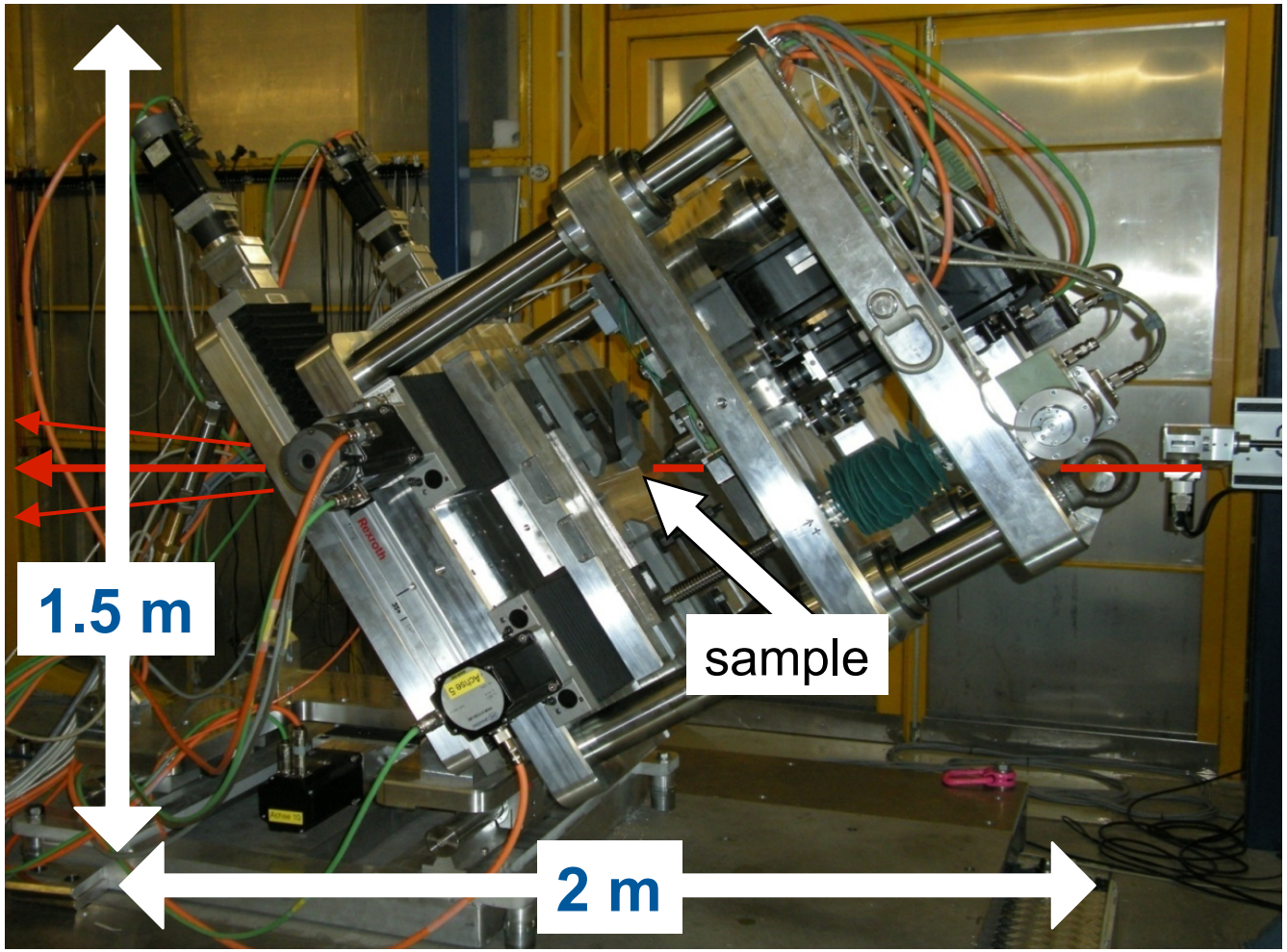




Sophisticated user experiments

In situ studies of the friction stir welding (FSW) process:

mass:
1400 kg



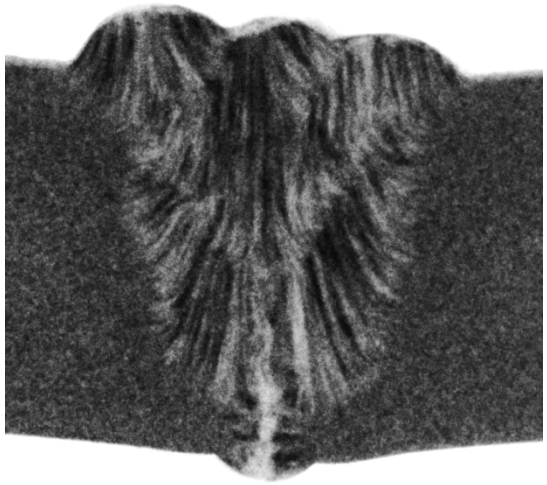
HZG friction stir welding machine for *in situ* studies
("FlexiStir" used at a HZG synchrotron beamline)

Develop robotics

Robotic sample holding and changing for large sample series:

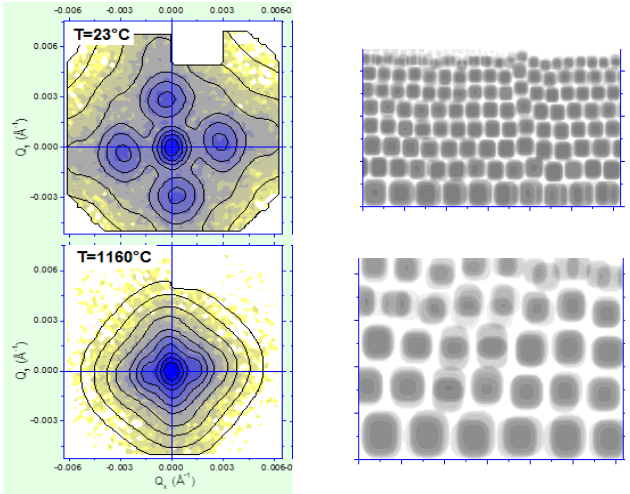
Six-axis robot at STRESS-SPEC (HZG/TUM)

Combining techniques



imaging

simultaneous diffraction and
small-angle scattering (SANS) or imaging
from engineering materials under extreme conditions providing in-situ information on precipitation, void nucleation, crystallization from liquid, sintering at high temperatures and external loads



