Australian Government

ansto

Nuclear-based science benefiting all Australians

Perspectives on Synchrotron Radiation Research and the AOFSRR

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2013 Cheiron School

AOF Synchrotron Radiation

Asia/Oceania Forum for Synchrotron Radiation Research

AOFSRR Objective

The objective of the AOFSRR is to encourage regional collaboration in, and to promote the advancement of, synchrotron radiation research and related subjects in Asia and Oceania.

Specific Activities:

(1) The annual workshop and Cheiron School, and organization of other scientific collaboration meetings;
(2) Exchange of information of facilities and user groups;
(3) Provision of a framework for cooperative activities;
(4) Any activities that promote and expand the role of synchrotron light source facilities and synchrotron based research in the Asia – Oceania region.

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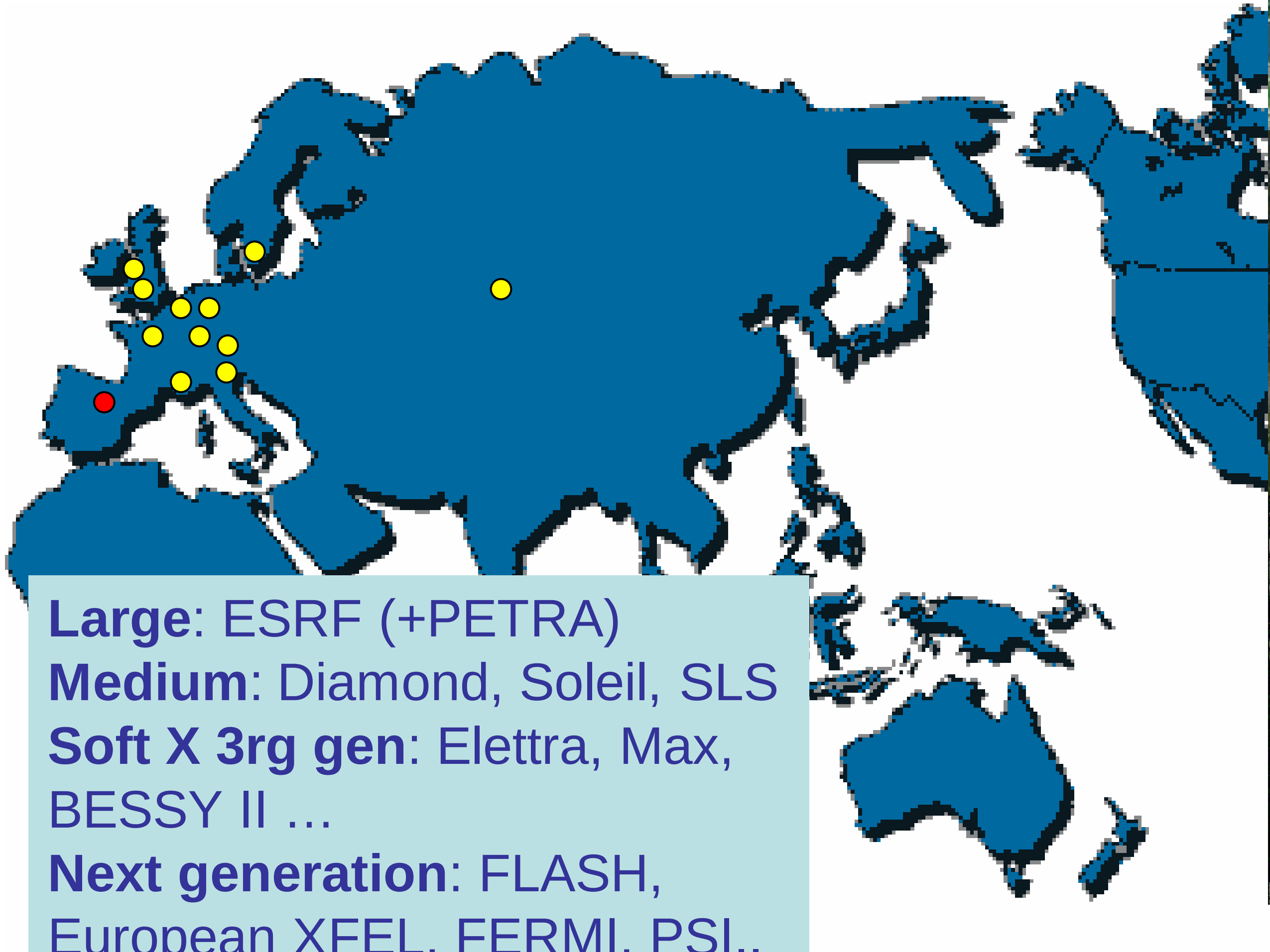
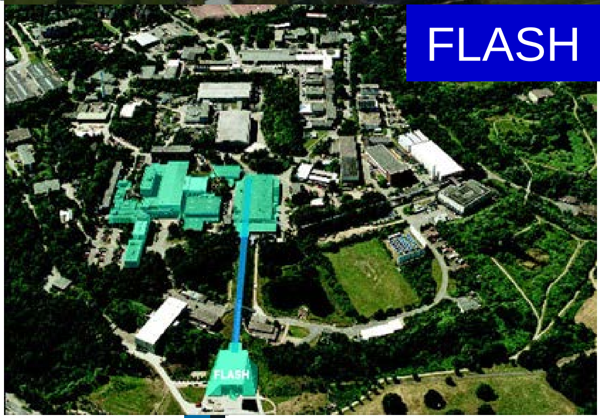
Synchrotron Radiation

European Union



Large: ESRF (+PETRA)
Medium: Diamond, Soleil, SLS
Soft X 3rg gen: Elettra, Max, BESSY II …
Next generation: FLASH, European XFEL, FERMI, PSI..

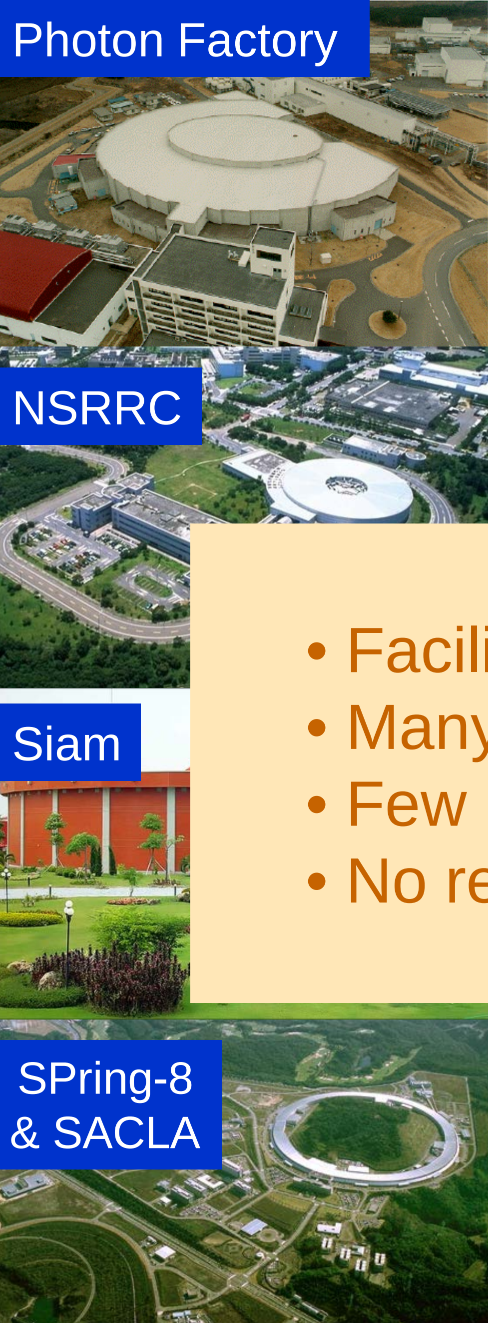


The Americas

Large: APS
Medium: CLS, NSLS II, SSRL
Soft X 3rd Gen: ALS
2nd gen: NSLS, CHESS, Brazil, Alladin…
Next generation: LCLS, JLab, Cornell ERL(?)

AOF Synchrotron Radiation

Asia Oceania & the AOFSRR



Large: SPring-8
Medium: AS, Indus II, PLS II, Shanghai, TPS..
ISRRC,
PF,
ore …
,
EL…

- Facilities equal or better than Europe & USA
- Many bi-lateral agreements between facilities
- Few relationships between user communities
- No real regional organisation

Members:

- Australia
- China
- India
- Japan
- South Korea
- Singapore
- Taiwan
- Thailand

Associate Members:

- Malaysia
- New Zealand
- Vietnam

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Synchrotron Radiation

AOFSRR Activities

Annual Workshop

Year	Host
2006	Tsukuba, Japan
2007	Hsinchu, Taiwan
2008	Melbourne, Australia
2009	Shanghai, China
2010	Pohang, South Korea
2011/12	Bangkok, Thailand
2013	Himeji, Japan
2014	Hsinchu, Taiwan

Cheiron School: Always SPring-8 !!

AOF Synchrotron Radiation

User Community Networking

- The AOF annual workshop
- Cheiron School
- Open access to facilities
- Special Access
- Multi-nation scientific collaborations
- Regional accelerator school
- Other workshops

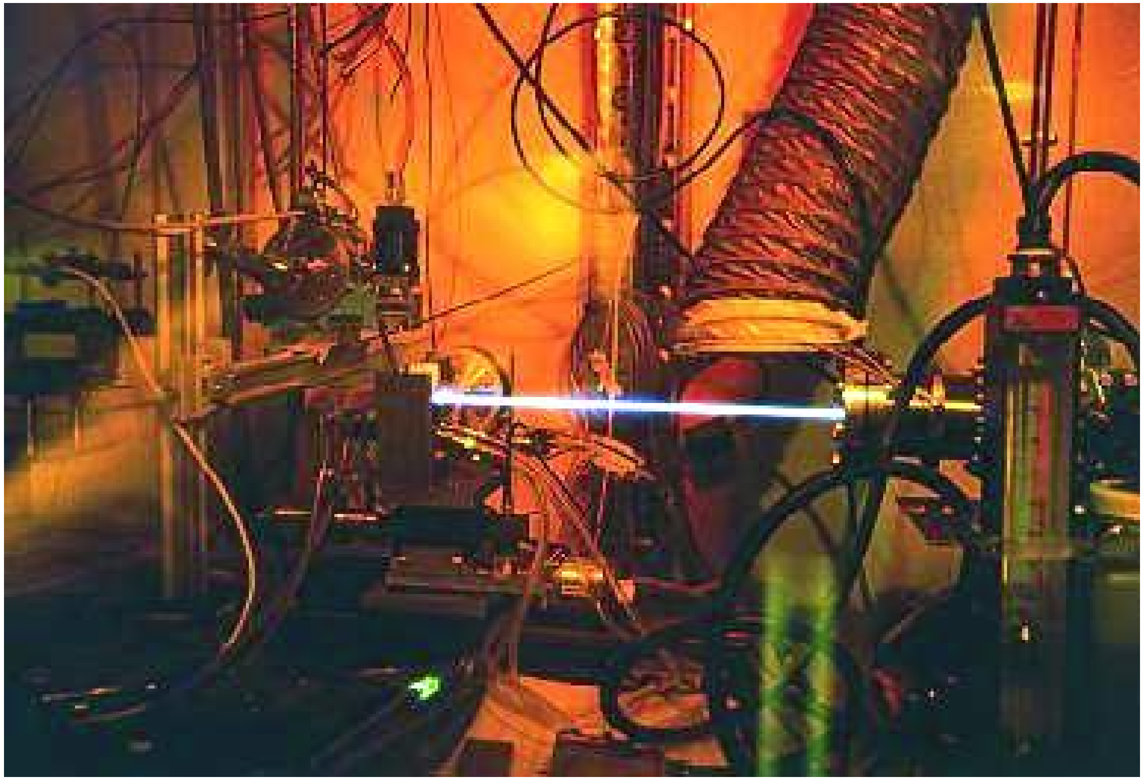
Promote Synchrotron Research

- Nations can build new communities at other facilities
  - Australian soft X-ray program at NSRRC and
  - NSRRC hard X-ray program at SPring-8
- Promote SR research in non-member nations in the A-O region
- Assist SR science in developing nations
  - Cheiron School
  - Assistance to attend conferences
  - Visiting scientists hosted at SR facilities
  - Work with other organisations (IUCr etc)

In the Future it is <u>your</u> AOF:

How Should it Develop ?

Synchrotron Radiation



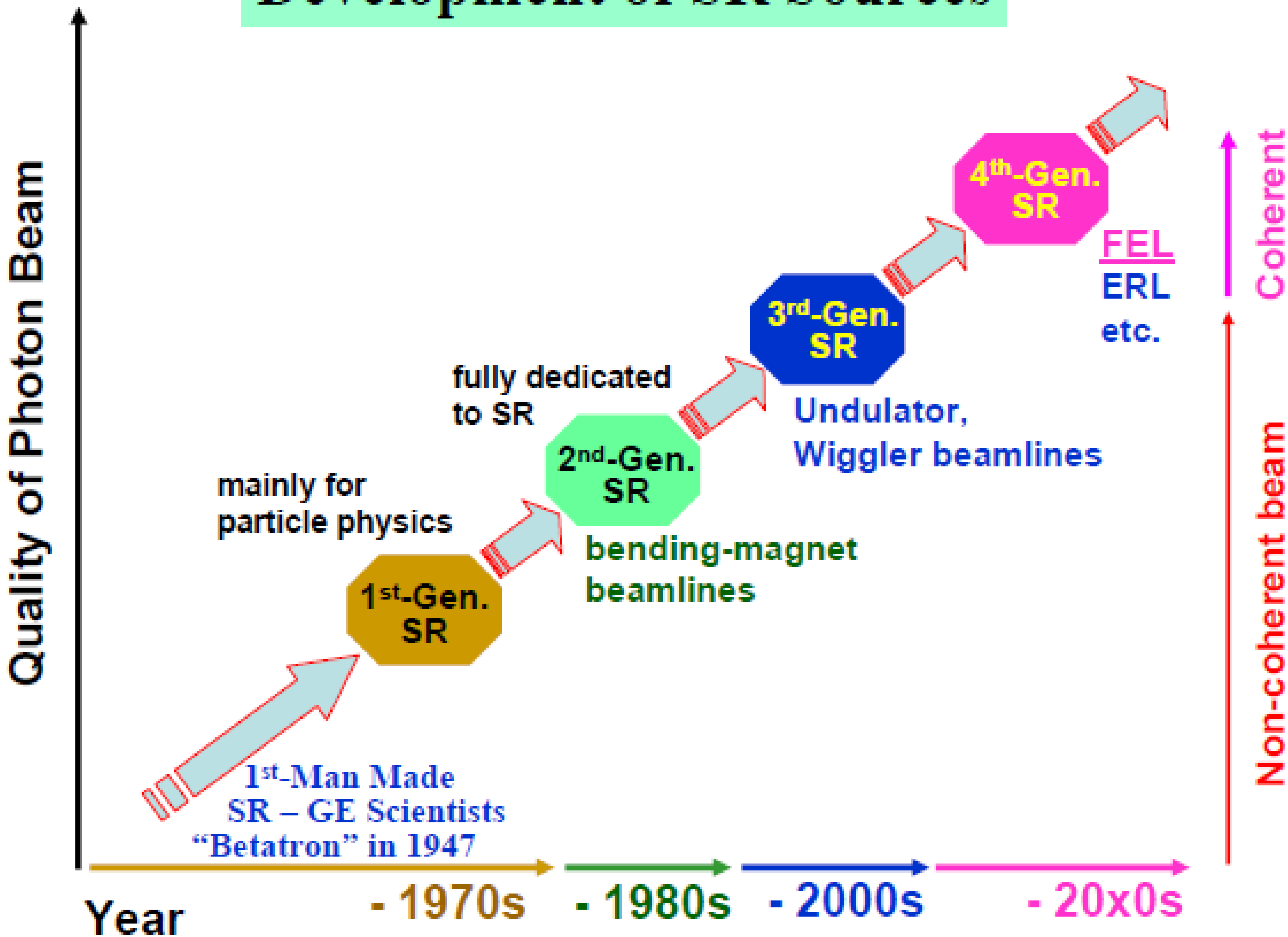
X25 wiggler beam, NSLS

Outline

- What is a synchrotron?
- How is the light produced & what are its characteristics?
- Brief Basics of Synchrotron Beamlines
- Some Applications
- The Future (is here already): “Next Generation Sources”
- Some Cool Stuff

