Synchrotron Light Generation, Manipulation and Applications

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Lead Physicist for Infrared Beamlines

National Synchrotron Light Source II

Outline: Producing Synchrotron Radiation (Light)

- Basics of Electromagnetic Radiation:
  - Accelerating charge (electrons)
  - Special Relativity – why it's important for producing X-rays
- How an Electron Synchrotron Works: achromatic "lattices", focusing and RF
- Magnetic Devices for Generating Synchrotron Light:

  Transverse (centripetal) acceleration in a magnetic field
  - Bending Magnets *See https://journals.iucr.org/s/issues/2018/04/00/yn5030/yn5030.pdf*
  - Insertion Devices (wigglers and undulators)

Outline: Applications of Synchrotron Light

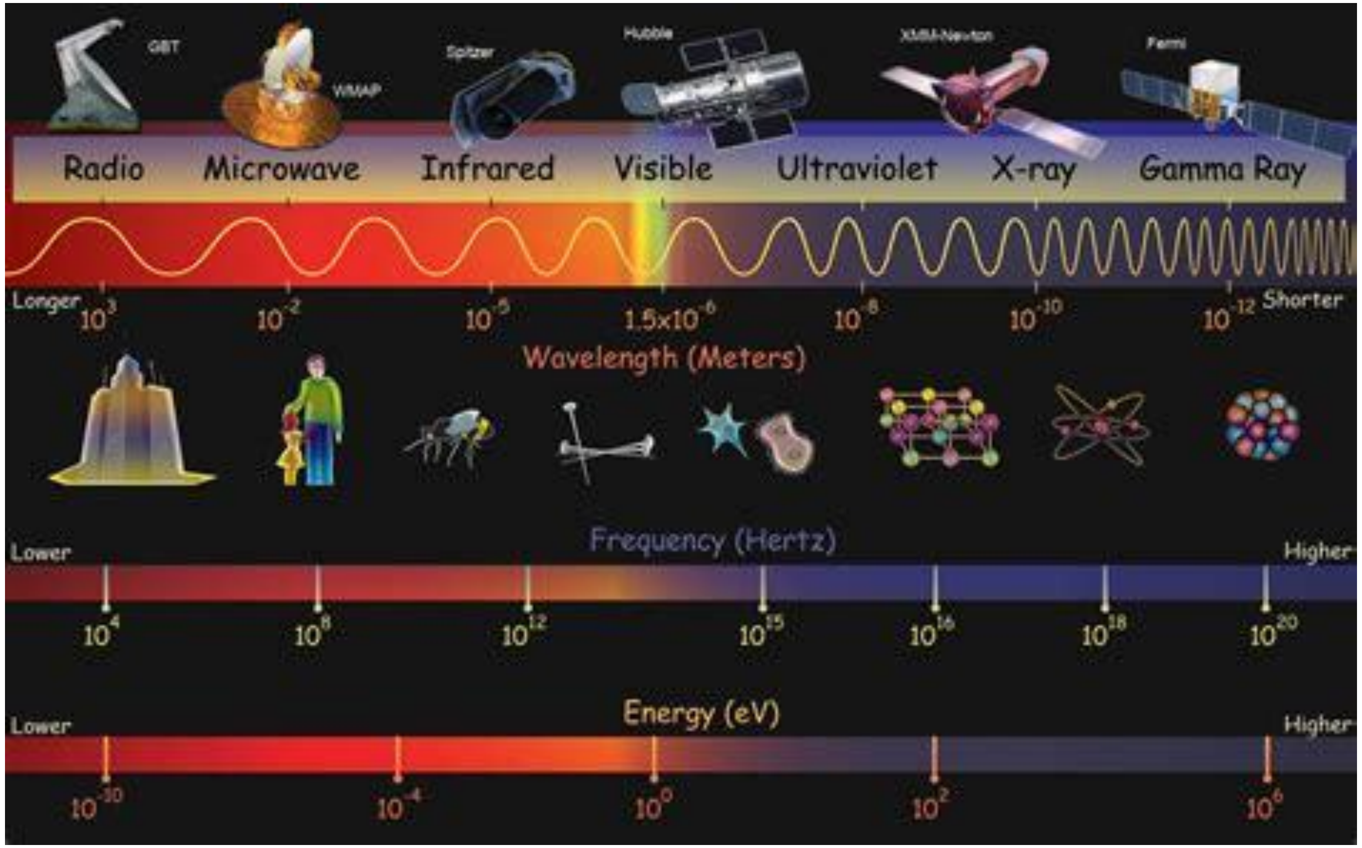
- Diffraction / Crystallography: “Hard” X-rays for crystal structure
  - Diffraction from Crystals and Periodic Structures
    - Powders (small crystals)
    - Single Crystals
    - Proteins
- Scattering:
  - Resonance, Inelastic (soft x-rays)
  - Small angle
- Spectroscopies
  - X-ray Absorption Spectroscopy (XAS) - excitations from electronic “core” levels: medium energies (soft & tender). Sense elemental content and local environment (EXAFS, XANES)
  - X-ray and UV Photoelectron Spectroscopy (XPS, UPS, ARPES): Absorbed x-ray ejects electron.

Our “Favorite” Unit for Energy: The electron Volt (eV)

- Energy an electron gains when crossing a 1V potential => 1.6×10^{-19} J/eV
  - Visible light photons span 1.7 (red) to 3 (violet) eV.
  - UV from 4 eV to ~100 eV
  - X-rays from a few hundred eV to ~100 keV
  - Infrared from ~1 meV to ~1 eV

  - Rest mass of an electron: 511 keV (0.511 MeV)
  - “ “ “ “ proton: 938 MeV
    (proton at rest is about 2000x more massive than electron at rest).

- Synchrotron light sources can produce photons with energies from ~ 1meV to 100 keV and beyond.

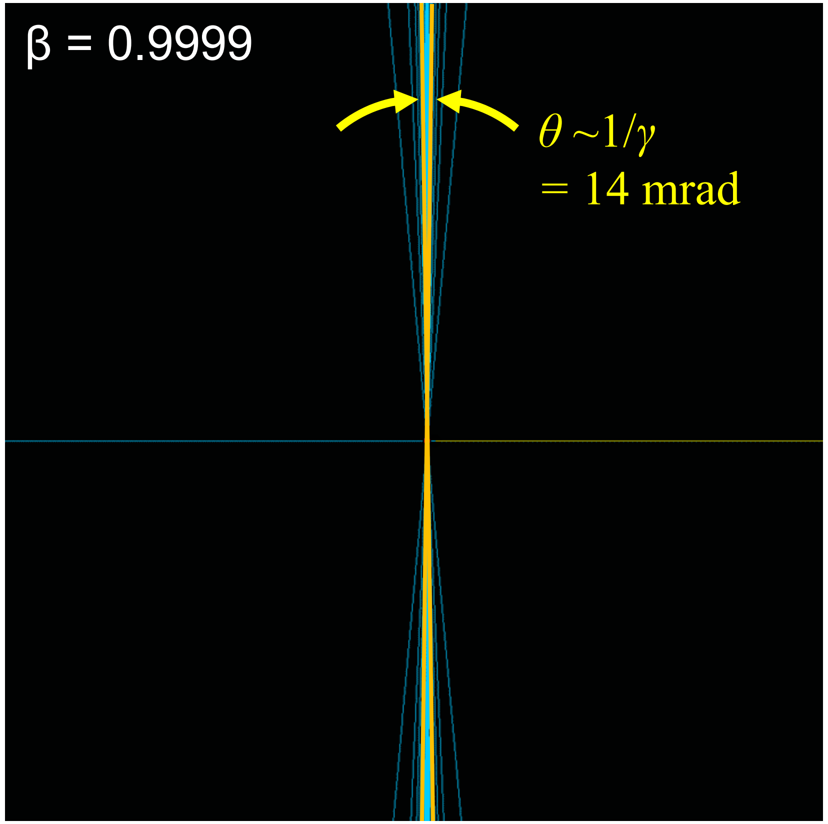


The Electromagnetic Spectrum | Physics LibreTexts

Relativity: E-Field of an electron moving at constant velocity

Velocity $v = \beta c$ (*i.e.* $\beta = v/c$)

Mass enhancement $m = \gamma \cdot m_0$; $\gamma = \sqrt{\frac{1}{(1-\beta^2)}}$



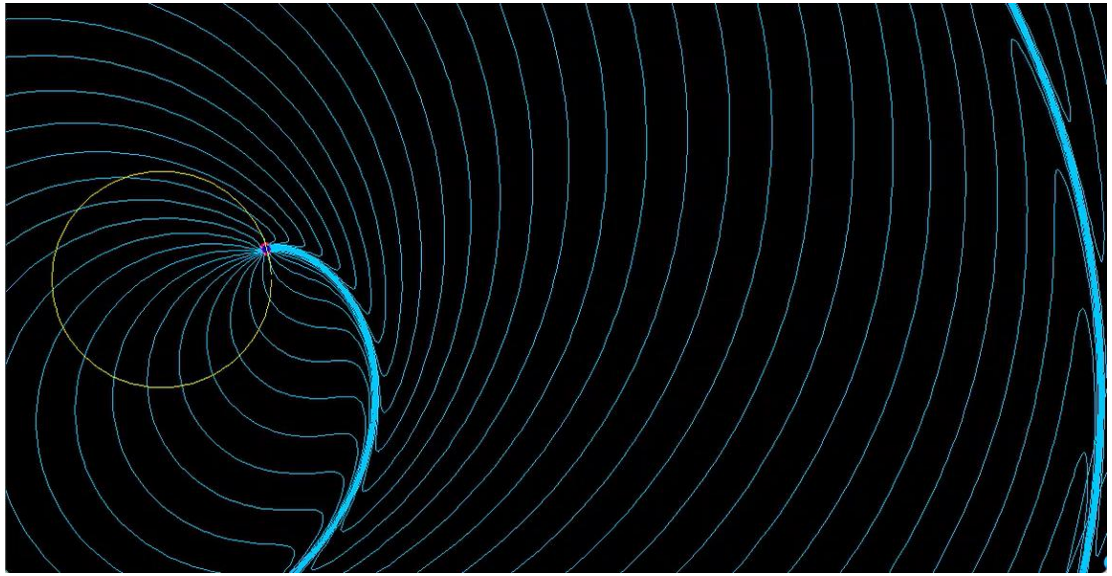
At NSLS-II, γ = 5871, β = 0.99999998549

At this velocity, electron mass is about 3X that of a proton at rest

Back to Emission of Electromagnetic Waves (Photons)

Charged particles emit when they are *accelerated*.

