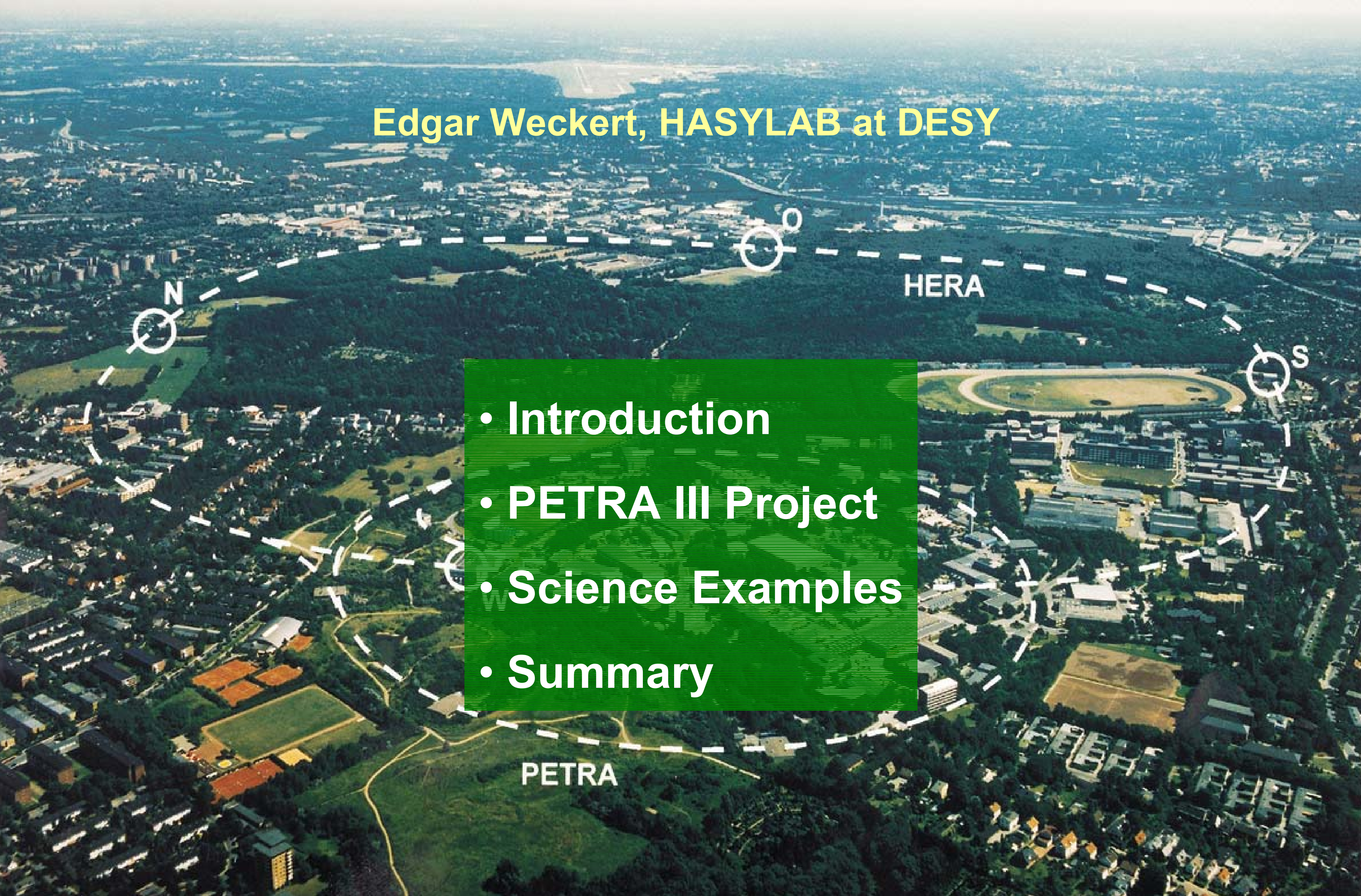
Science at PETRA III

Edgar Weckert, HASYLAB at DESY



- Introduction
- PETRA III Project
- Science Examples
- Summary

Introduction

Radiation source properties:

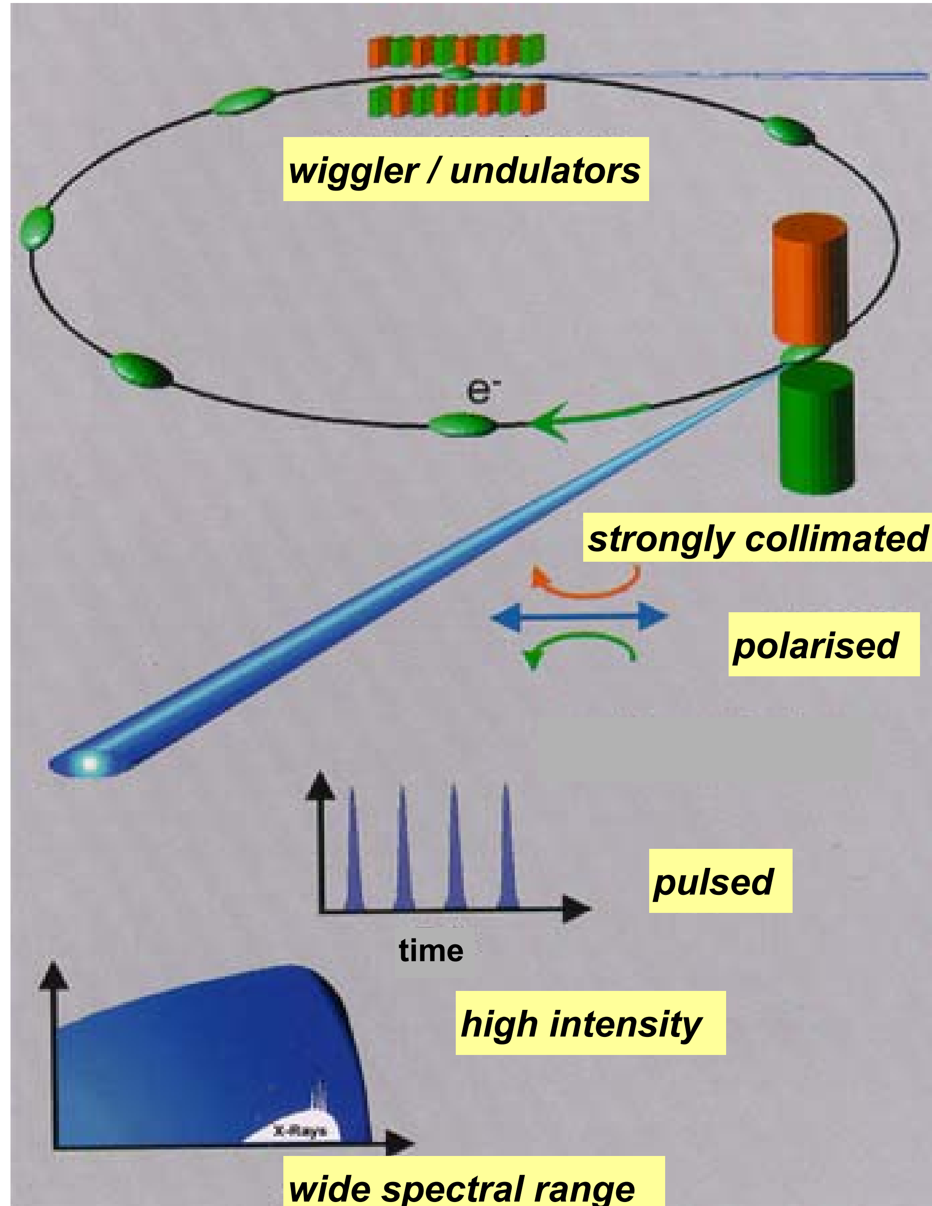
- **flux:**
  F [ph/(s 0.1%BW)]

- **brilliance:**
  $B = F/((2\pi)^2 \sigma_{Tx}\sigma_{Tx'}\sigma_{Ty}\sigma_{Ty'})$
  [ph/(s mm²mrad²0.1%BW)]

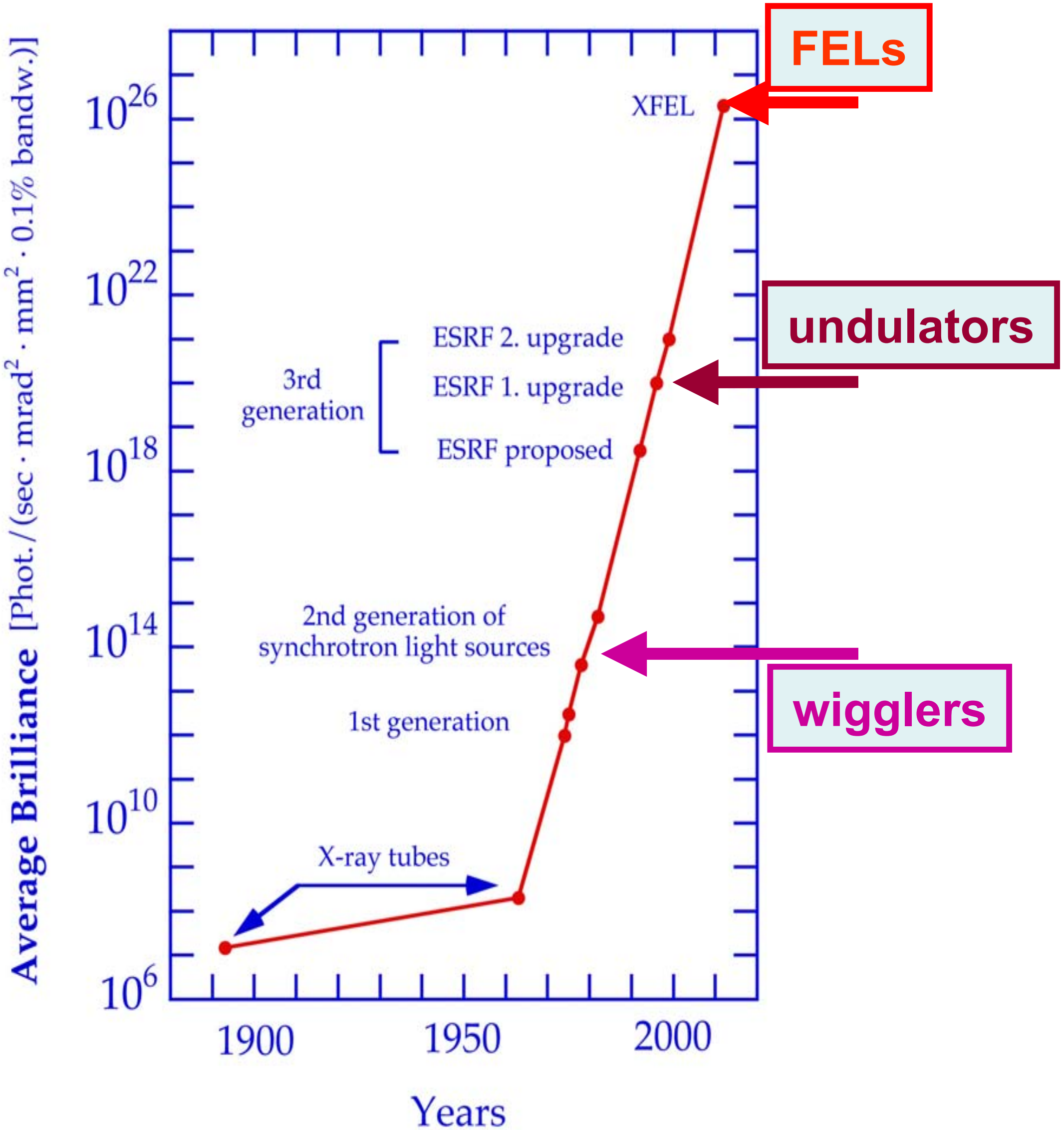
- **coherent flux:**
  $F_c = B(\lambda/2)^2$ [ph/(s 0.1% BW)]

