

# A Diffraction Beamline Supporting Materials Science for Sustainability

With input from the OPERA Expression of Interest

# Scientific Background

## MAX IV proposal to WISE

**A beamline that extends our capabilities for grazing-incidence X-ray diffraction experiments and fast operando experiments, especially on industrial processes.**

Surfaces and coatings

Industrial processes

Energy Materials

# Scientific Background

Surface diffraction

X-ray reflectivity

X-ray scattering

Powder diffraction

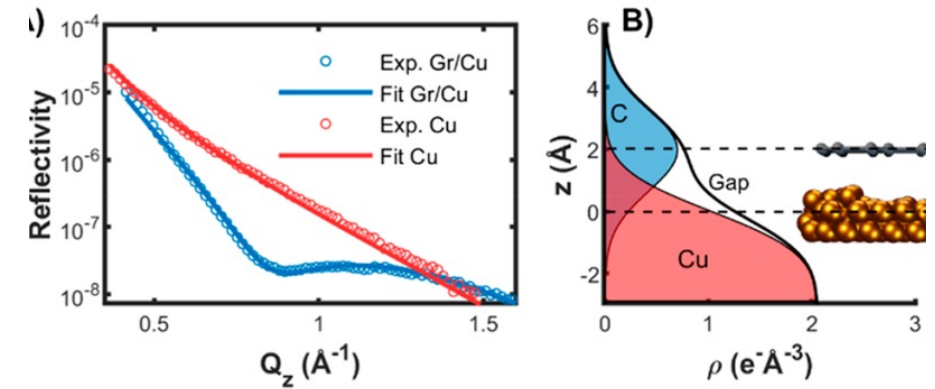
Microsecond X-ray diffraction

Surface catalysis  
Thin-film electrochemistry  
Liquid-metal catalysis  
Nanomaterial growth  
Surface dynamics

Cutting-tool coatings  
Operando deposition  
Welding and brazing  
Additive manufacturing  
Tribology

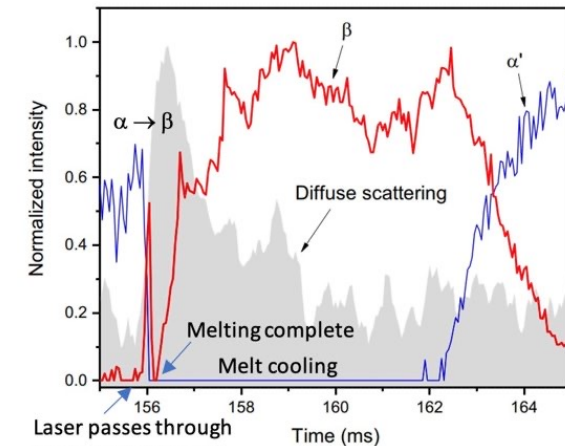
Battery materials  
Fuel cells  
Solar-cell materials  
Critical raw materials