Example: circular motion (centripetal acceleration)



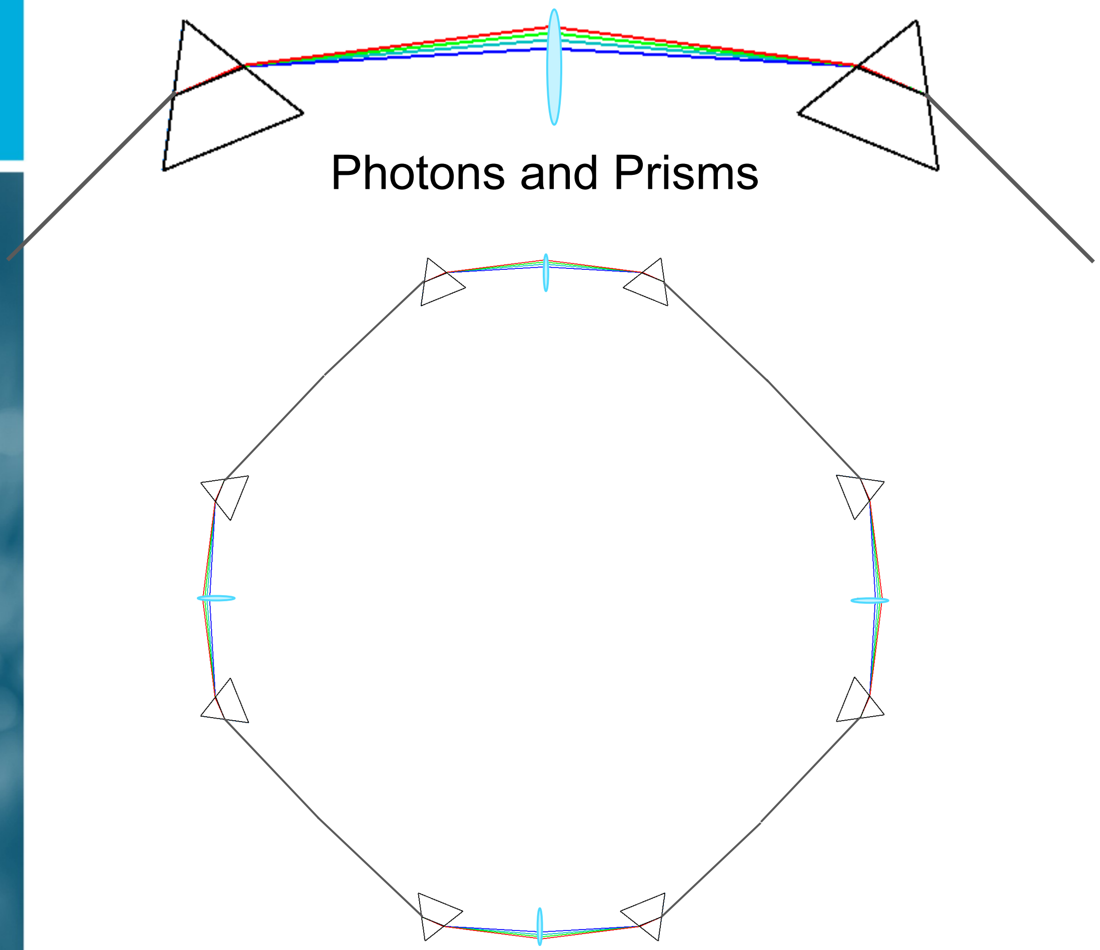
Relativistic electron at 98% of c (β = 0.98)

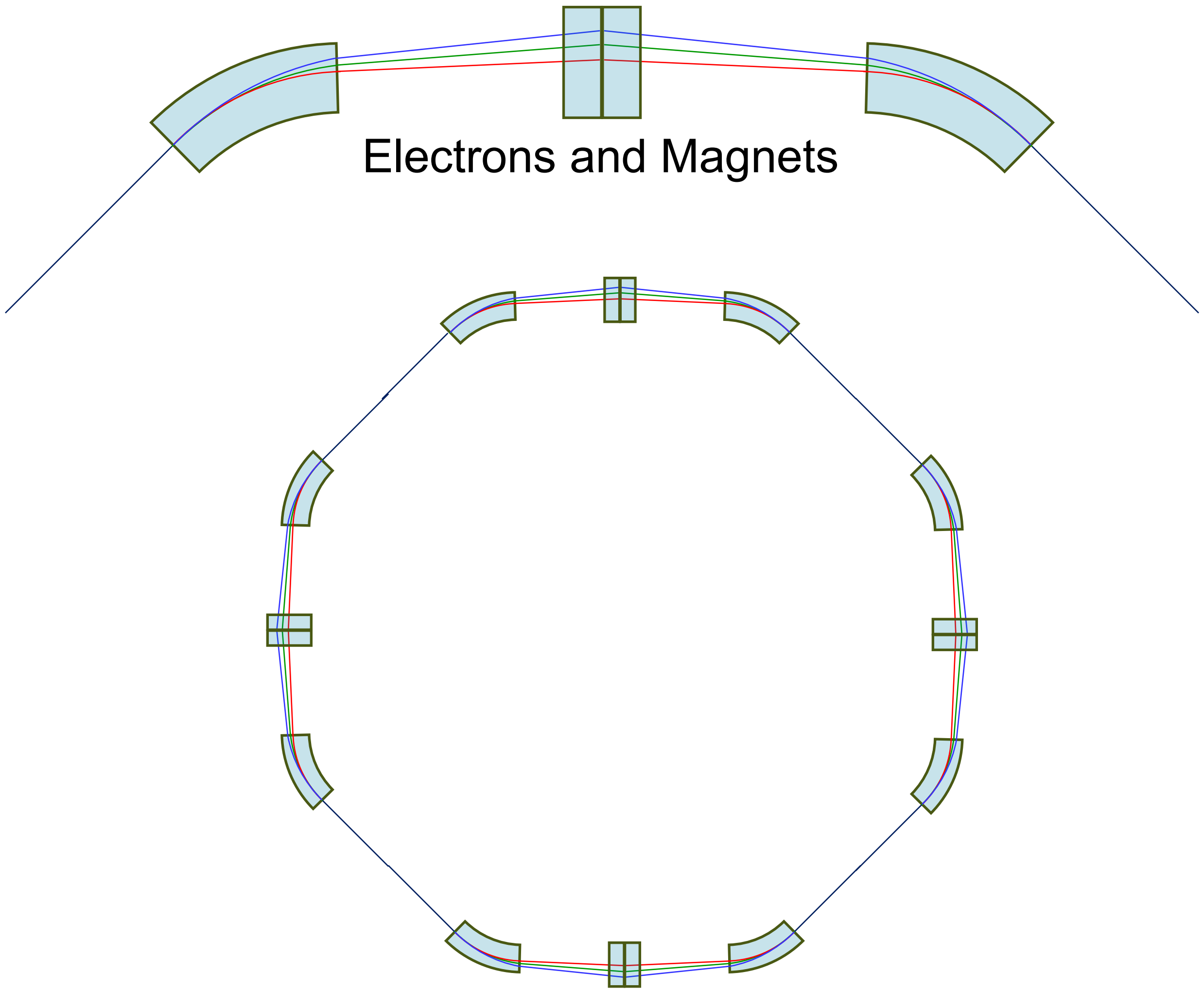
Radiated fields have a sharp (fast) “kink” due to the relativistically compressed Coulomb field PLUS Doppler effect.