- **horizontal emittance:**
  $\varepsilon_x = \sigma_x\sigma_{x'} \heartsuit E^2/N_B{}^3$

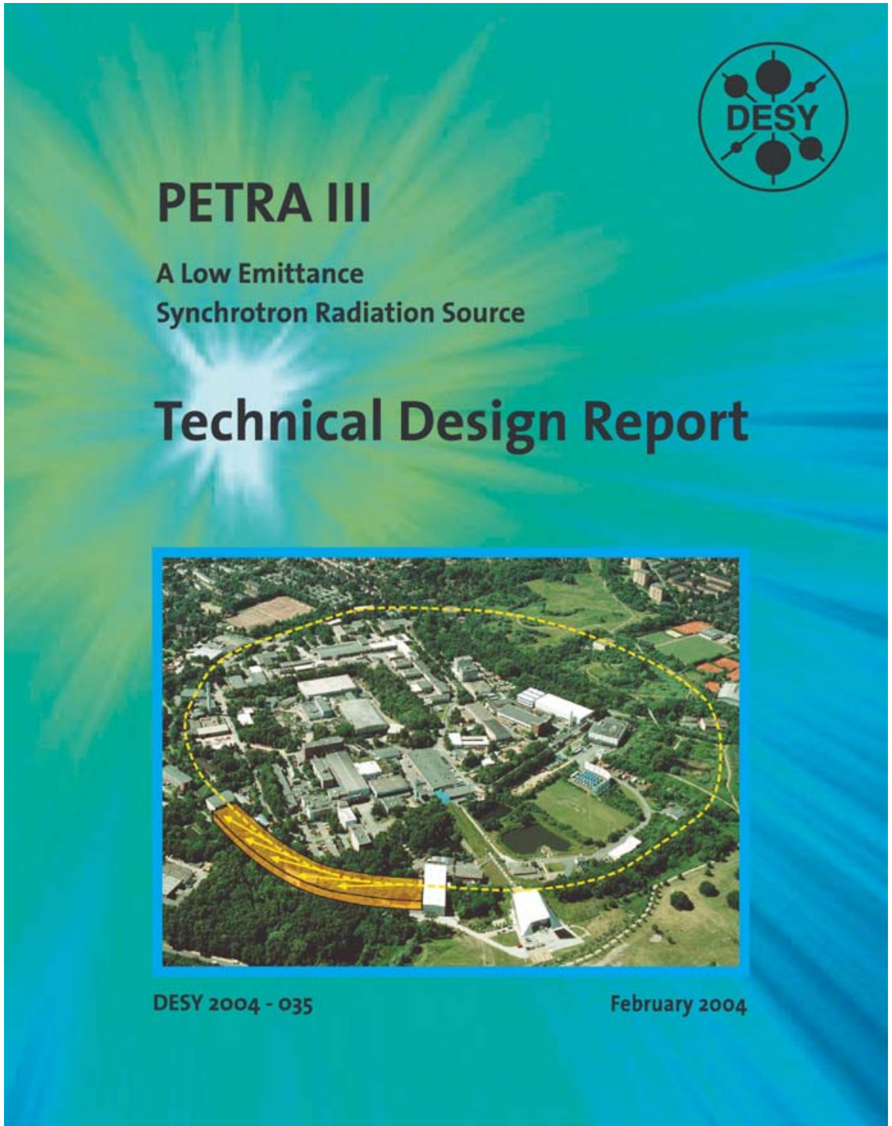
- **vertical emittance:**
  $\varepsilon_y = \sigma_y\sigma_{y'} = \kappa\varepsilon_x$;
  κ: horiz./vert. coupling



Brilliance

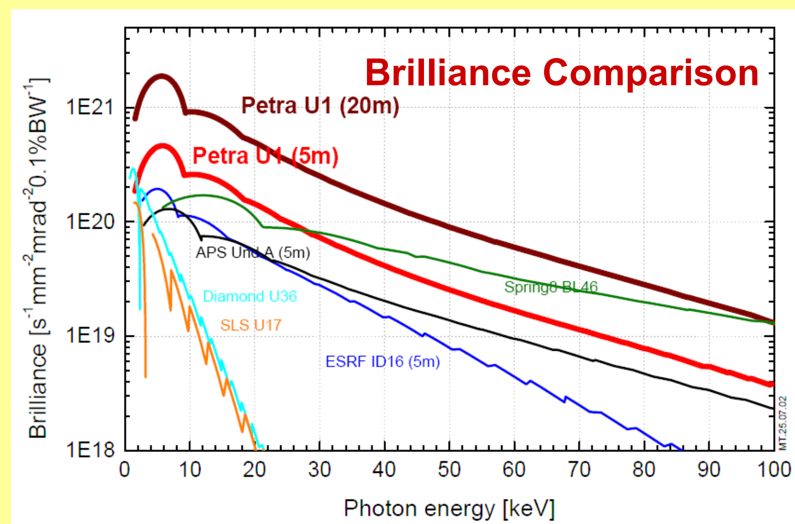

FELs
undulators
wigglers
XFEL
ESRF 2. upgrade
ESRF 1. upgrade
ESRF proposed
3rd generation
2nd generation of synchrotron light sources
1st generation
X-ray tubes
10^{26}
10^{22}
10^{18}
10^{14}
10^{10}
10^{6}
1900
1950
2000
Years
Average Brilliance [Phot./(sec · mrad^2 · mm^2 · 0.1% bandw.)]

PETRA III Project

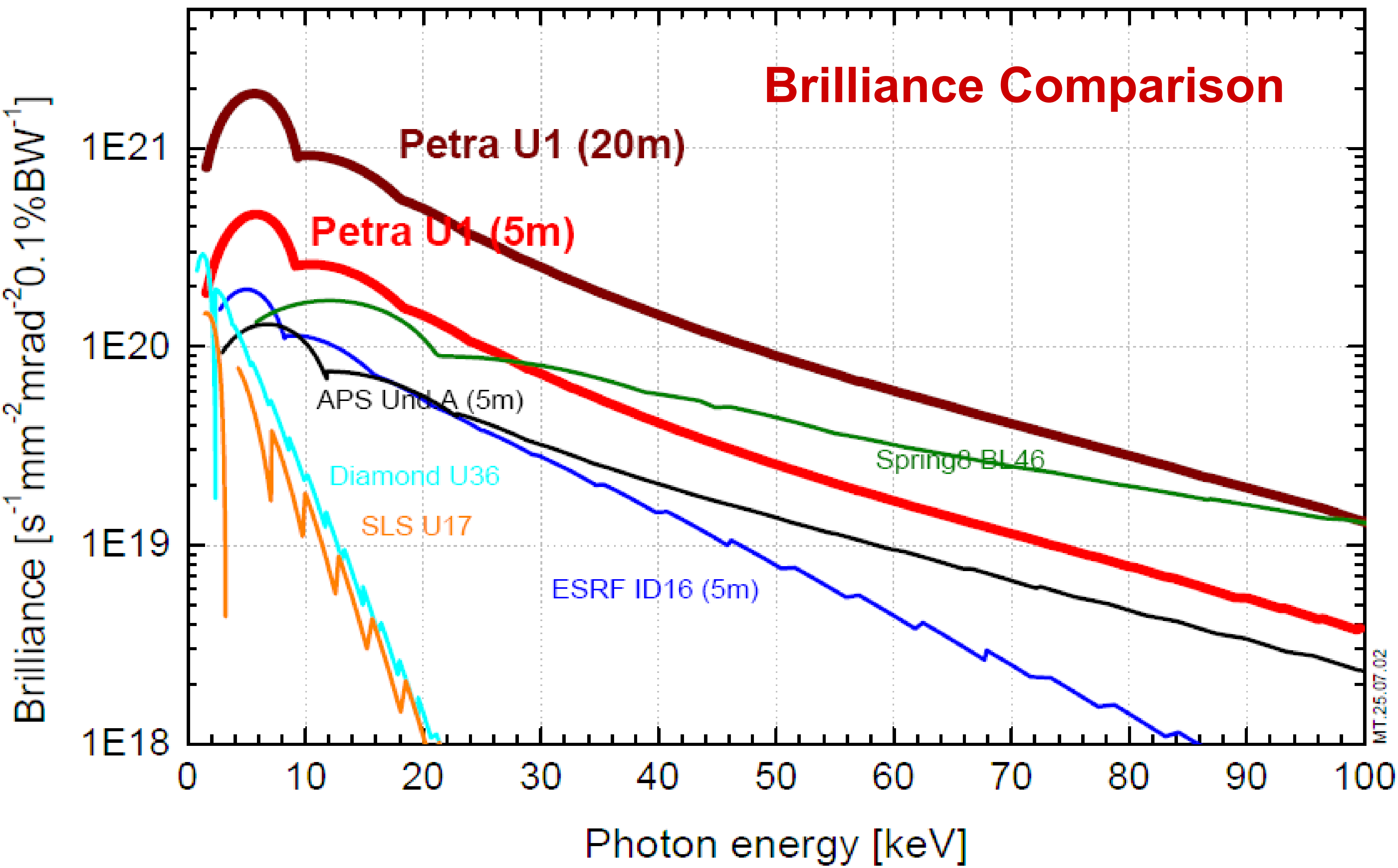


Parameters:

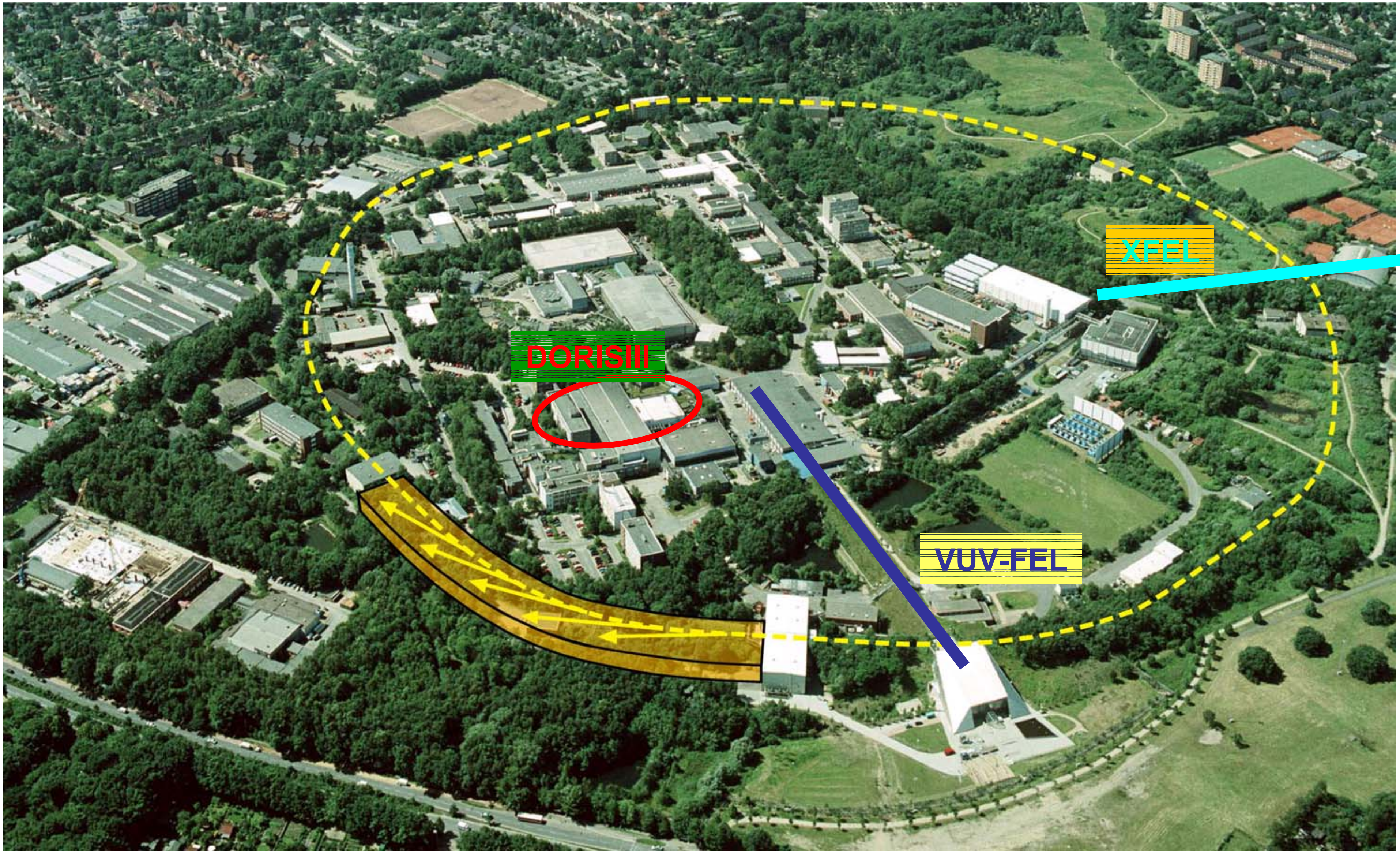
- rebuild of 1/8 of PETRA
- refurbishment of 7/8 of PETRA
- circumference: 2304 m
- energy: 6 GeV
- current: 100 mA
- emittance: 1 nmrad
- straight sections: 9
- undulators: 13
- undulator length: 2, 5, 20 m
- top up operation mode



PETRA III Proiect



PETRA III Project



Photon beam parameters

Comparison of photon beam sizes and divergences (@ 12keV)

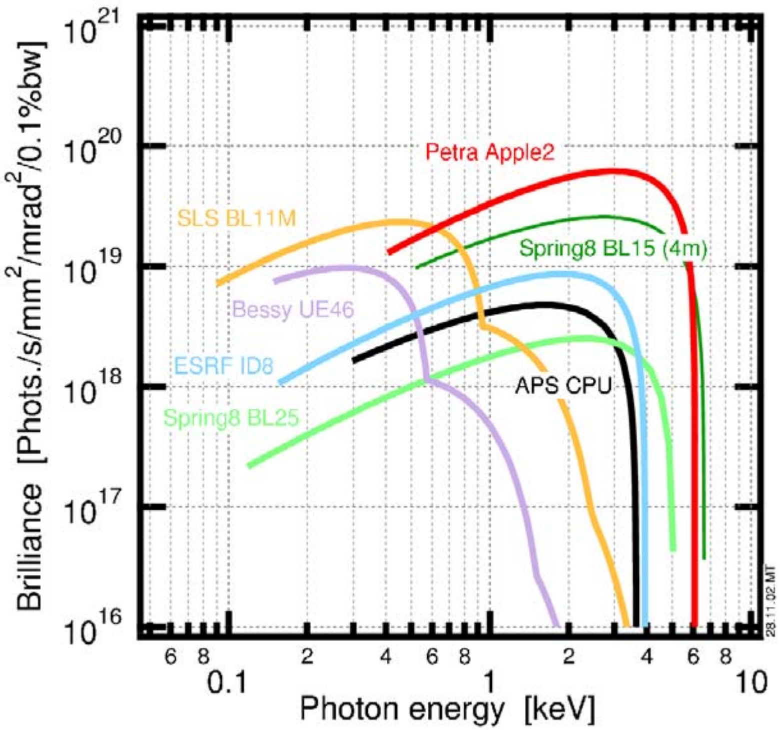
	β_x [m]	β_y [m]	σ_x [μm]	σ_y [μm]	$\sigma_{x'}$ [μrad]	$\sigma_{y'}$ [μrad]	ID-length [m]
low-β 5 m	1.3	3	35.9	5.7	28	5.0	5
high-β 5 m	20	2.38	141	5.2	8.6	5.2	5
low-β 2×2 m	1.4	3	37	5.6	28	7.7	2
high-β 2×2 m	16.2	2.6	127	5.2	10.8	7.7	2
20 m-ID	16	5	126	7.5	8.6	3.6	10
DW-drift	16	16	126	12.7	10.5	4.4	5
ESRF low-β	0.5	2.73	60	8.4	89.3	6	5
ESRF high-β	35.2	2.52	403	8.2	11.8	6	5
Spring-8	22.6	5.6	277	6.4	13	5	4.5
APS	15.9	5.3	217	12.6	15.3	5.7	4

- two β-function values possible in the new eighth of the storage ring (can be changed)
- main gain in performance of PETRAIII is in the horizontal direction
- transverse coherence length $\xi \sim L\,\lambda/S$ (low-β FWHM @ 60m, 1Å): ξ_h ~70μm, ξ_v ~450μm

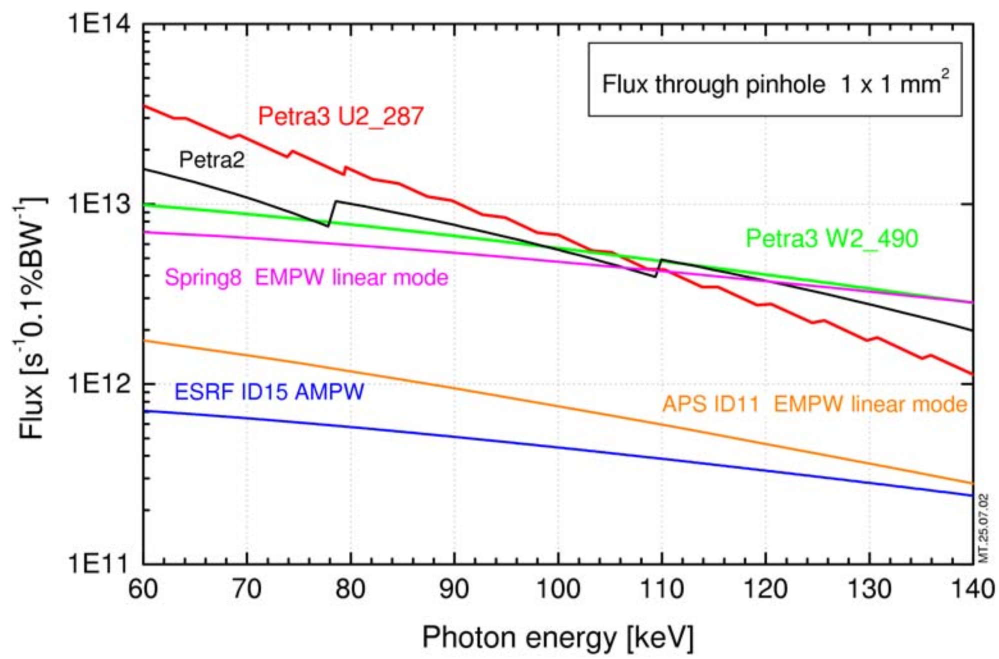
  (high-β FWHM @ 60m, 1Å): ξ_h ~18μm, ξ_v ~490μm
- horizontal beam size (FWHM@12keV) in 100m distance: low-β: 6.7mm high-β: 2mm
- vertical beam size : 1.2mm