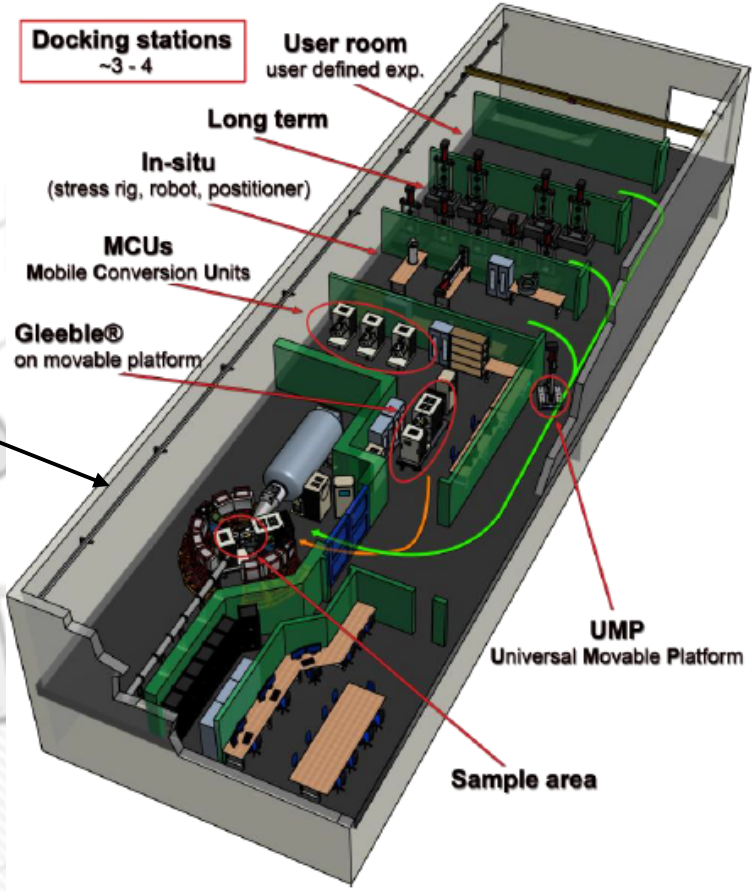
SANS

The Materials Engineering Diffractometer for ESS

— *Part II: Instrument concept* —

engineering lab

experimental area



neutron guides (150 m)

frame chopper

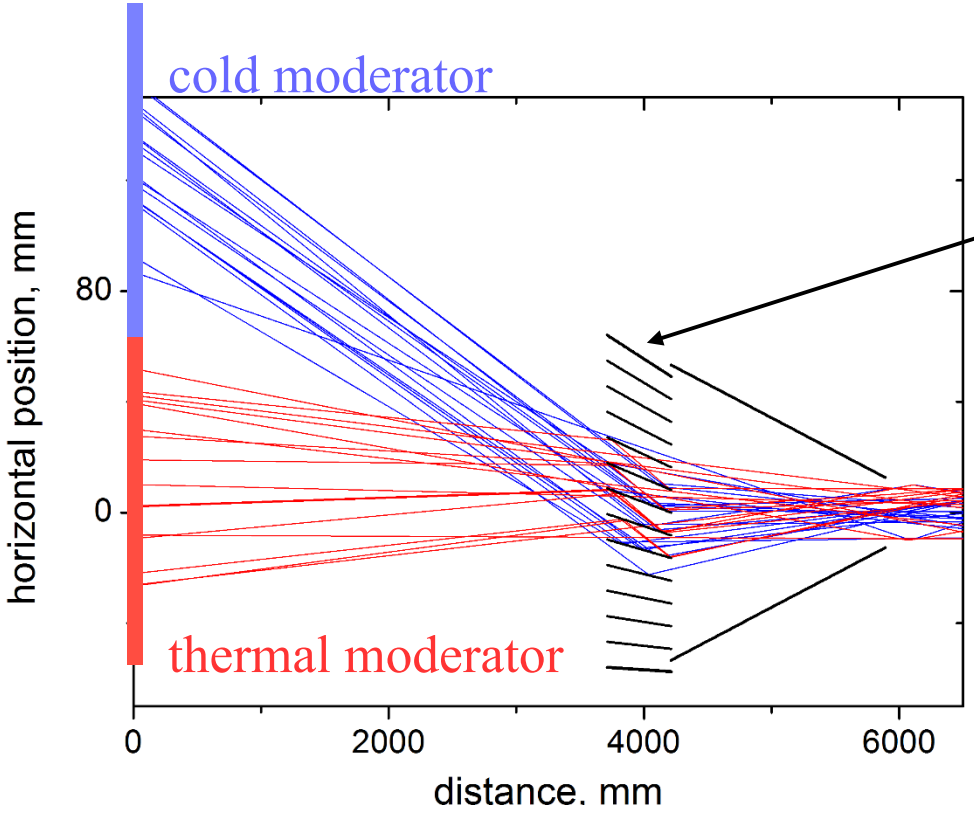
target &
moderators

chopper cave

bi-spectral
extraction optics

proton beam

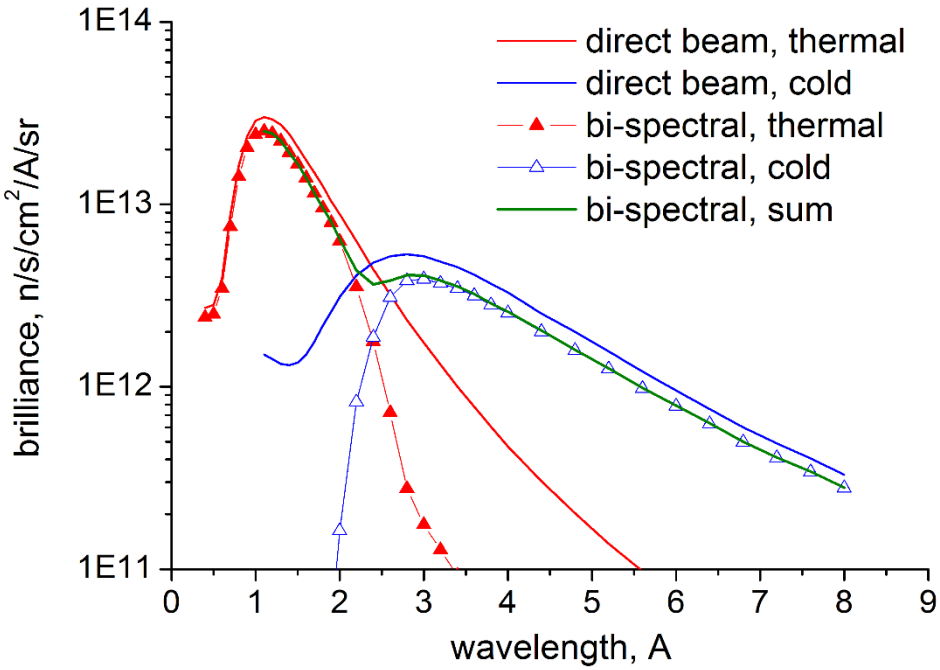
Bi-spectral extraction



semi-transparent supermirror blades
cut-off wavelength ~ 2.35 Å

Sample of trajectories through the extraction optics from the cold (blue) and thermal (red) moderators.