Rapidly changing radiated fields
=> emission to very high frequencies (i.e. x-rays)

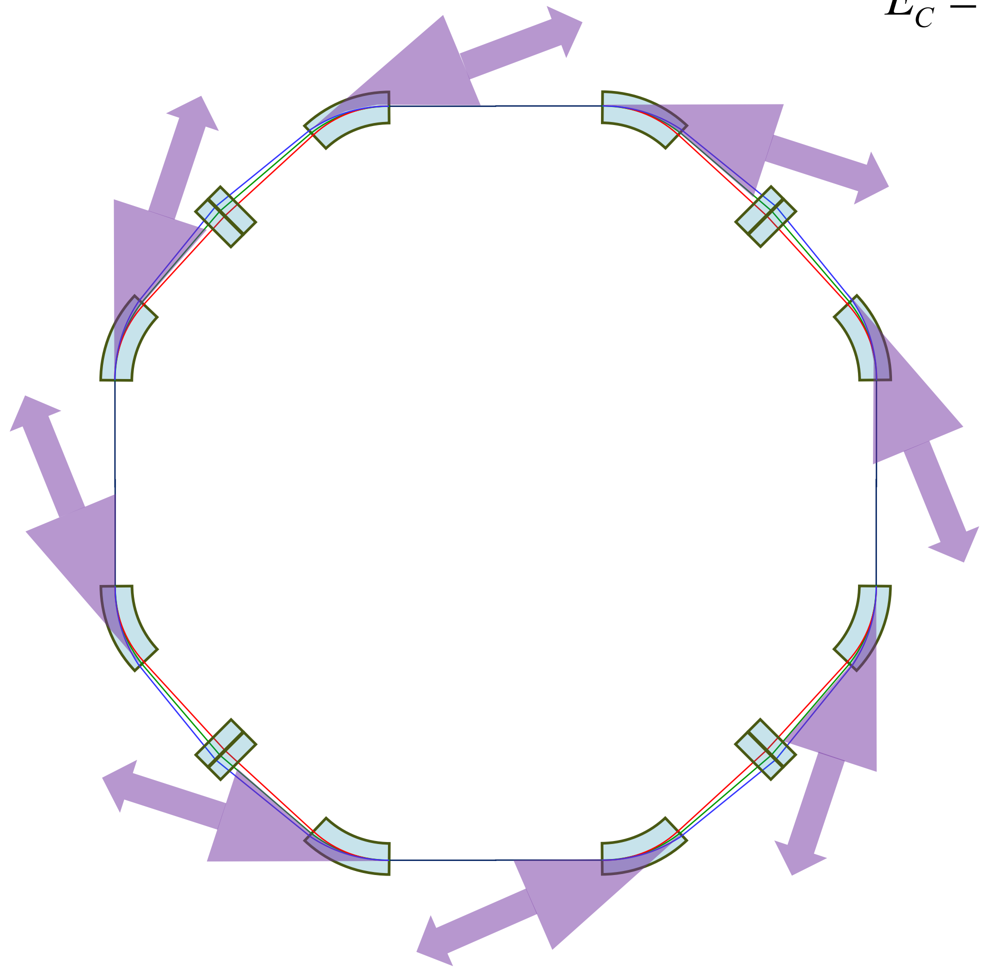
Emission is from very small electron beam into narrow angle
=> Very high brightness/brilliance/radiance

Electron Synchrotrons (and Storage Rings) as Light Sources



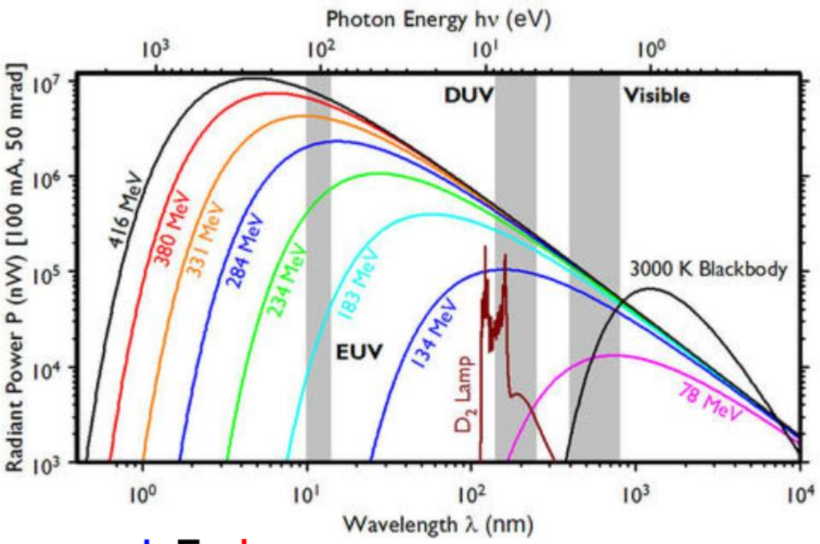


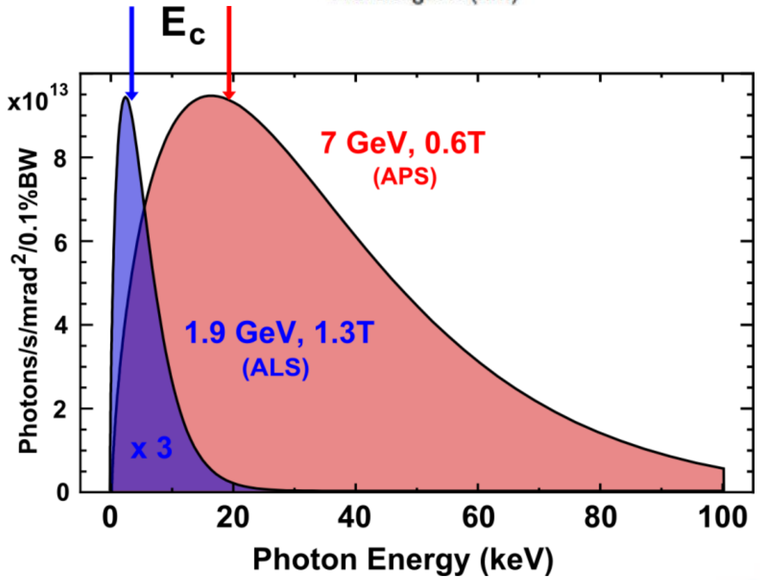
Electron Synchrotrons (and Storage Rings) as Light Sources



$$E_C = h\nu_C = \frac{3h}{4\pi}\frac{c}{\rho}\gamma^3$$

Bending Magnet Radiated Output

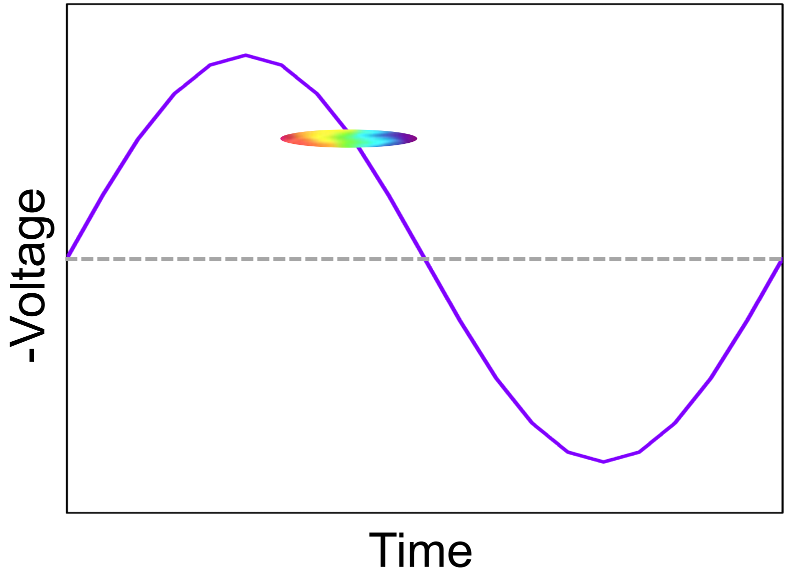




Electrons Emit EM radiation (what we want!)

- Electrons lose energy => Needs to be restored.

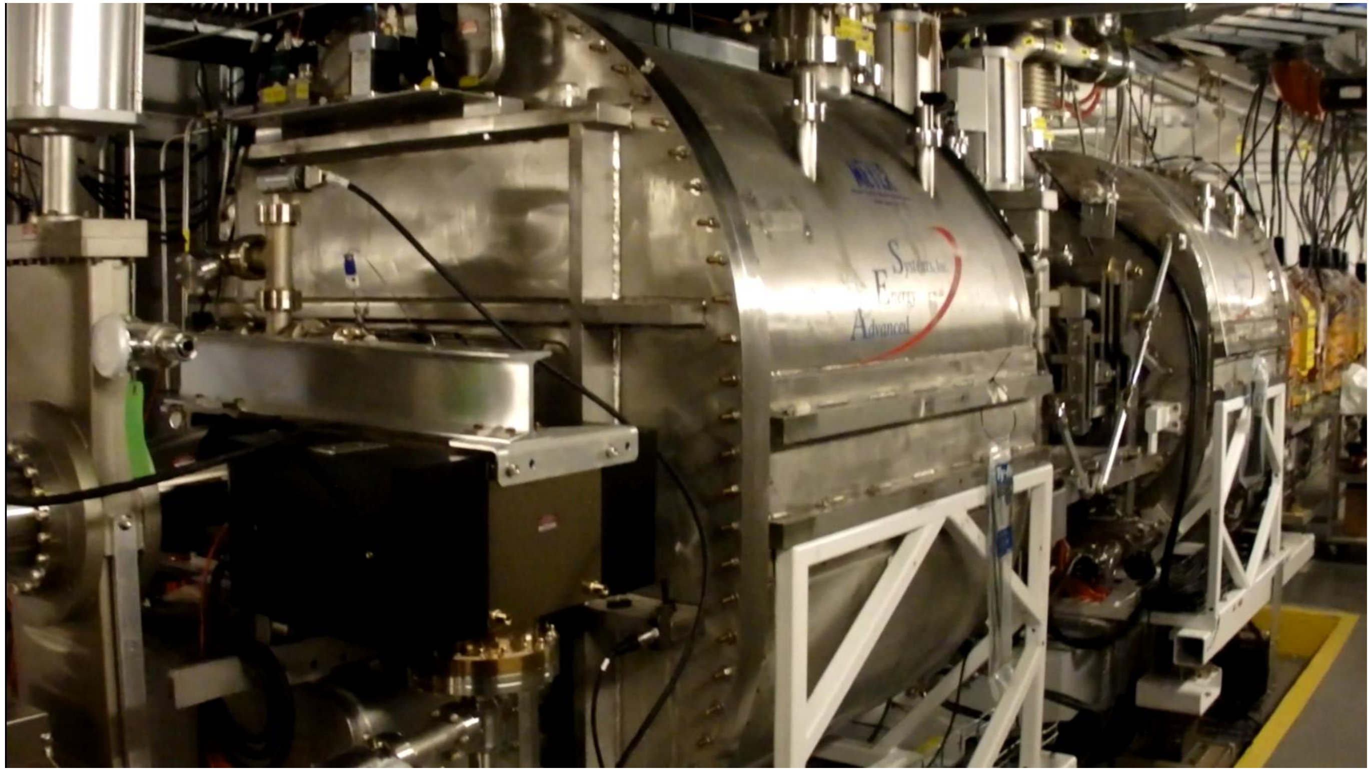
- Use time-varying E-field (voltage) from a powered radio-frequency (RF) cavity
  - Electrons circulate in ***bunches*** to arrive at the correct RF voltage (time or phase) to restore the lost energy. $V(t \text{ or } \phi) = \Delta E_{avg}/e$
  - Note: Electrons do not all have the exact same energy.
    - ► Electrons with energy excess (heavier) follow longer orbit, arrive later.
    - ► Electrons with energy deficit (lighter) take shorter orbit, arriver earlier.