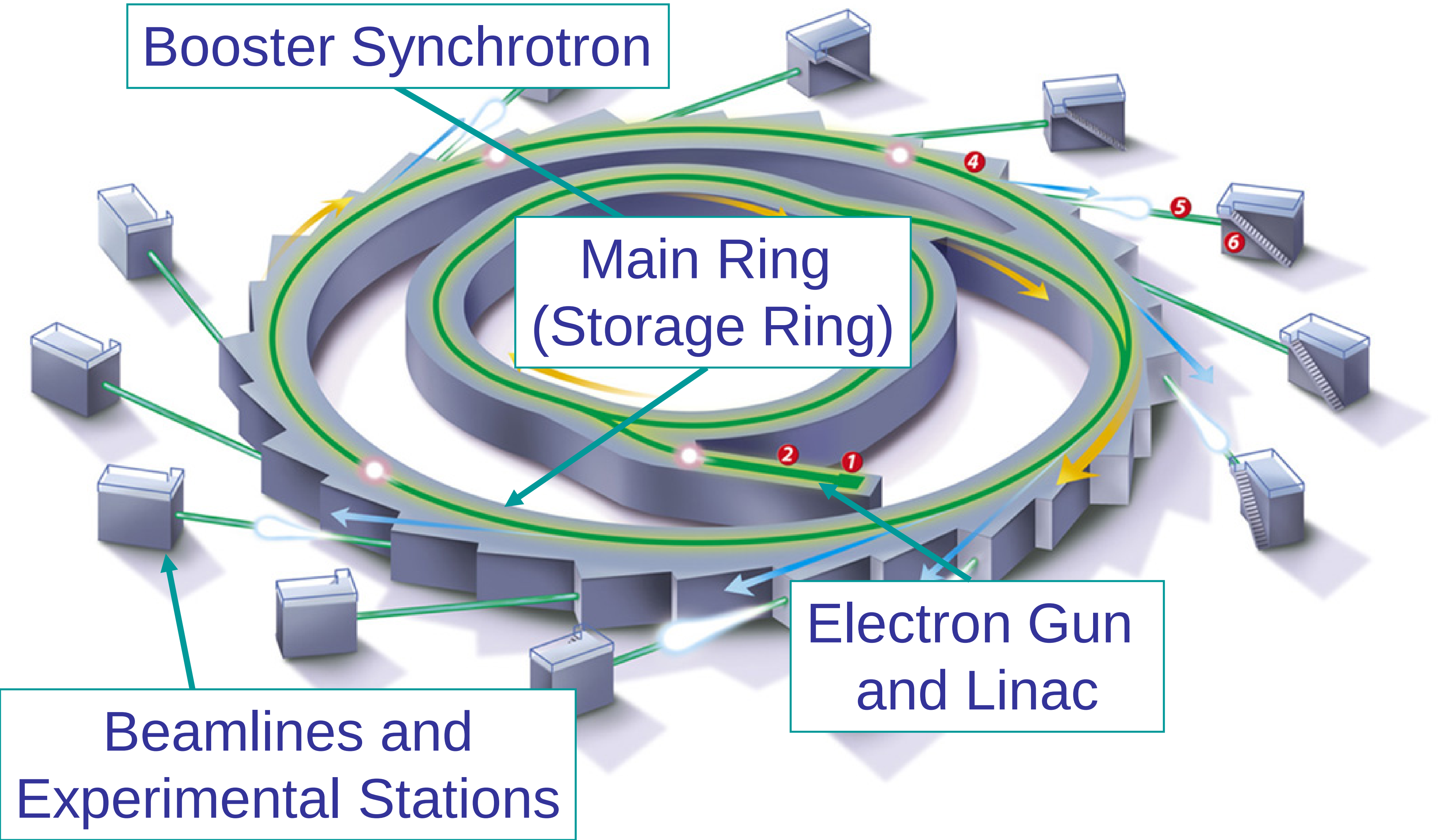
AOF Synchrotron Radiation

Development of SR Sources

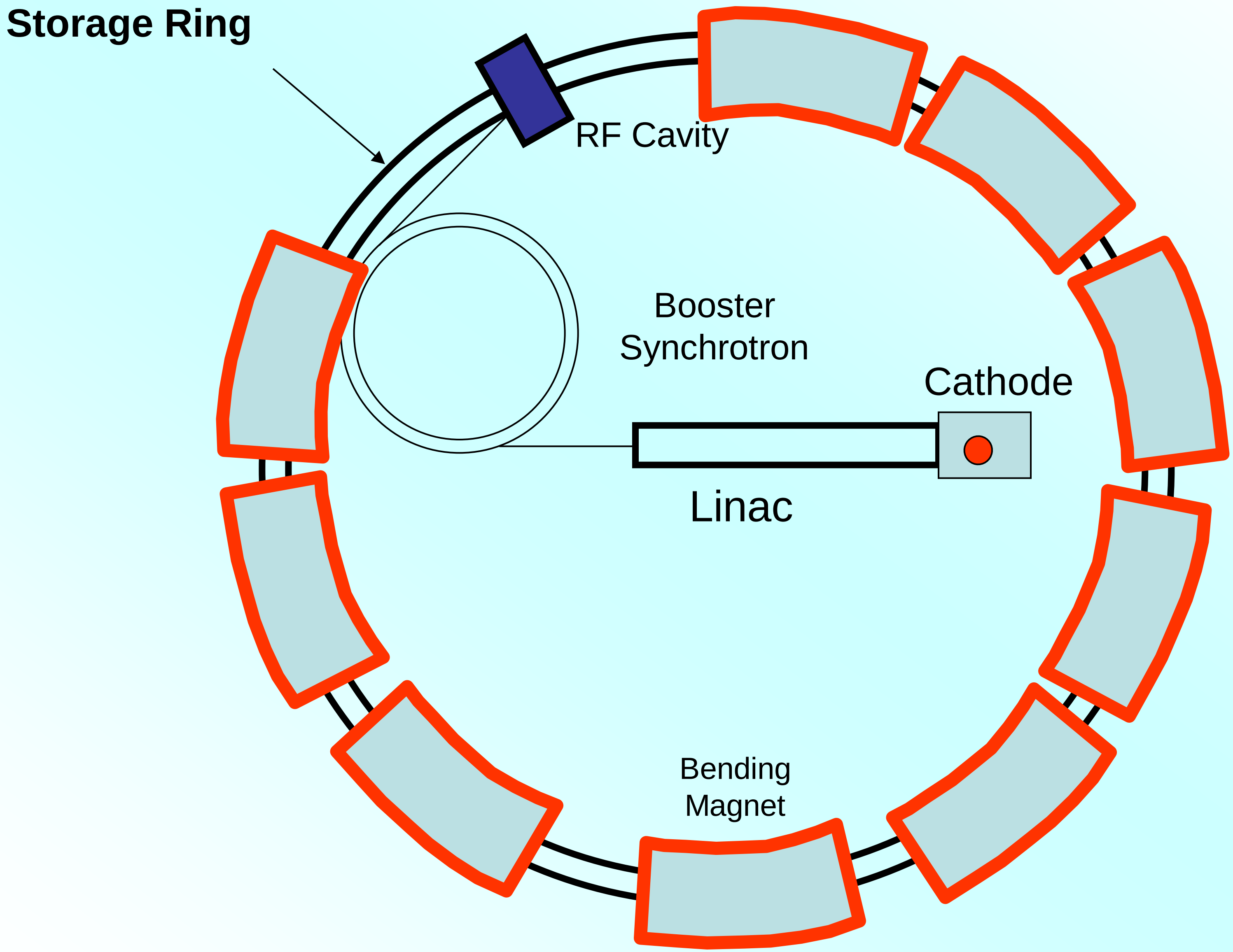


Courtesy M. Ree, PLS

A Synchrotron Step by Step

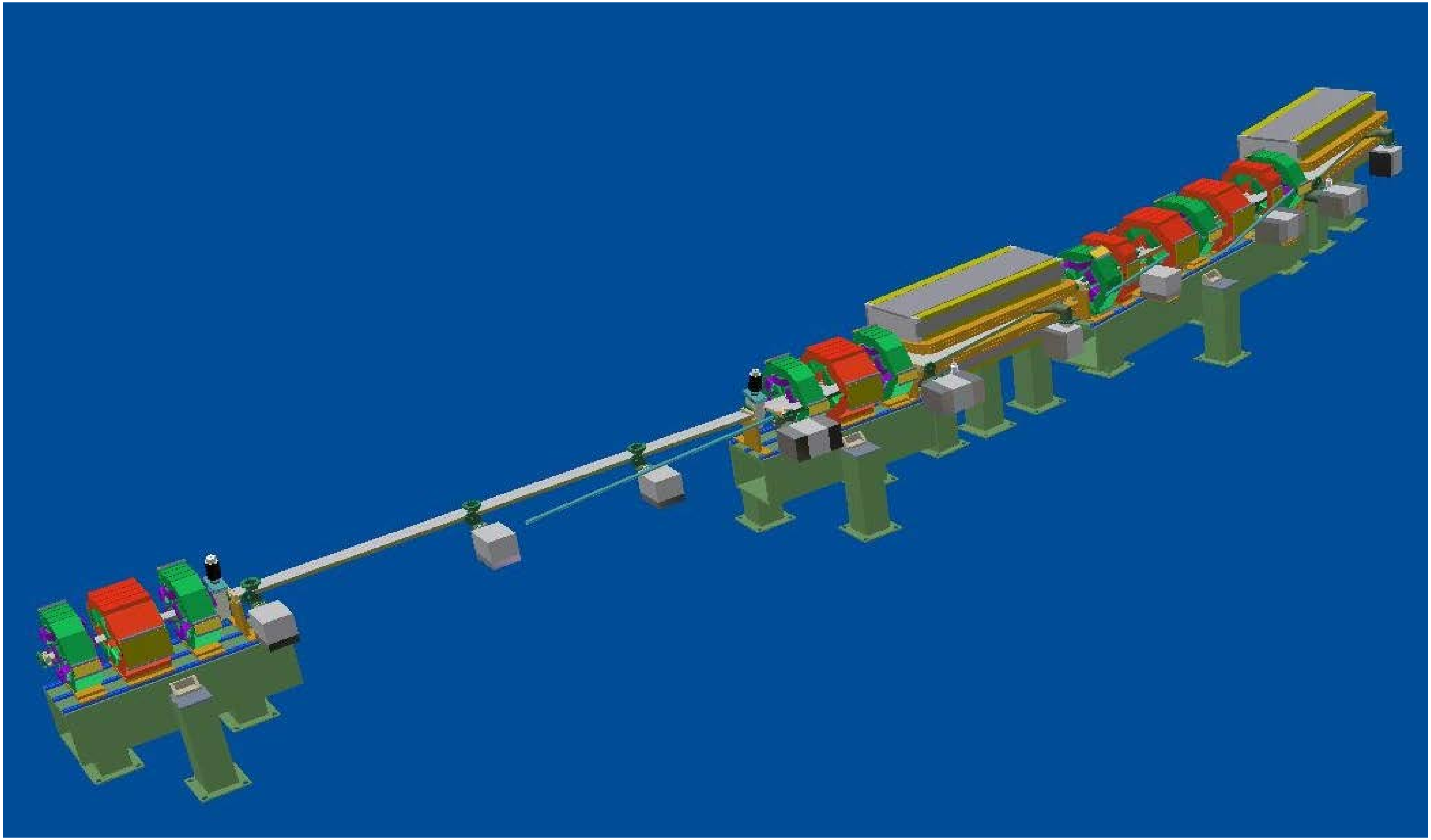


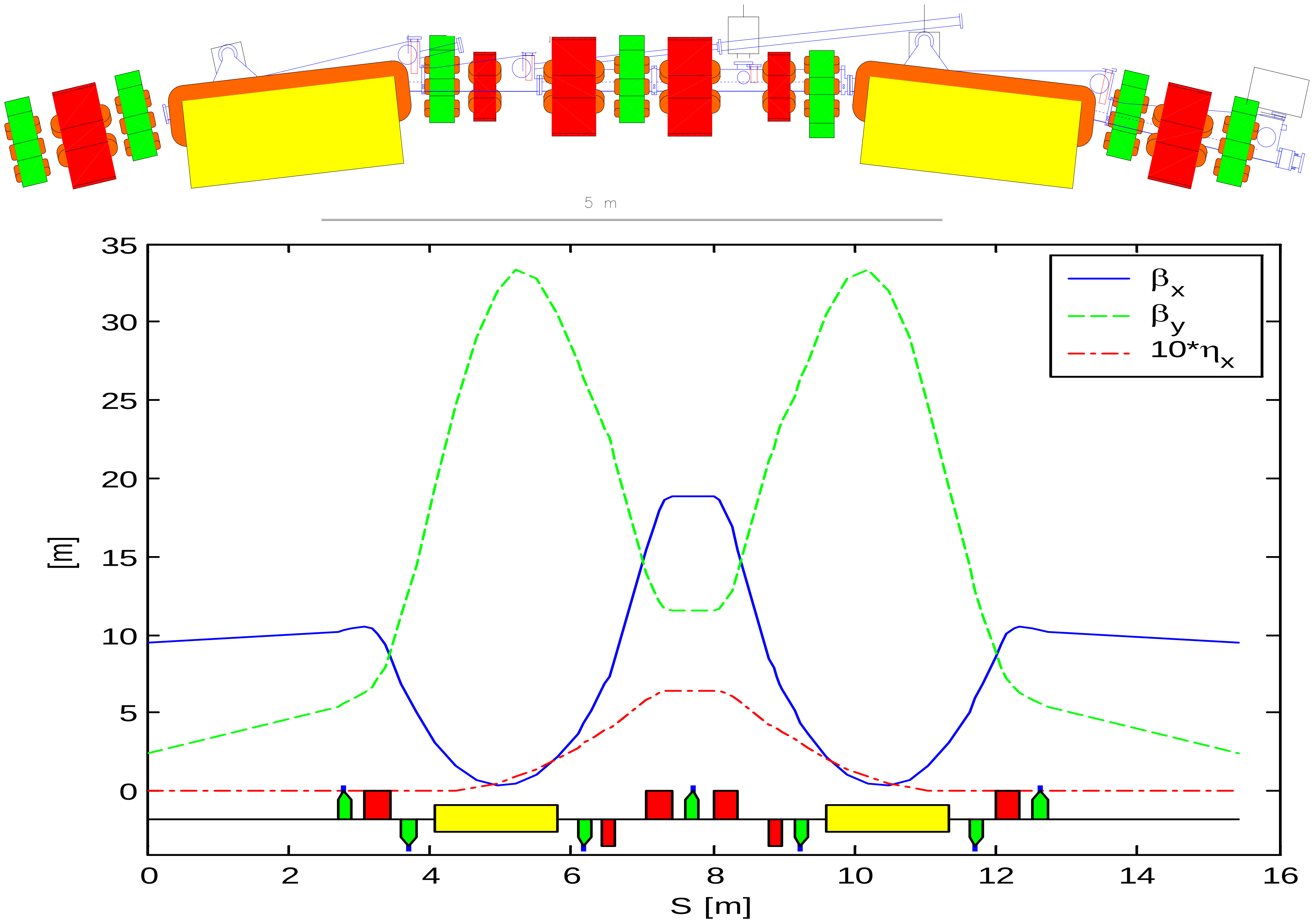
Synchrotron Animation



Courtesy T. Graber, ChemMatCARS

Section of the Australian Synchrotron





5 m
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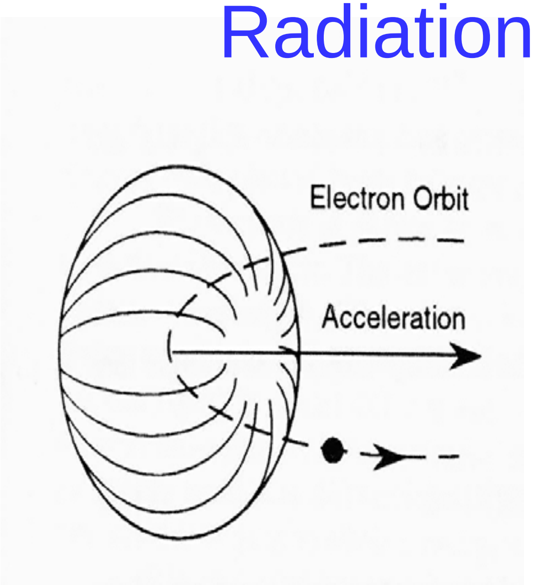
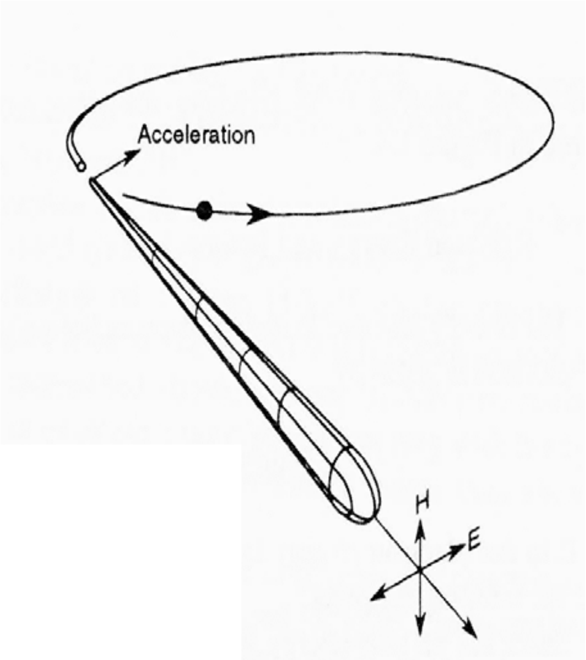
Generation of Synchrotron Radiation: Radiation from Accelerating Charge



Low energy electrons:

Radiation in all directions

Example: Radio waves from a transmitter.



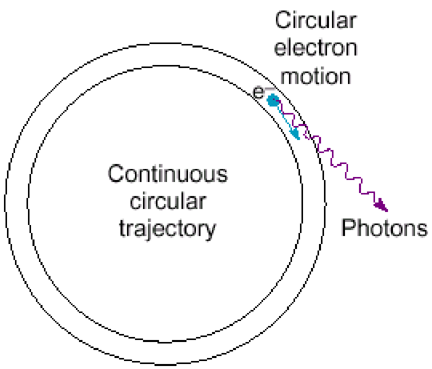
High energy (relativistic) electrons:

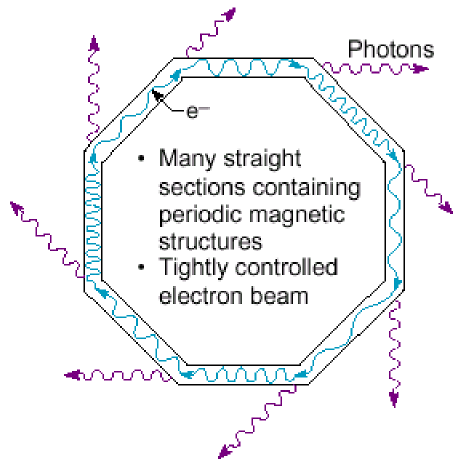
Radiation pattern swept into a narrow cone in the forward direction = High brightness!

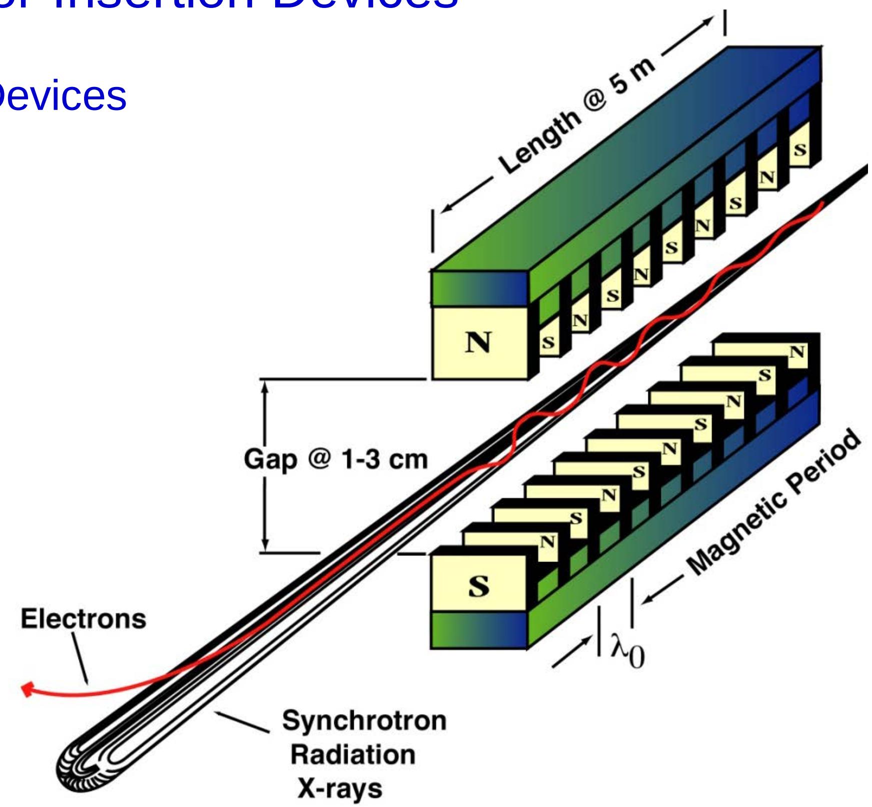
Third Generation Sources: Undulator Insertion Devices

1st, 2nd Generation

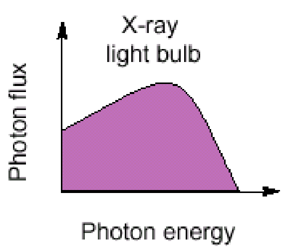
3rd Generation: Insertion Devices



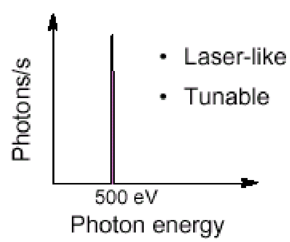


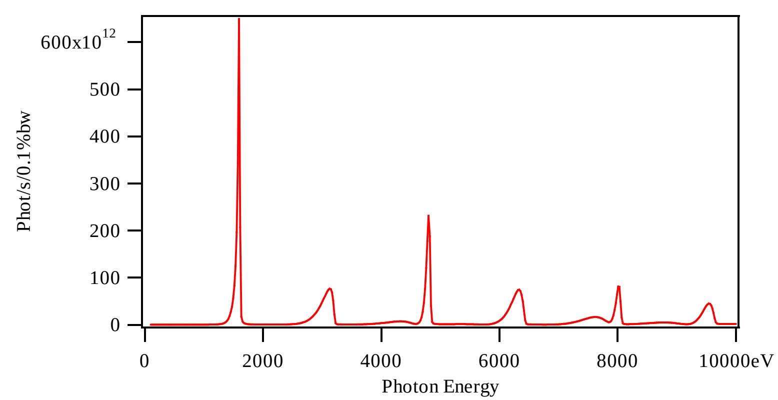


Bend Magnet Radiation

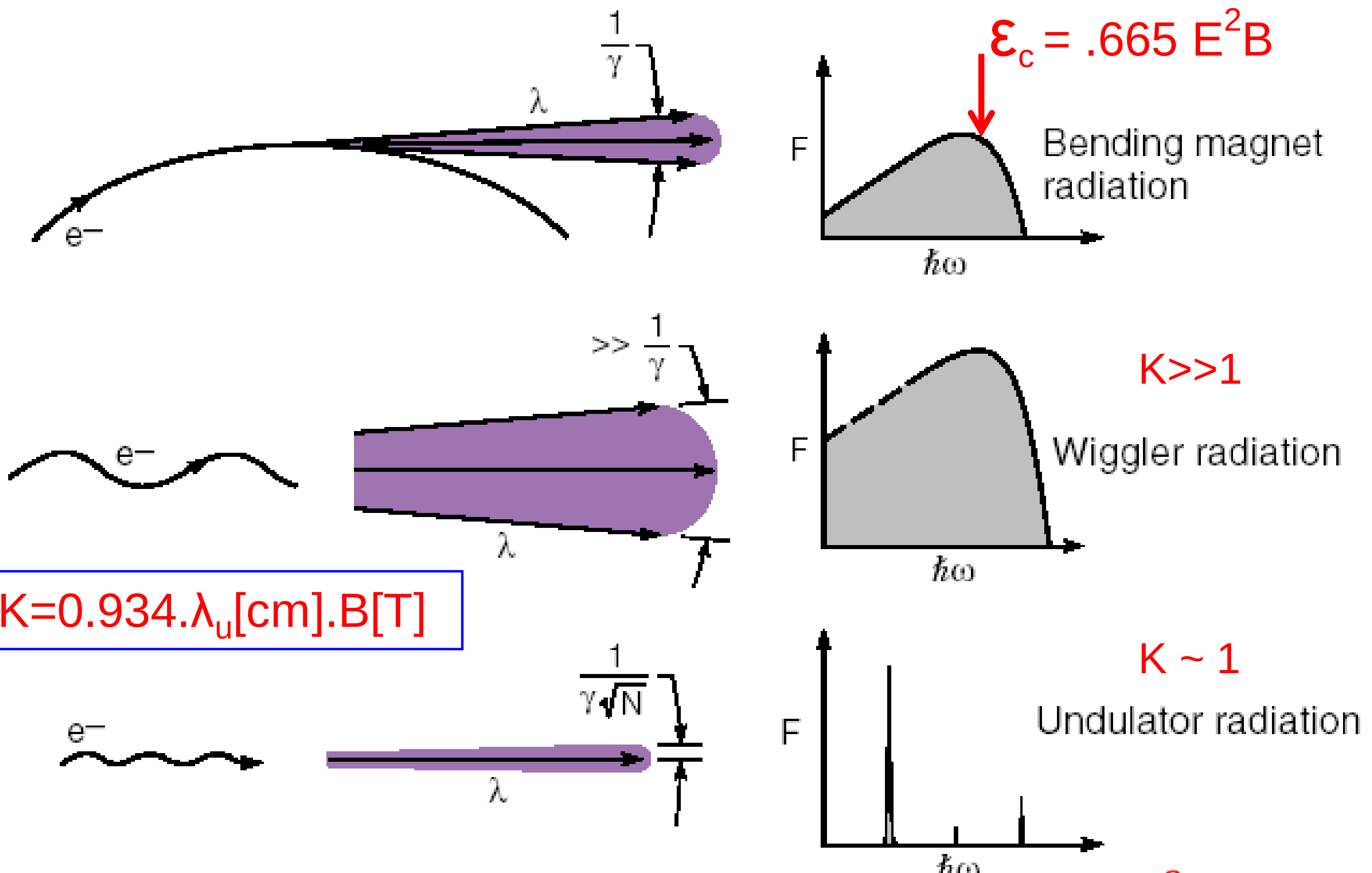


Undulator Radiation





Three Forms of Synchrotron Radiation



K=0.934.λ_u[cm].B[T]