Graphene layers on liquid-Cu surface



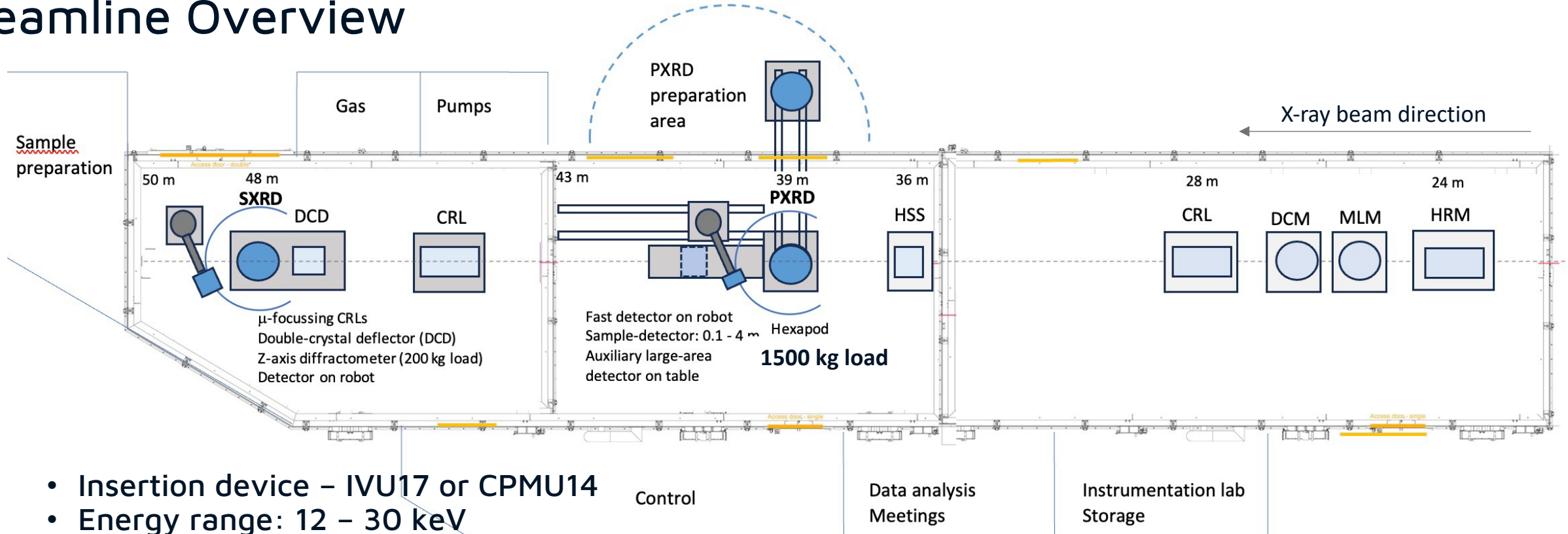
Jankowski et al. *ACS Nano* **15** (2021) 9638–9648

Selective laser melting in additive manufacturing with Ti-6Al-4V alloy.



Hocine et al. *Materials Today* **34** (2020) 30 - 40.