  - Have electrons arrive on the correct $V(t)$ slope.
    - ► Early (lower energy) electrons cross a larger potential
    - ► Late (higher energy) electrons cross a smaller potential
    - ⇒ Energy correction and orbit stability.
    - ⇒ Electrons intrinsically “find” the appropriate potential, follow the RF synchronously -> *synchrotron*

NSLS-II Superconducting RF Cavities

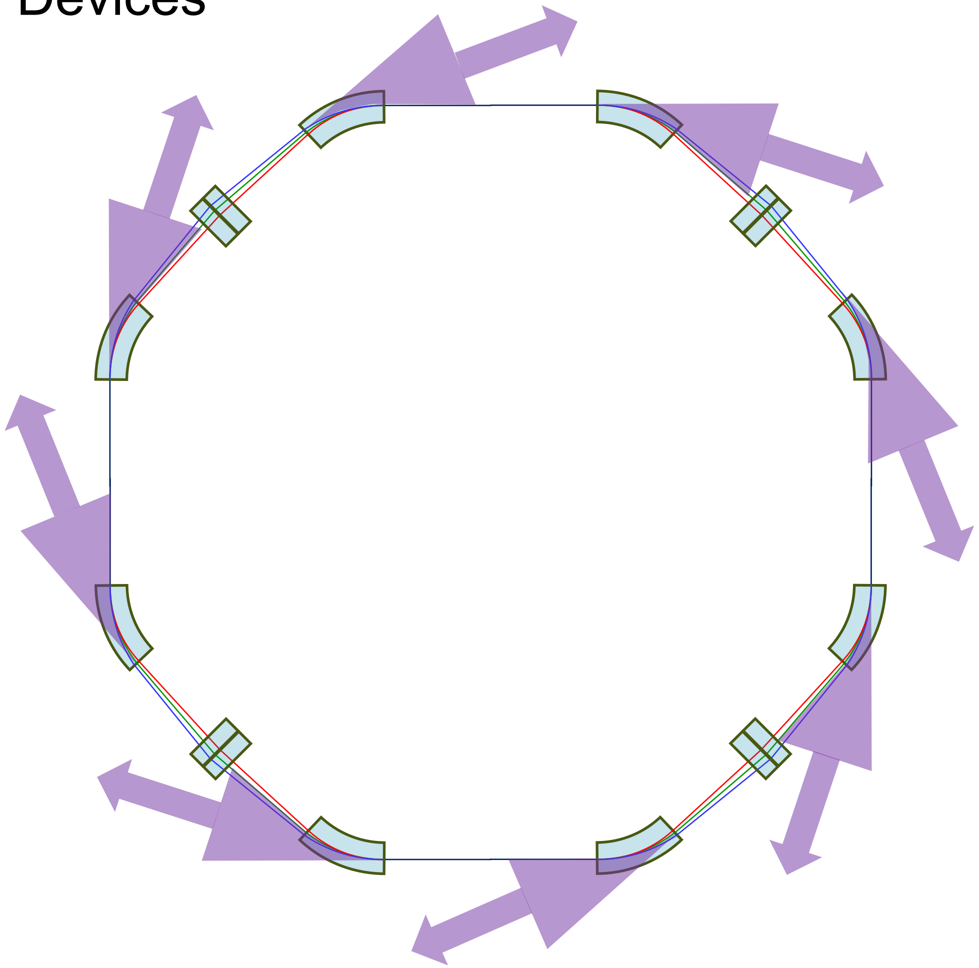
- 1.2 MV during normal operations
- ~150 kW of radiated power from dipoles alone (IDs add a lot more …)
- Presently three RF cavities, plans for a total of four.



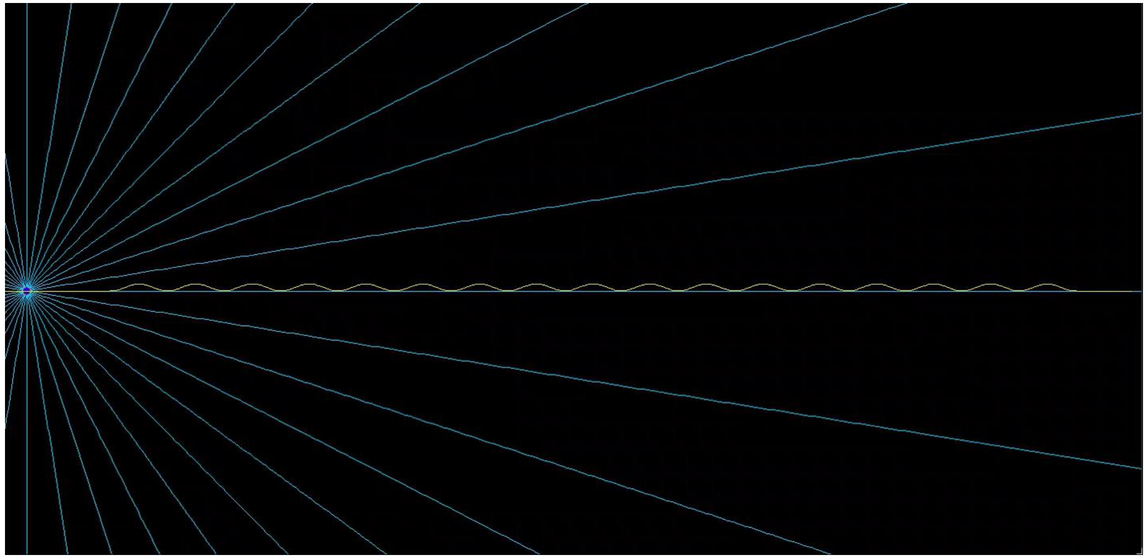
Electron Synchrotrons (and Storage Rings) as Light Sources

Can insert more magnets in the straight sections if electrons remain on orbit => periodic magnet structures

“Insertion Devices”