$$\lambda = \lambda_u\left(1 + \frac{K^2}{2} + \gamma^2\theta^2\right)$$

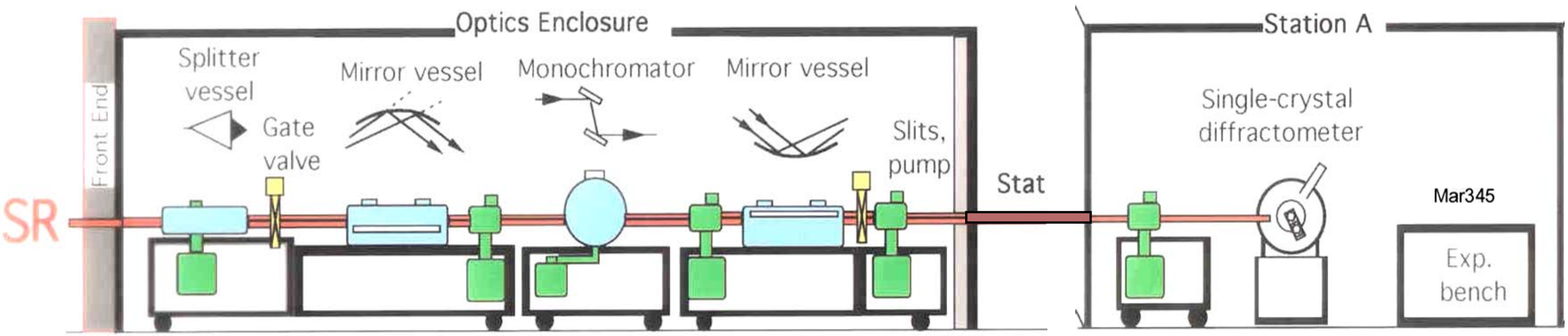
Beamline Design Goals

- Deliver the required X-ray beam to the experiment:
  - Energy and bandwidth
  - Spot size
  - Divergence/convergence
- Preserve source characteristics eg intensity, coherence
- Optimise signal / background
- Be very stable and reproducible, in position, intensity and energy
- Be safe to operate
- Be user friendly to operate
- Achieve all the above within a reasonable budget !

(Good Luck!)

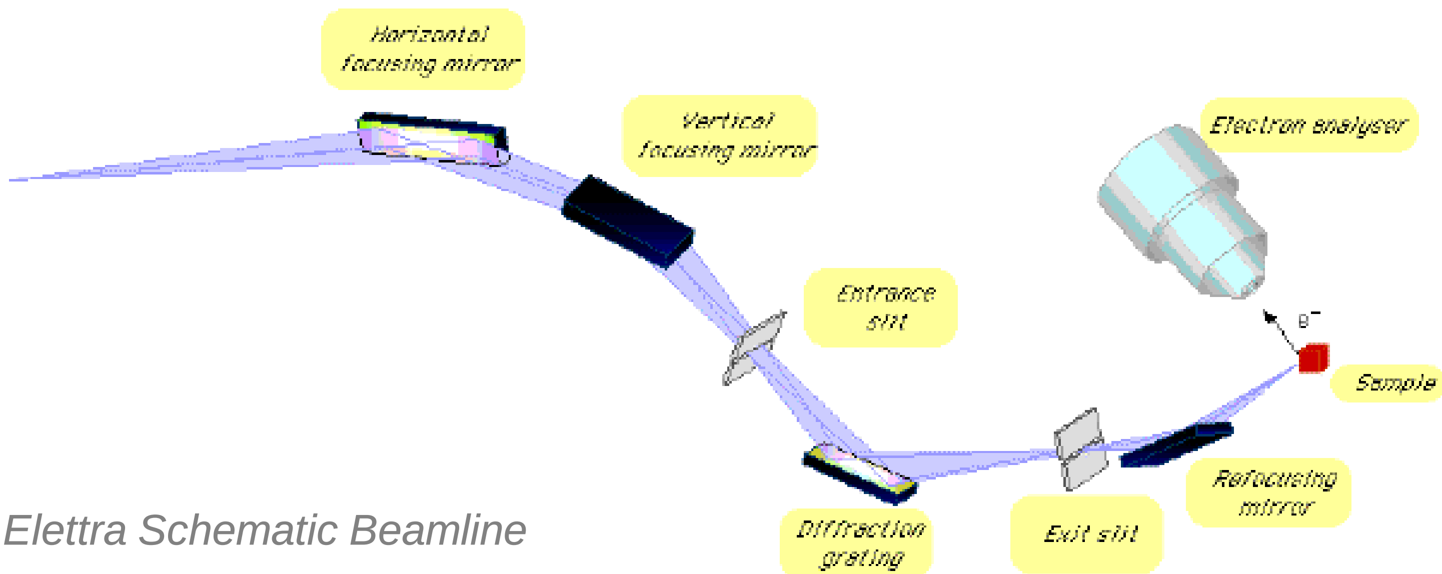
AOF Synchrotron Radiation

Hard X-ray Beamline: Si crystal monochromator E > 4 keV



(Swiss-Norwegian beamline, ESRF)

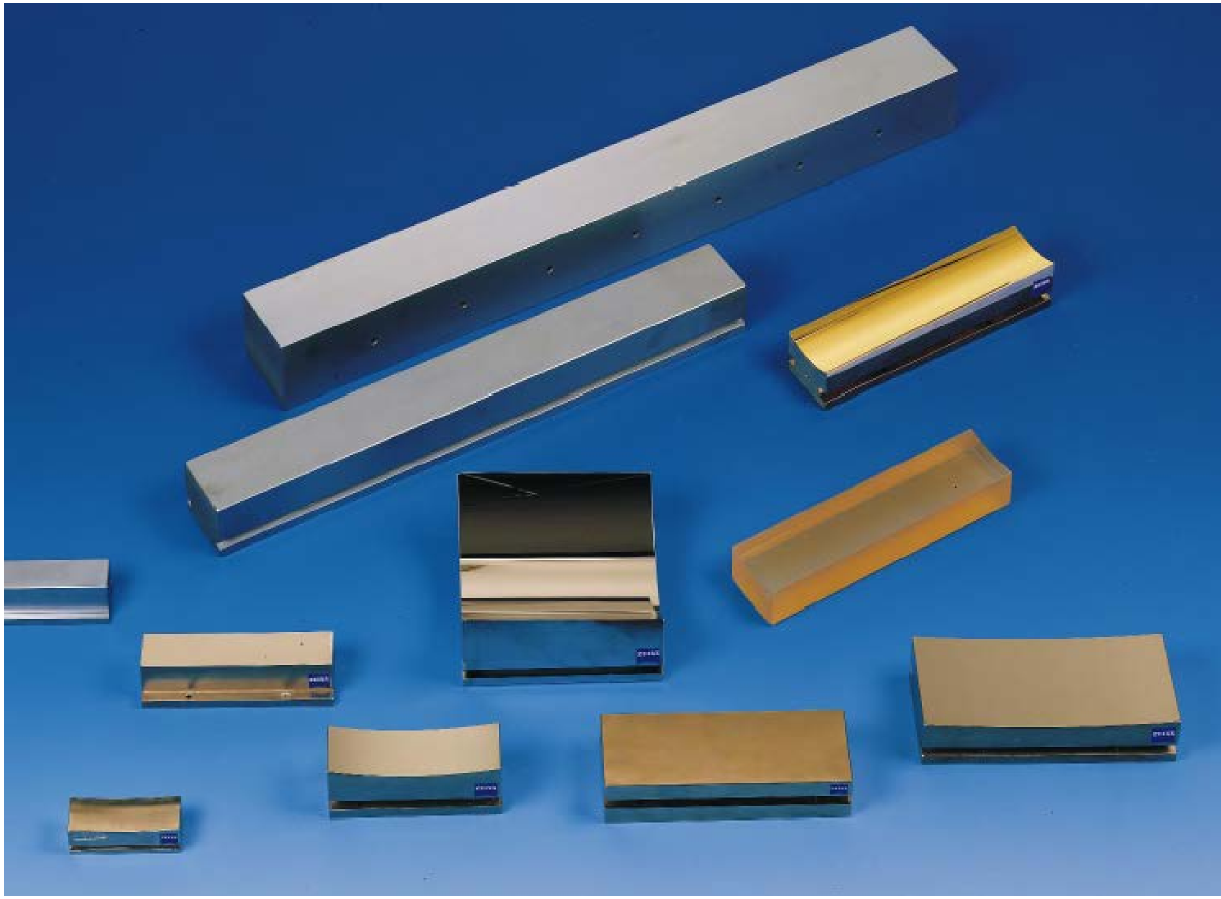
Soft X-ray Beamline: Grating monochromator E < 2 keV



Elettra Schematic Beamline

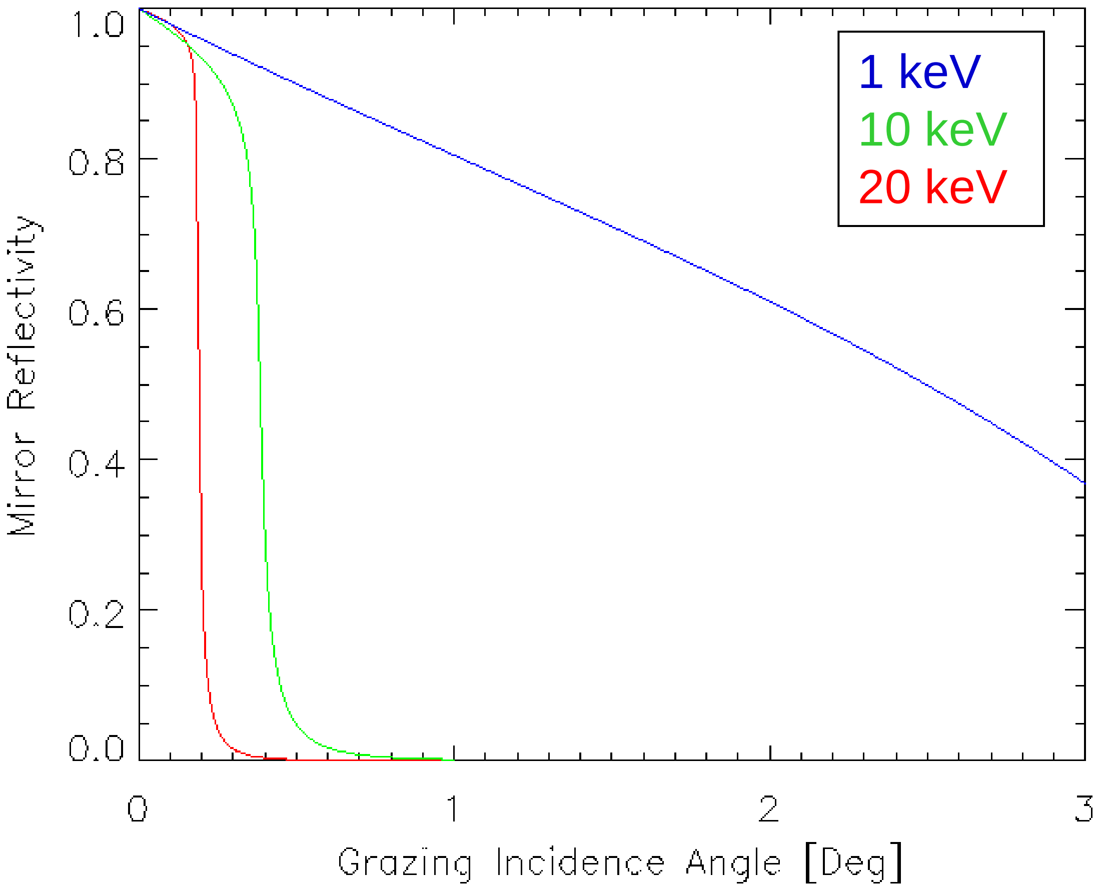
Mirrors for Synchrotron Beamlines

- Deflection
- Focusing
- Harmonic Rejection
- Power Reduction



AOF Synchrotron Radiation

Critical Angle/Reflectivity with Energy: Rhodium Coated Mirror Example

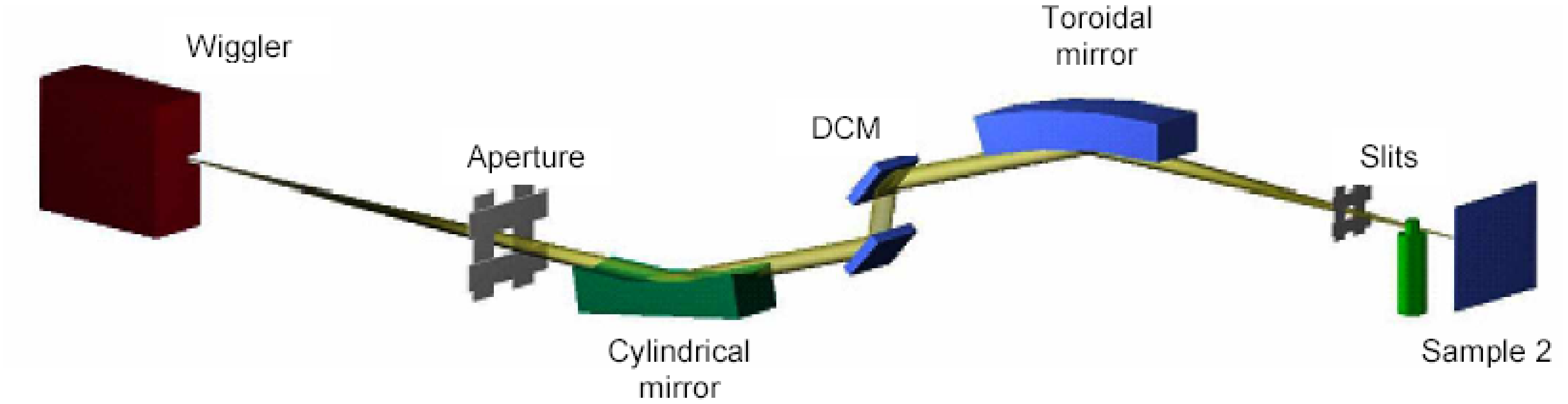


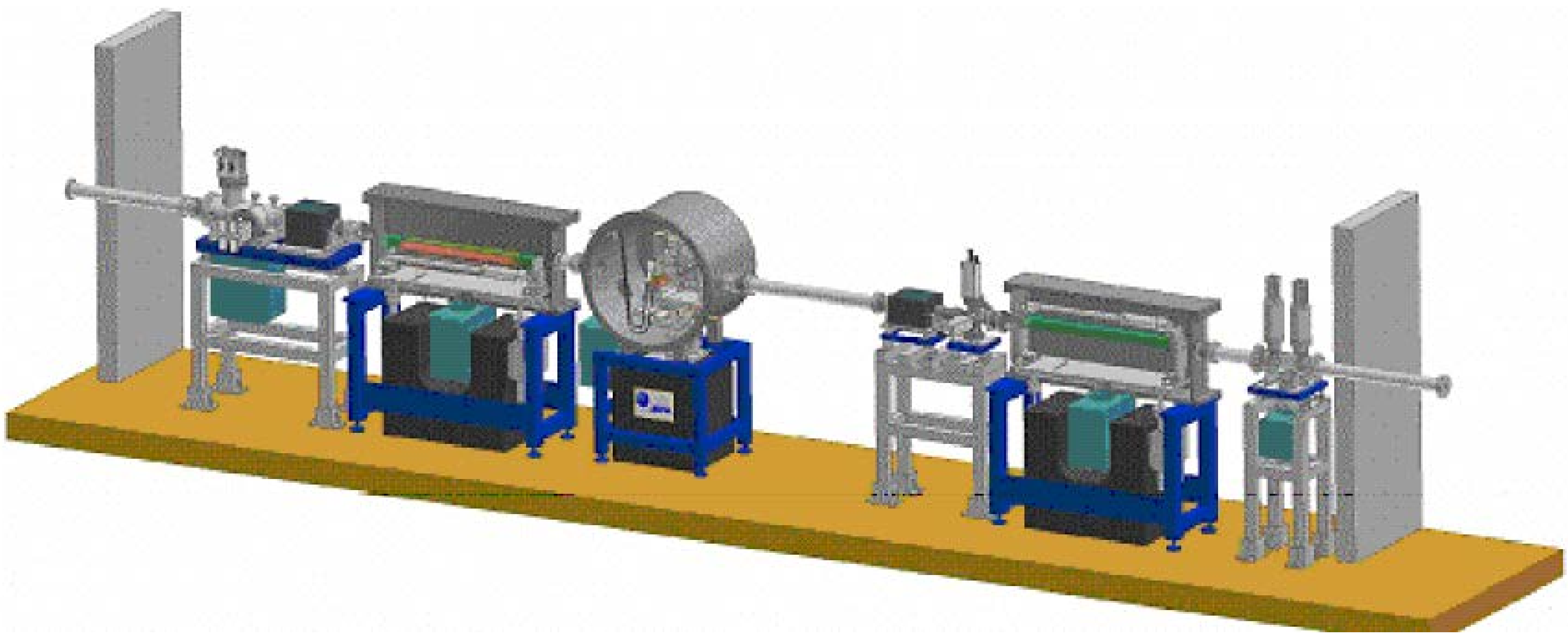
Harder X-rays need more grazing angles and longer mirrors:

2 mm high beam needs:

≤ 10 cm mirror at 1 keV
≥ 80 cm mirror at 20 keV

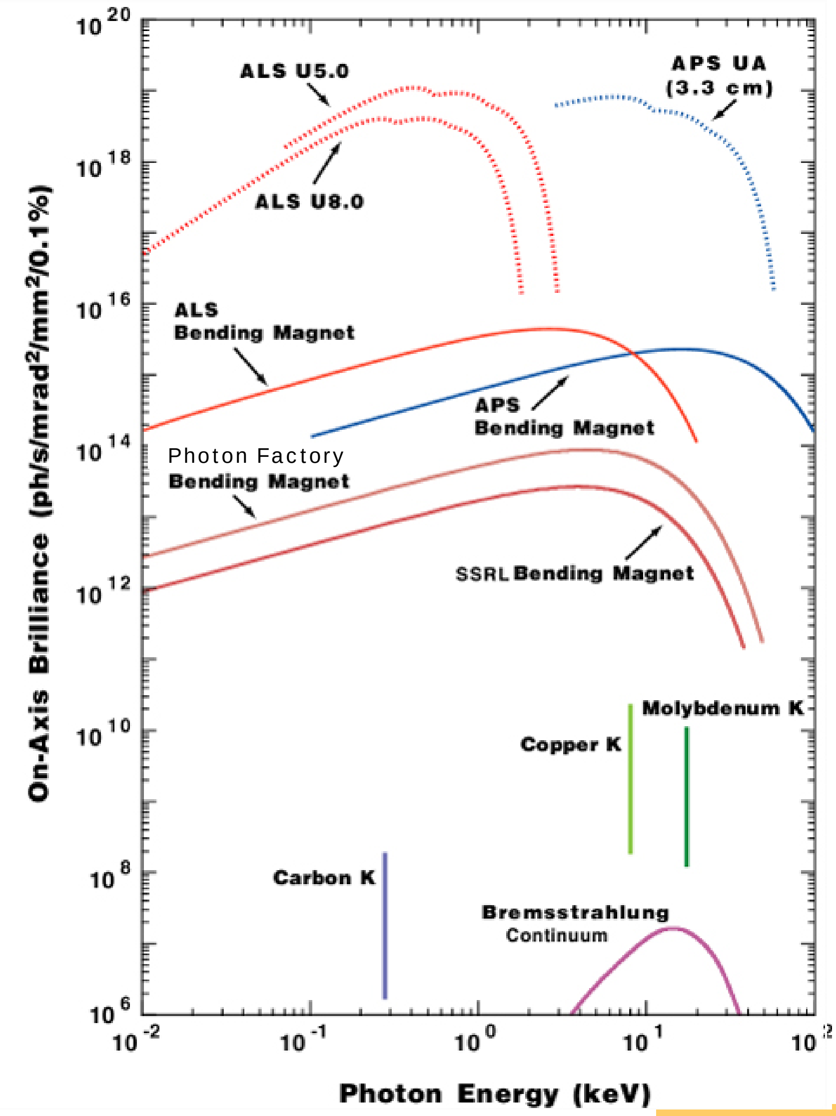
An example beamline:
the AS Xray Absorption Spectroscopy Beamline

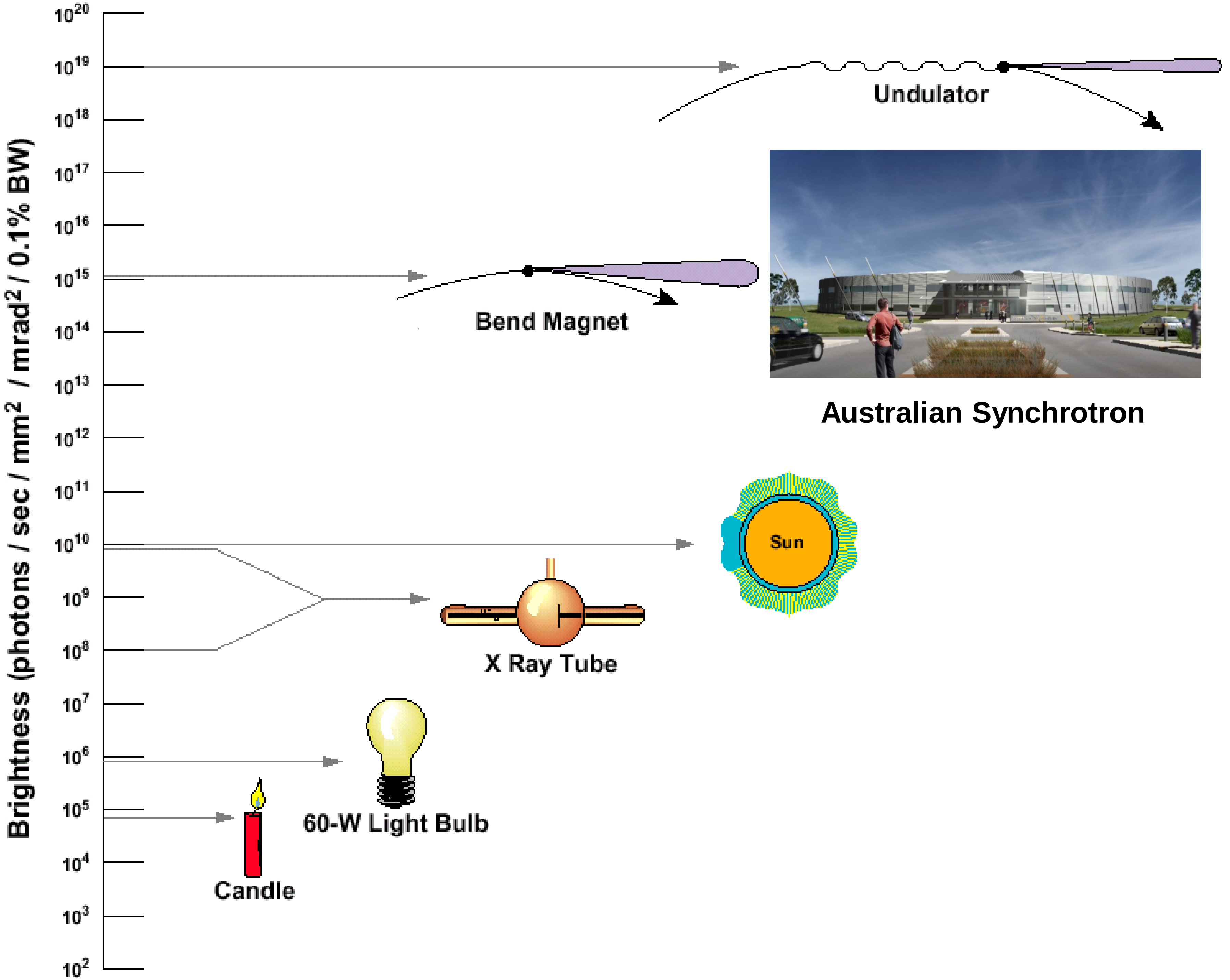




Characteristics of Synchrotron Radiation

- ✓ High brightness/flux
- ✓ Wide energy spectrum
- ✓ Plane polarised
- ✓ Pulsed





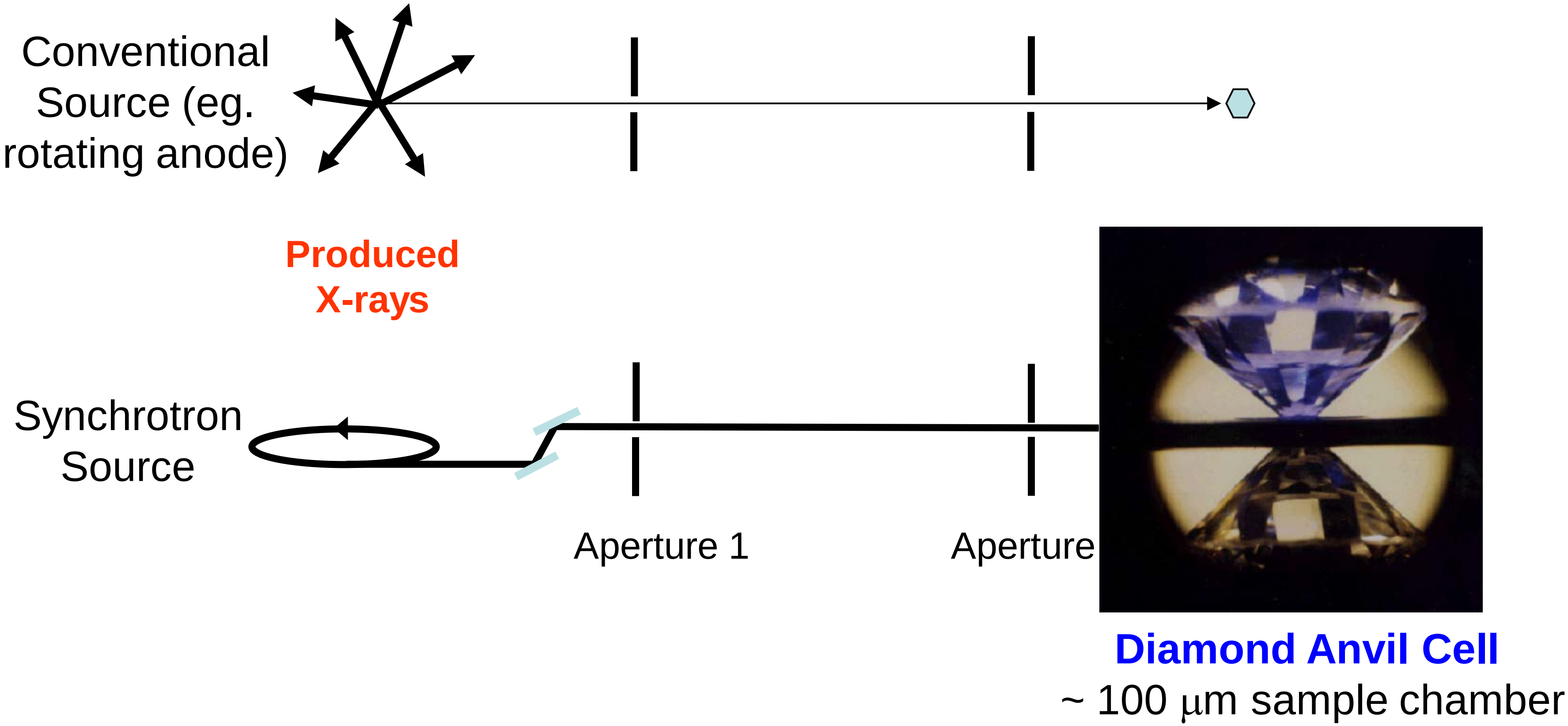
Brightness (photons / sec / mm^2 / mrad^2 / 0.1% BW)
10^{20}
10^{19}
10^{18}
10^{17}
10^{16}
10^{15}
10^{14}
10^{13}
10^{12}
10^{11}
10^{10}
10^{9}
10^{8}
10^{7}
10^{6}
10^{5}
10^{4}
10^{3}
10^{2}
Undulator
Bend Magnet
Australian Synchrotron
Sun
X Ray Tube
60-W Light Bulb
Candle

Unique Characteristics of Synchrotron Radiation

- Extremely high brightness. Modern synchrotron sources are about 10 billion times as intense as a laboratory X-ray generator: dilute samples; fast measurements; trace elements;
  - Low divergence: high intensity can be focussed onto tiny samples: Microscopies
- Wide X-ray energy spectrum:
  - the optimum X-ray energy to be chosen for each experiment;
  - X-ray spectroscopies are possible eg EXAFS
- Polarisation: various dichroisms; magnetic imaging; molecular orientation;
- Time structure: time of flight and very fast timing.

AOF Synchrotron Radiation

Why Brightness is Important

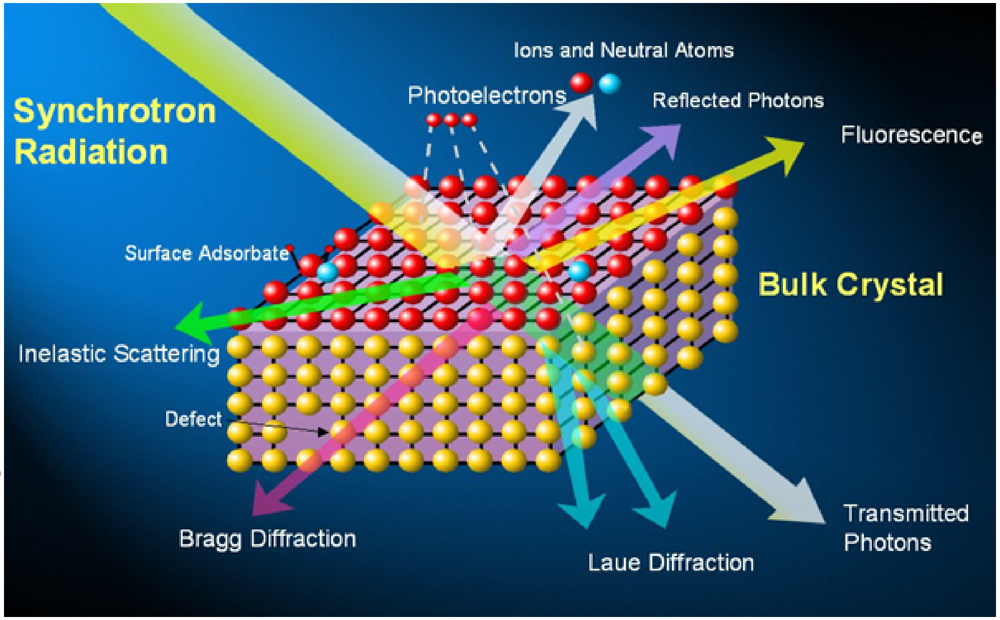


Brilliance of a synchrotron (flux/source size/divergence) gives more usable x-rays or effective intensity

AOF Synchrotron Radiation

X-rays and their Interaction with Matter

Courtesy SRRC, Taiwan



X-ray Fluorescence
➔ trace element analysis

X-ray Diffraction ➔ Structure

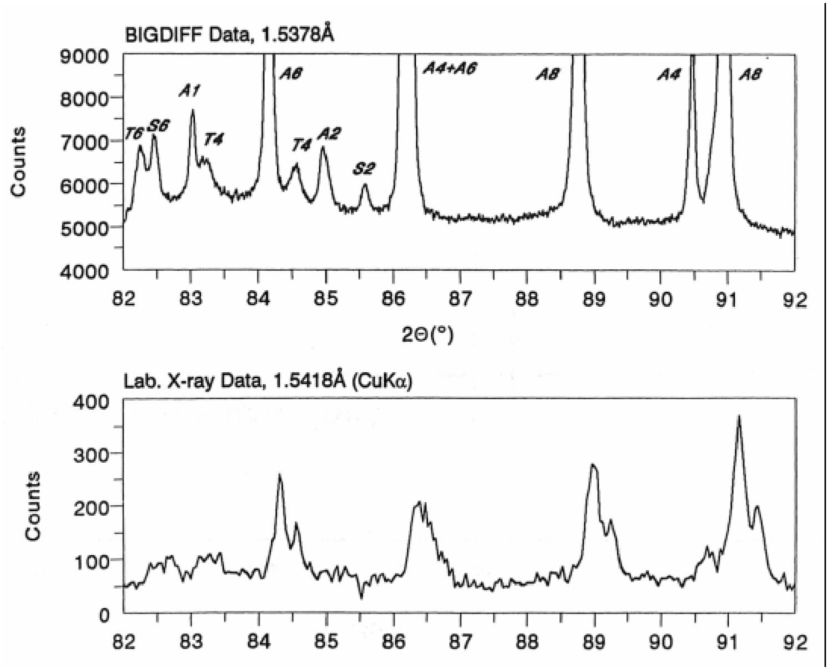
Transmitted Photons:
➔ Imaging
Absorption Spectroscopy
➔ Chemical information

AOF Synchrotron Radiation

	Synchrotron	Proton	Electron Microscope	SIMS	Neutron
Sensitivity	✓	●	✗	✓	✗
Sub micron	✓	●	✓	✗	✗
Chemical Information	✓	✗	●	●	✗
In-situ	✓	●	✗	✗	✓
Atomic Structure	✓	✗	✓	✗	✓

AOF Synchrotron Radiation

Sometimes High Intensity = Better Data
Synchrotron Powder XRD

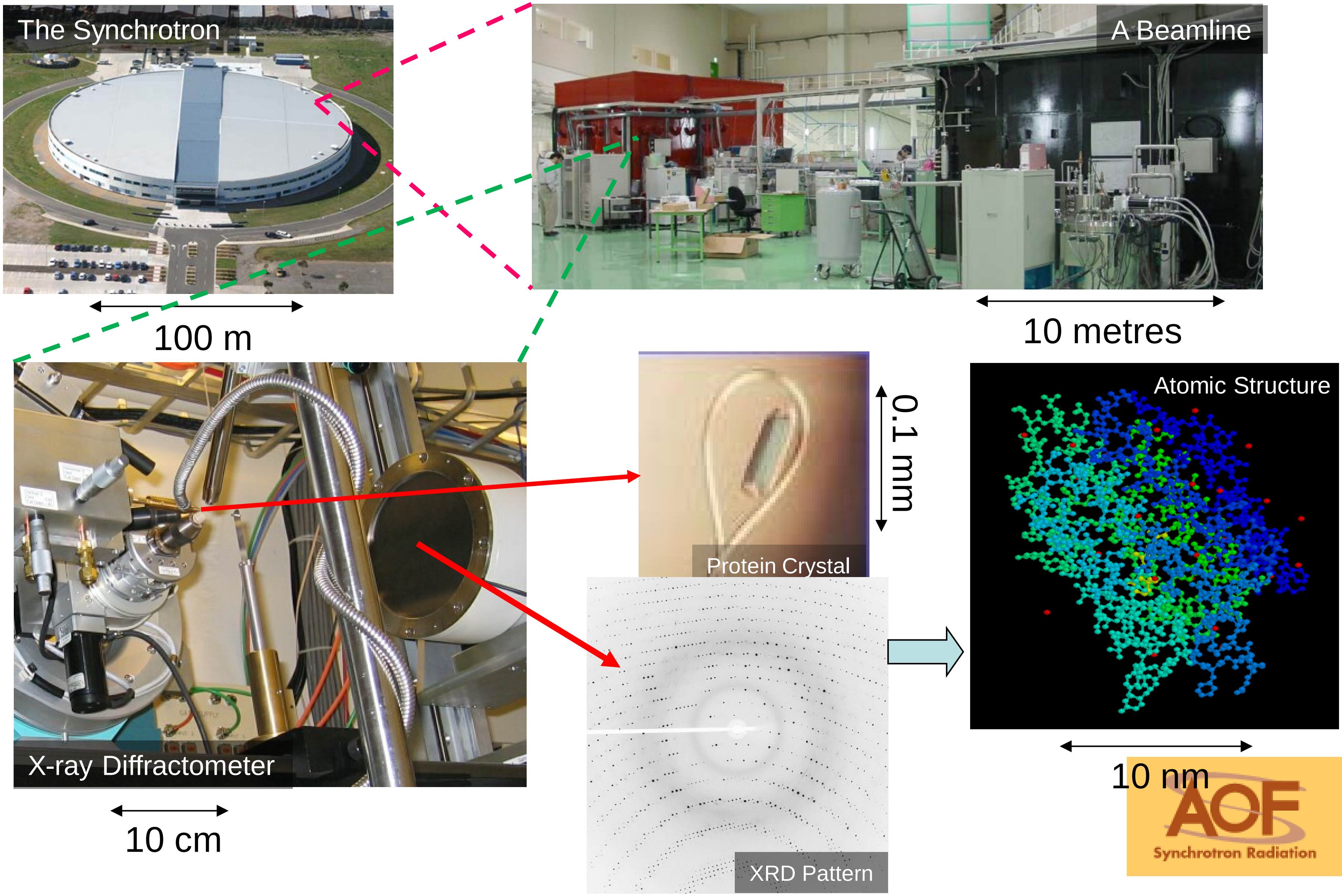


Multi-phase ceramic: α Al_2O_3, ZrO_2, MgO-Al_2O_3 (spinel).
Top synchrotron data; Bottom: lab data.