# Beamline Overview



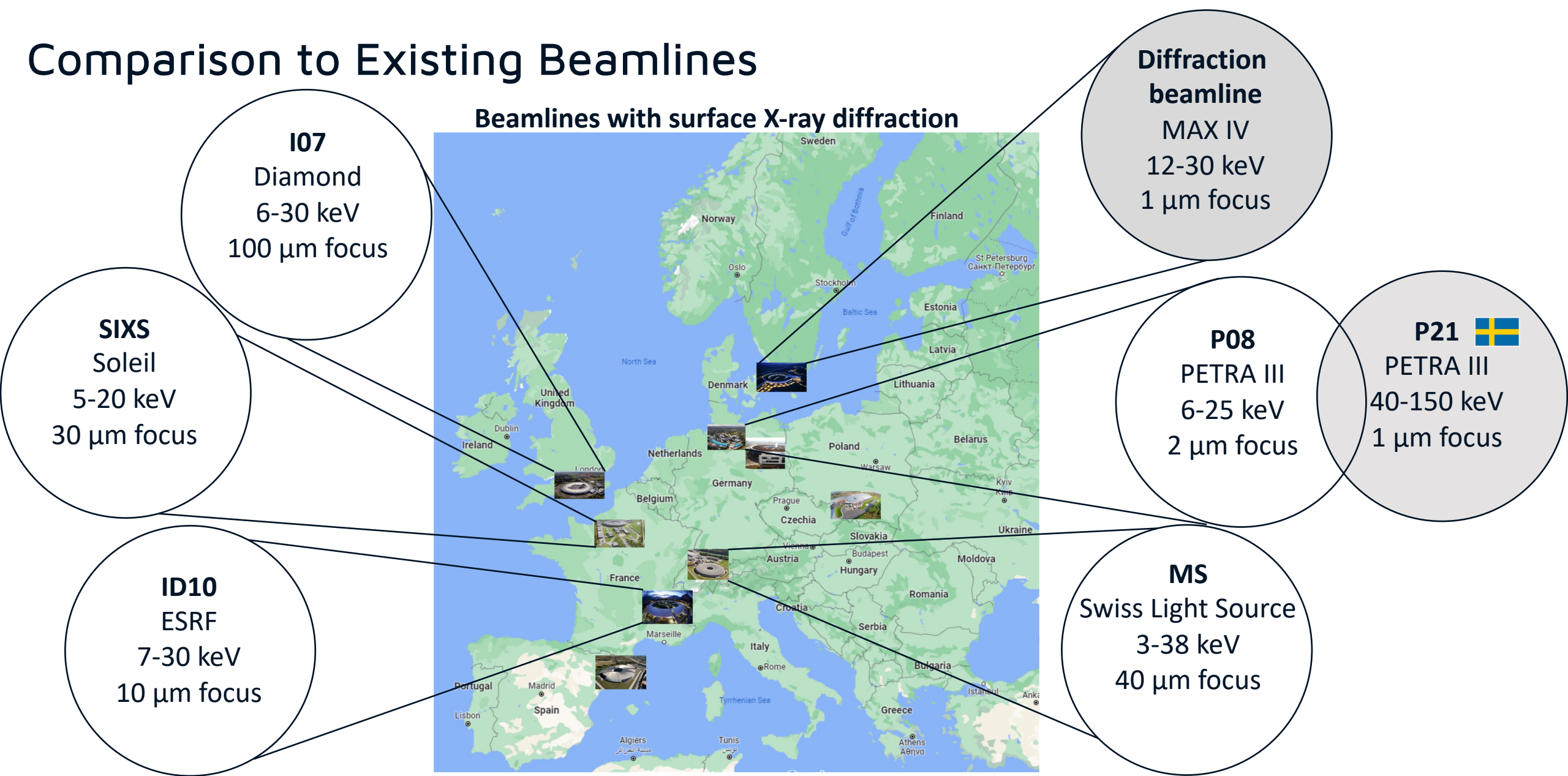
- Insertion device – IVU17 or CPMU14
- Energy range: 12 – 30 keV
- Horizontally collimating mirror
- Multilayer monochromator ( $\Delta E/E = 10^{-2}$ ,  $10^{14}$  ph/s)
- Double-crystal monochromator ( $\Delta E/E = 10^{-4}$ ,  $10^{13}$  ph/s)
- In-line optics (compound refractive lenses)
- Horizontal secondary-source
- $\mu\text{m}$  to mm spot size

# Beamlines in the MAX IV Portfolio

	Proposed beamline	DanMAX	Balder	NanoMAX	CoSAXS
Energy range (keV)	12 – 30	15 – 35	4 – 40	5 – 28	8 – 25
Focus range (μm)	1 – 1000	10 – 1000	50 – 2000	0.05 – 0.2	1 - 4000
Time resolution	microsecond	millisecond	millisecond	millisecond	millisecond
Research focus	Surfaces, interfaces, thin films, liquids in grazing-incidence XRD mode. Powder XRD on energy materials and industrial processes. In-situ/operando XRD studies. <b>Fast time resolution.</b>	High-resolution powder XRD. Full-field imaging and tomography. In-situ/operando experiments.	Operando XAFS. Catalytic materials, environmental samples, electrochemistry.	Nano-focused XRD and imaging.	SAXS/WAXS on soft matter. Polymers, medicine, drug delivery.