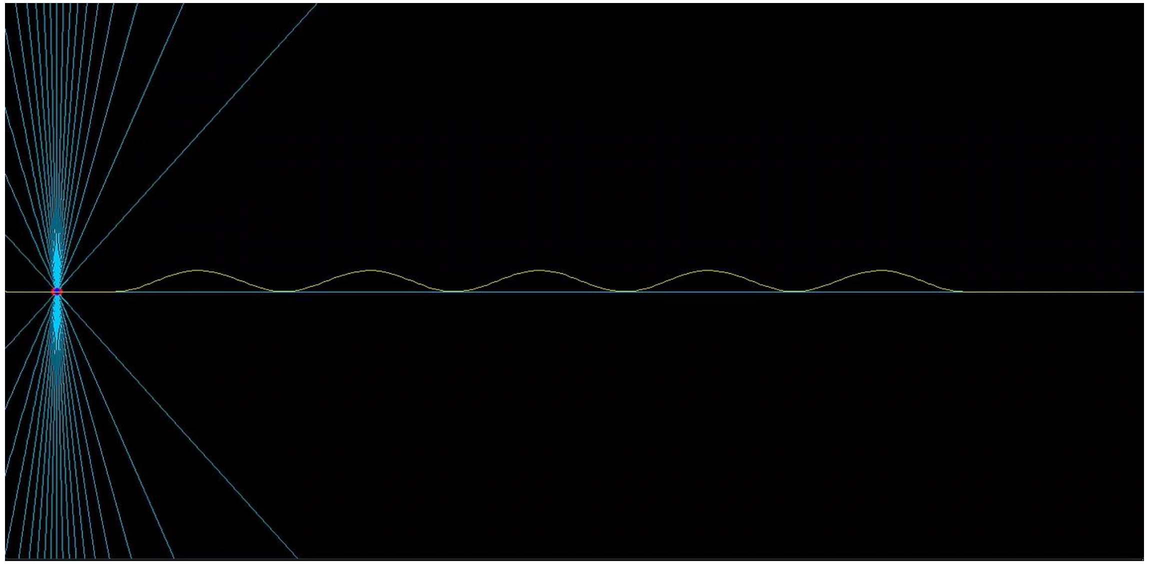


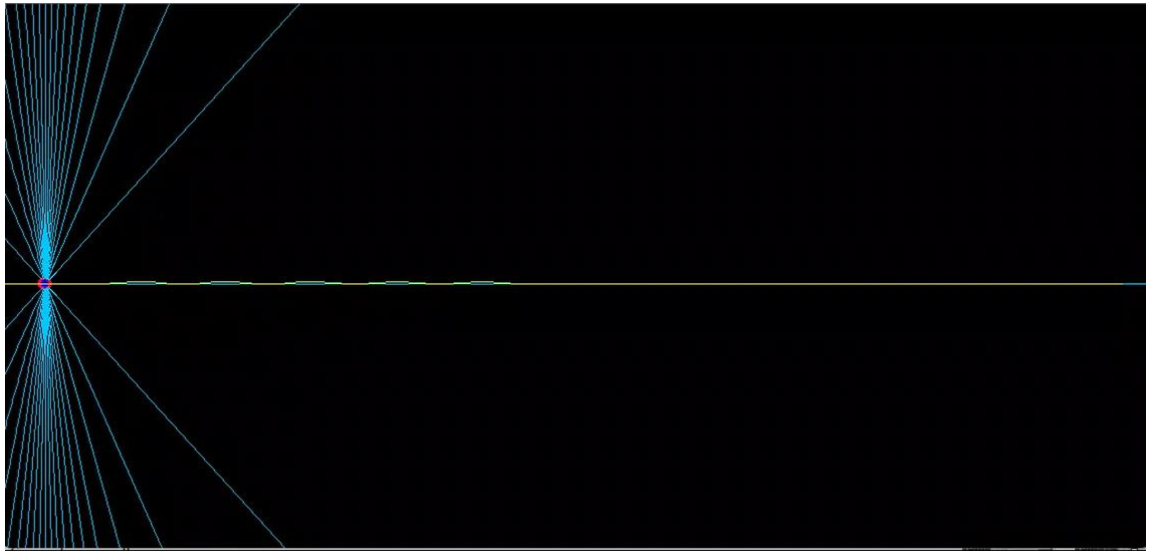
Insertion Devices for Synchrotron Light Sources



Non-relativistic

Relativistic - Wiggler





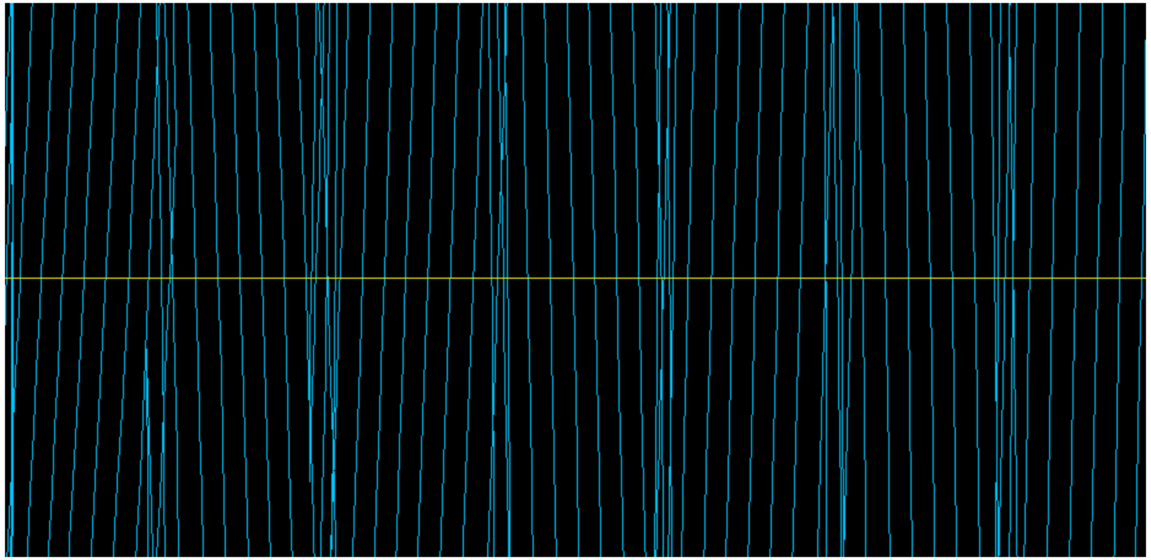
Relativistic - Undulator

Undulators and Wigglers

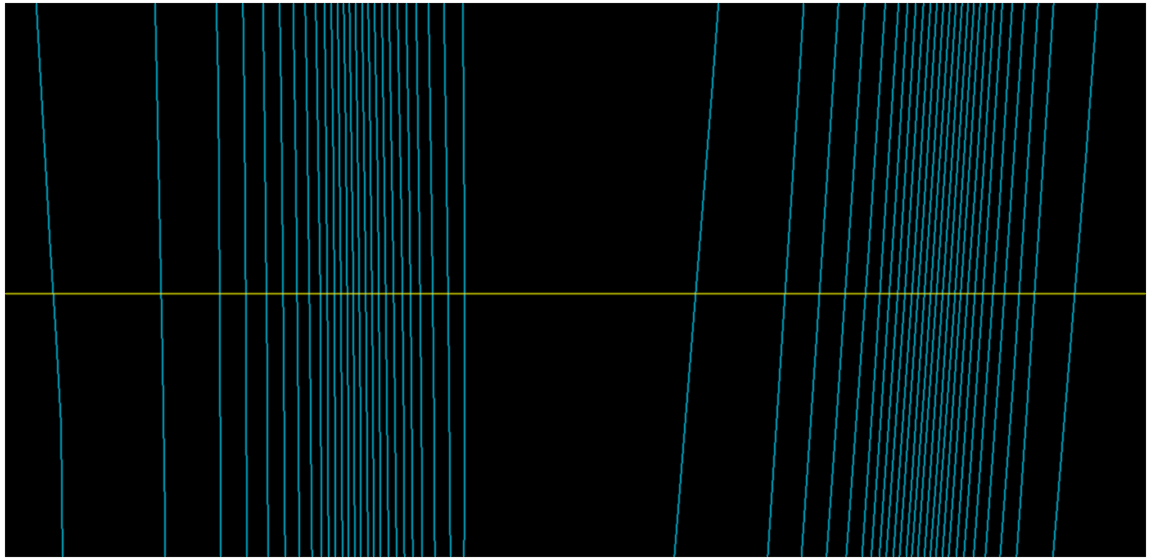
$$\lambda_{on-axis} = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right)$$

$$K(B) = \frac{eB\lambda_u}{2\pi mc} = 0.934\lambda_u[cm]B[T]$$

Undulators:
Waveform with somewhat evenly spaced E-field cycles
=> Moderately discrete frequencies and wavelengths



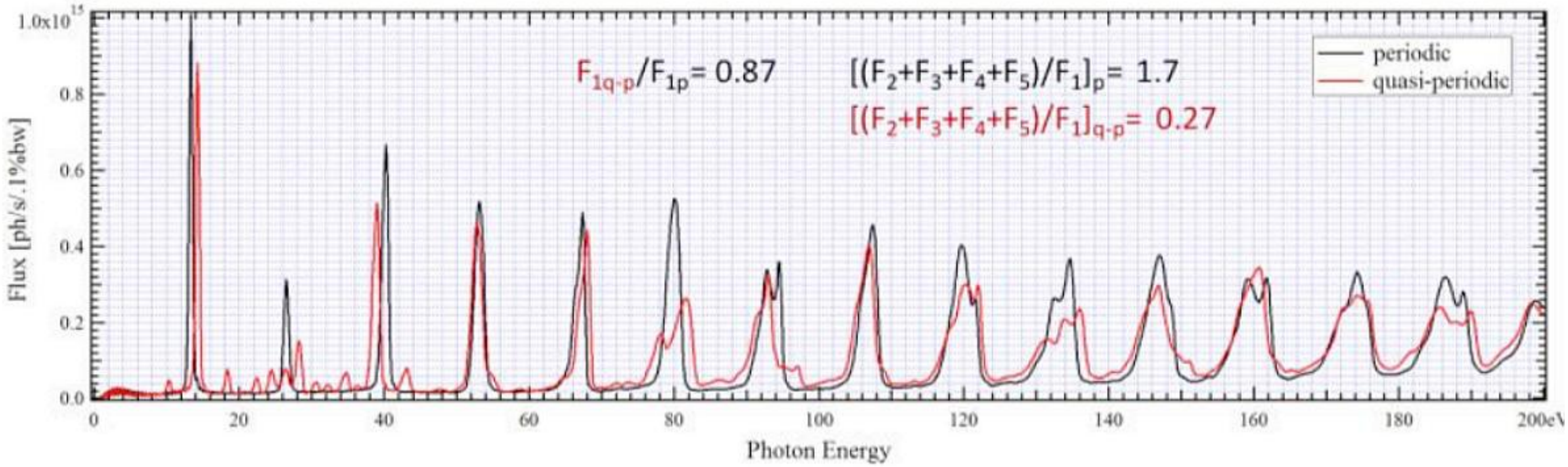
Wigglers:
E-field has less well-defined periodicity
=> Smoother spectral output, reaches higher frequencies



Undulator Spectral Output

$$\lambda_{on-axis} = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right)$$