About 80 % efficiency

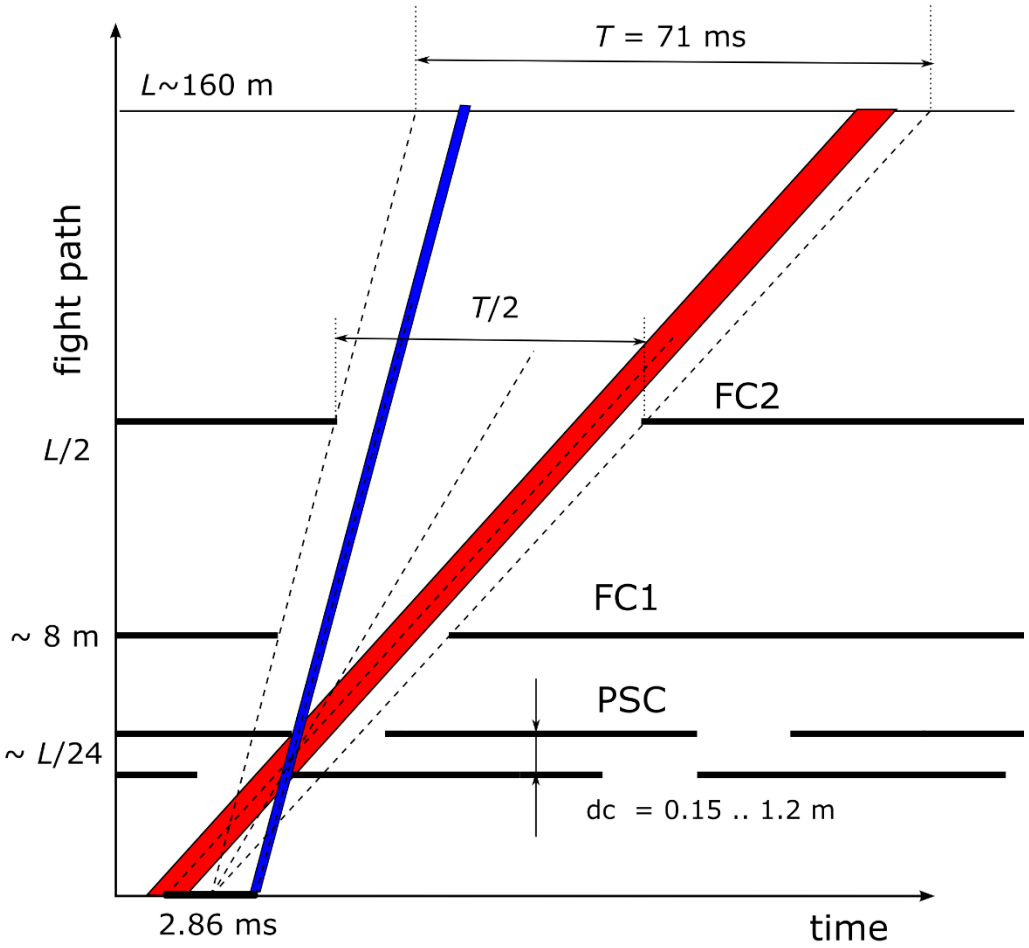


Simulated beam brilliance at the sample position

Why:

- access to large *d* (*d*=2.5 Å => λ=3.5 .. 5 Å)
- Bragg edge (*d*=2λ)

Pulse shaping



Pulse length definition

Pulse shaping choppers (PSC) in blind mode
used at ILL/D33, ANSTO/PLATYPUS, FRMII / REFSANS, …

Source: Astrium

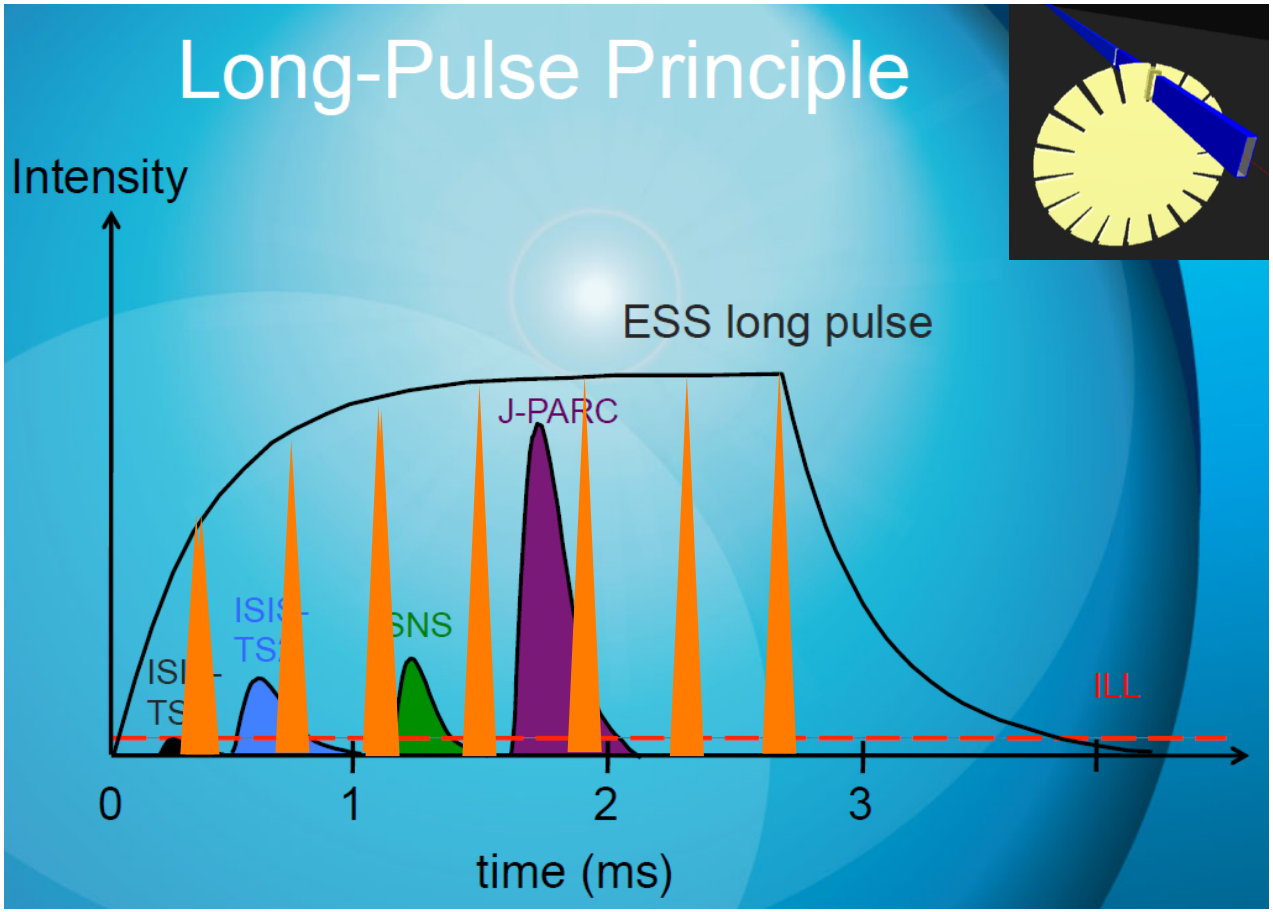
For ESS, we require fast-rotating (168 Hz) choppers with magnetic bearings

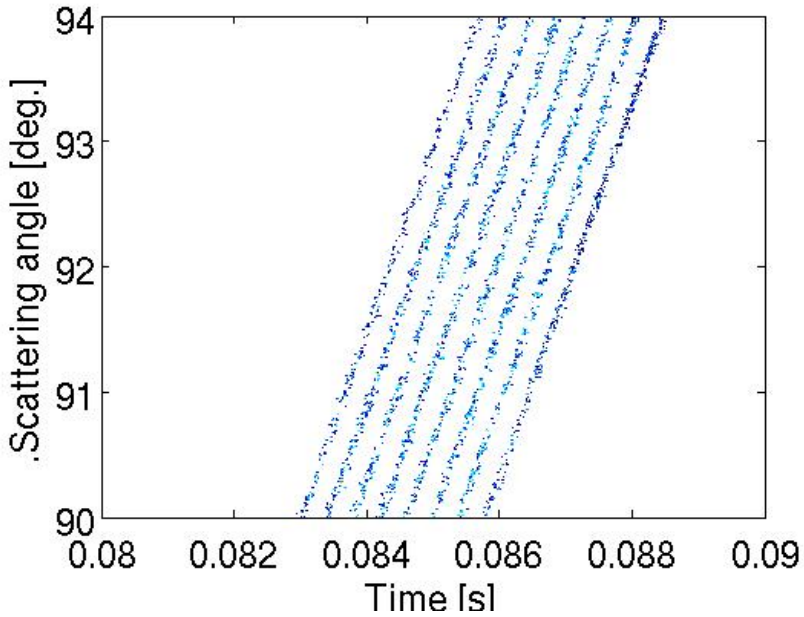
- constant $\Delta t/t = \Delta\lambda/\lambda$ resolution
- tunable (see the table)