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# Comparison to Existing Beamlines



# Strategic Relevance

Added MAX IV capabilities	Strategic benefits for MAX IV
Dedicated setup for grazing-incidence X-ray diffraction.	Studies of catalytic, electrochemical, and nano materials on surfaces and thin films.
Liquid-surface X-ray scattering experiments.	Surface melting, liquid-metal surfaces, gels and fluid systems.
Strengthening operando X-ray diffraction on industrial processes	Heavy industrial equipment. Real operando conditions in layer deposition or metal cutting.
Microsecond detection mode for operando studies.	Fast heating and quenching, meta-stable intermediates, electronic switching.

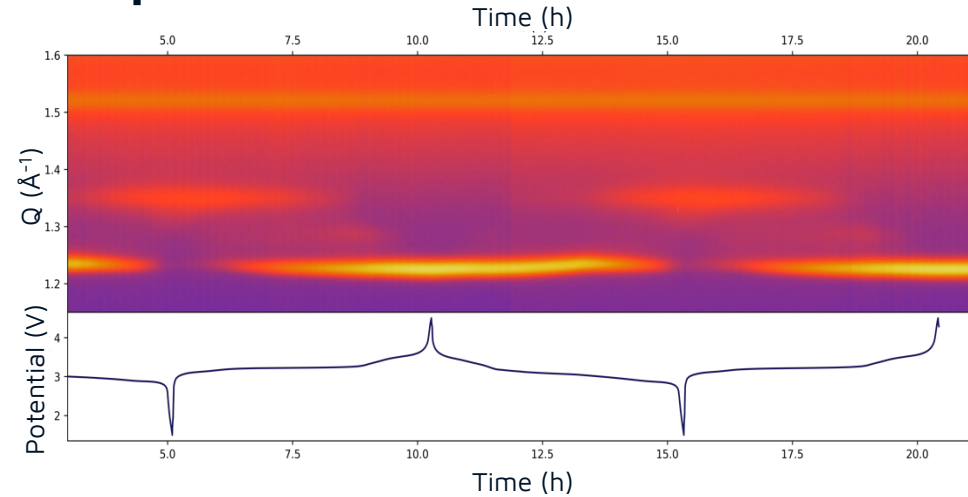




# Backup slide

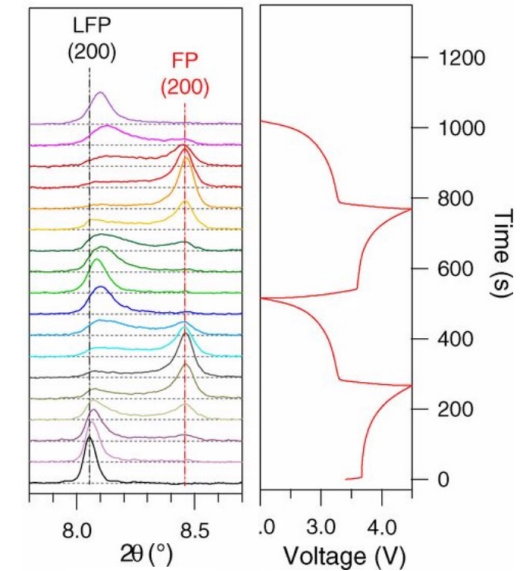
Facility	Beamline	Energy (keV)	Flux (ph/sec)	Min. spot size ( $\mu\text{m}^2$ ), (h x v)	Techniques
MAX IV	OPERA	10 – 30	$10^{12}$ - $10^{13}$ , $10^{16}$ MLM	1 x 1	Fast operando XRD, PXRD, surface- and interface XRD, XRR
	DanMAX	8 - 35	$10^{10}$ - $10^{13}$ , $10^{15}$ MLM	60 x 7	Full-field Imaging and PXRD, time resolved, in situ
ESRF	ID31	20 -150	$5 \times 10^{12}$	20 x 3	XRR, WAXS, GI-WAXS, SAXS, imaging
	ID11	18-140		0.2 x 0.07	3D-XRD, PDF, PXRD, time-resolved diffraction.
	ID10	7 - 30	$2 \times 10^{13}$	30 x 100	Grazing-incidence XRD, XRR, and GISAXS on solid and liquid surfaces.
	ID15A	40-120	$1.5 \times 10^{12}$	0.3 x 0.3	Fast operando XRD, diffraction tomography, PDF
	ID01	6 - 24	$1 \times 10^{12}$	120 x 25 (TF)	Micro-XRD, GISAXS, CDI, Ptychography
	ID03	5 - 30	$10^{12}$	3 x 2	Surface- and interface XRD, XRR, DAFS
	ID13	7 - 30		1 x 1	Micro branch, Micro-XRD, Ptychography, XRF, SAXS
	BM28	2 – 40	$10^{13}$	60 x 70	SXRD, PXRD, operando
	BM32	5 - 27	$3 \times 10^{11}$	0.5 x 0.25	Integrated UHV-diffractometer, MBE, PVD
PETRA3	P07	50-200	$5 \times 10^{12}$	1 x 1	Solid and liquid interface XRD