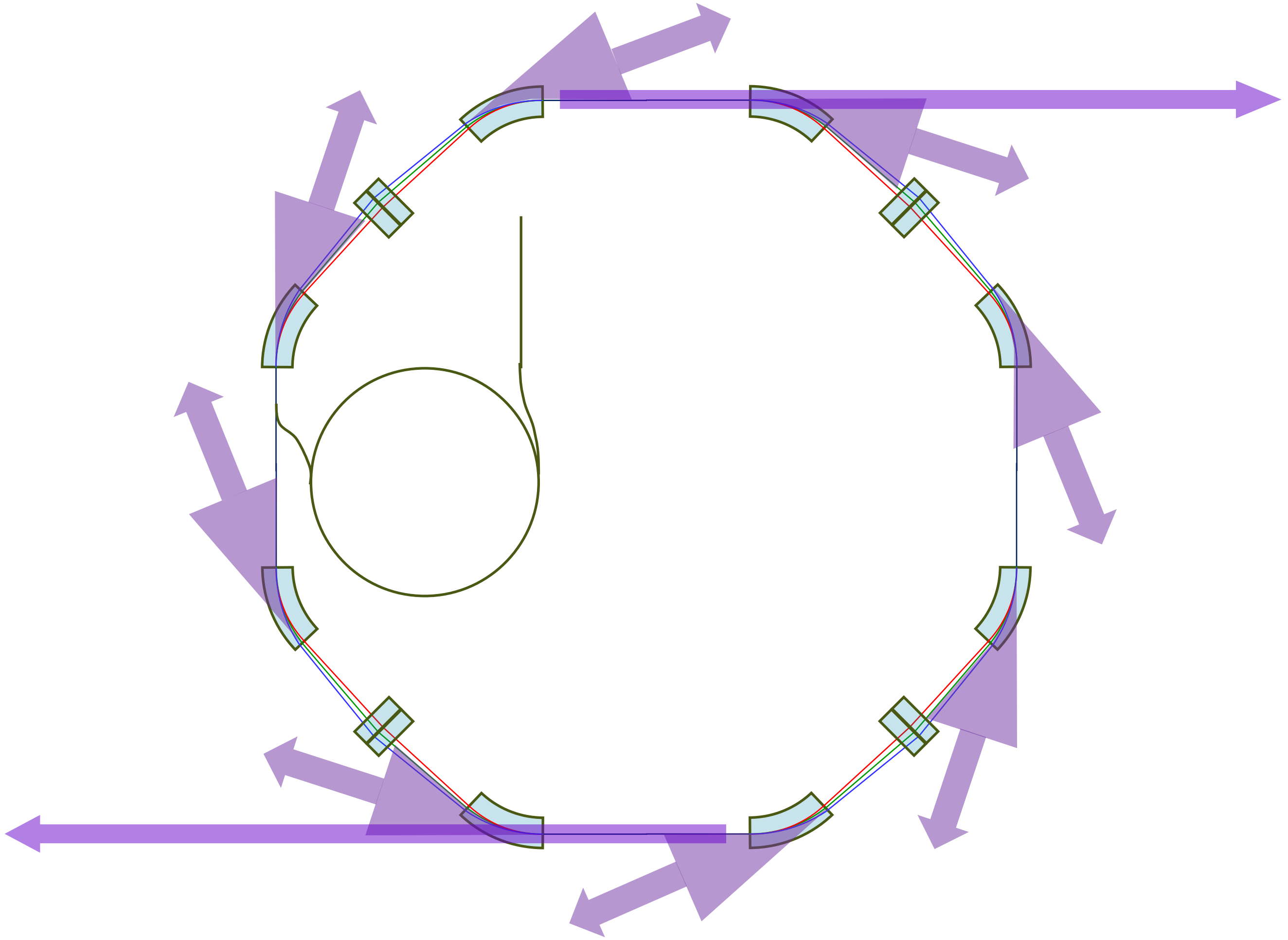
$$K(B) = \frac{eB\lambda_u}{2\pi mc} = 0.934\lambda_u[cm]B[T]$$



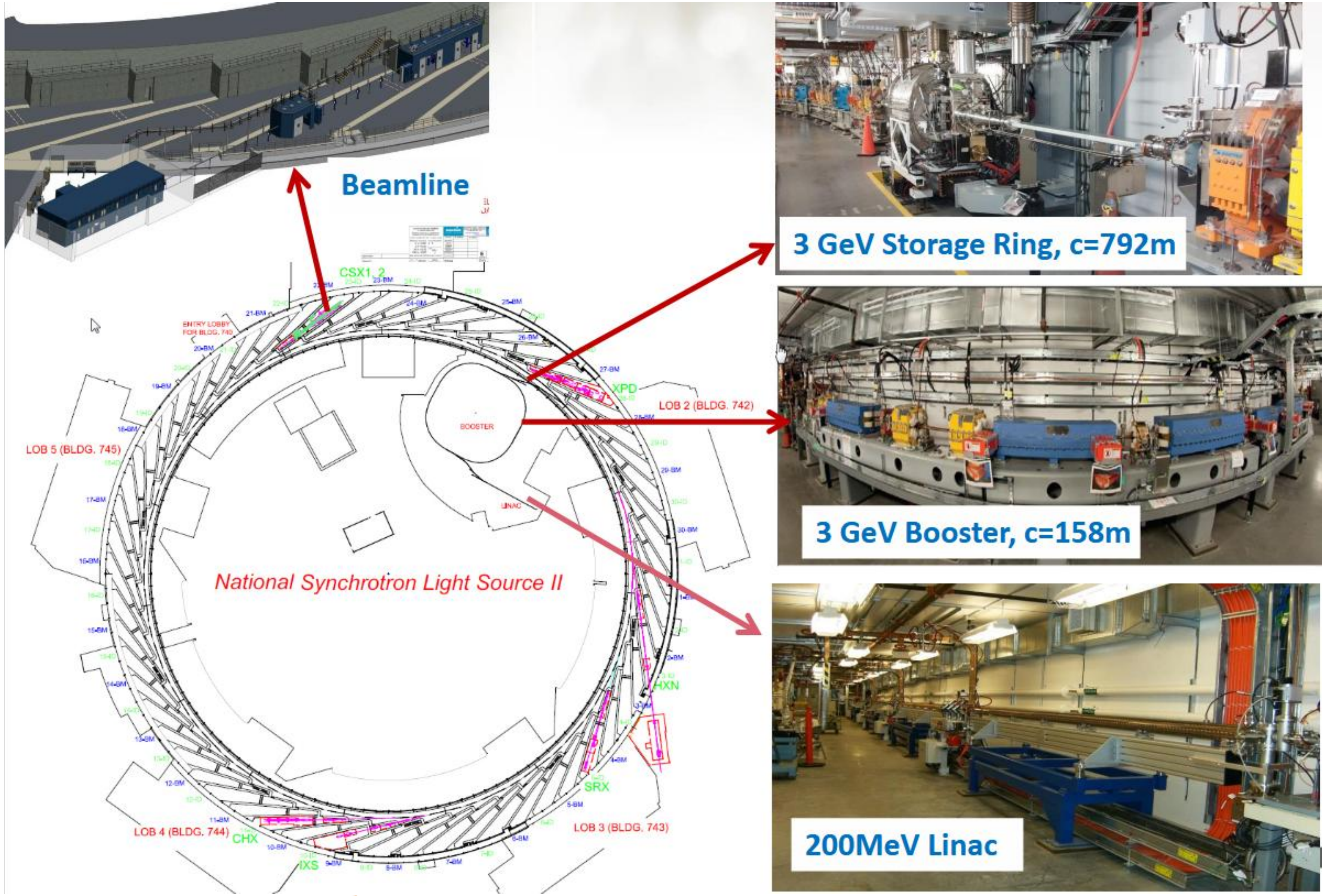
Insertion Devices at NSLS-II

Electron Synchrotrons (and Storage Rings) as Light Sources

Can insert more magnets in the straight sections if electrons emerge on same orbit => periodic magnet structures