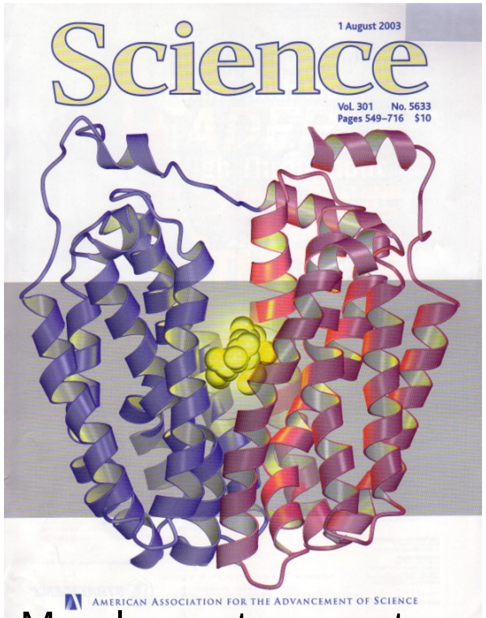
B. H. Oconnor, A. van Riessen, J. Carter, G. Burton, R. F. Garrett and D. J. Cookson,
J. American Chemical Soc. 80 (1997) 1373

AOF Synchrotron Radiation

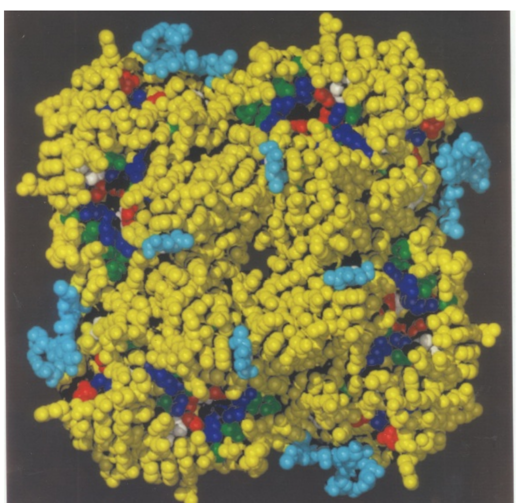
X-ray Diffraction at a Synchrotron



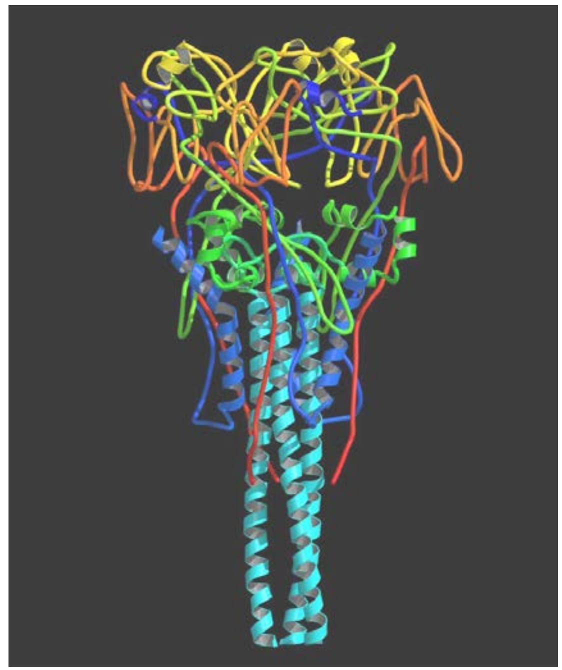
Most Significant Macromolecular Structures Solved using Synchrotron X-rays



Membrane transporter



Neuraminidase: Colman & Varghese, CSIRO

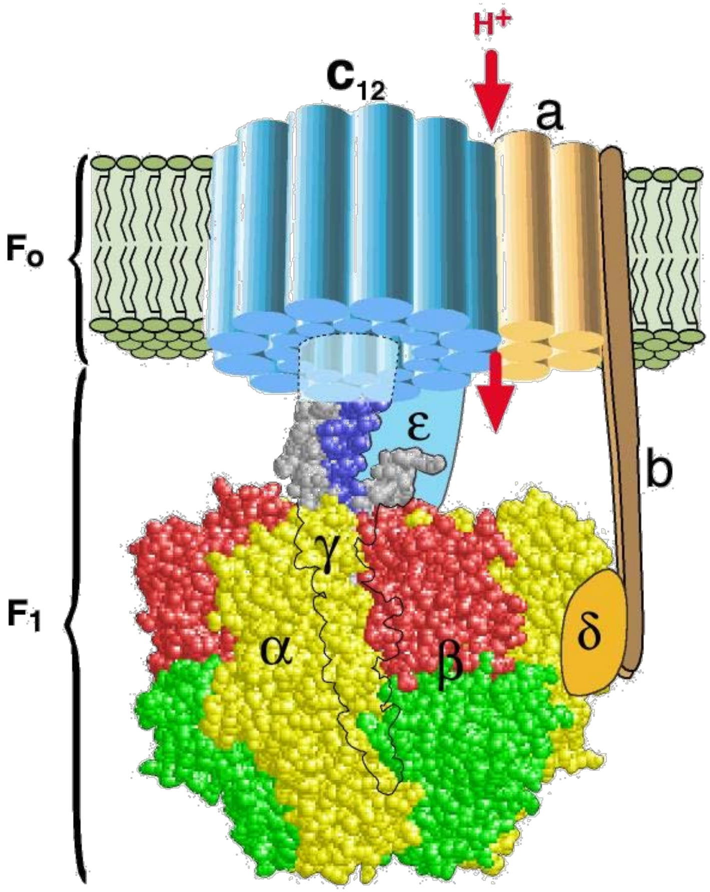


The fusion protein from Newcastle Disease Virus. ©Structure
M. Lawrence, CSIRO

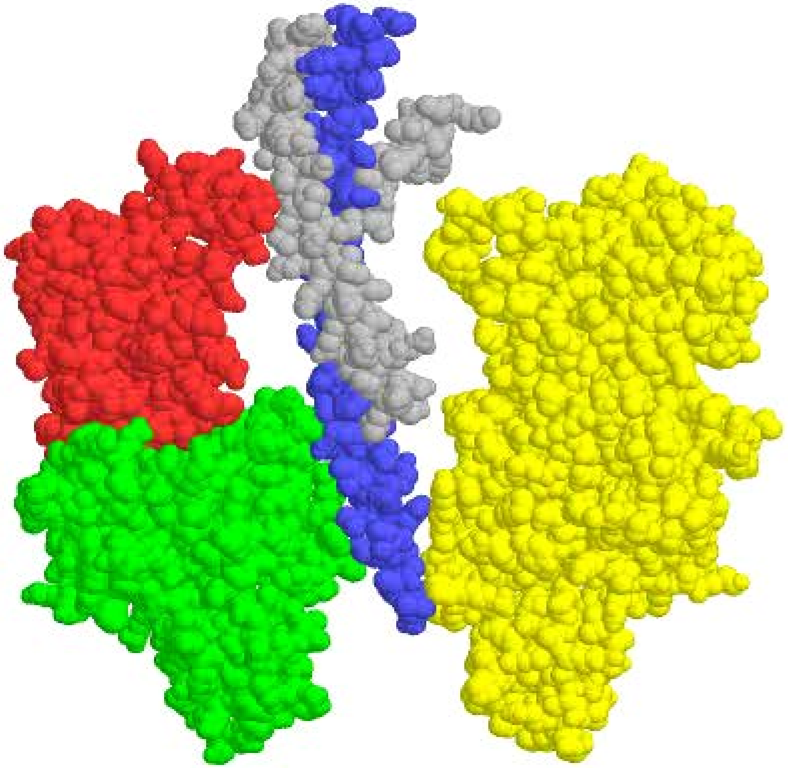
Virus

Ribosome

ATP Synthase: a Molecular Motor



H. Wang and G. Oster (1998). Nature 396:279-282.



John Walker won the 1997 Nobel Chemistry prize for solving the F1 catalytic domain using synchrotron radiation at Daresbury, UK.

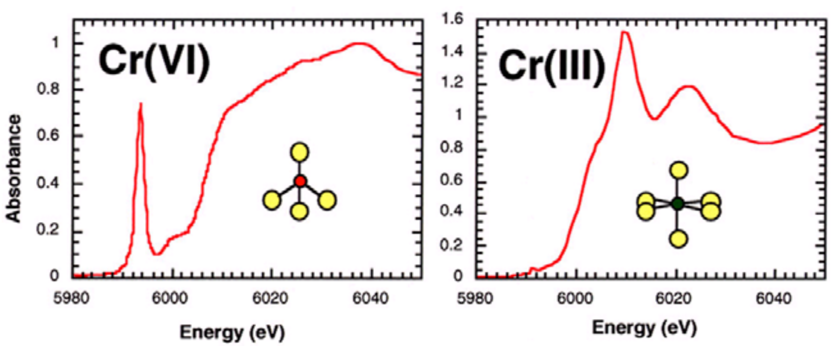
Atomic structure informs biological function

AOF Synchrotron Radiation

Broad Energy Spectrum: SR Only Spectroscopies eg Xray Absorption Spectroscopy

XANES: near edge structure

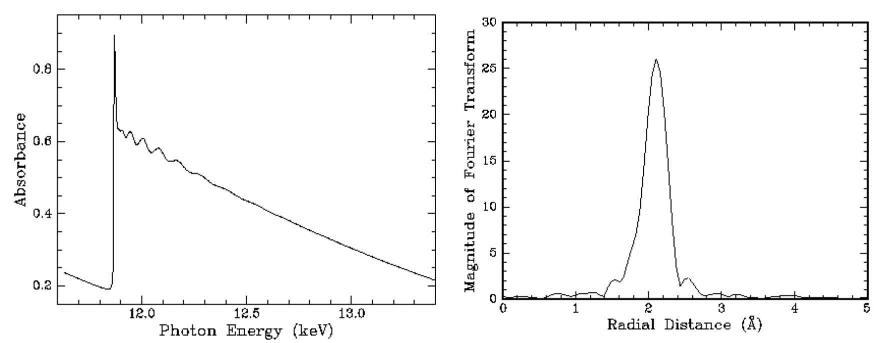
Sensitive to chemical environment of absorbing element.
Often different valence states have markedly different XANES spectra.



XANES spectra of Cr III (relatively benign) and Cr VI, a known carcinogen.

EXAFS: extended structure to ~1 keV above an absorption edge

Nearest neighbour atomic distances, coordination etc. Crystals not required: disordered systems like solution species can be measured.



Amorphous GaAs EXAFS and Fourier transform.

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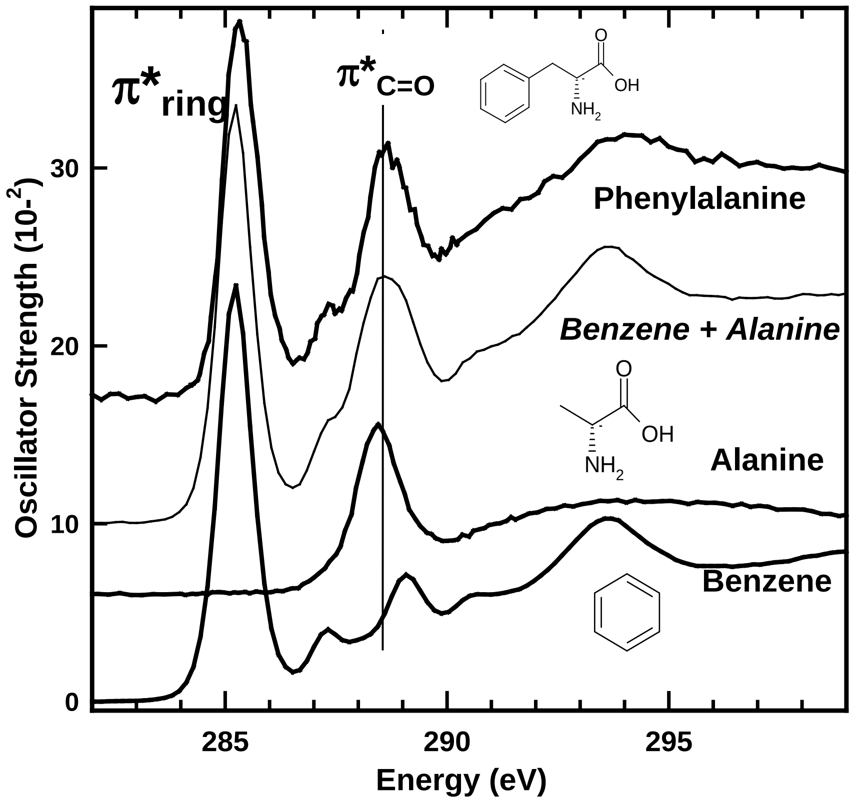
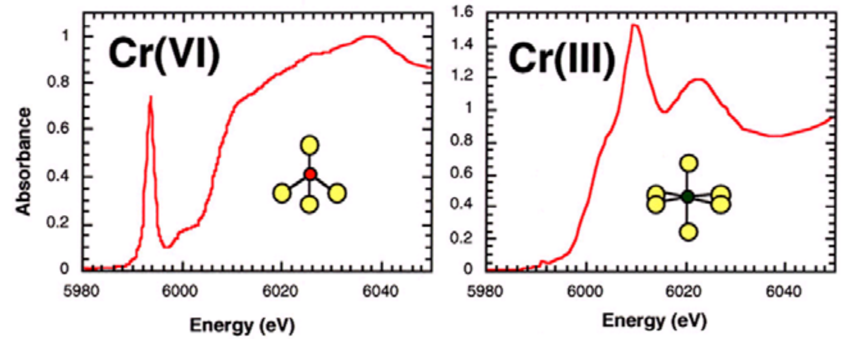
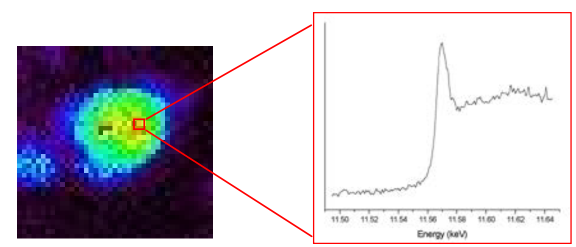
Near Edge Spectroscopy: Chemical Sensitivity

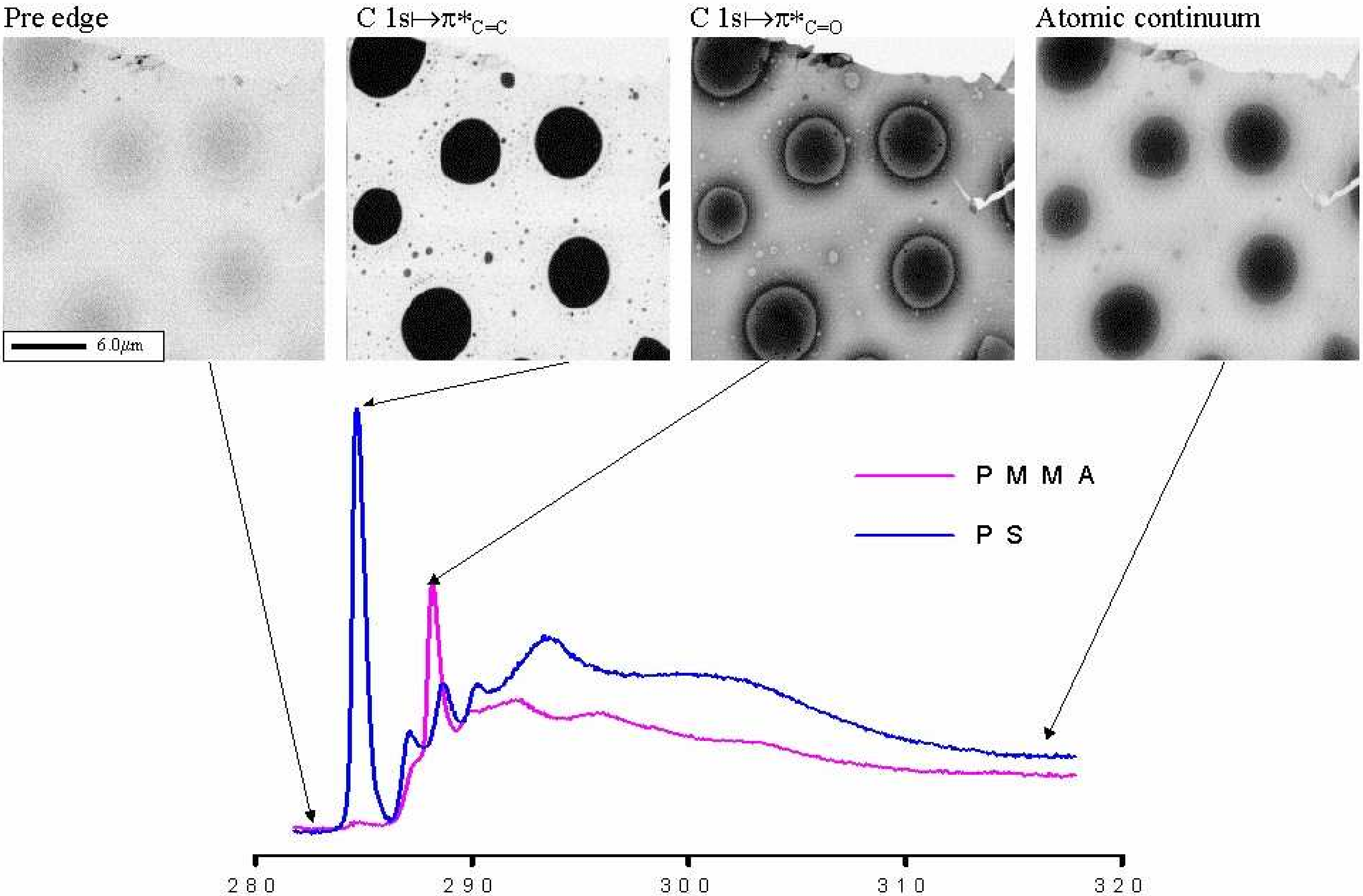


Carbon K-edge Spectra





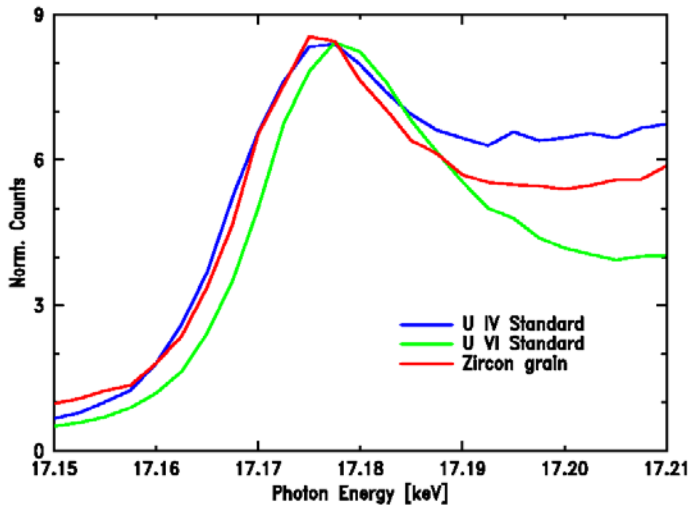
Pt spectrum located in a tumour cell Hambley, U Syd



Courtesy H Ade, NC State Univ.