Parameters:

R=300 mm, *window*=40% , *frequency*=168 Hz (12 x f_{src}) for max. λ=8 Å.
Distance ~ L_{det}/24 ~ 6.5 m

Pulse multiplexing





factor ~ 5–10 gain in count rate

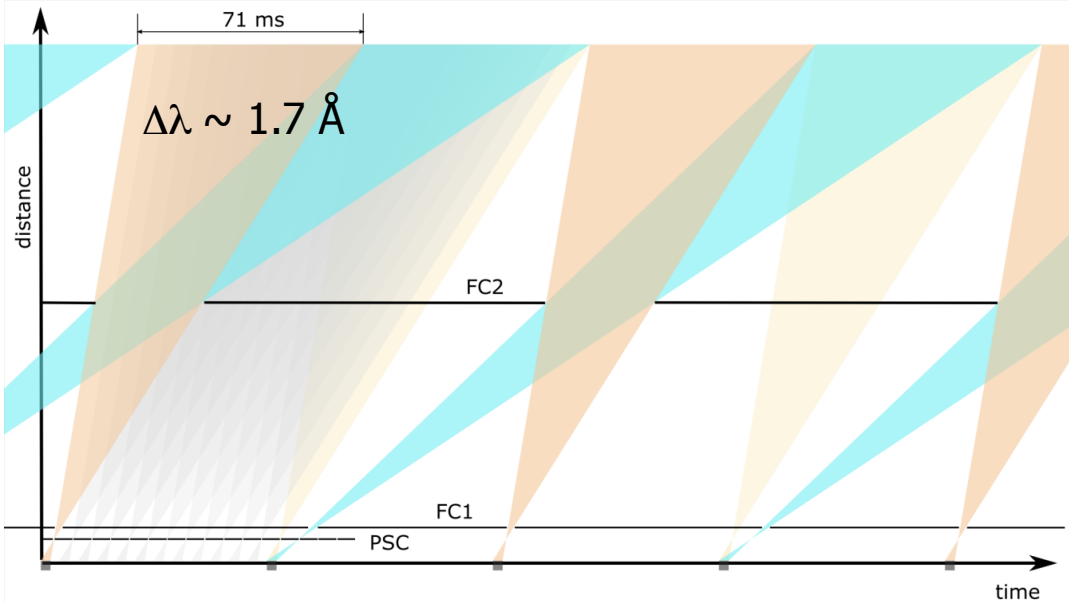
Modulation chopper:
- several wavelengths at the detector at the same time
- distinguished by scattering angle

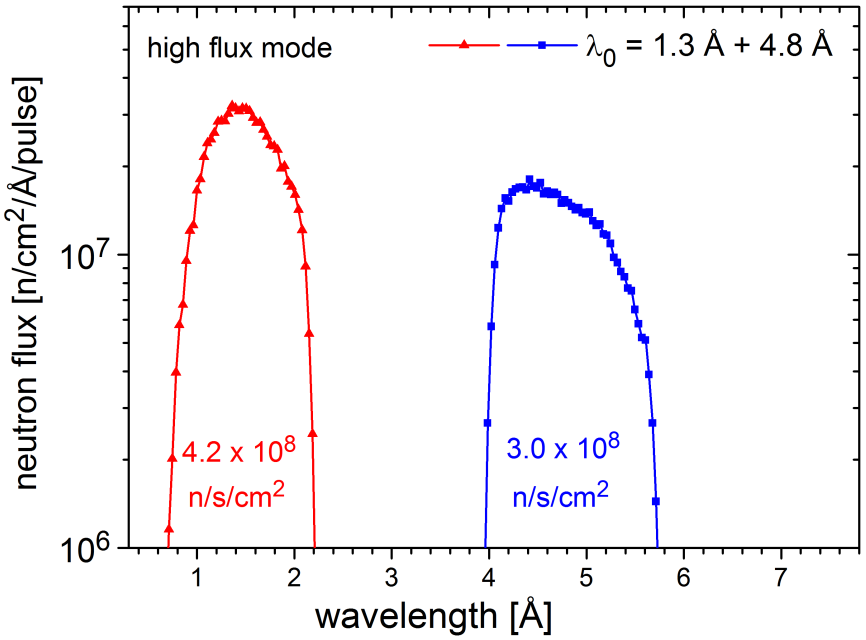
- decouple resolution and intensity
- for well separated lines in crystals with high symmetry