PETRAIII: Energy Range

VUV and XUV

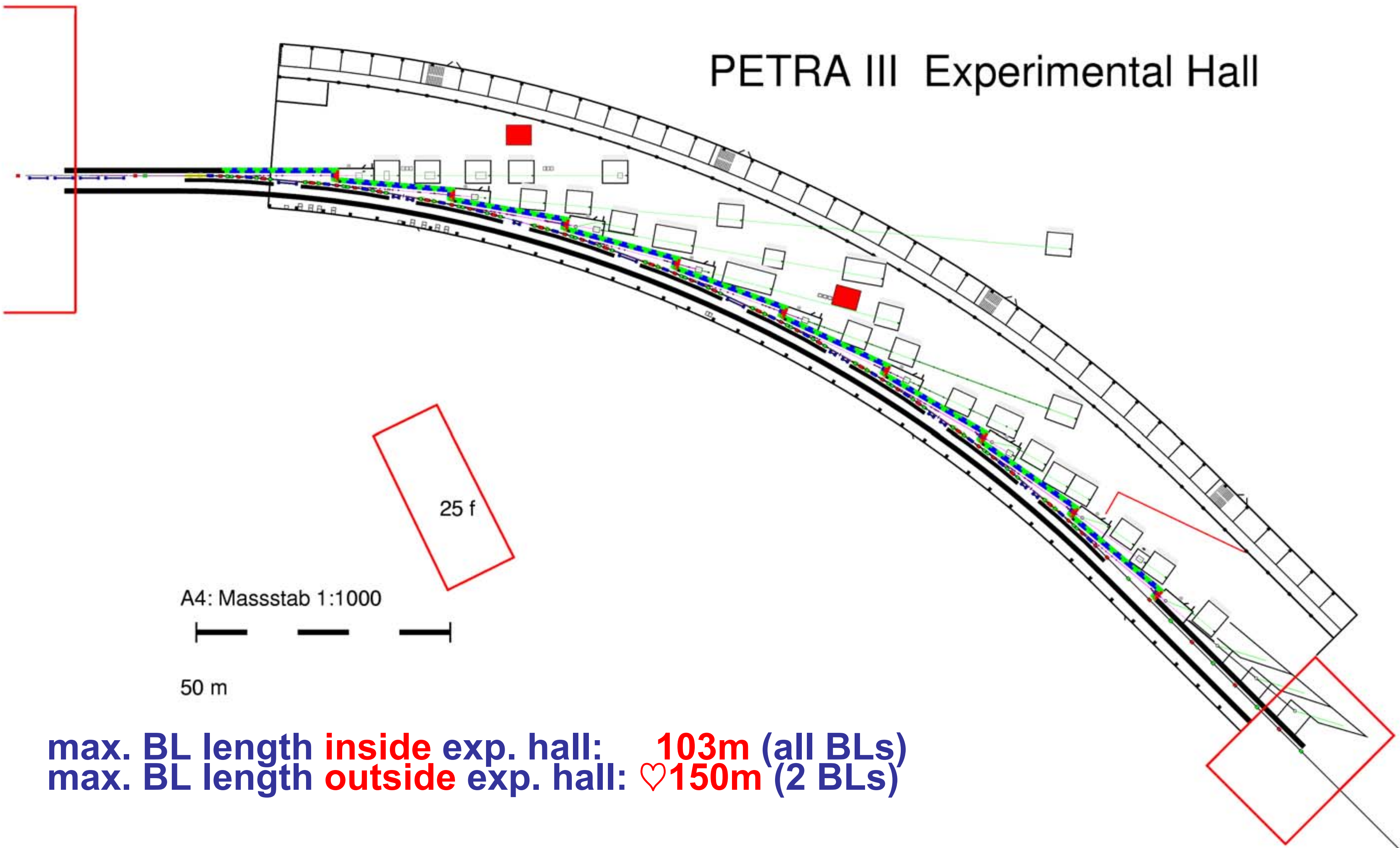


hard X-rays




HERA
Hallen N
EXPO-Halle
DESY-Sportplatz
HERA Halle West
Halle NW
Halle NO
Halle W
Halle O
PETRA
Nebeneingang
Side Gate
Halle SW
Halle SO
HERA
Hallen S

Tentative layout of the experimental floor



max. BL length inside exp. hall: 103m (all BLs)
max. BL length outside exp. hall: ♡150m (2 BLs)

Schedule

- Submission of the TDR: Feb. 2004
- Selection of the phase I beamlines: Summer 2004
- Start of beamline R&D, prototyping: 2004
- Start detailed beamline planning: end 2004/2005

  ➔ user workshops on detailed beamline design
- Start of component production: 2006
- Start of reconstruction: mid 2007
- Installation of first beamlines: mid 2008
- Start of user operation: 2009

TDR: Proposed Beamlines I

X-ray diffraction and imaging

- <u>High energy X-ray diffraction</u>
- Coherent X-ray beamline
- Micro- and nanotomography
- High resolution diffraction

High energy resolution spectroscopy

- Inelastic scattering
- Nuclear resonant scattering

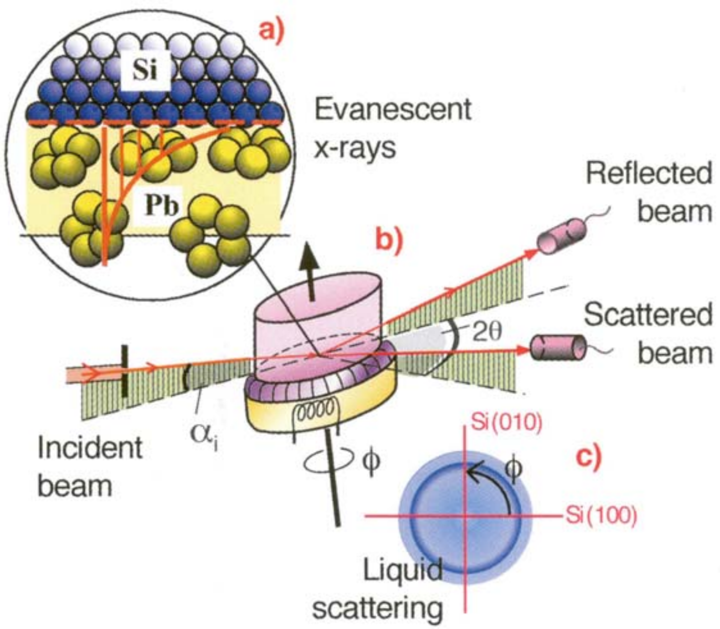
Materials science

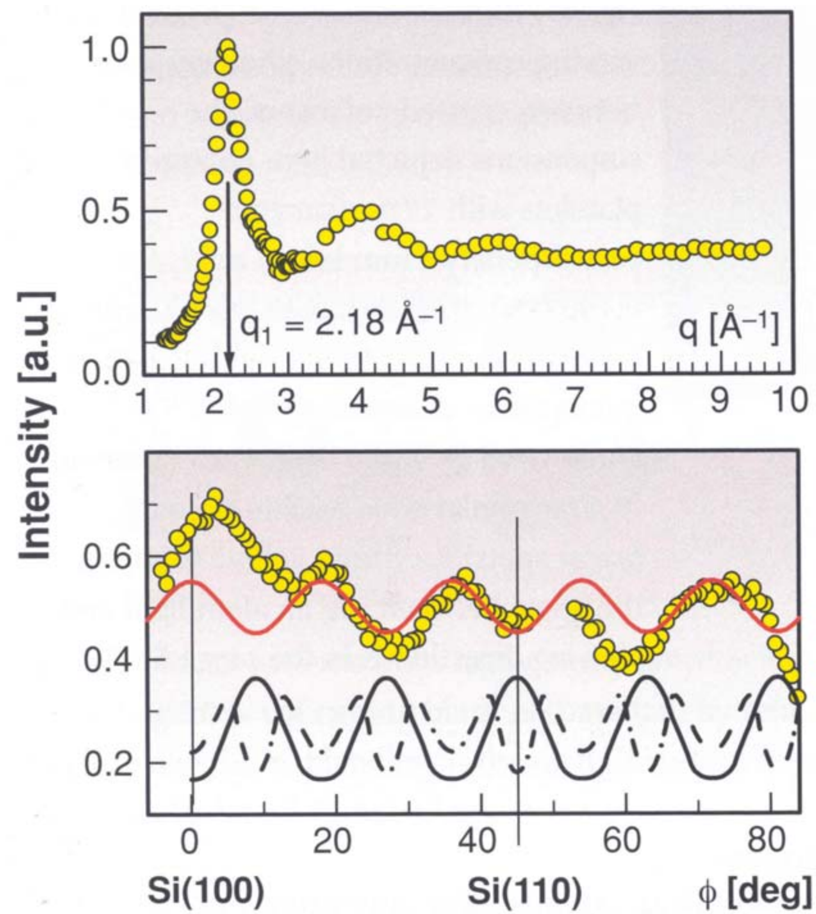
- High energy X-ray materials science
- Powder diffraction
- (U,A)-SAXS
- Microfocus scattering

Structure of the solid liquid interface

System: Si(001)-Pb(lq. ; T_M+10K)