	P08	5.4 - 29	$2 \times 10^{12}$	30 x 2	XRD, grazing incidence, solids, liquids, Langmuir
	P21	40-150	$10^{12}$	6 x 1	SAXS, PDF, PXRD, XRD
	P23	5-35	$6 \times 10^{12}$	5.2 x 1.6	XRD, XRR, resonant XRD, GI-XRD, XSW.
SLS	X04SA	5 – 38	$2.5 \times 10^{13}$	130 x 40	PXRD, in-situ surface XRD
	X05LA	3 - 23	$2 \times 10^{12}$	1 x 1	Micro-XRD-XRF-XAS, fs-laser pulses
SOLEIL	Cristal	5 - 30		30 x 30	SC-XRD, PXRD, coherent XRD, time-resolved XRD
	Diffabs	3 - 23	$10^9$ - $10^{10}$	10 x 10	XRD, XANES, EXAFS, XRF, DAFS, XRR.
	Sirius	1.4 - 13	$2 \times 10^{13}$	1700 x 1000	GIXRD, GISAXS), XRF, anomalous XRD, GI-XAFS.
	Sixs	5 - 20	$3 \times 10^{12}$	30 x 30	Surface and interface XRD (solid-solid or solid-liquid)
DLS	I07	6 - 30	$10^{14}$	300 x 100	Surface and Interface Diffraction, GI-XRD, GISAXS, XRR
	I12	53-150	$10^{11}$	50 x 50	Imaging and XRD, heavy sample environments
	Diad	7 - 38		13 x 2	Dual imaging and diffraction, in situ/operando XRD
APS	6-ID-B,C	4 - 38	$7 \times 10^{12}$	1500 x 150	XRD, magnetic XRD, SXRD, resonant scattering
	6-ID-D	50-130	$10^{11}$	1000 x 1000	Single-crystal XRD, PXRD
	11-ID-D	26-120	$10^{13}$	0.5 x 0.5	In construction, XRD, SAXS, PDF, SXRD
	33-ID-D,E	5 - 30	$10^{13}$	70 x 30	XRD, SXRD, XRR, in situ UHV
	CSSI	6 - 25	$10^{13}$	0.75 x 0.42	APS-U beamline, “Pink beam”, Coherent SXRD, GISAXS, GI-XPCS
	CHEX	15 - 60	$4 \times 10^{12}$	0.8 x 0.3	APS-U beamlines (8 endstations), in situ chemistry, surface coherent scattering
NSLS-II	4-ID ISR	2.5 - 23	$5 \times 10^{12}$	45 x 25	Resonant XRD, CTR, XRR, GI-SAXS, GI-XRD, in situ.
	XPD	40 - 70	$6 \times 10^{13}$	600 x 200	PXRD, sub-minute resolution
Spring-8	BL11XU	6 - 70			Surface XRD, Inelastic scattering, Mössbauer
	BL13XU	5 - 72	$10^7$ - $10^{10}$	2 x 2	Surface-, Thin film XRD, PXRD, in situ/operando
	BL19B2	5 - 72	$10^9$		XRD, GI-XRD, CTR, XRR, SAXS, USAXS
CLS	BXDS-IVU	5 - 24	$10^{11}$ - $10^{13}$	170 x 50	XRD, GI-XRD, GI-SAXS, XRR, DAFS, XES.