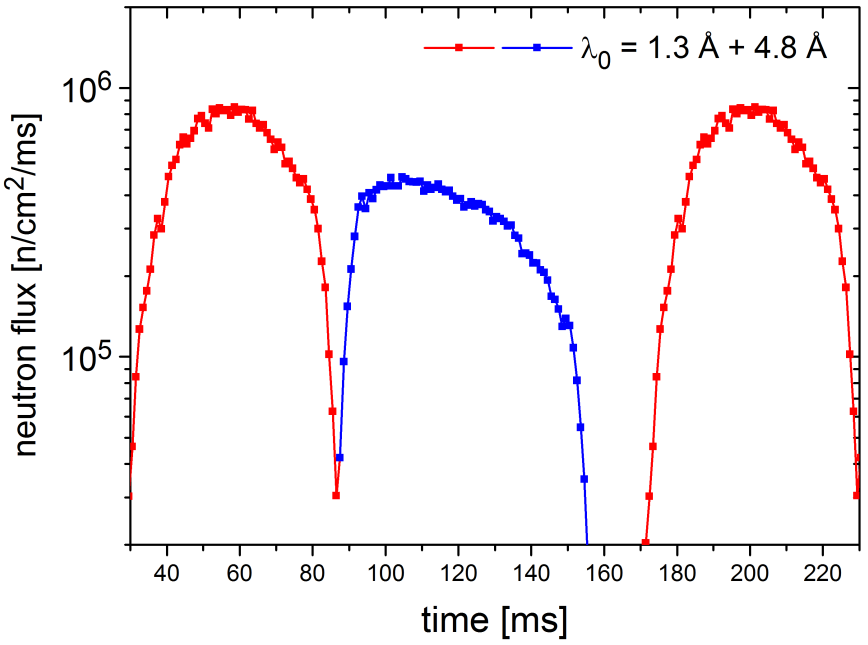
Pulse suppression

Use thermal and cold neutrons simultaneously

1. pulse suppression
2. phase modulation



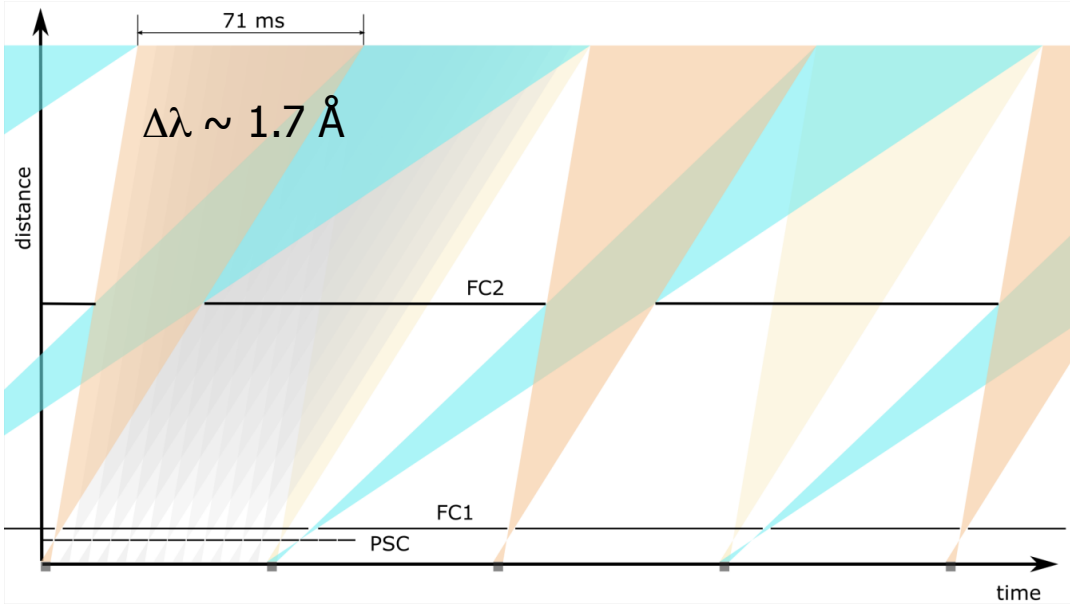


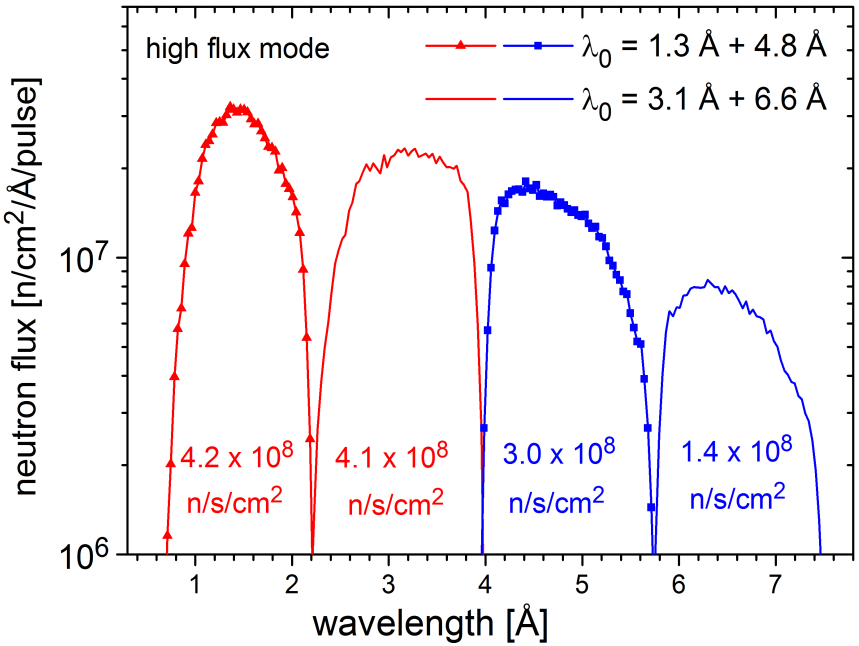


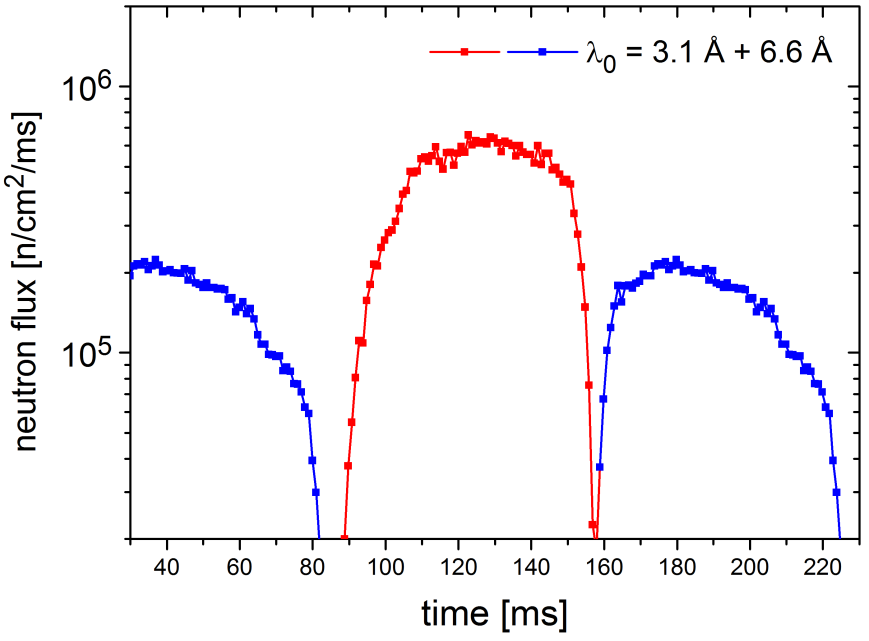
Pulse suppression

Use thermal and cold neutrons simultaneously

1. pulse suppression
2. phase modulation

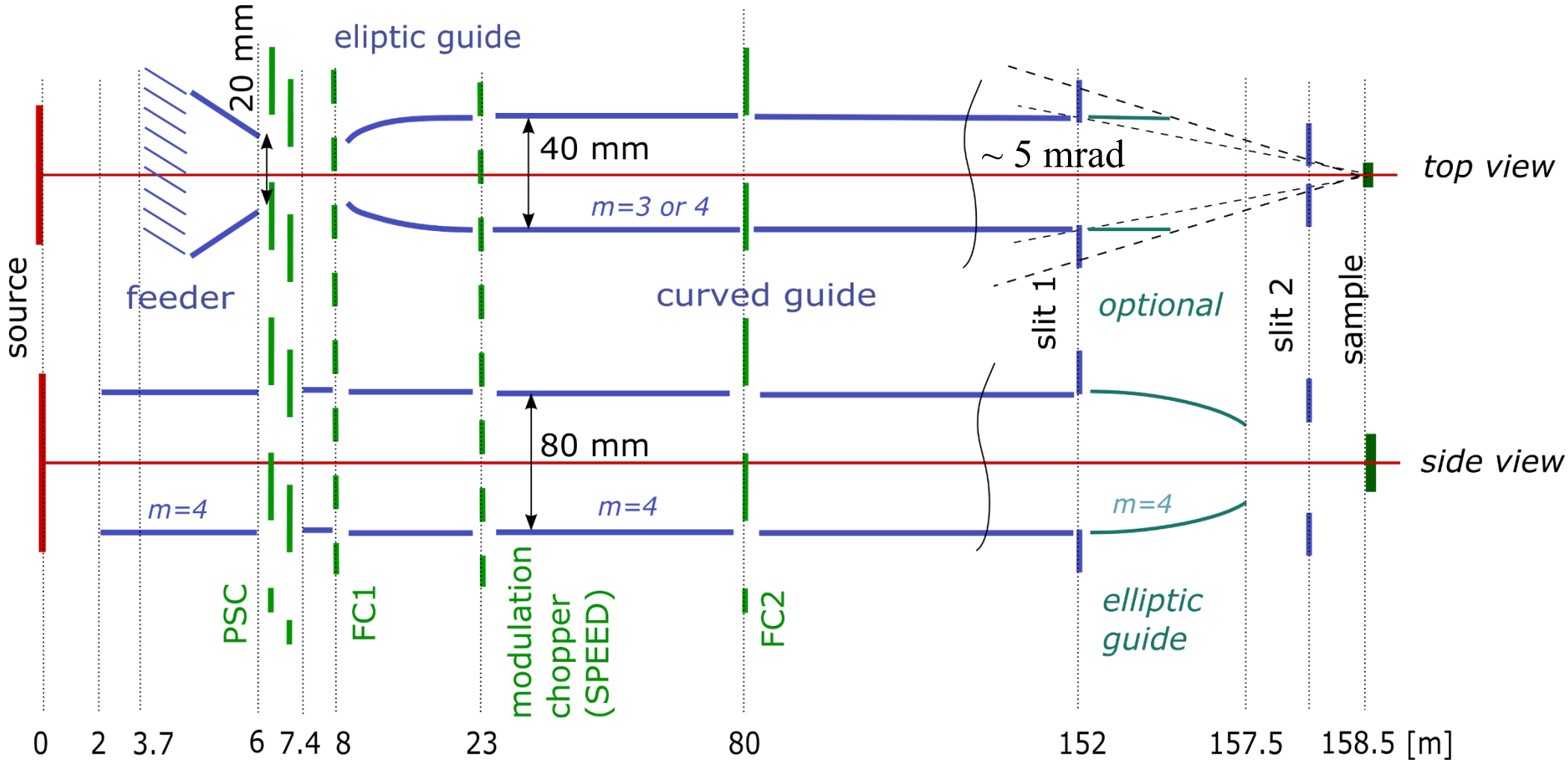