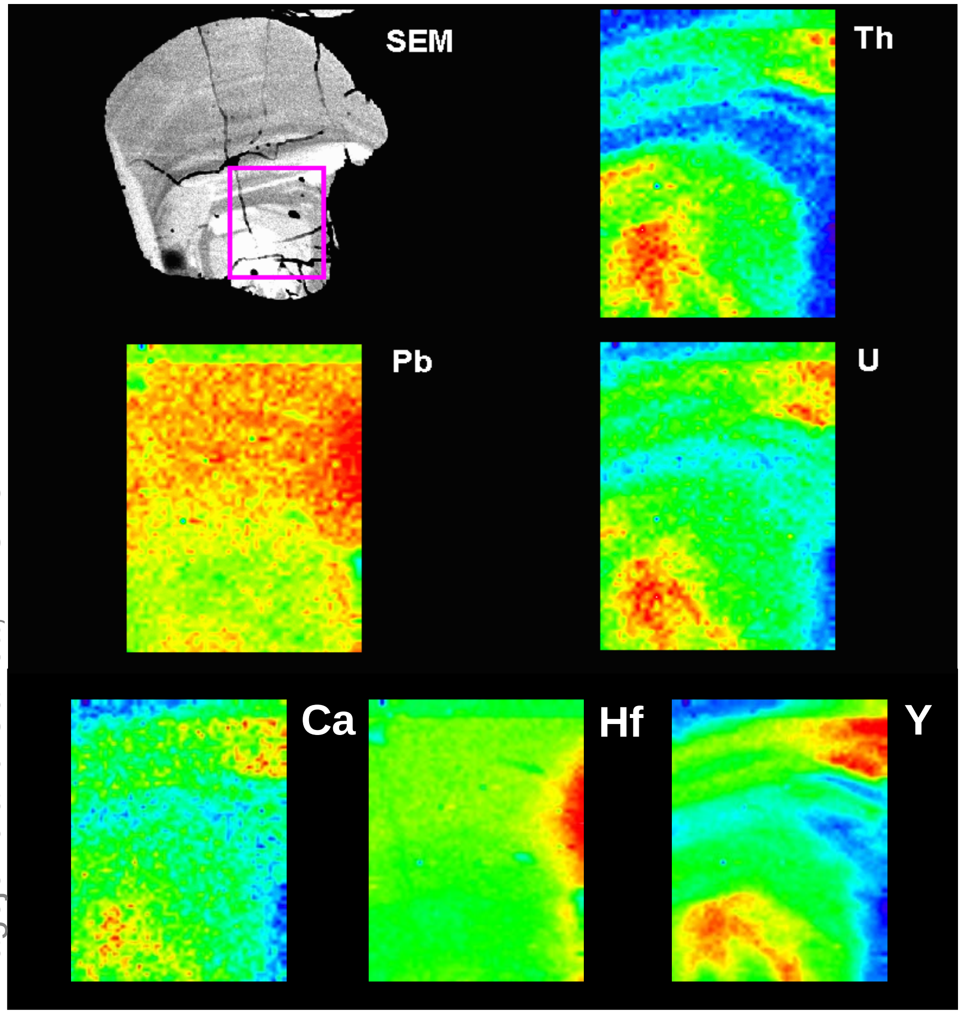
Micro-imaging and XANES from Mineral Sands

- Aim: to image and analyse chemical state of radioactive trace elements Zircon mineral grains
- X-ray Absorption Near Edge Spectroscopy (XANES) determined uranium is present as U_{IV}
- Chemical state is needed to design process to remove these elements



Zr K-edge 18.0 keV
U L3-edge 17.2 keV

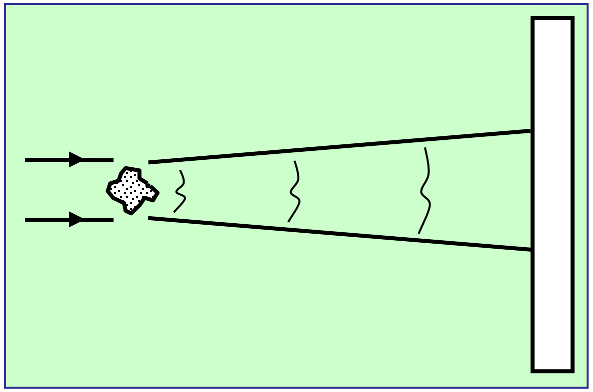
Blagojevic and Garrett, ANSTO



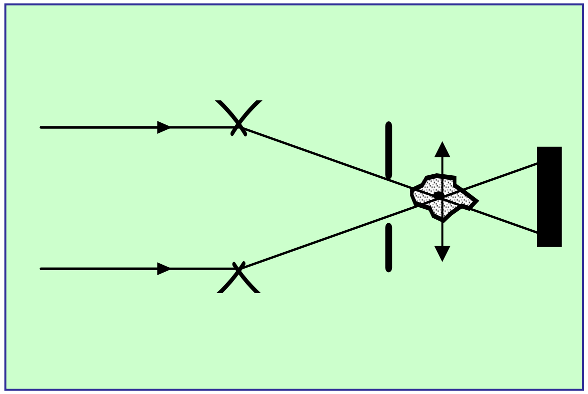
Concentration ranges: U 13 ppm to 33 ppm
Th 3 ppm to 11 ppm
Pb 3 to 4 ppm

Imaging

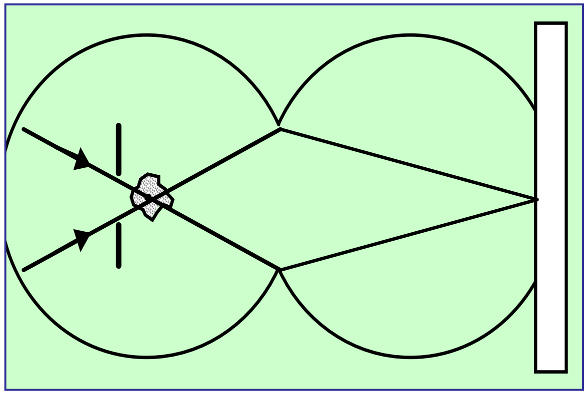
Mapping



Radiography



Scanning



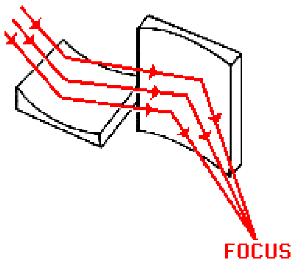
Imaging

Various Imaging Techniques have become more and more important in synchrotron research over the last 10 years

Some Imaging Needs Focusing optics

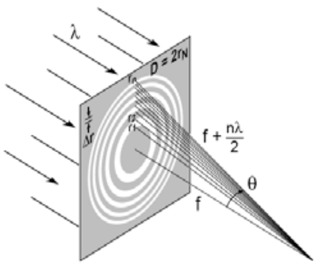
Reflective (Kirkpatrick-Baez mirrors) **typical ~1 µm**

High efficiency, achromatic, limited to ~10 nm



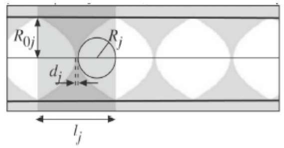
Diffractive (Fresnel zone plates) **typical ~ 100 nm**

Moderate efficiency, limited to ~10 nm



Refractive (compound refractive lenses) **10s µm - ~ 50 nm**

Low efficiency, highly chromatic, aberrations



AOF Synchrotron Radiation

Contrast mechanisms in x-ray imaging

➢ **Absorption**	measure electron density; can be element specific
➢ **Fluorescence**	measure elemental distribution
➢ **Spectroscopy**	extract chemical state, spin state
➢ **Diffraction**	reveal structure, strain, magnetism, charge…
➢ **Phase**	measure real part of refractive index

In general with X-rays:

- **Natural sample contrast is possible; staining not required**
- **Image structure of thick samples, sectioning not required**
- **More penetrating, less damage, less charging than with electrons**

AOF Synchrotron Radiation

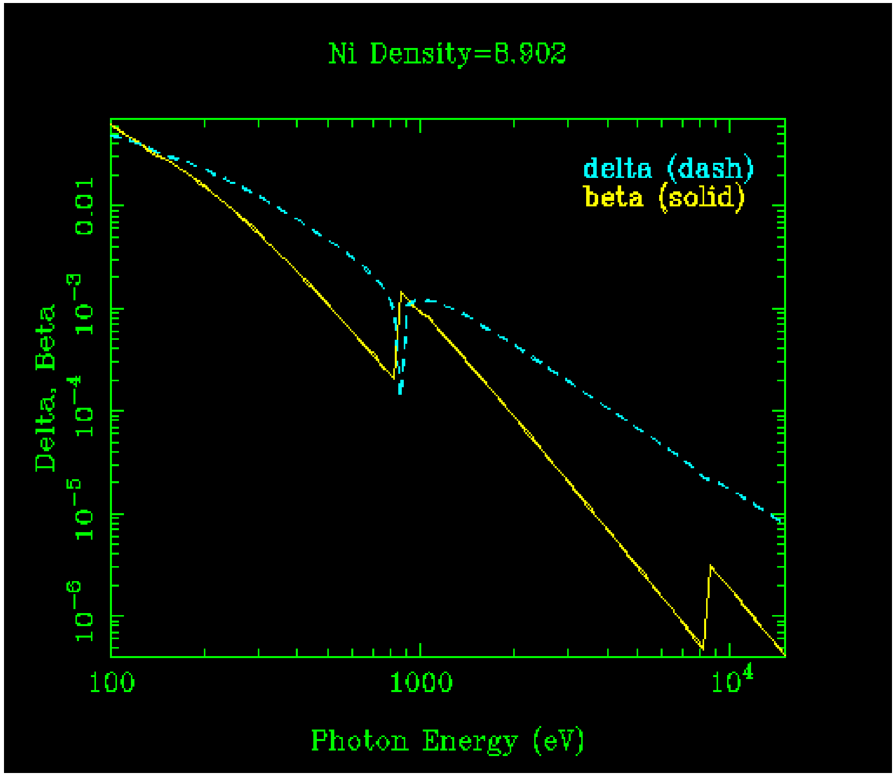
Phase Contrast

Refractive index:

for X-rays it is less than 1 by about 1 part in a million

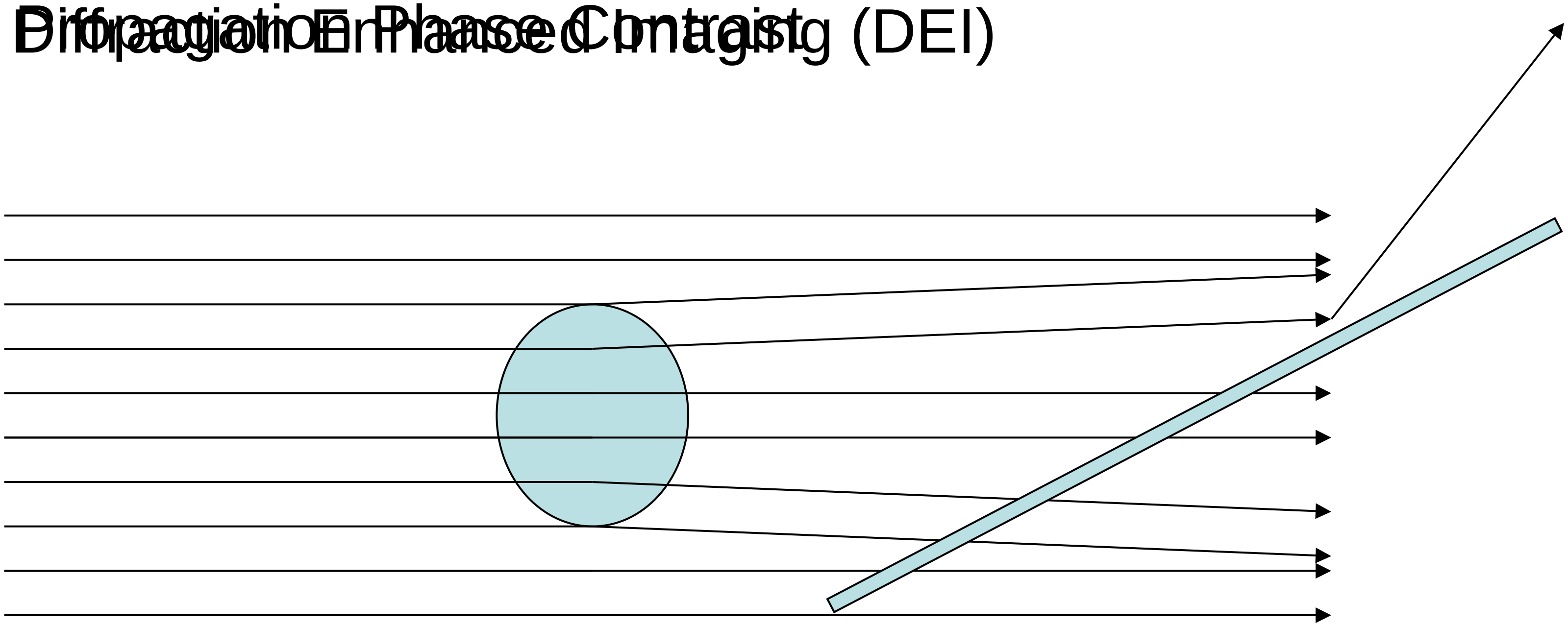
$$n = 1 - \delta - i\beta = 1 - \frac{r_e}{2\pi}\lambda^2 \sum_i n_i f_i(0)$$

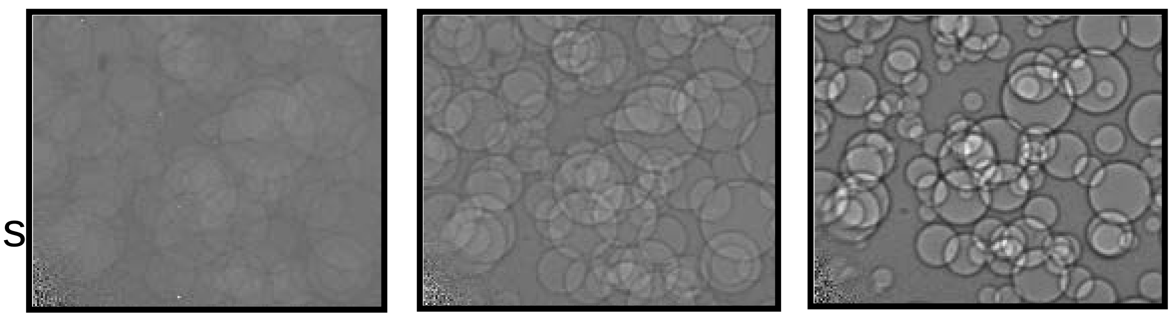
- Absorption contrast: sensitive to *Im(n)*
- Phase contrast: sensitive to *Re(n)*
- At high X-ray energies, phase contrast wins



Phase Contrast

1. Diffraction Enhanced Imaging (DEI)
2. Propagation Phase Contrast

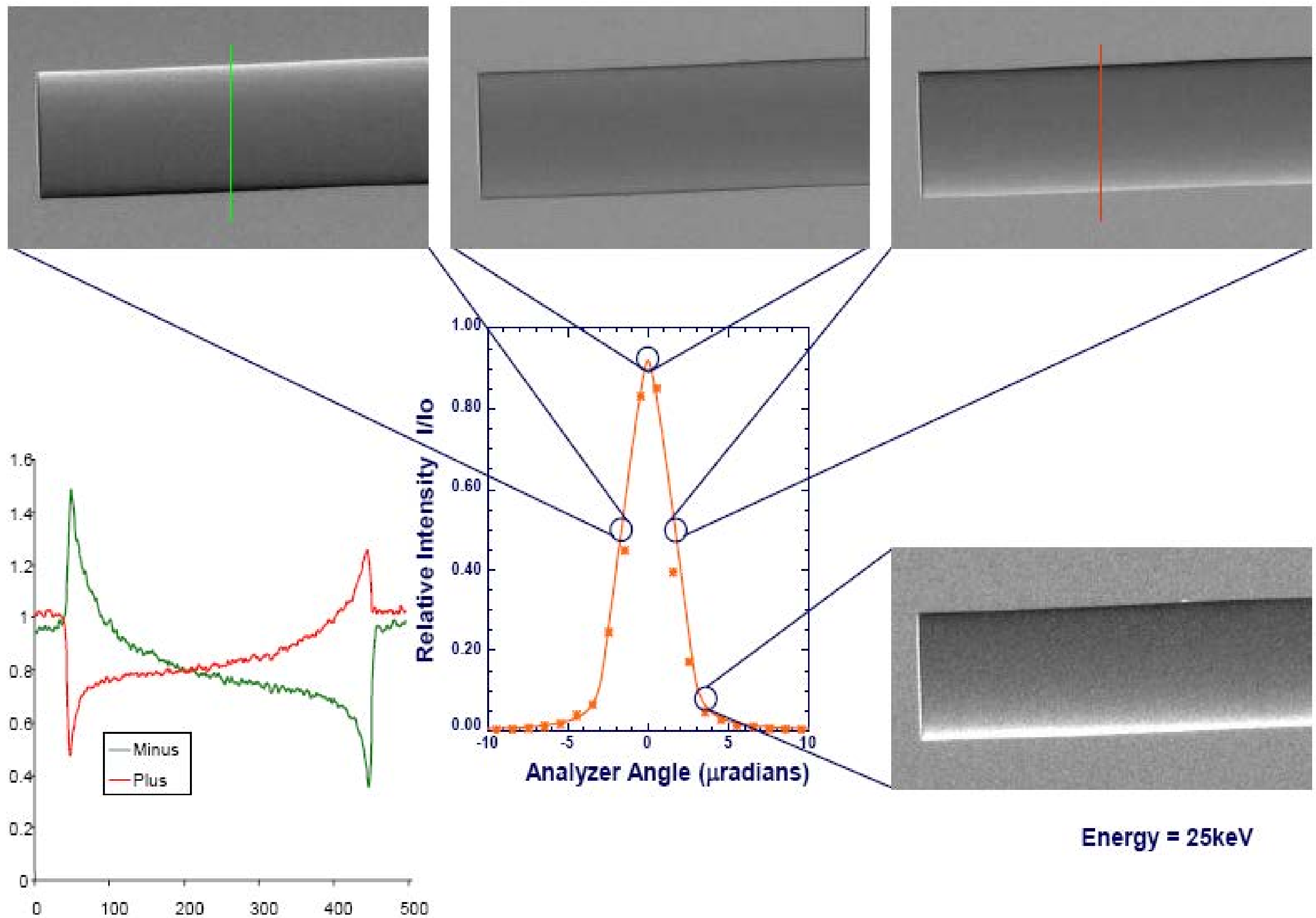




AS Medical Beamline
Wiggler Source
Phase contrast simulations
(Can recover phase shift)

Diffraction Enhanced Imaging

- Edge/density gradient sensitive
- Move on rocking curve to change contrast



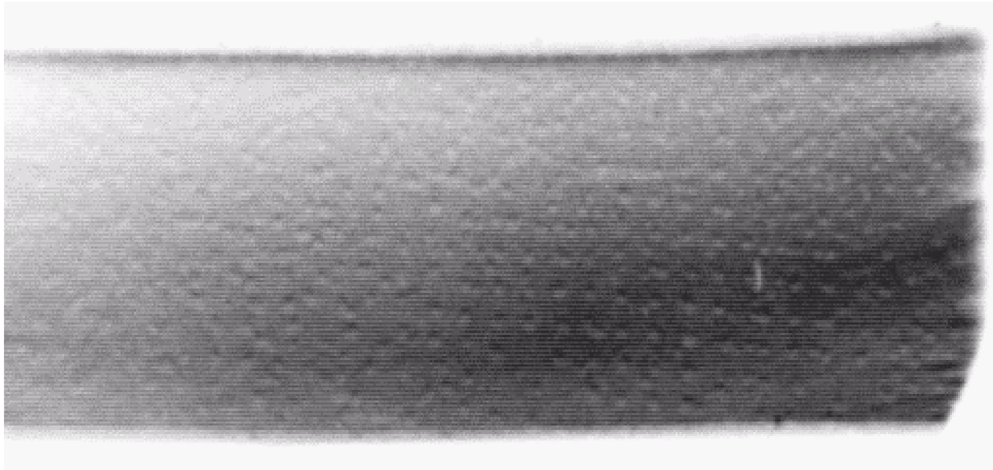
X-ray phase imaging: Biology and Materials

Conventional X-ray

Synchrotron

Synchrotron: propagation phase contrast

Rob Lewis, Monash University/
Energy = 20keV

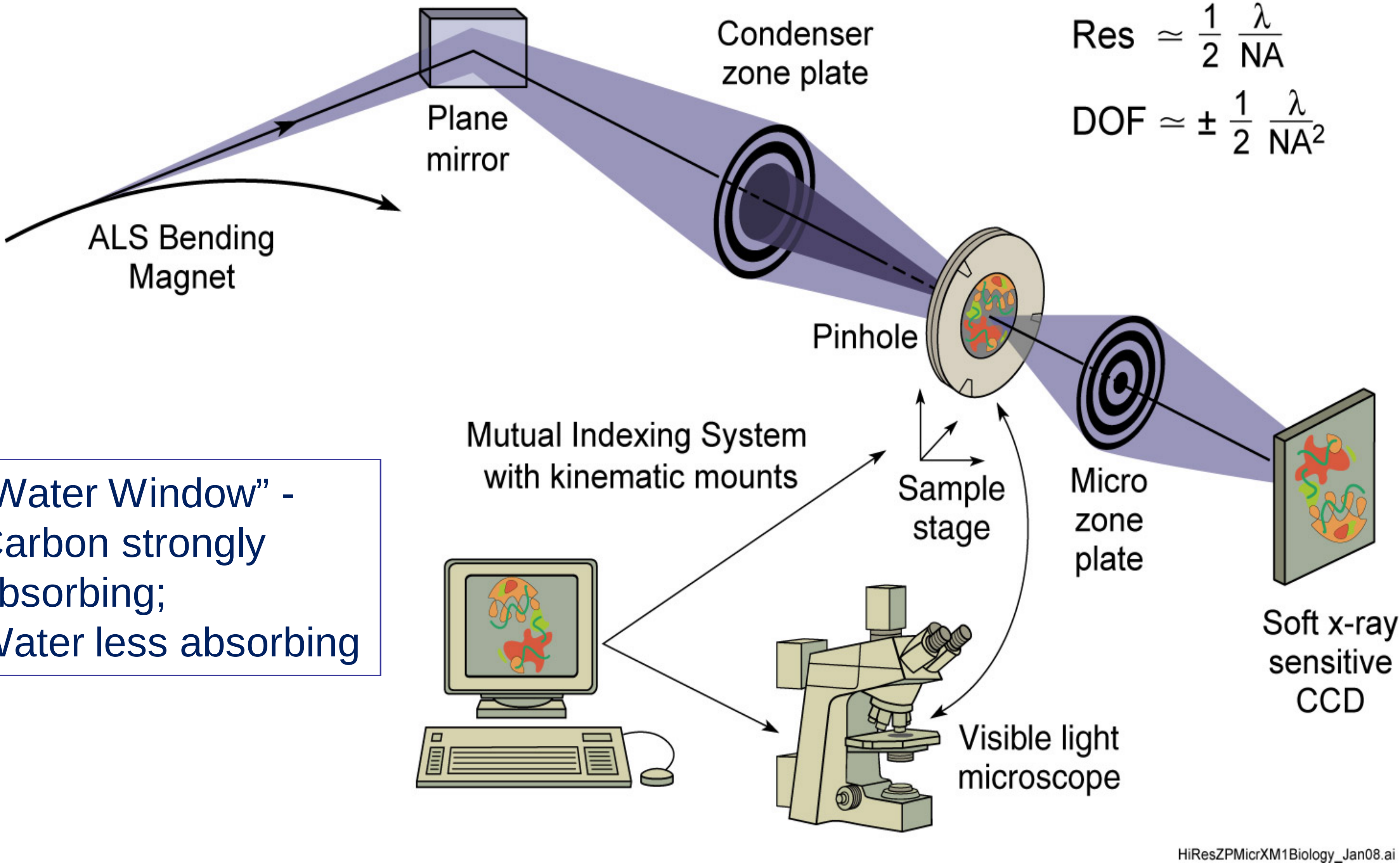


DEI “Dark field” phase image of bonded aluminium sheets @ 33 keV
Dots are bubbles in the epoxy bond.