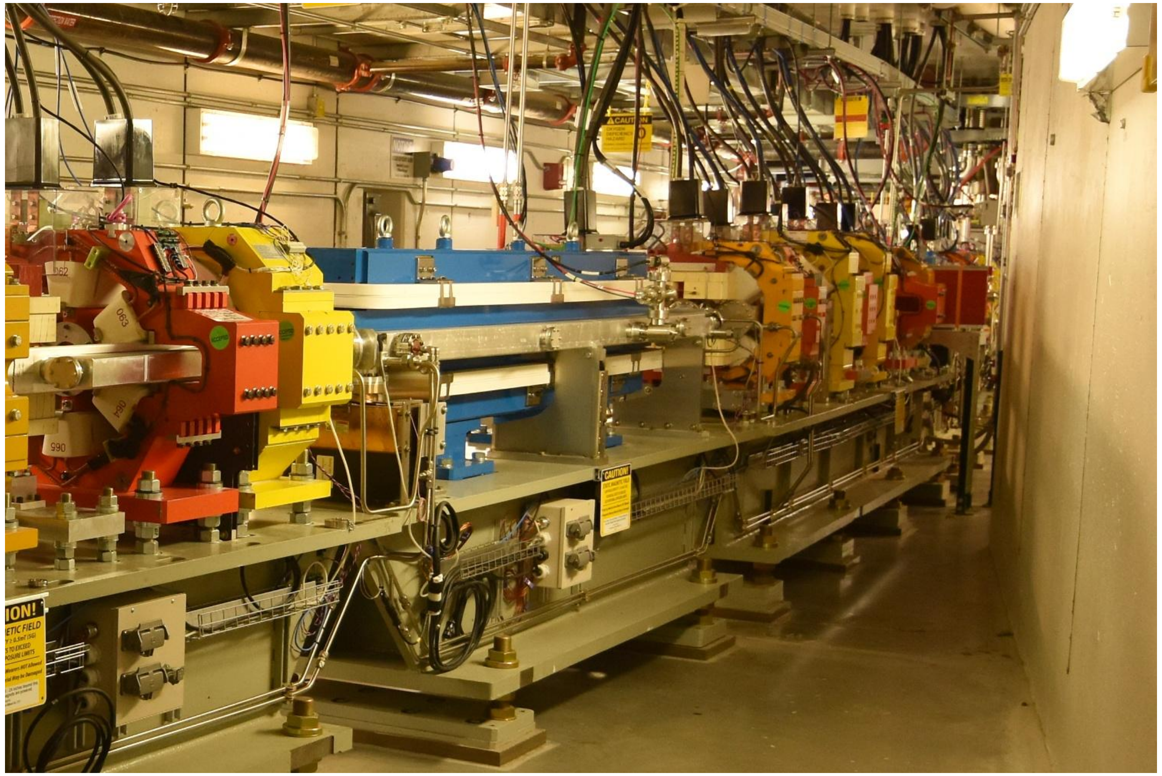


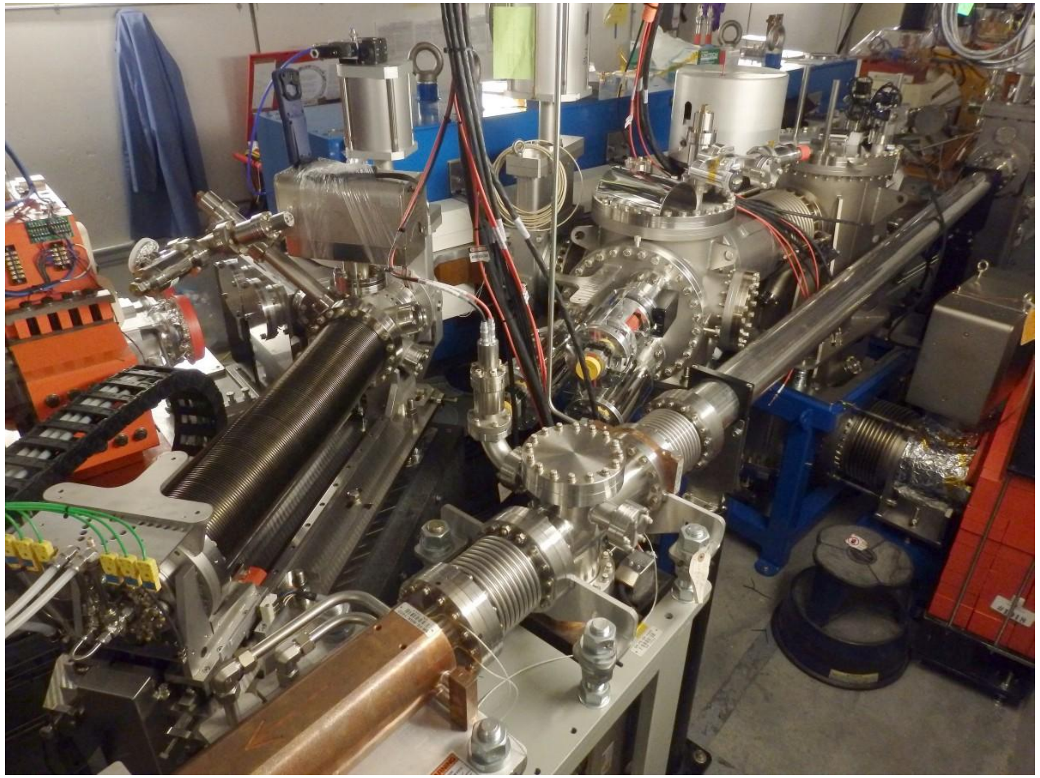
National Synchrotron Light Source II: Accelerator Components



Dipole Bend Source: 90mm gap, 0.4T (ρ =25m for E=3 GeV)

NSLS-II, Dipole





Optics for X-Rays: Needed for beam Steering and Focusing

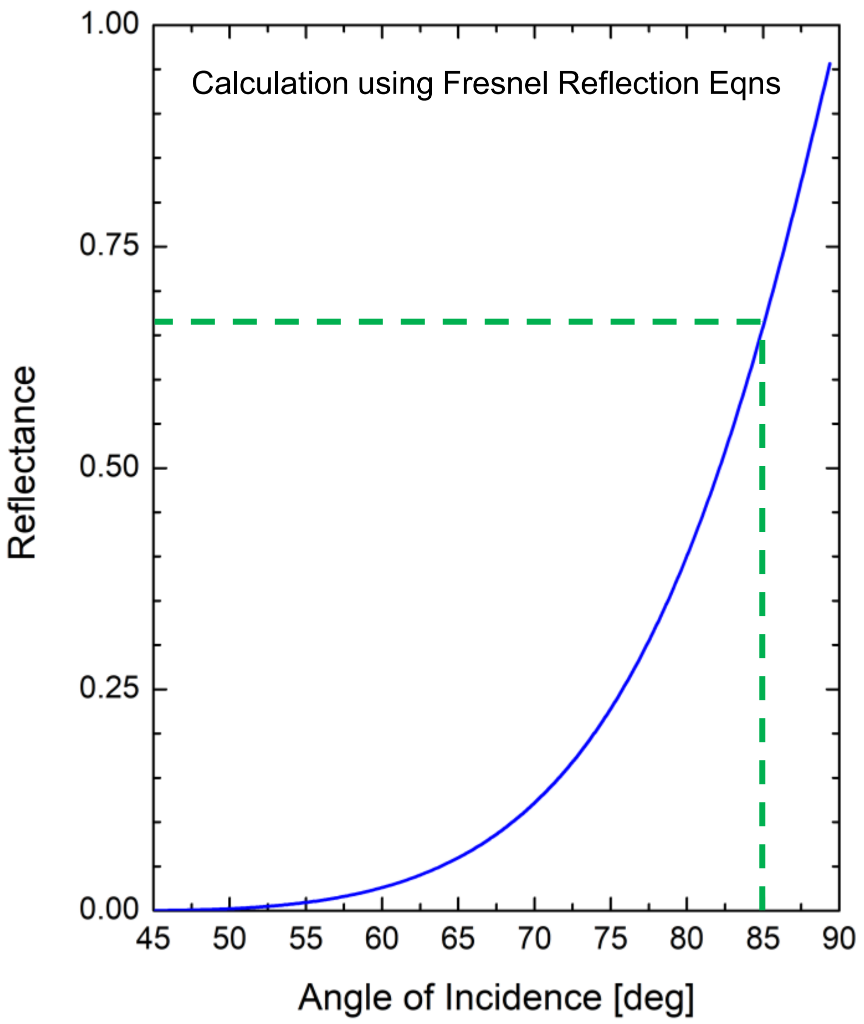
Reflection: Mostly metals at near grazing incidence

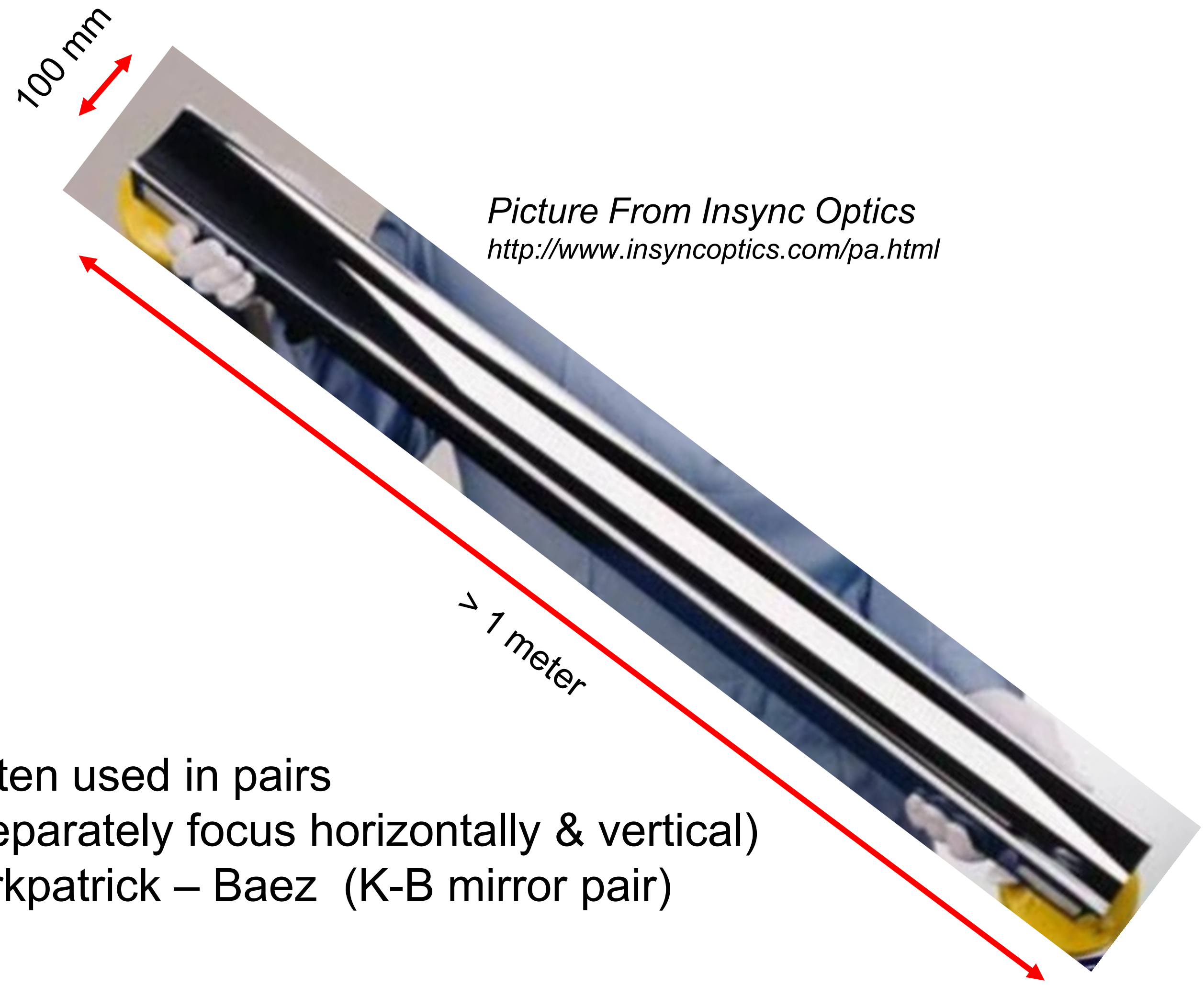
- Kirkpatrick-Baez (KB) mirror pairs
  - Grazing incidence
  - Focus vertical and horizontal separately