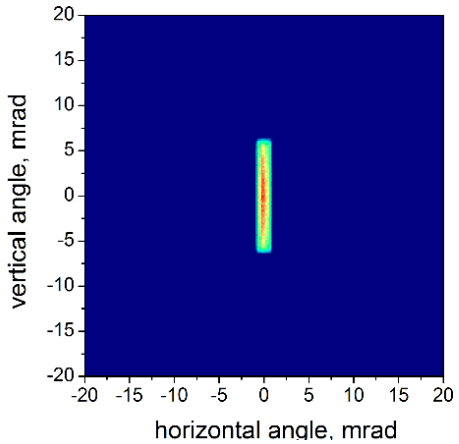
Neutron transport

divergence transported through the long guide ~ 5 mrad (*fwhm*)



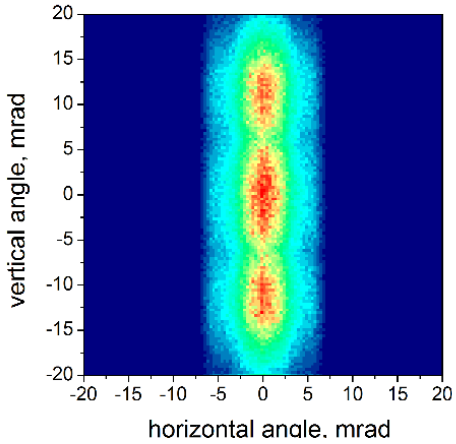
Focusing optics

high resolution mode, slit 1x8 cm², no focusing
divergences 1.3 x 8 mrad²



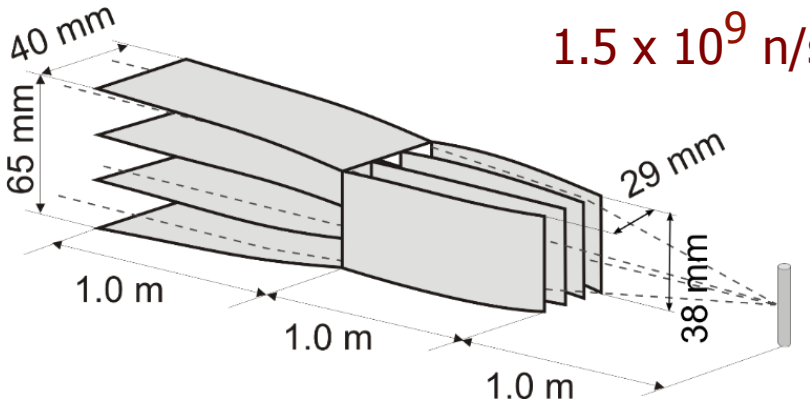
8.6 x 10^6 n/s/cm²

high flux mode – vertical focusing
divergences 6 x 32 mrad²



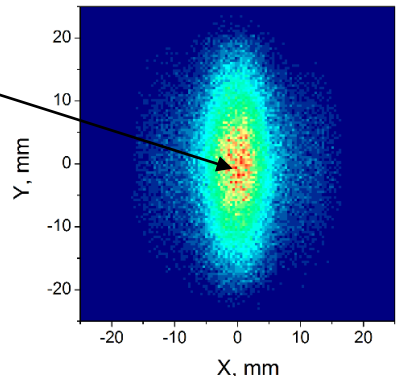
4.8 x 10^8 n/s/cm²

Multichannel optics\:

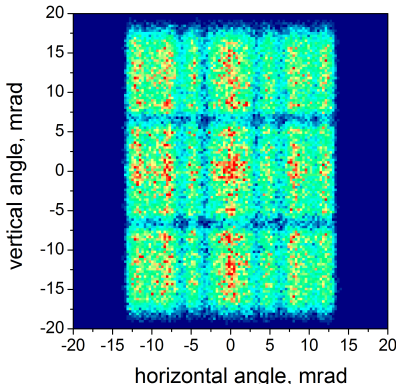


1.5 x 10^9 n/s/cm²

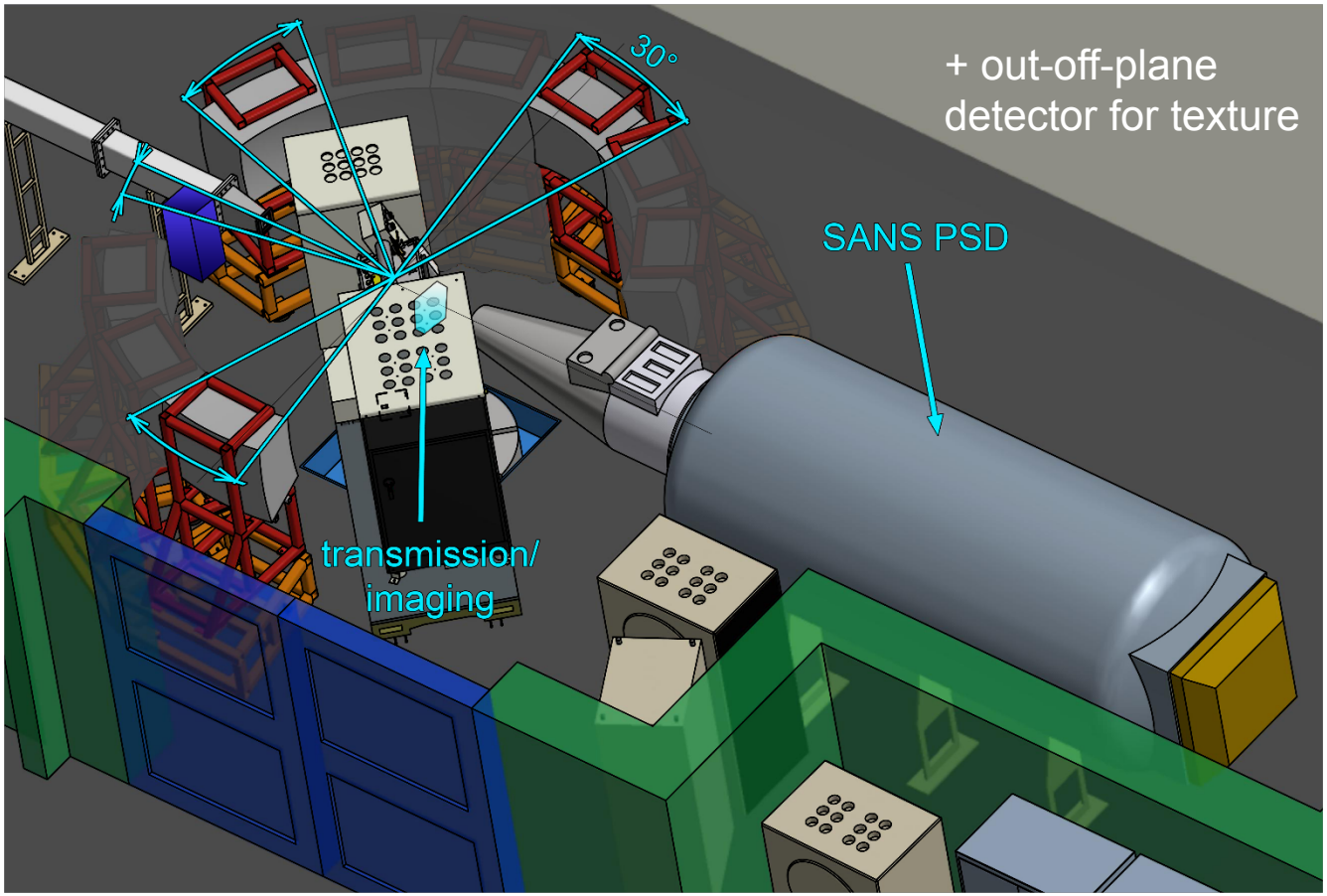
fwhm = 8 x 21 mm²



divergence 20 x 30 mrad²



Detectors

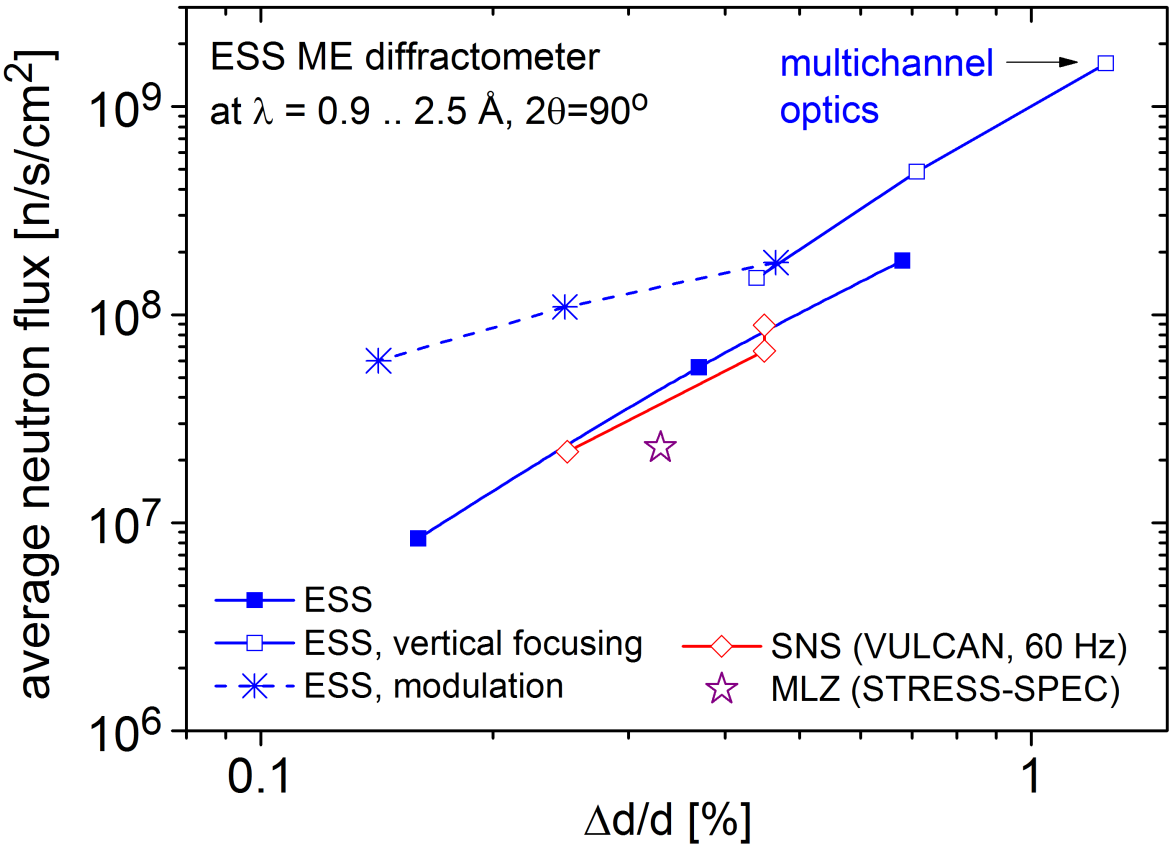


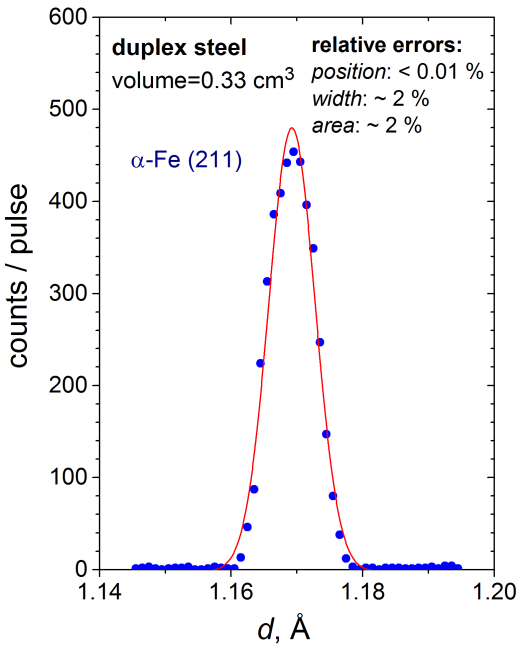
Required parameters
distance: 2 m
resolution: < 2 x 5 mm ^{2}