Energy: 80 keV





H. Reichert et al., Nature, 408, 839 (2000)

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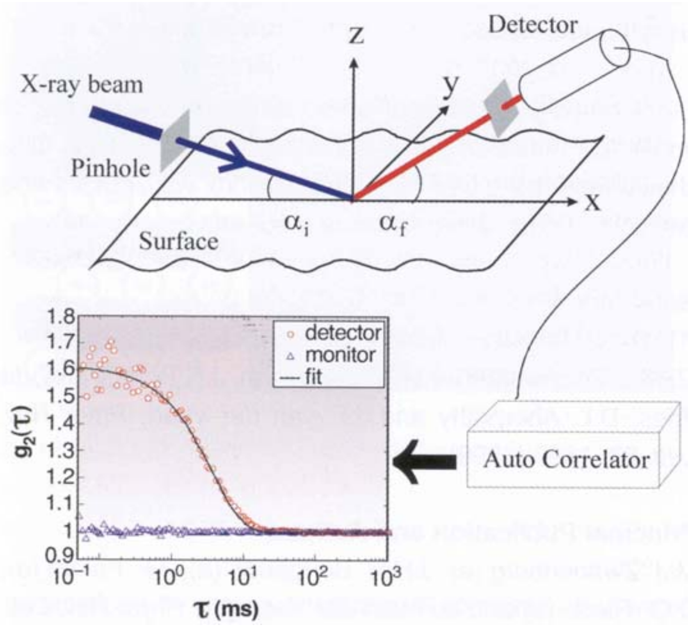
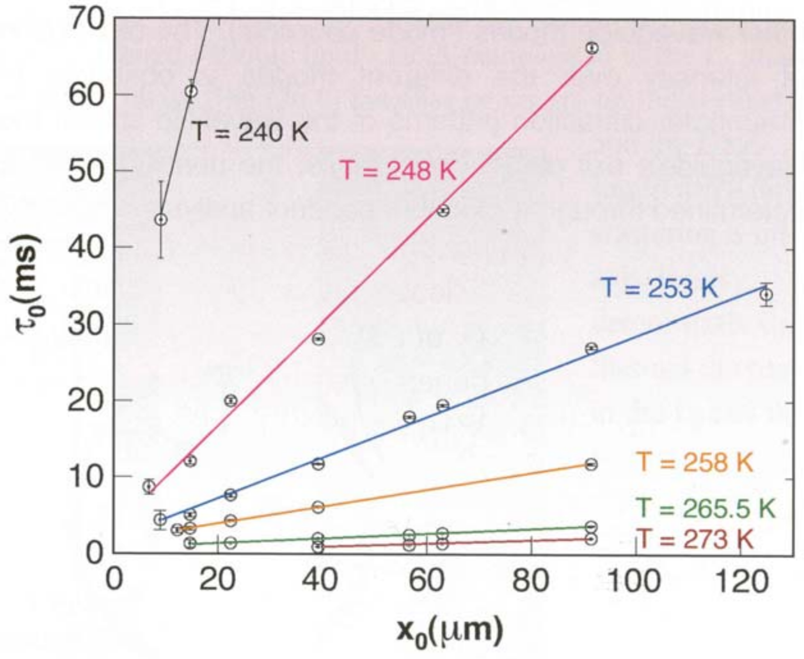
XPCS (X-ray photon correlation spectroscopy)

requirement: coherent radiation

5-10 µm pinhole to mask the coherent part of the radiation





$$g_2(\tau) = \langle I(t+\tau)I(t)\rangle / \langle I(t)\rangle^2 = g_0 \exp(-\tau/\tau_0) + 1;\; \tau_0 = x_0\eta(T)/\pi\gamma(T)$$

$\eta(T)$: **dyn. Viscosity**

$\gamma(T)$: **surface tension**

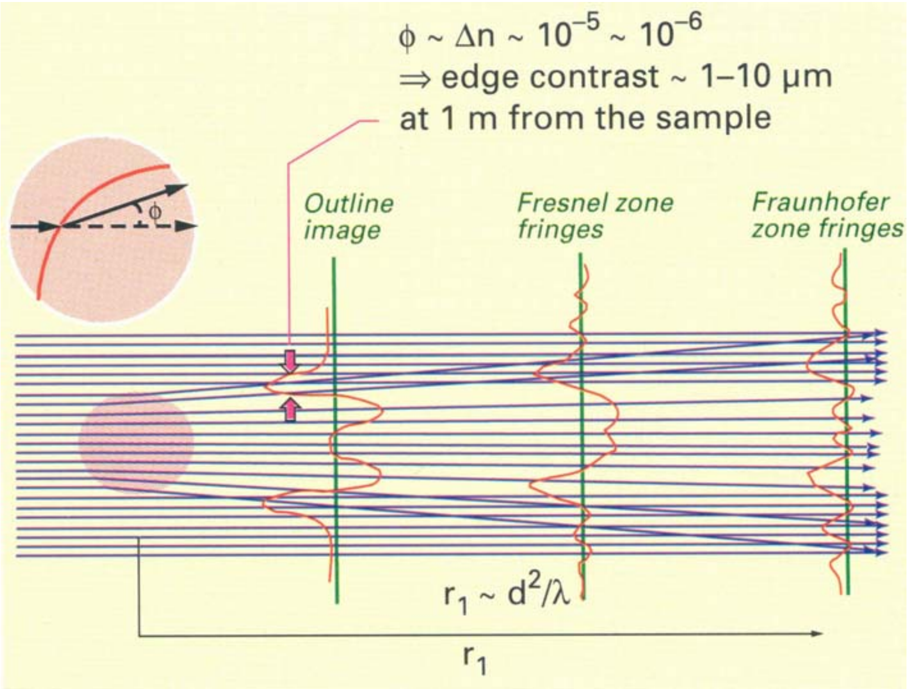
T. Seydel et al., Phys. Rev. B 63(7), (2001)

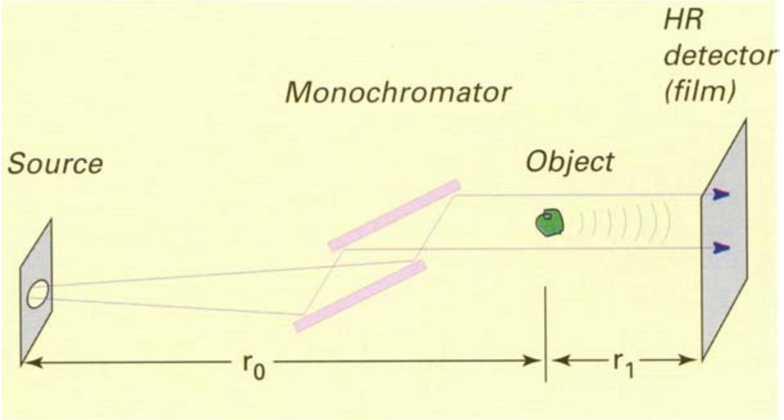
Phase contrast imaging

requirement: lateral partially coherent radiation

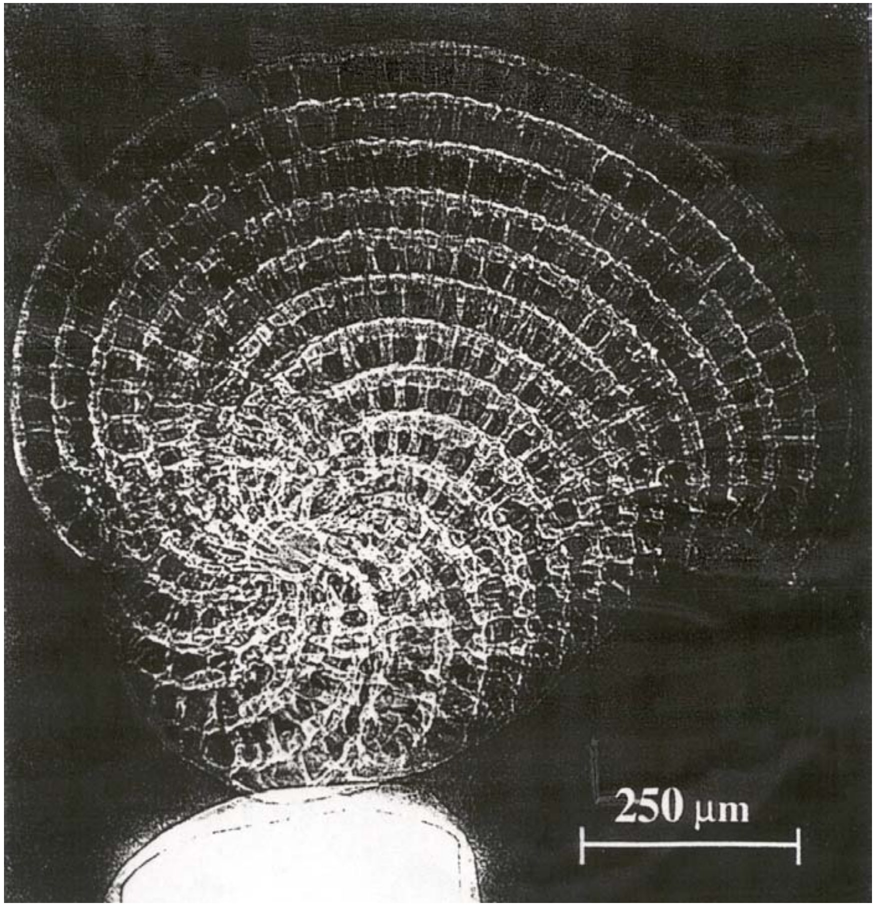
Lateral coherence length: $\xi \propto \lambda L/s$

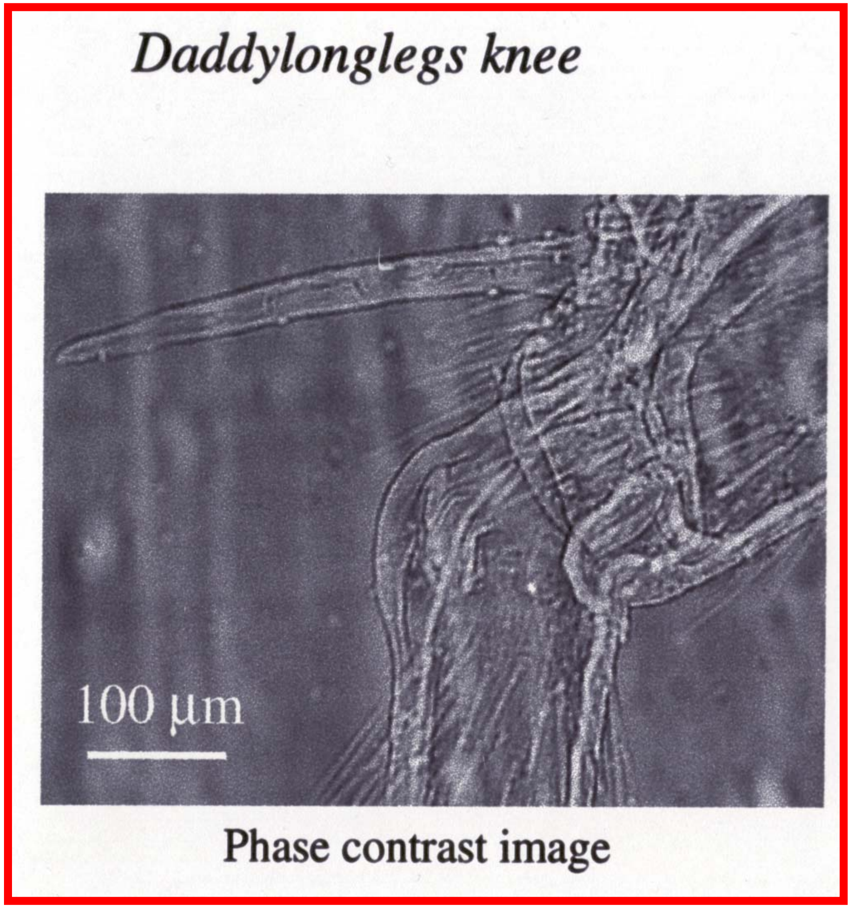
L: distance from the source; s: source size





