Swedish Materials Science Beamline (SMS) at PETRA III: In-line branch (P21.2).

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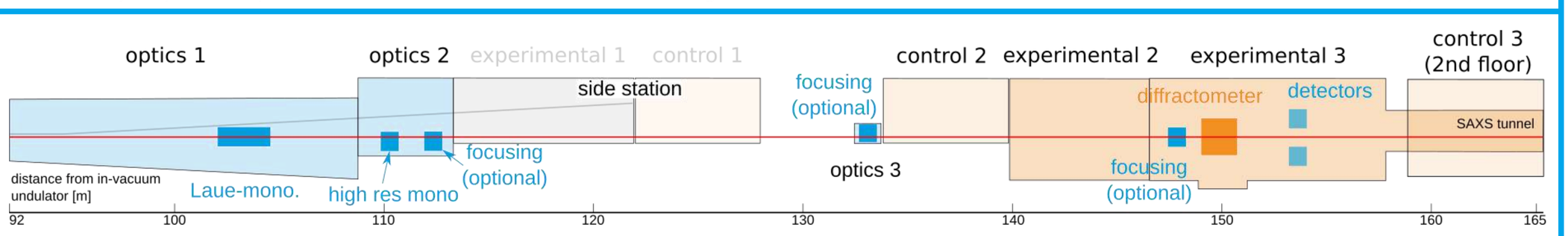
ID card

- Energy range 38 – 150 keV
- *In situ* materials characterization
- Combination of WAXS (bulk & interfaces) with SAXS & imaging
- Beam size (h × v, FWHM): 6 µm × 1 µm ↔ 6 mm × 2 mm
- “zoom-in” data acquisition
- Broad band diffraction side-station P21.1
- Funded by Swedish Research Council & administered through the Center for X-rays in Swedish Materials Science (CeXS)
- Privileged beamtime access for Swedish users (all DESY beamlines)

Beamline layout



Optics

In-vacuum undulator (IVU)

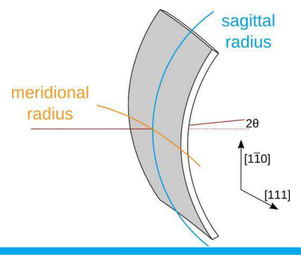
- Minimum gap: 7.0 mm
- Period: 21.2 mm, length: 4 m
- B_0 = 0.76 T, K = 1.49, E_1 = 7.8 keV
- Total power: 5.2 kW