# Backup slide: Cool experiments



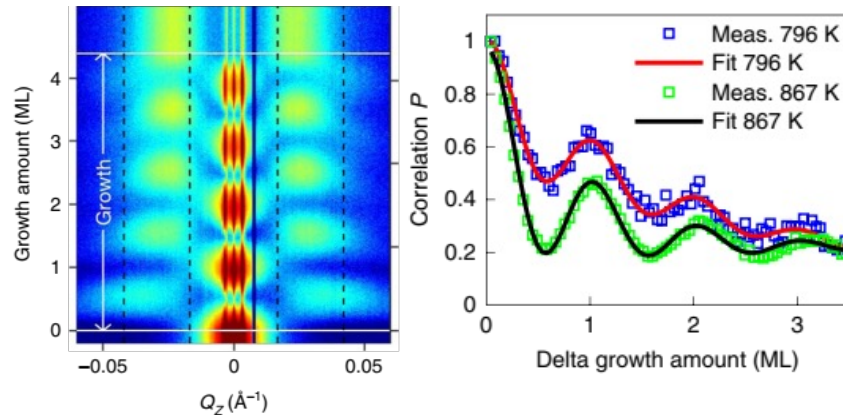
X-ray  
Diffraction

Electro-  
chemistry



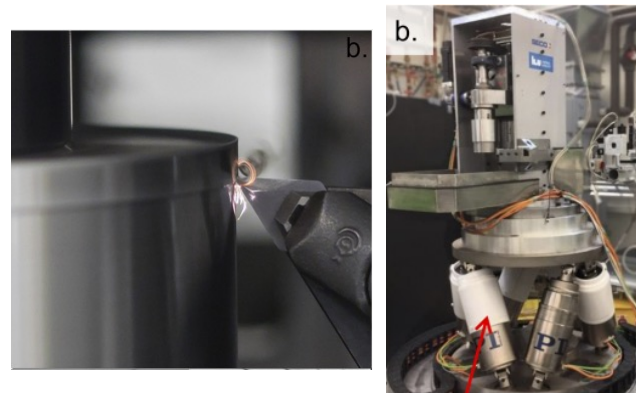
Liu et al. *Science* **344** (2024) 1252817.

Coherent photon correlation spectroscopy  
during epitaxial growth of GaN

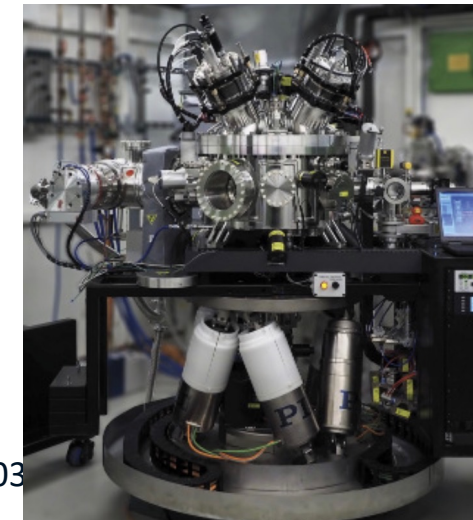


Guangxu Ju et al. *Nature Physics* **15** (2019) 589–594.

Lathe setup for tool-wear studies  
during turning (P07, Petra3).



Rogström et al. *Rev. Sci. Instrum.* **90** (2019) 103



UHV deposition  
system at P07,  
Petra3.

Schroeder et al. *Rev. Sci. Instrum.* **86** (2015) 095113.