Phase contrast images





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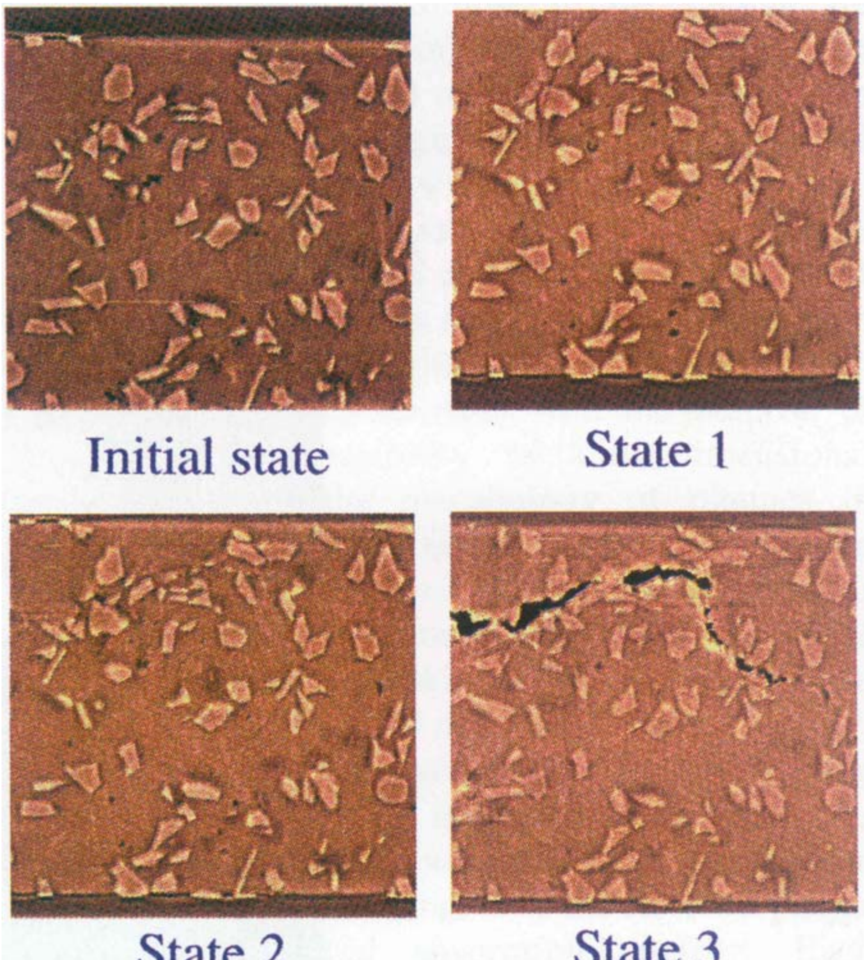
Phase contrast tomography



example: SiC in Al:

Micro tomographic reconstructions for different strains.

Energy: 25 keV

Distance sample-detector: 82 cm

P. Cloetens, R. Barret, J. Baruchel, J. Guigay, M. Schlenker, J. Phys. D, 29,133-145 (1996)

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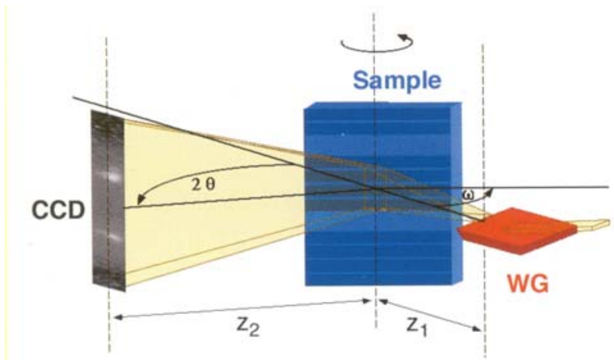
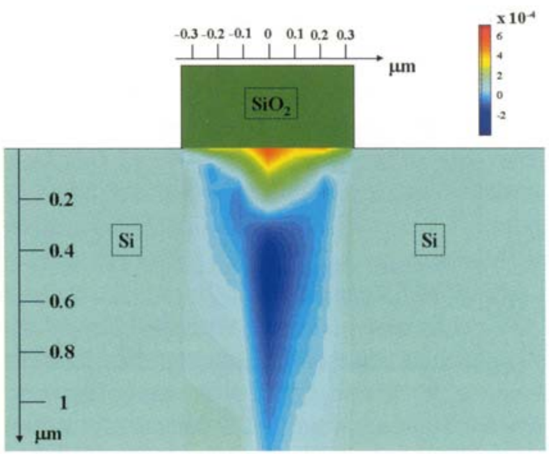
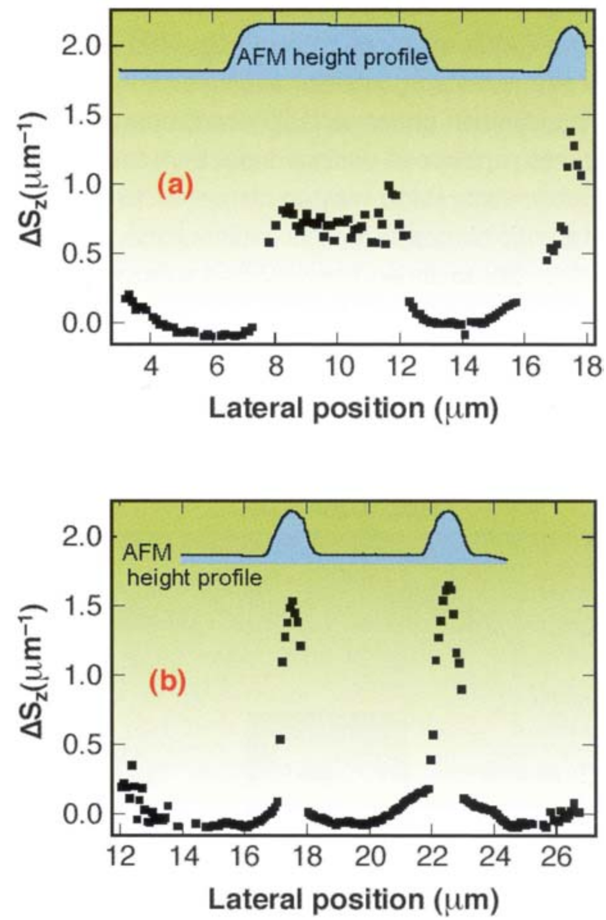
Diffraction with nm spatial resolution

Investigation of the strain of SiO_2 on Si

Focussing by wave guides







S. Di Fonzo et al. Nature, 403, 638 (2000)

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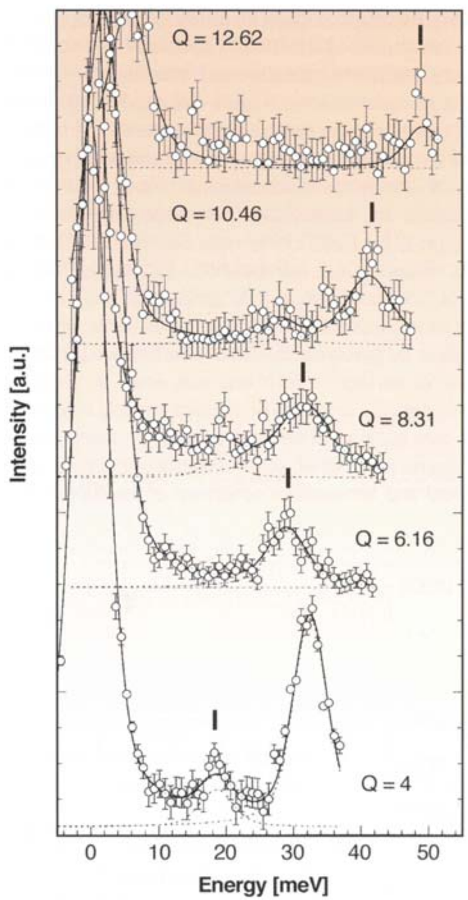
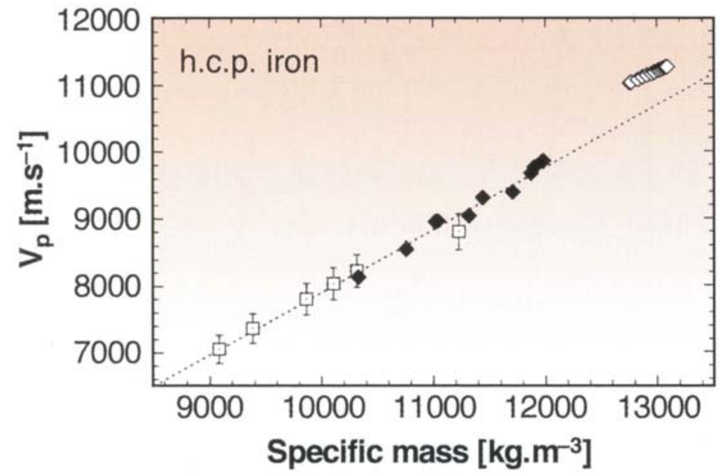
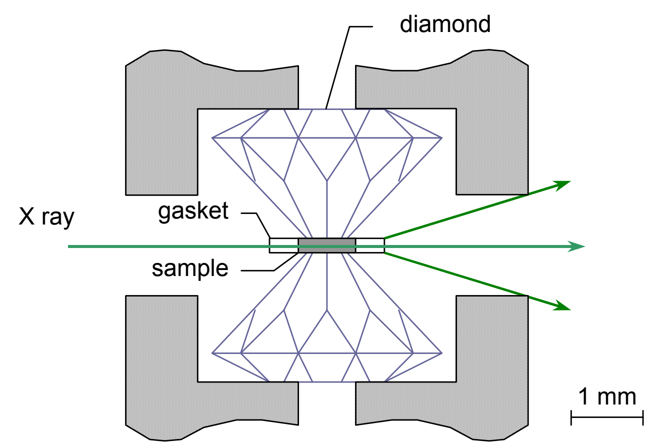
Inelastic scattering under high pressure