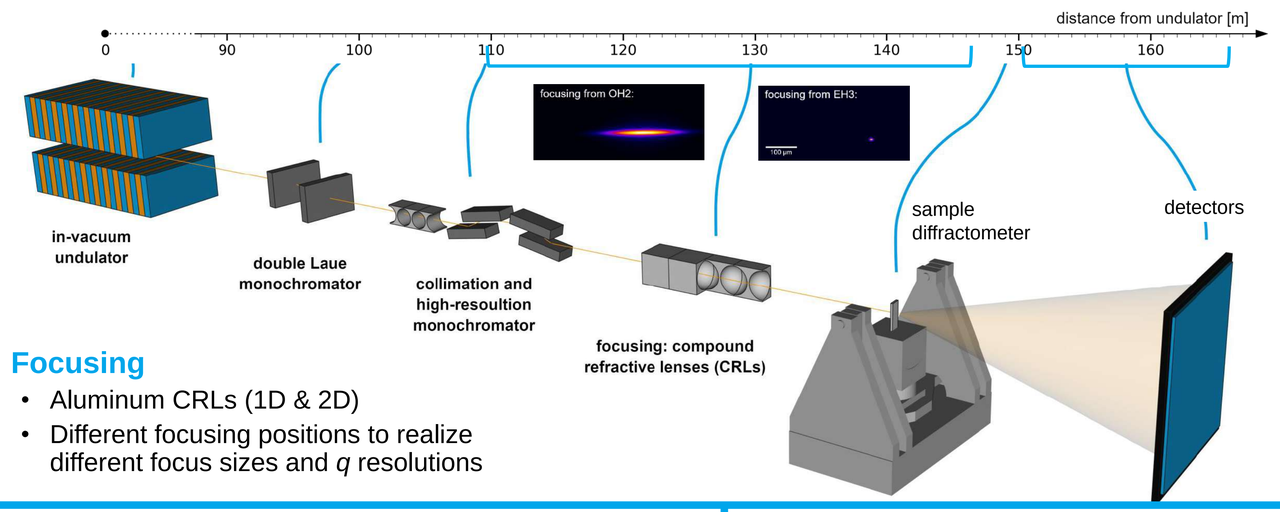
Broad band monochromator

- Double bent Laue Si (111)
- Horizontal diffraction plane
- Rowland circle bending
- Indirect cryogenic cooling
- Bandwidth 50 µrad:
  ΔE/E = 0.1% (0.2%) at 40 keV (80 keV)

High resolution monochromator (optional)

- Two Si (111) Bragg channel cuts
- Collimation with 1D Al CRLs
- Energy range: 38 – 100 keV
- Bandwidth: ΔE/E = 0.01%

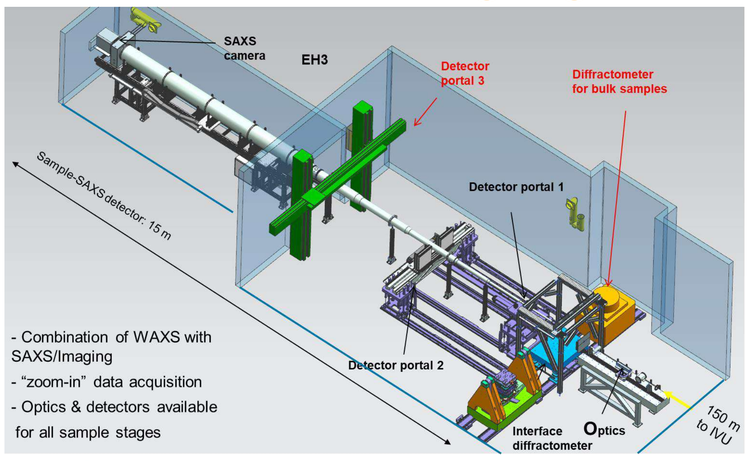




Focusing

- Aluminum CRLs (1D & 2D)
- Different focusing positions to realize different focus sizes and *q* resolutions

Diffraction & imaging station EH3



Detectors

Area detectors

- Up to four Varex XRD4343CT
- Dectris Pilatus X CdTe 2M (pool device, 25% time share)
- LuAG & GGG scintillator with Allied Vision Manta or with pco.edge 5.5 (imaging detector)

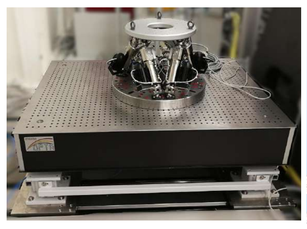
Point detectors:

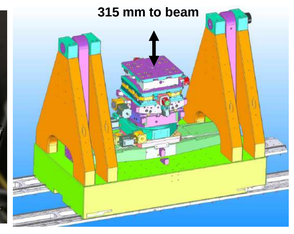
- Amptek XR-100T-CdTe (fluorescence detector)
- FMB Oxford Cyberstar YAP scintillation detector

Diffractometers

8-axis interface diffractometer

- Precise setting of incidence angle with rotation and translation stages
- Maximum load: 200 kg
- Heavy load table (up to 1 t) with hexapod (up to 400 kg)