Stevenson, Garrett, Hyodo et.al.

Two Famous Microscopes

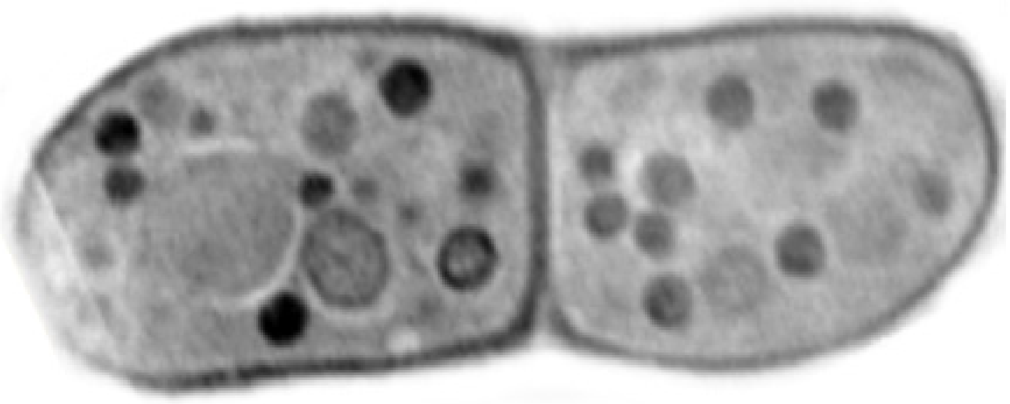
First: ALS XM-1 Microscope



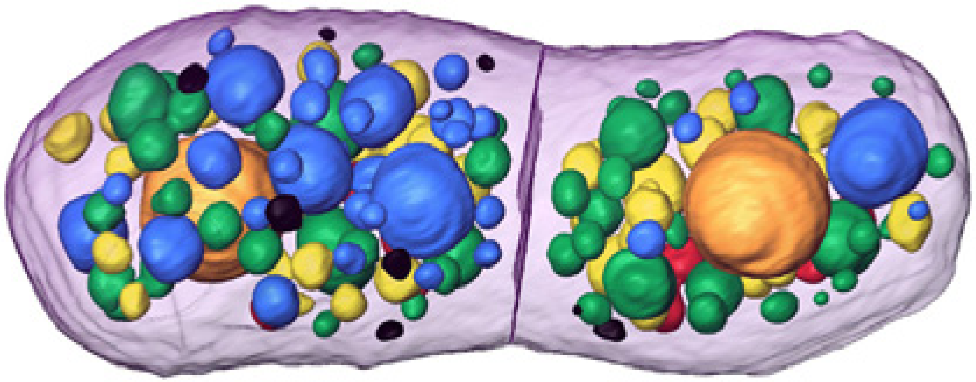
"Water Window" -
Carbon strongly absorbing;
Water less absorbing

Nanoscale 3-D biotomography

Mother daughter yeast cells just before separation



2-D slice from 3-D Tomogram. Images every 2°, 180° data set, several minutes. Δr = 45 nm

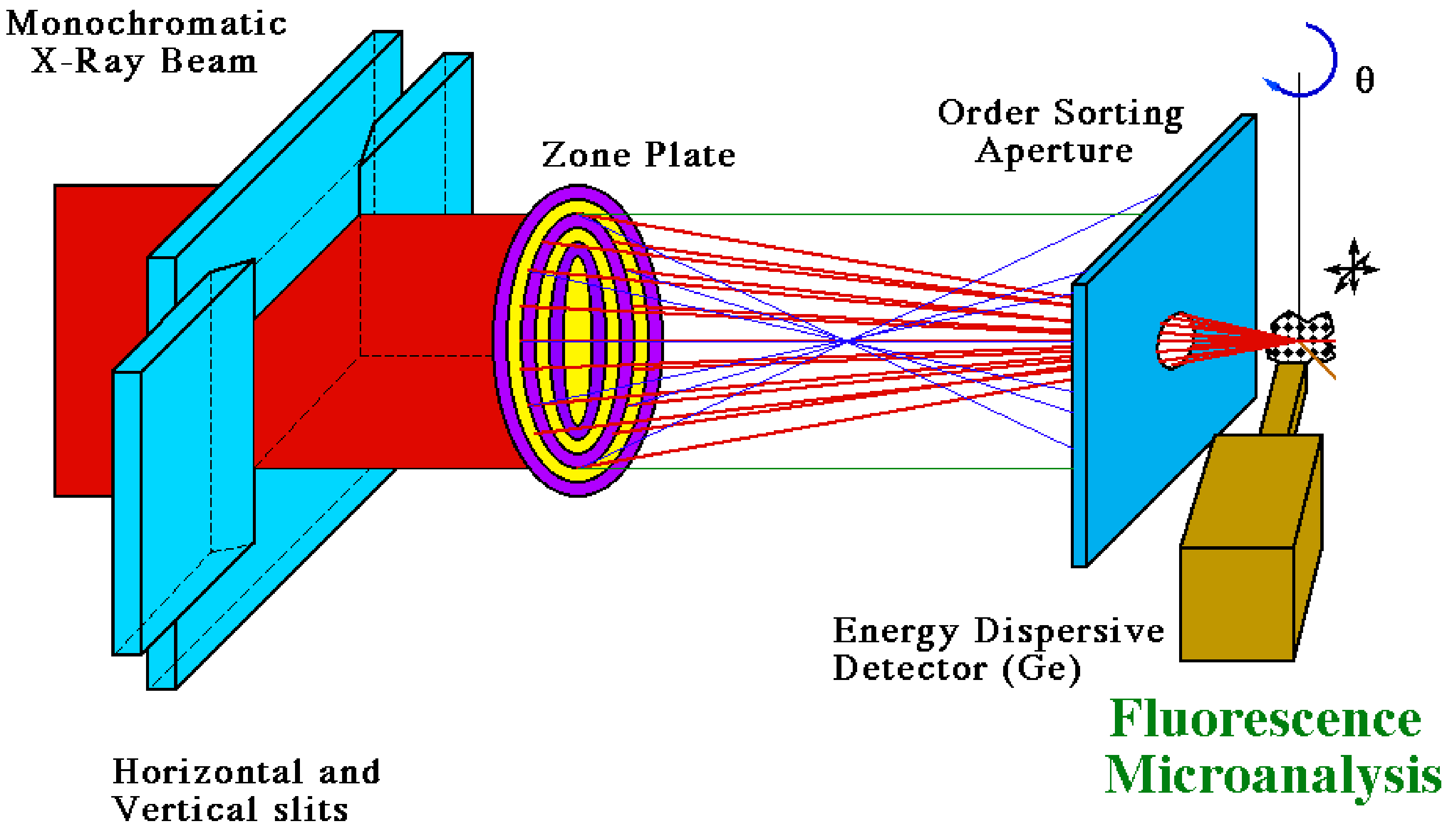


Color coding identifies subcellular components by their x-ray absorption coefficients

Courtesy of Carolyn Larabell, UCSF/LBNL

AOF Synchrotron Radiation

Second:
The X-ray Fluorescence Microscope Beamline at the AS



Conventional Fluorescence Microscope: APS 2ID-D

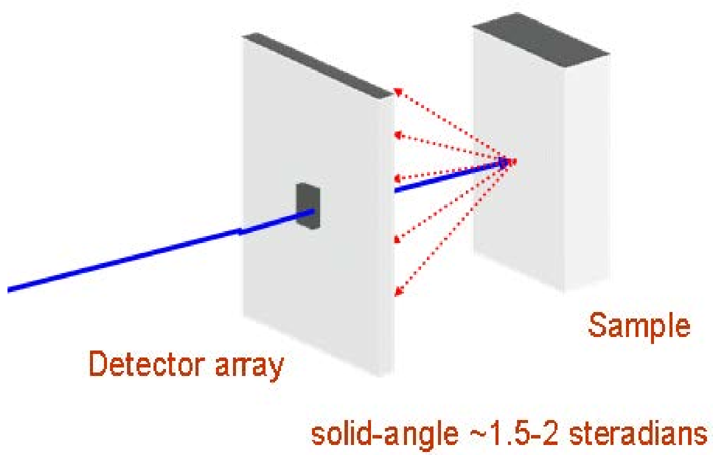
Advanced fluorescence detector at the AS

Annular geometry

•Maximises solid angle, sample @ 90˚

•384 Si pixel detector array (BNL, Siddons etal)

• No constraint on lateral sample size and scan range



+ Parallel data processing

• CSIRO: HYMOD2 pipelined, parallel processor (Ryan etal)

• Whole XRF spectrum acquired and analysed in real time

+ Fast Scanning Stage

•Data acquired "on the fly"

•milli-second dwell times

cf 1 second or greater normally

= New micro-XRF capability at the AS X-ray Fluorescence Microscope beamline

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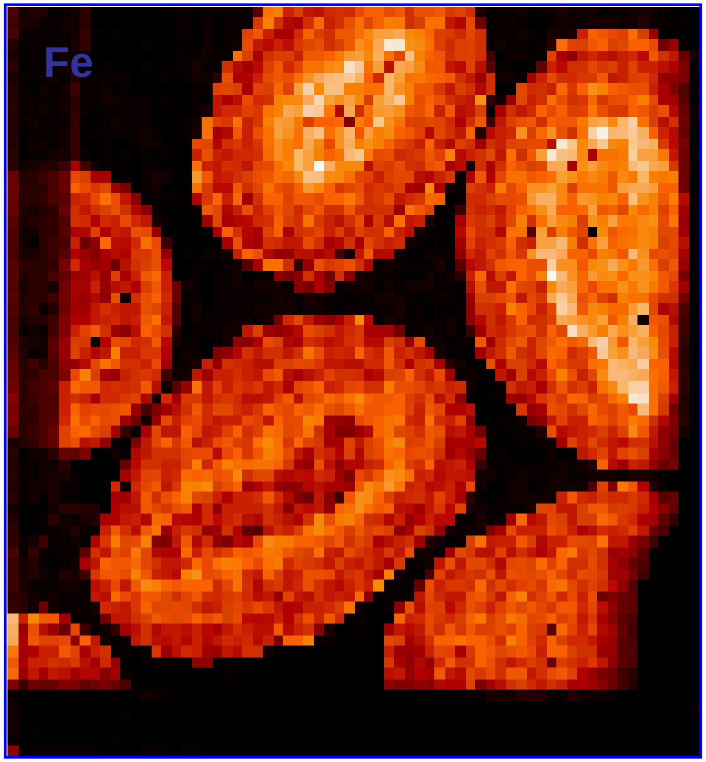
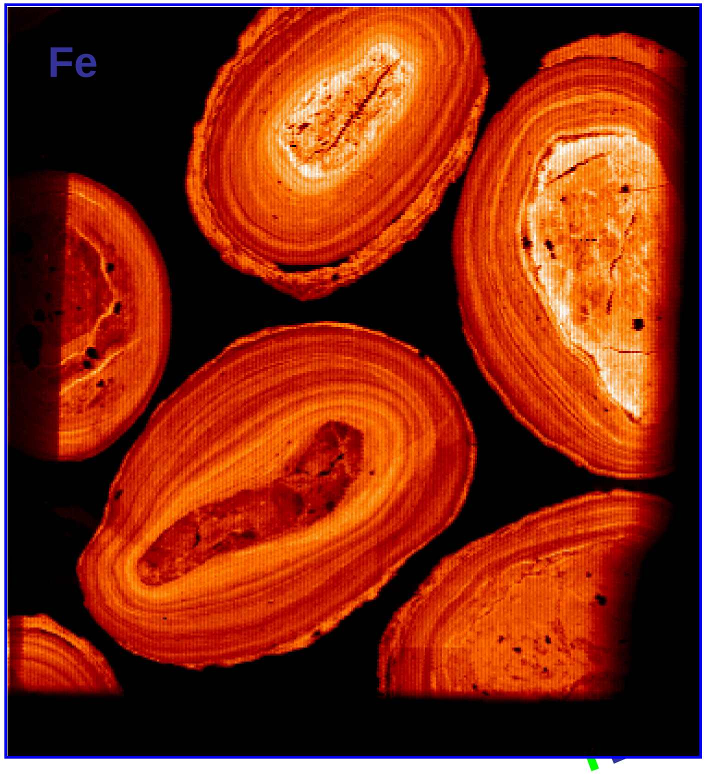
XFM image definition (number of pixels) limited by dwell time

Long dwell → Low Image Definition

- **~1 s / pixel** (for readout of 1-16 detector spectra)
- 1.3 hours → 67 x 67 pixels





Short dwell → Good image definition

- 32 ms / pixel
- 1.3 hours → 375 x 375 pixels (30 fold increase)
- New Maia-32 prototype detector, NSLS X27A

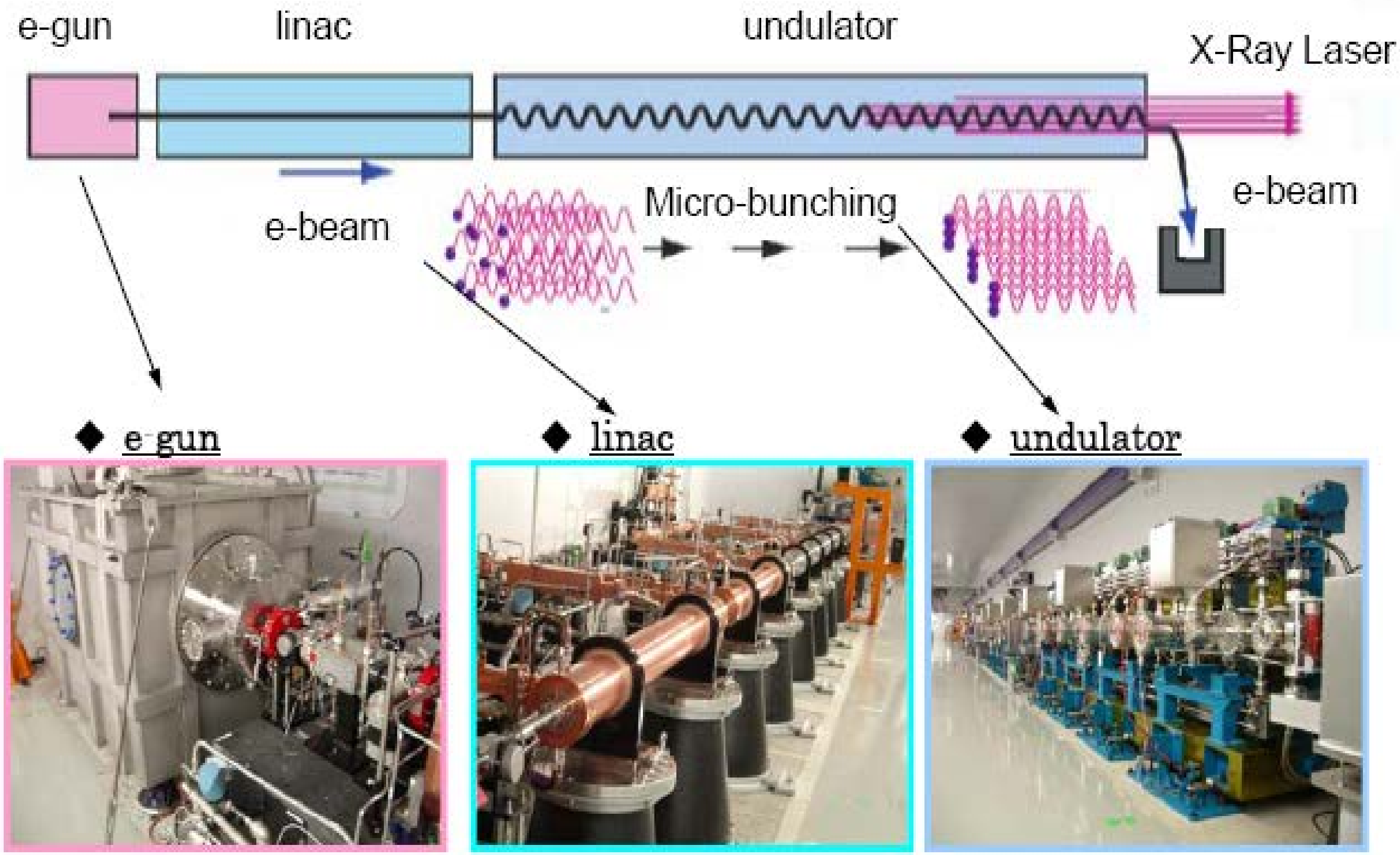
Courtesy C. Ryan, CSIRO

Synchrotron Radiation

New Sources:

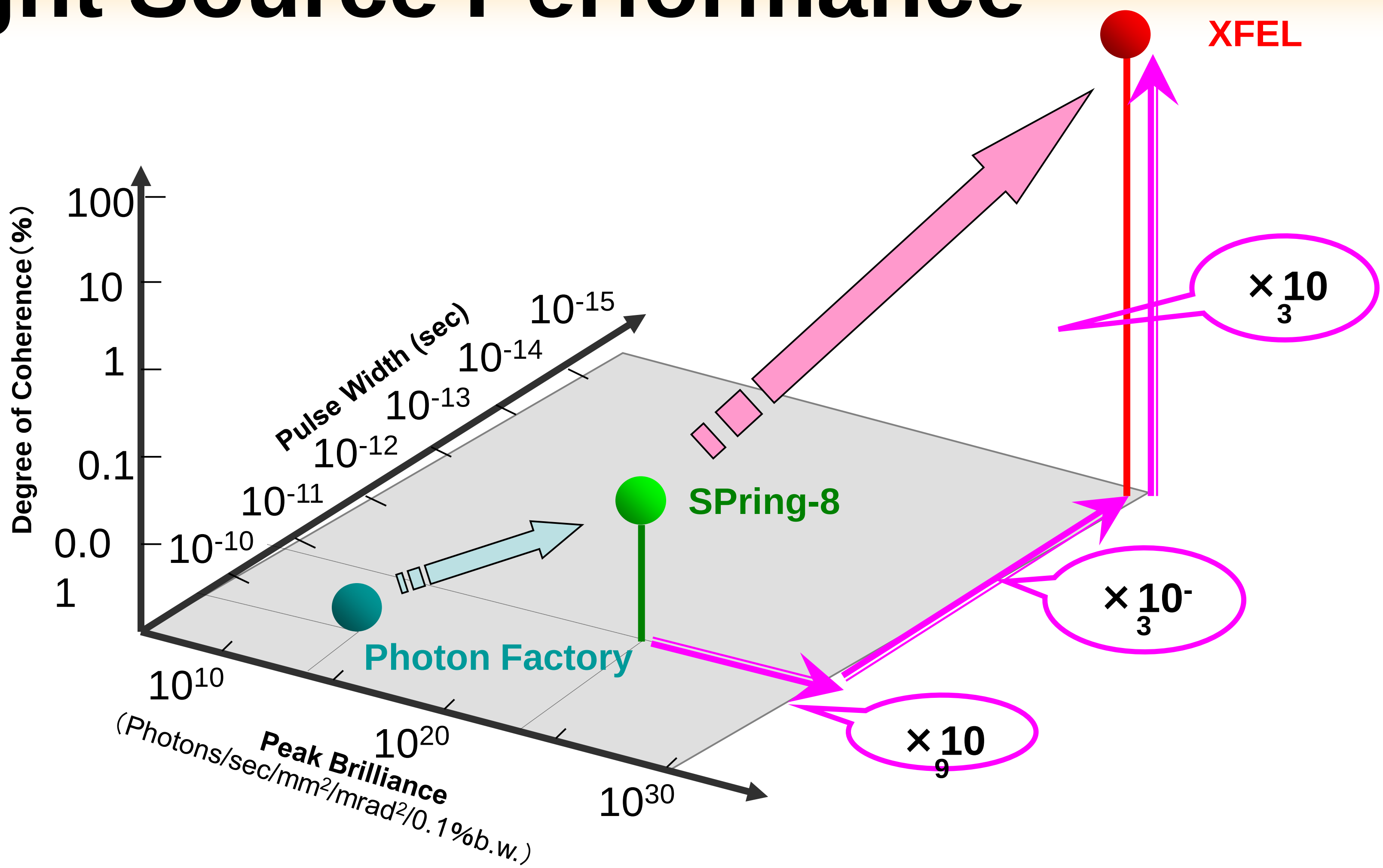
XFELs

Linac-Based Free Electron Laser
Self-Amplified Spontaneous Emission (SASE)