Technology
^{10}B plates
^{3}He (small detectors)

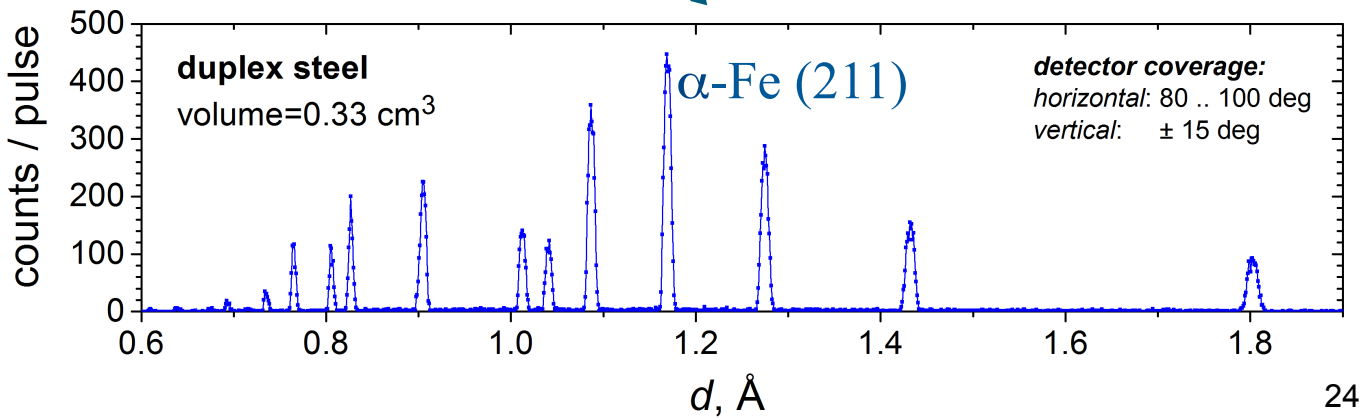
priority:
detectors at 2θ~90^O and 160^O

Instrument performance





Simulation: data collected in **one pulse**
Exposure time for Fe 211: 10 ms



Concluding remarks

Preliminary cost estimate (MEUR)

total	23.0
neutron guides	6.7
choppers	1.5
detectors, electronics, radial collimators	5.2
shielding	2.6
sample stage and sample environment	2.8
manpower	3.0
other (building, instrument infrastructure, ...)	1.2

To be shared 50:50 by the in-kind partners

Maturity

No high-risk components

Prepared to build the instrument if approved

Collaborators

Helmholtz-Zentrum Geesthacht

H.G. Brokmeier, J. Fenske, R. Kampmann, M. Müller, G. Nowak, M. Rouijaa, A. Schreyer, P. Staron

Nuclear Physics Institute, ASCR

P. Beran, L. Kadeřávek, P. Lukáš, P. Mikula, J. Navrátil, J. Pilch, V. Ryukhtin, P. Strunz, J. Šaroun

Institute of Physics, ASCR

P. Šittner

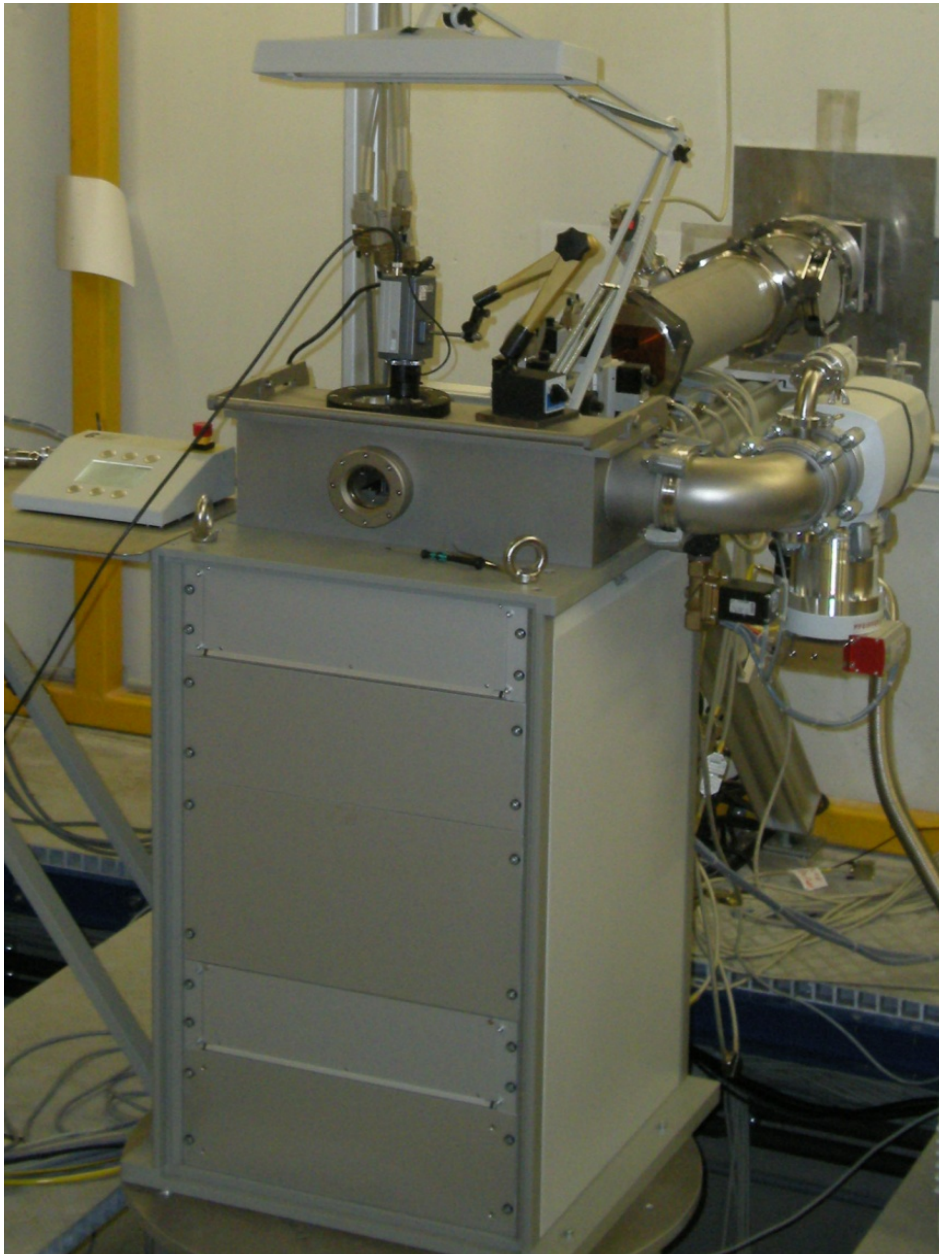
European Spallation Source

M. Strobl, ESS coordinator

Faculty of Mathematics and Physics, Charles University

P. Javorský, V. Sechovský, P. Svoboda

Sample environment



Quenching and deformation dilatometer Bähr 805 A/D for the simulation of thermo-mechanical treatments

- induction heating:
  – max. heating rate 4000 K/s
  – max. cooling rate 2500 K/s
- DSC unit
- deformation units
  (compr., tension; 25 kN)