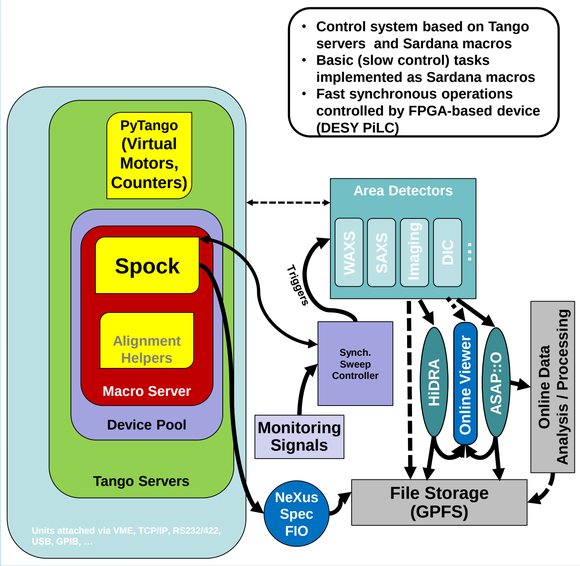




Sample environments

- Compact load frame: uniaxial tension / compression, max. 5 kN
- Linkam furnace (pool device, cryo to < 600 °C & ambient to 1500 °C)
- Induction furnace (under development): inert atmosphere / sample rotation / 1500 °C

Beamline control



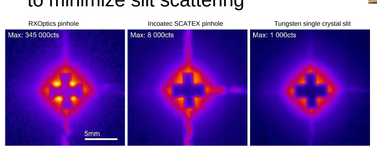
Case studies

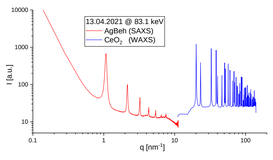
Optimizing SAXS

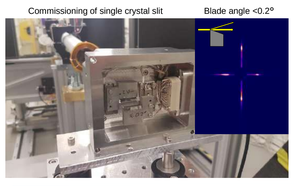
- evacuated flight path to sample to minimize air scattering

- conical flight tube to minimize SAXS/WAXS gap

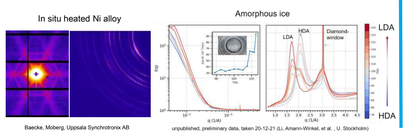
- single crystal slit to minimize slit scattering





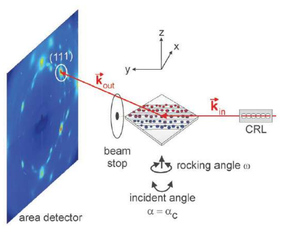


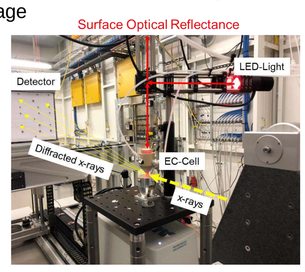
SAXS/WAXS



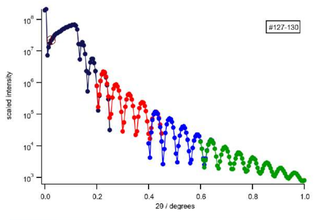
Surface diffraction

- sample environments
- large reciprocal space coverage
- catalysis &
- electrochemistry