T. Ishikawa, RIKEN SPring-8 Center

Light Source Performance



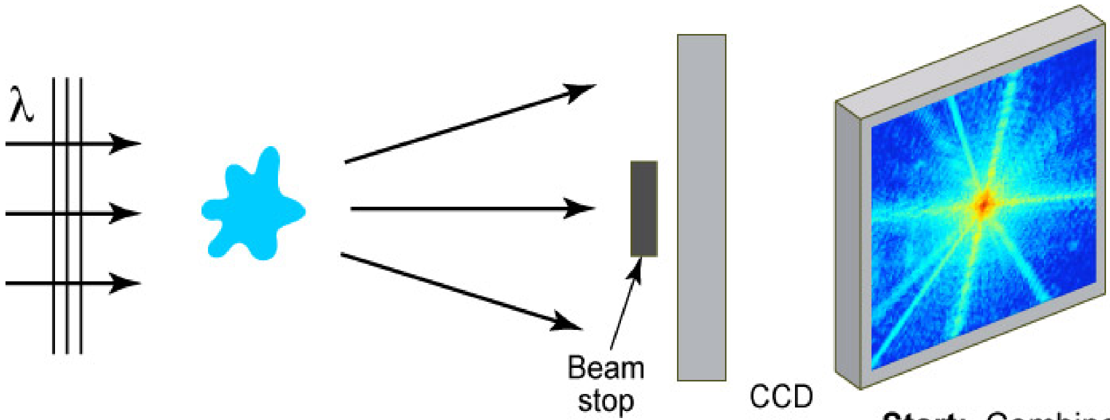
<u>Remarkable Features of XFEL producing λ<0.1 nm X-Rays</u>

◎ <u>High Peak Brilliance</u>
◎ <u>Narrow Pulse Width</u>
◎ <u>High Degree of Coherence</u>

RIKEN

SACLA 1st beamline: 90m Undulator

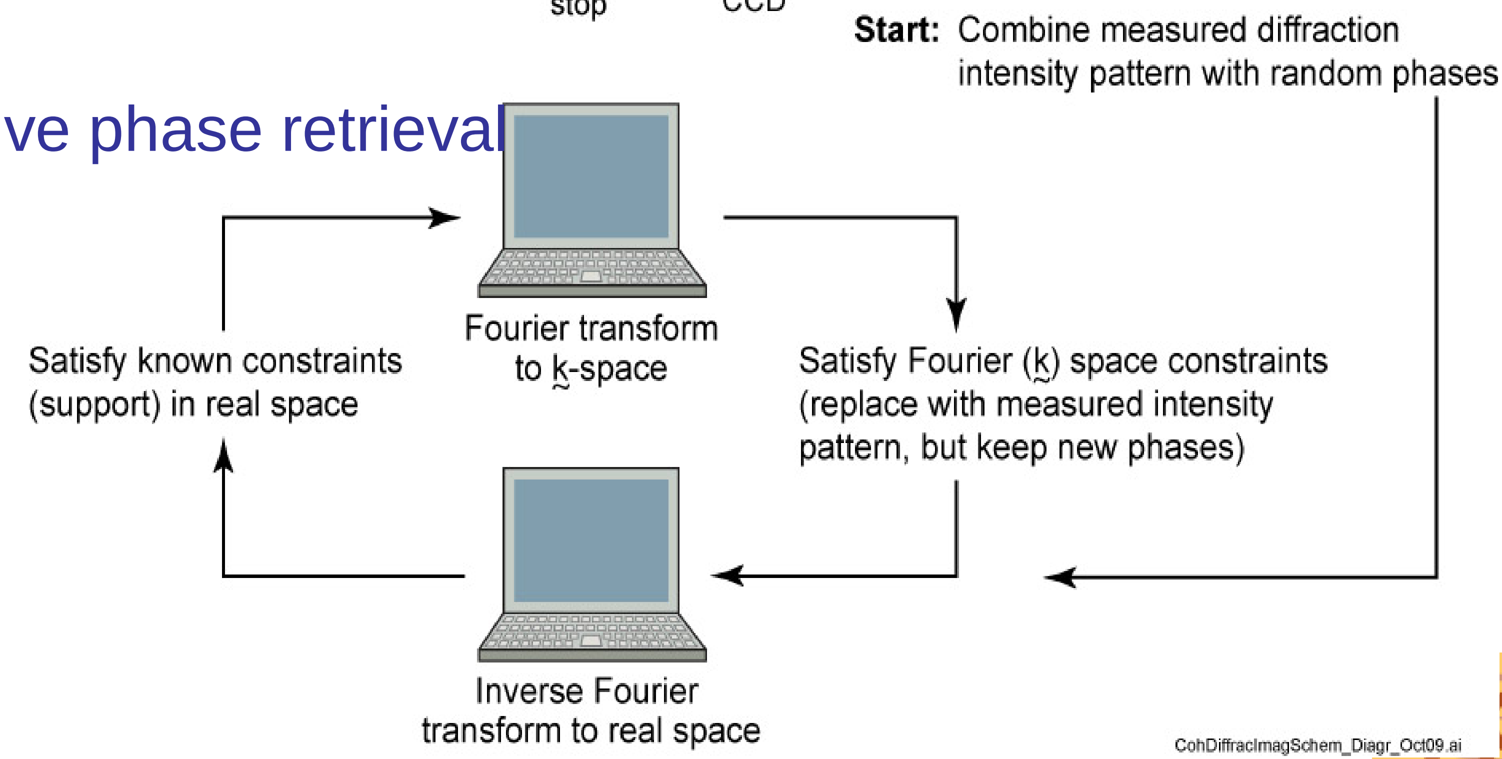
Coherent Diffractive Imaging: no lens, no crystal



Resolution = k λ / NA

Currently to ~20nm

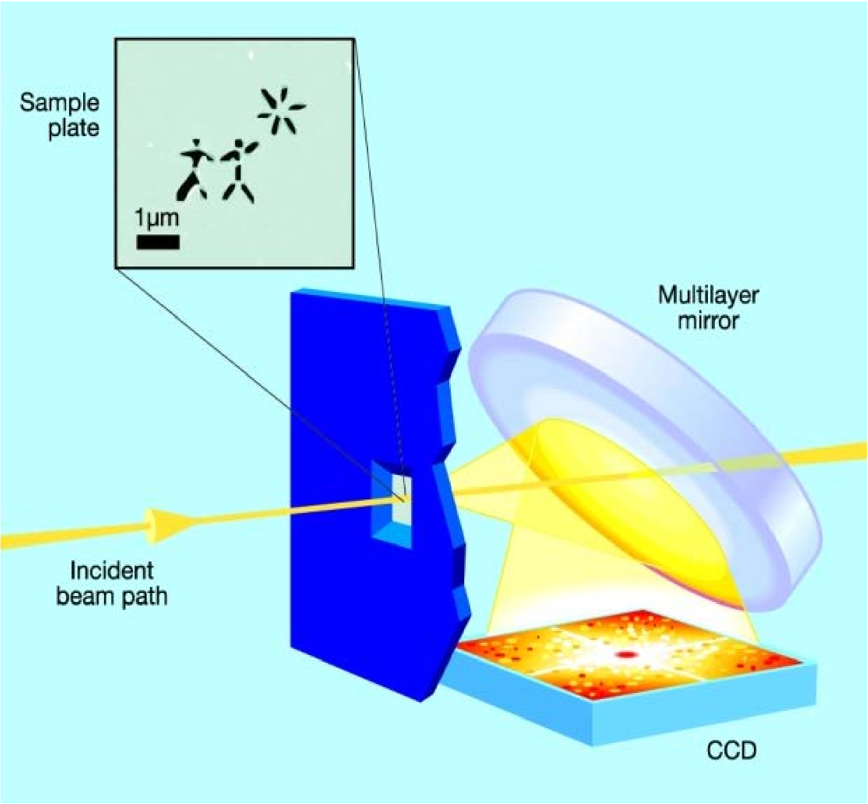
Iterative phase retrieval

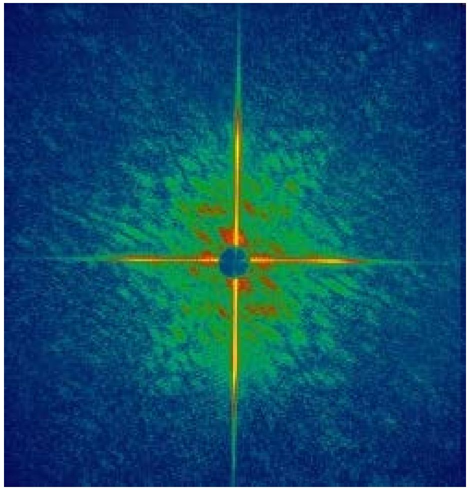


R. Gerchberg and W. Saxton, *Optik* 35, 237 (1972); J.R. Fienup, *Appl. Opt.* 21, 2758 (1982)

Synchrotron Radiation

Single Shot Imaging at the FLASH Soft X-ray FEL



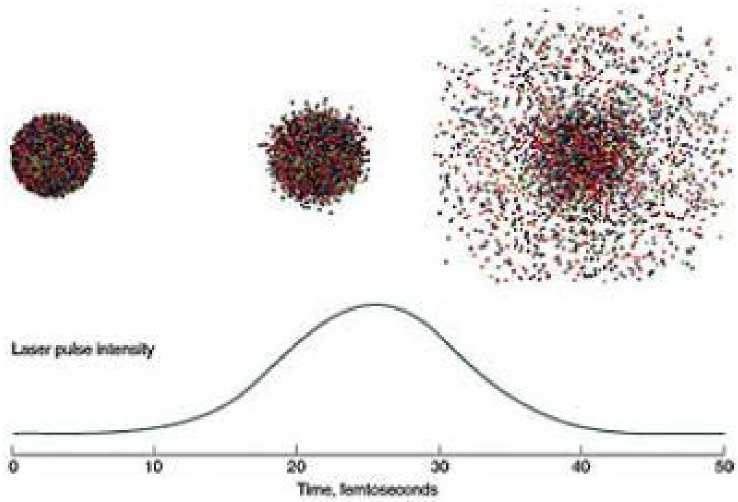


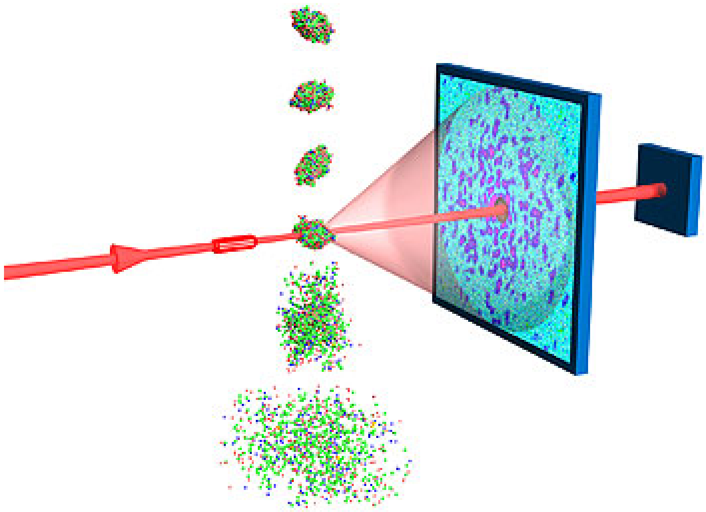
A coherent diffraction pattern of the object recorded from a single 25-femtosecond FEL pulse.

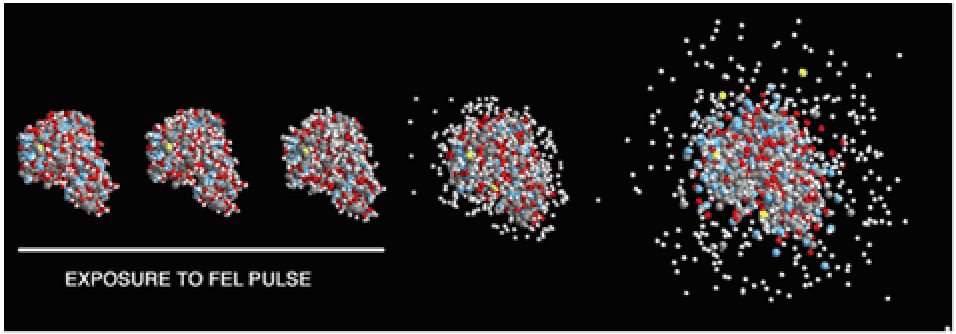
Reconstructed image: no signs of damage caused by the pulse.

H. Chapman et al., *Nature Physics* 2, 839 (2006)

XFEL Holy Grail?: Single Molecule Imaging



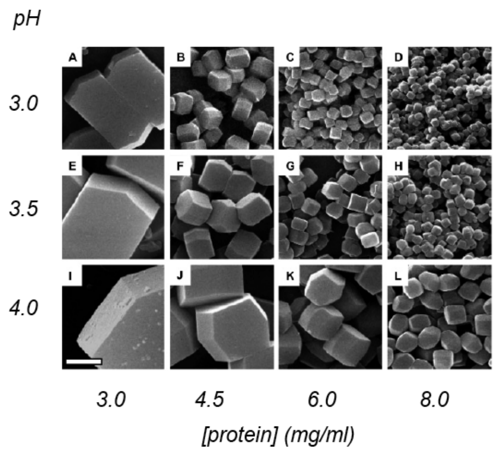


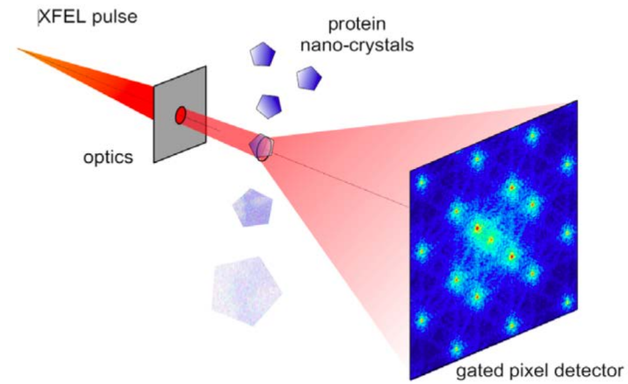


Neutze etal, Nature 406, (2000) 752-757

Nano Crystallography
- seems most promising so far

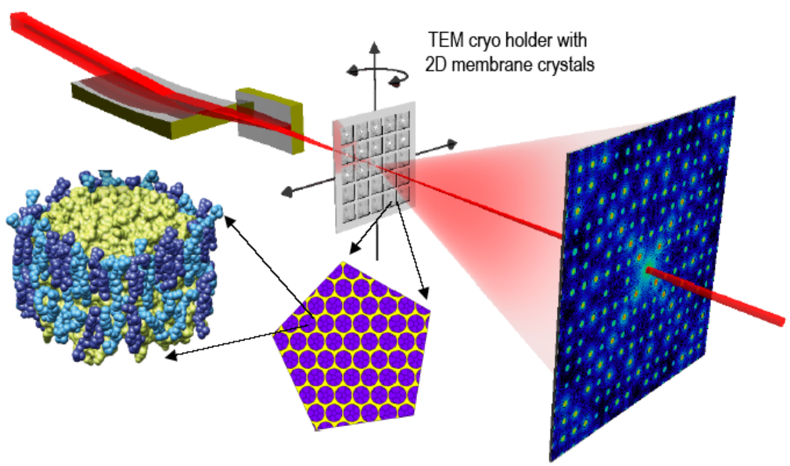
3d protein
nano-crystals

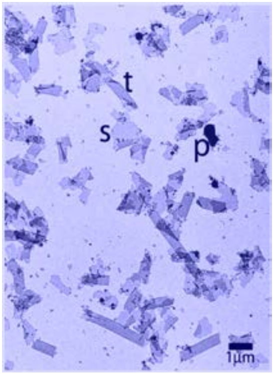




avoid damage
⇒ pulse < 20
fs

2D membrane
protein crystals





R. Abela, PSI

Two Cool Examples to Finish

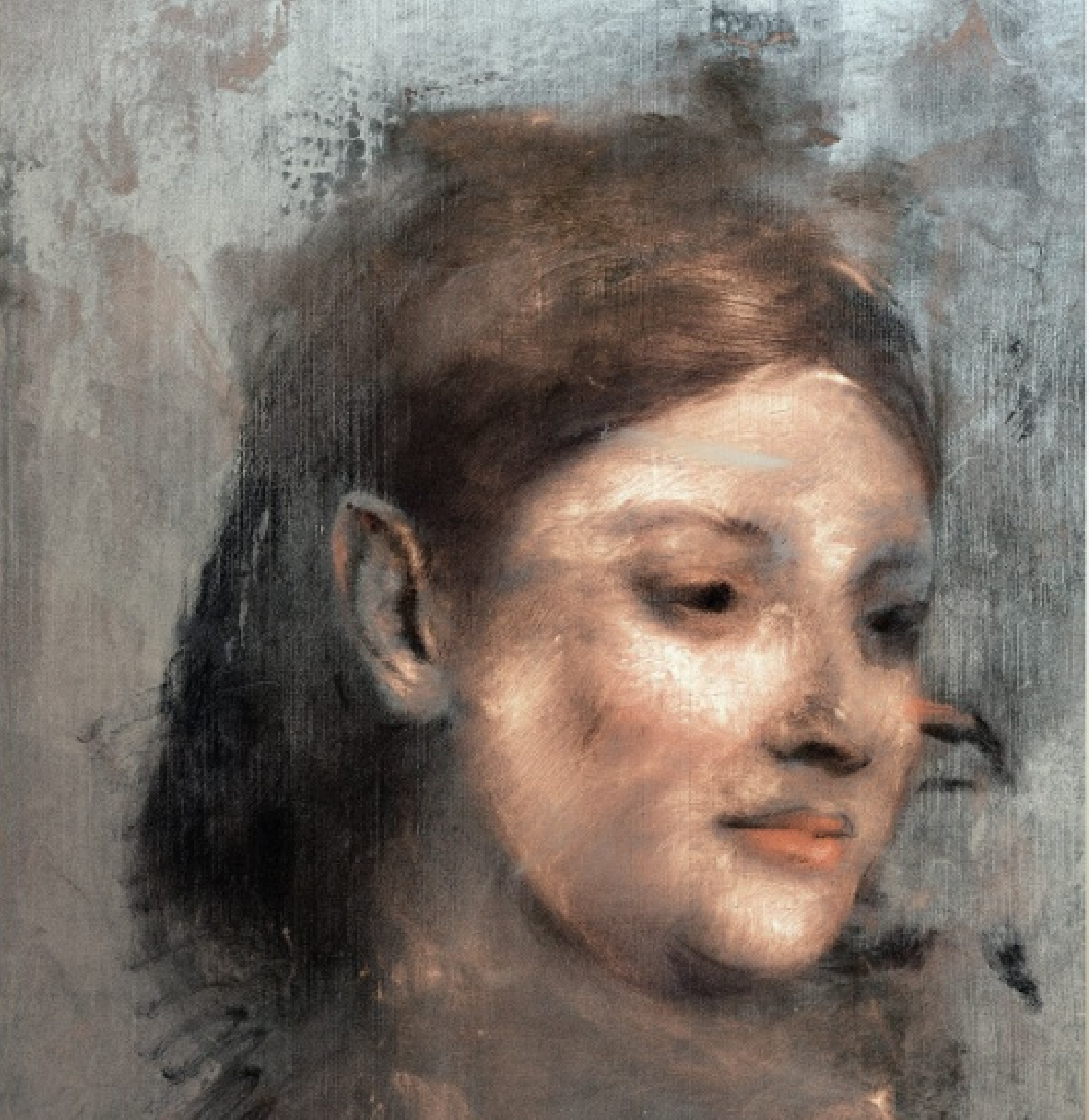
Exploring Cultural Heritage

Portrait of a Woman
By
Edgar Degas
1876-1880

Courtesy David Thurrowgood (National Gallery of Victoria)

AOF Synchrotron Radiation

Exploring Our Cultural Heritage



3.7 ms per 60 × 60 μm2
pixel

32 megapixel dataset

AOF Synchrotron Radiation

Phase Contrast CT: Fossils in Amber

Courtesy P Tafforeau, ESRF