Speed of sound of Fe under pressure (ESRF: 2 ph/min)



P=28GPa





G. Fiquet et al., Science (accepted)

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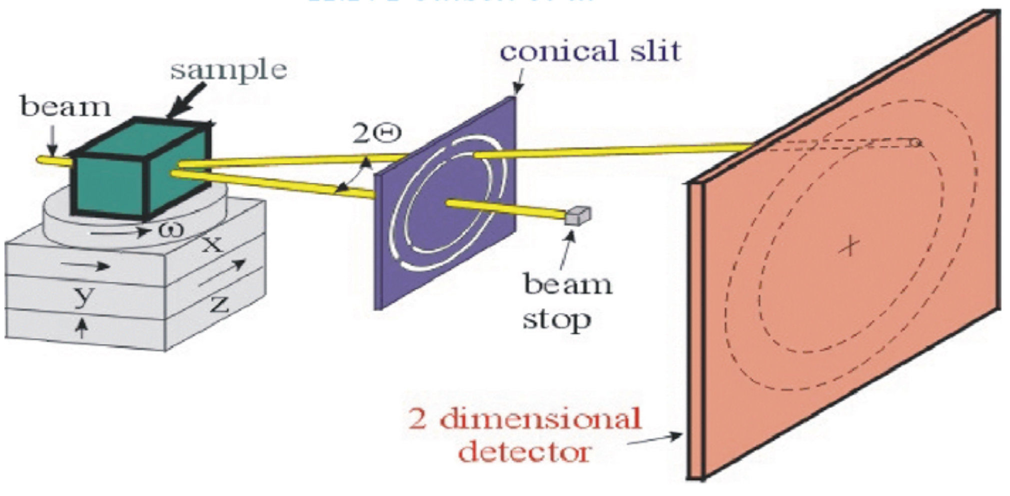
Example: Materials Science

Energy range: 50-100 keV; 5cm in Al

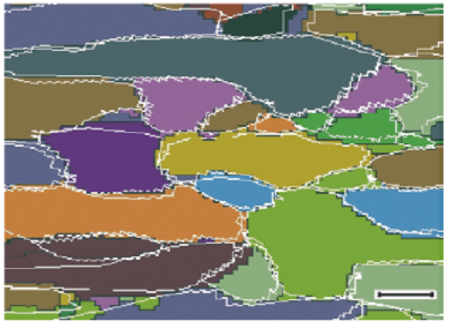
Accessible quantities: position, morphology, orientation, deformation (plastic/elastic), composition

3D X-ray microscope

H.F. Poulsen et al



Grain mapping in Al



Achiveable resolution today: 1.5 x 5 x 50 µm (ESRF)

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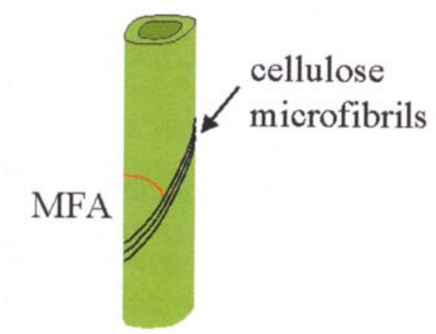
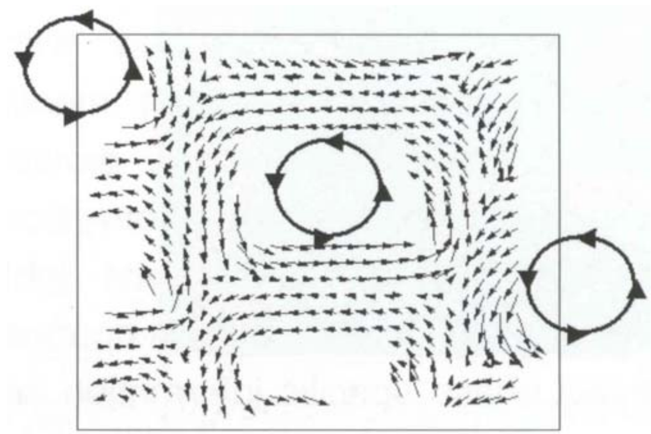
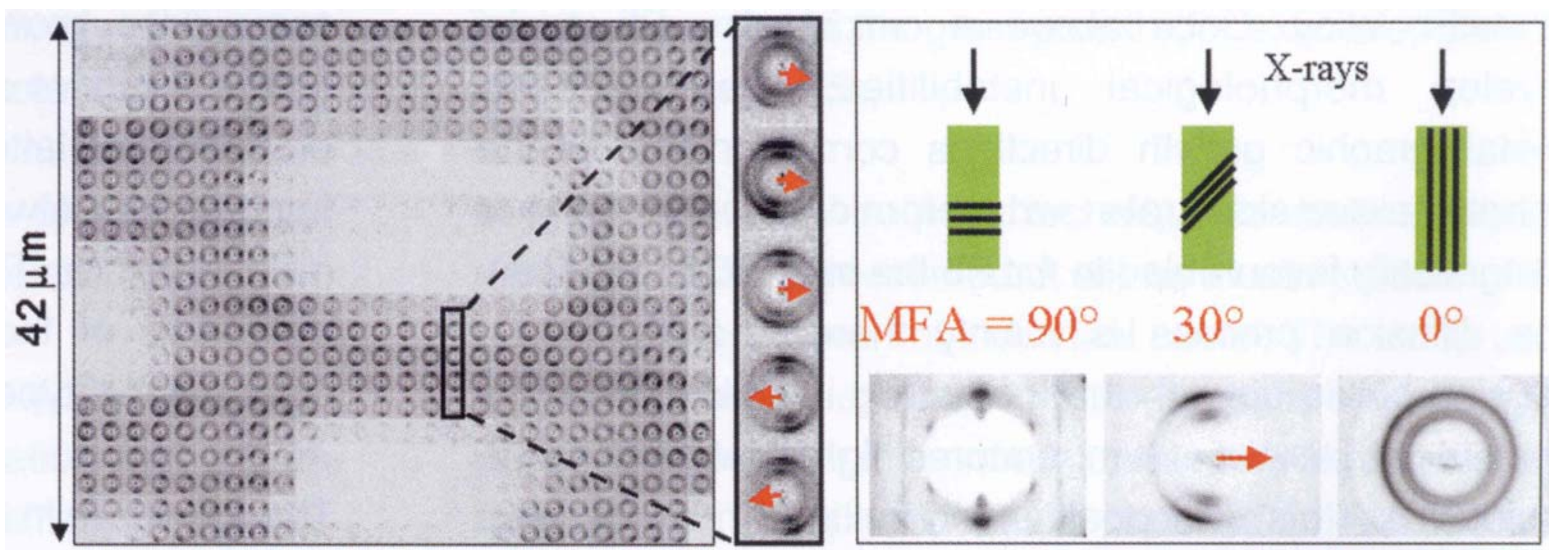
Micro SAXS





Orientation of micro fibrils in wood cells.

Spatial resolution: 2 µm



TDR: Proposed Beamlines II

X-ray absorption and resonant scattering

- Absorption spectroscopy
- Hard X-ray microprobe
- High energy photo electron spectroscopy
- Variable polarization XUV-beamline
- Resonant scattering beamline

Structural biology

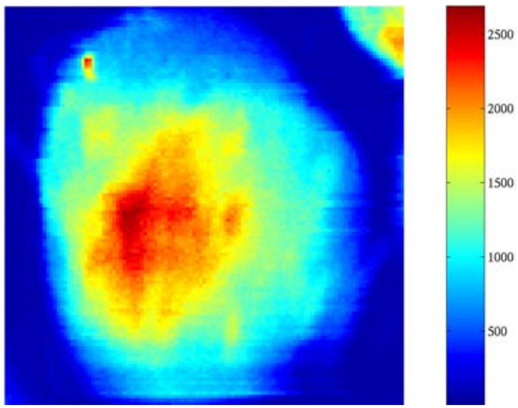
- Protein crystallography
- Bio-XAFS
- Bio-SAXS