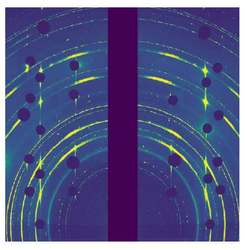




Reflectivity signal of 5 nm Pd and 15 nm Au on a sapphire 0001

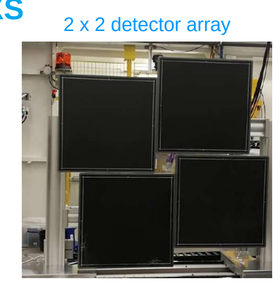


CTRs of Al_2O_3 on Pd surface

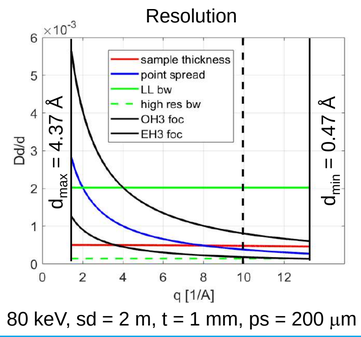


WAXS

2 x 2 detector array



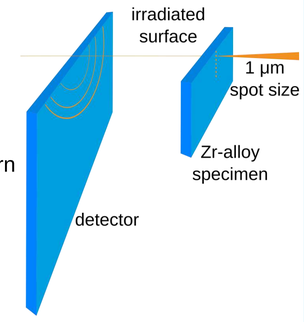
Resolution



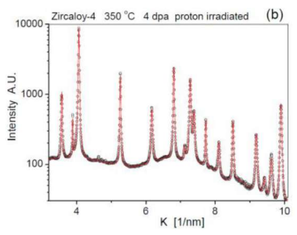
80 keV, sd = 2 m, t = 1 mm, ps = 200 µm

Depth profiling

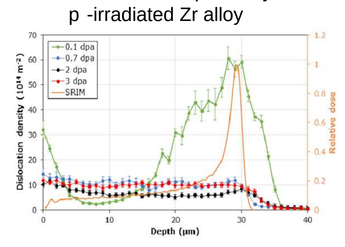
- p^+ irradiated Zr-alloy
- 1 µm vertical spot size at 67.5 keV
- 2 µm depth resolution (step size)
- Convolutional Multiple Whole Pattern line profile fitting
- density and character of dislocation loops



CMWP fitted diffractogram

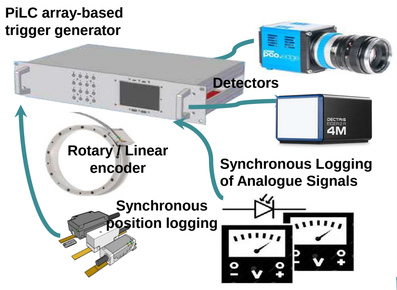


Dislocation loop density in a p -irradiated Zr alloy



Hardware based Synchronized Sweep Scans

(Thomas Bäcker)

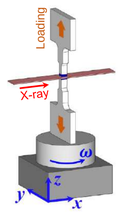


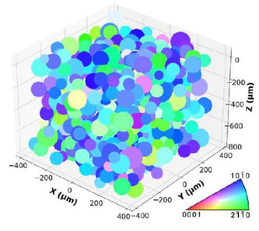
‘sweep’ macro family (Sardana)

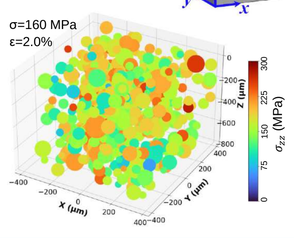
- Encoder-based trigger arrays for up to four detector & encoder channels + fast shutter
- Motor movement configuration
- Acquisition parameter configuration for all detector channels
- Synchronous logging
- Hardware synchronized time scan capability
- Flexible configuration capabilities

Multi-grain diffraction

- Extruded Mg-3Al (wt.%) alloy
- Far field grain reconstruction
- Stress tensors after deformation

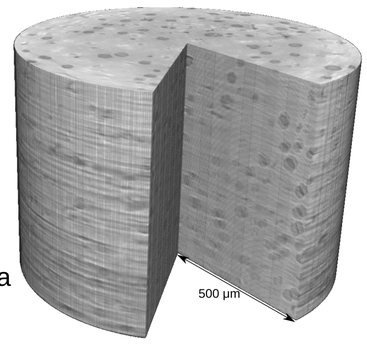






Tomography

- Cast iron with spherical graphite inclusions
- Reconstruction of 1800 images over 360° rotation
- Detector: LuAG scintillator with Allied Vision Manta CCD



Ongoing developments

- SAXS: Reduce q_{min} & SAXS/WAXS q-gap
- Bulk diffractometer: precise rotation of sample environments
- Fast temperature gradient furnace (dilatometer)
- Online data reduction: Integration of array detectors
- Data pipeline for Line Profile Analysis
- EH2 instrumentation for industrial use

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