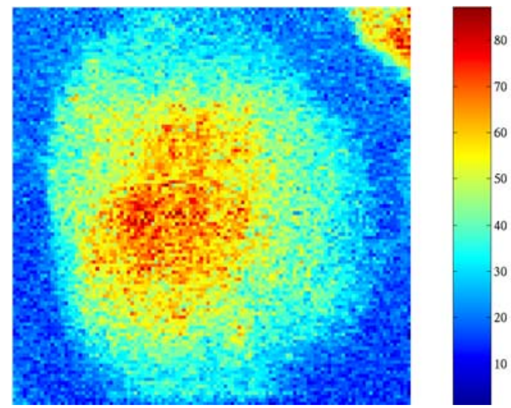
Example: µ-Fluorescence of Cancer Cells

Step = 0.3 µm, 0.9 sec/pt

40 µm

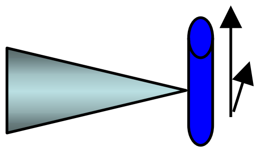
K



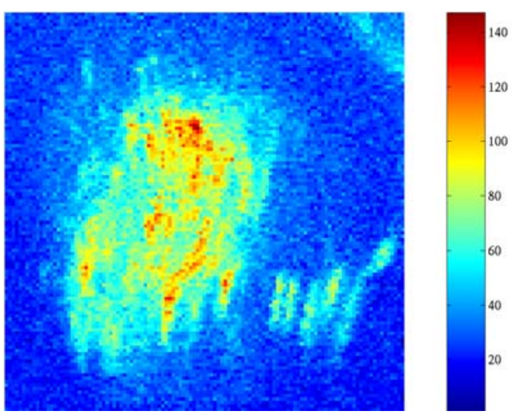


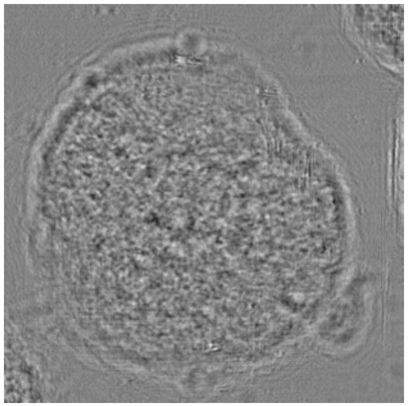
Pt

Cancerous cells



Fe





Phase-Contrast

P. Cloetens, W. Ludwig, S. Bohic

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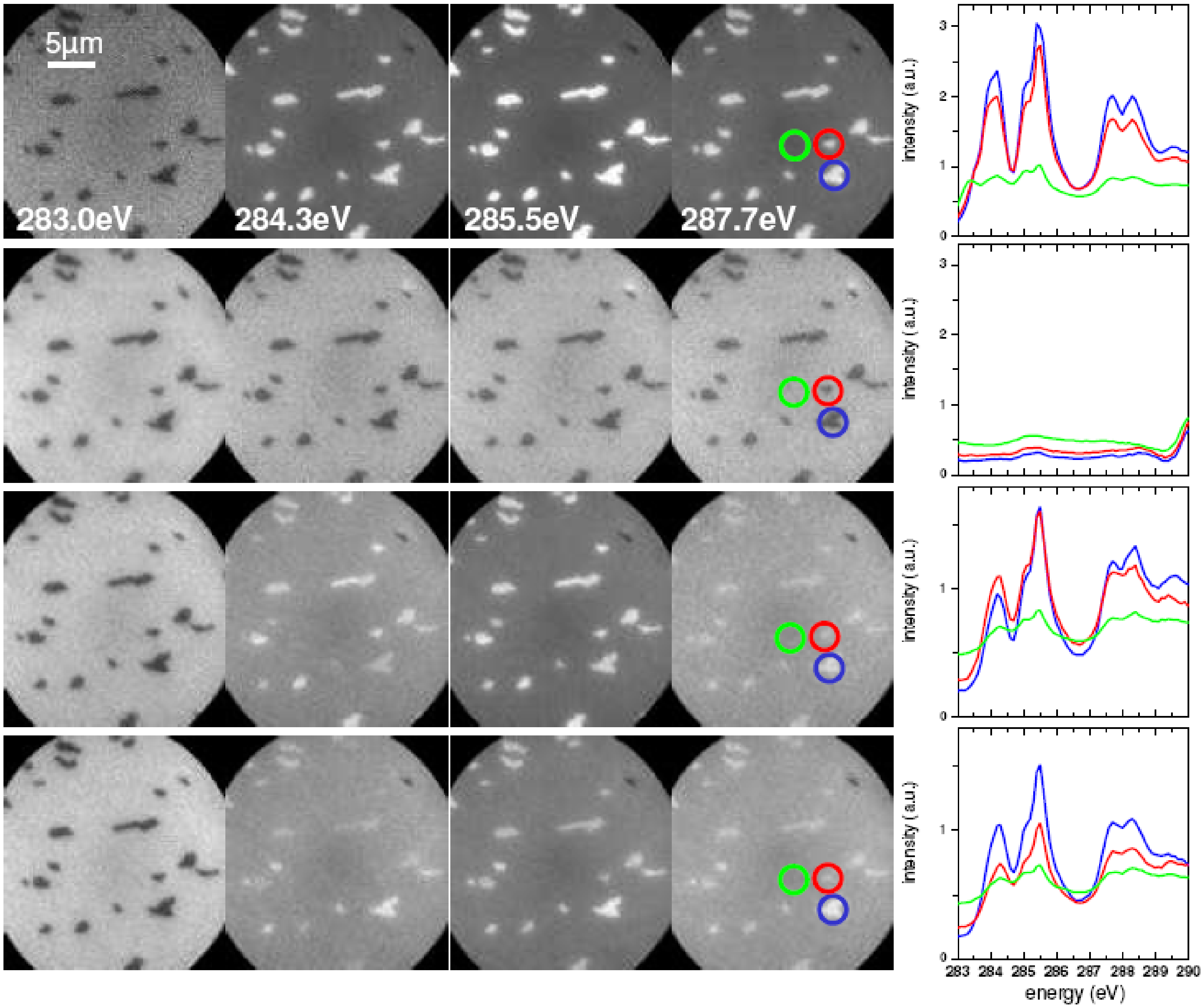
Spatially resolved VUV spectroscopy



Example:
NEXAFS-PEEM
near C 1s edge of 5ML PTCDA on Ag(111)

polarizations:
- linear 70deg
- linear ||
- left circ.
- right circ.

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Life sciences/Structural Biology

30S ribosomal subunit:
F. Schlünzen, R. Zarivach, J. Harms,
A. Bashan, A. Tocilj, R. Albrecht,
A. Yonath, Nature 413 (2001) 814-821

Small crystals:

- Micro focus and still small divergence

Large complexes:

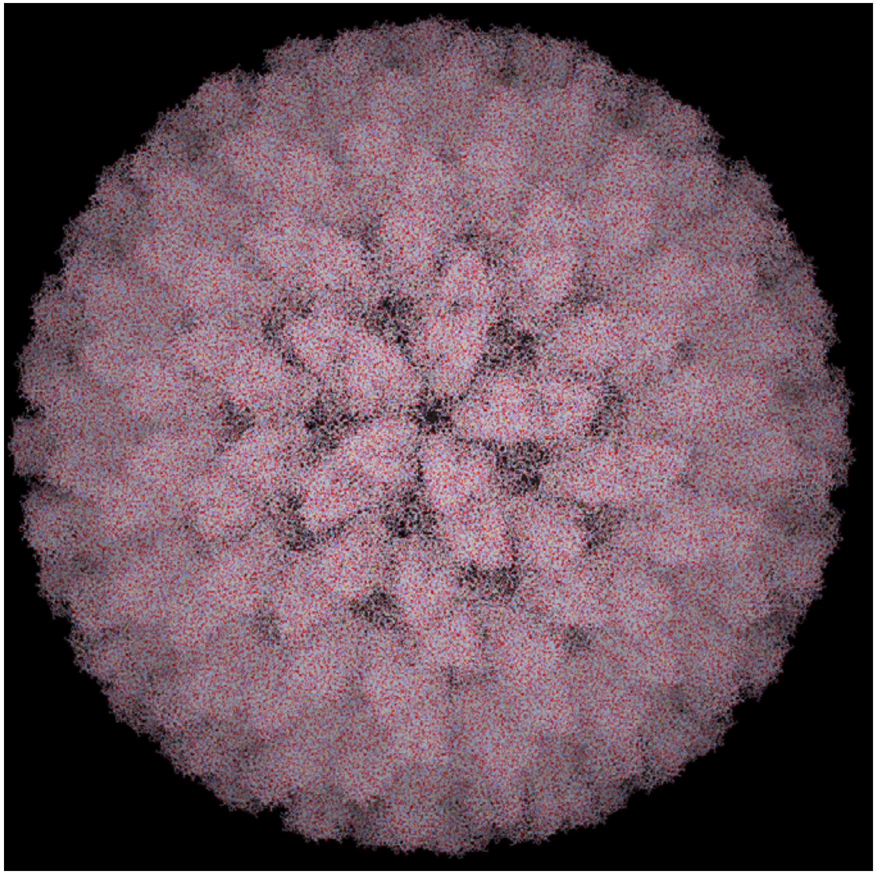
- Extremely intense and parallel radiation

Optimum anomalous signal:

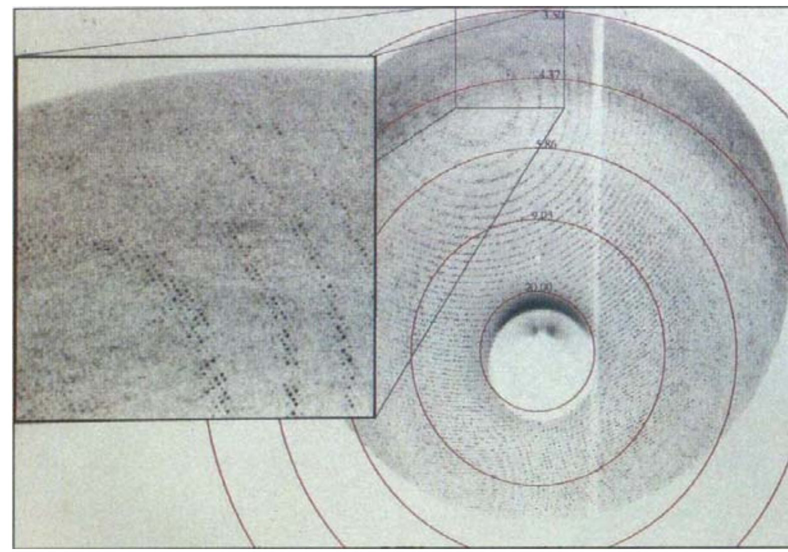
- High energy resolution and stability

Final experiments carried out mainly at ESRF and APS.

Extremely large complexes



example: Blue Tongue Virus



J.M. Grimes, J.N. Burroughs, P. Guet, J.M. Diprose, R. Malby, S. Zientra, P. Mertens, D.I. Stuart, Nature, 395, 470-478 (1998)

Summary

- The PETRA-III upgrade project is well on its way
- PETRA-III: one of the most brilliant storage ring based high energy X-ray source
- 13 undulator beamlines
- and quite a number of future upgrade possibilities
- exciting new possibilities for photon based research
- PETRA III will be complementary to the FEL sources

Thank you for your attention !!