Transmission: Low *Z* elements

- Compound lenses (beryllium, diamond)
- Fresnel Zone Plates

X-ray Mirrors: Grazing Incidence





Picture From Insync Optics
http://www.insyncoptics.com/pa.html

Often used in pairs
(separately focus horizontally & vertical)
Kirkpatrick – Baez (K-B mirror pair)

X-ray Lenses: Compound Refractive Len (CRL)

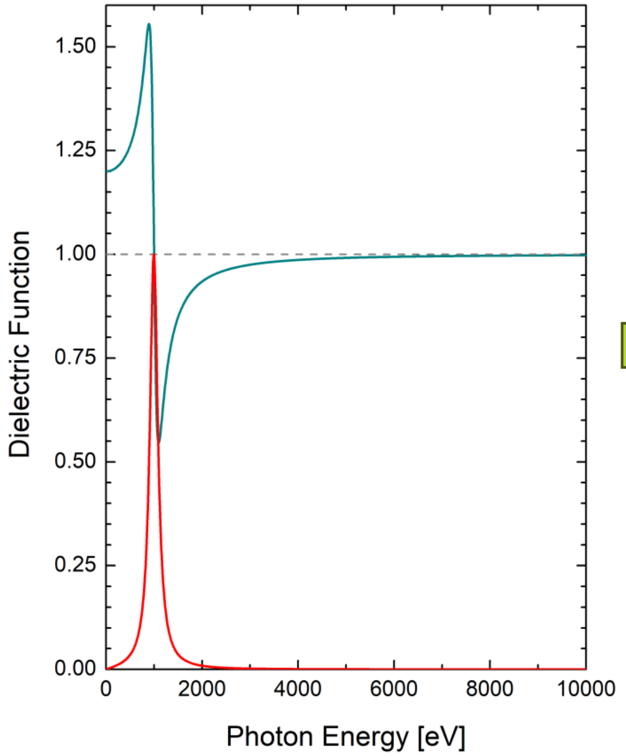
"Conventional" -> use low absorbing material
=> low *Z* elements: Beryllium, Carbon (Diamond)

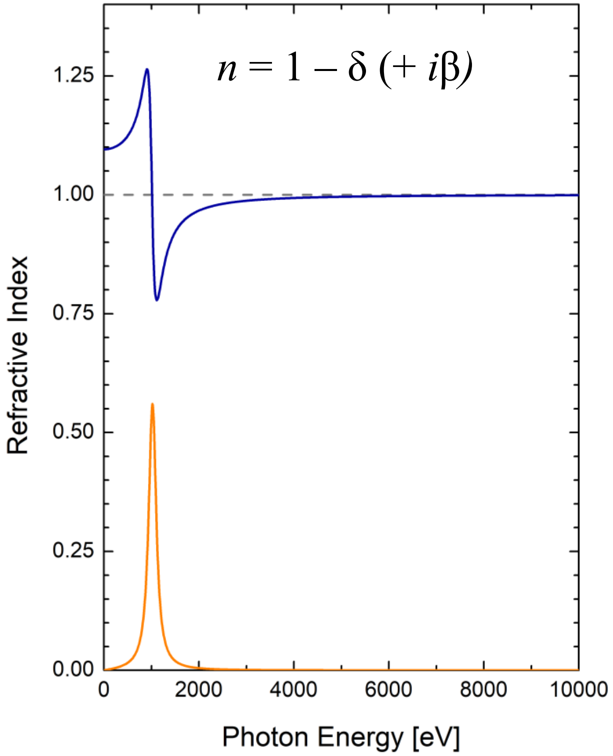
$$f = \frac{R}{2(n-1)} = \frac{R}{2\delta} \qquad \delta \sim 10^{-6}$$

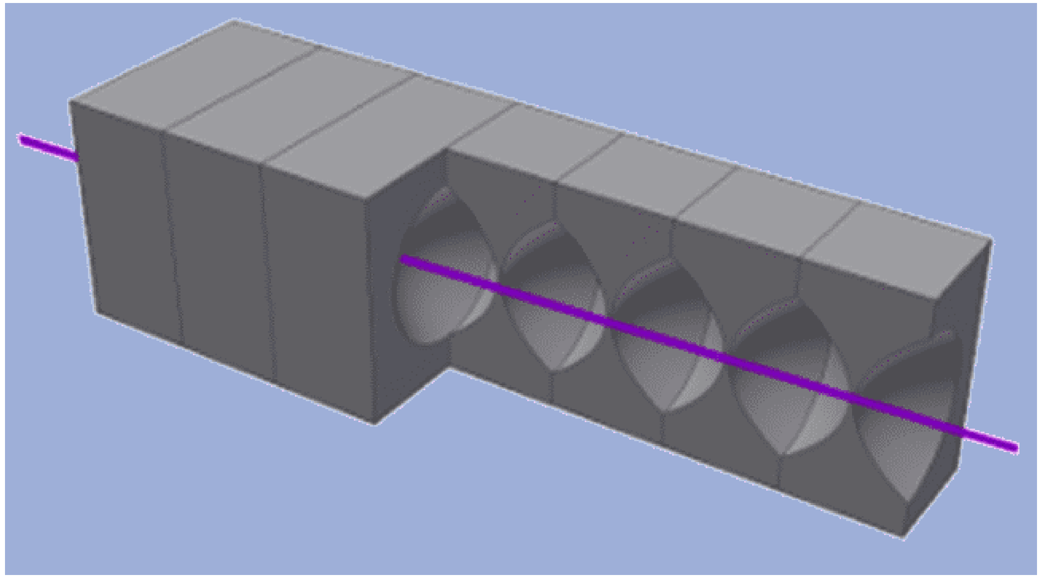
but can stack *many* (e.g. N) lenses in series

$$f = \frac{R}{2\delta \cdot N}$$

Can get f < 4 m and spotsize < 1 μm with N = 30 and R = 200 μm





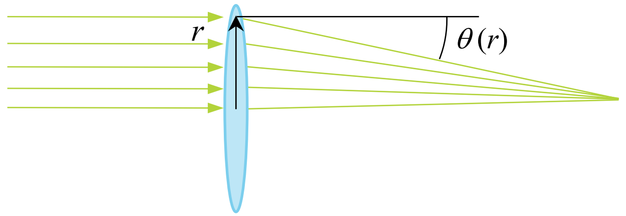


X-ray Lenses: Zone Plates

Grating with groove spacing d diffracts light of wavelength λ into an angle θ according to

$$d\sin(\theta) = n\lambda \quad \text{or} \quad \theta \cong \frac{n\lambda}{d} \quad \text{(small angle approx.)}$$

A convex lens bends light at an angle proportional to radial distance from center

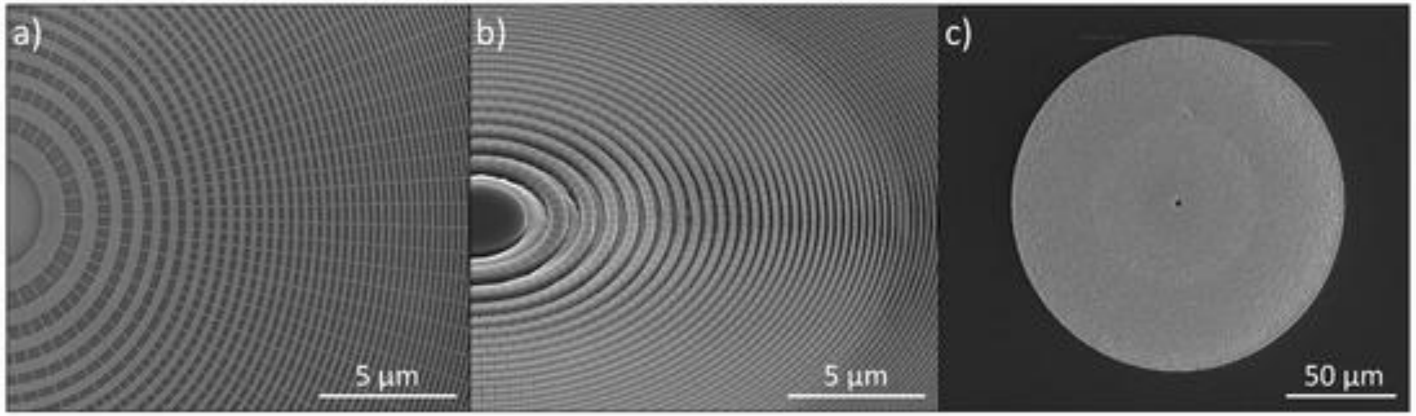


⇒ make a "circular" diffraction grating with groove spacing $d \sim 1/r$ –> "Zone Plate"

Spotsize (Airy disk) $D = 1.22\lambda/\sin(\theta_{MAX})$

⇒ Special lithography methods needed make the small grating spacing d needed for D to reach nanoscale.

Micromachines **2020**, *11*(3), 301; https://doi.org/10.3390/mi11030301



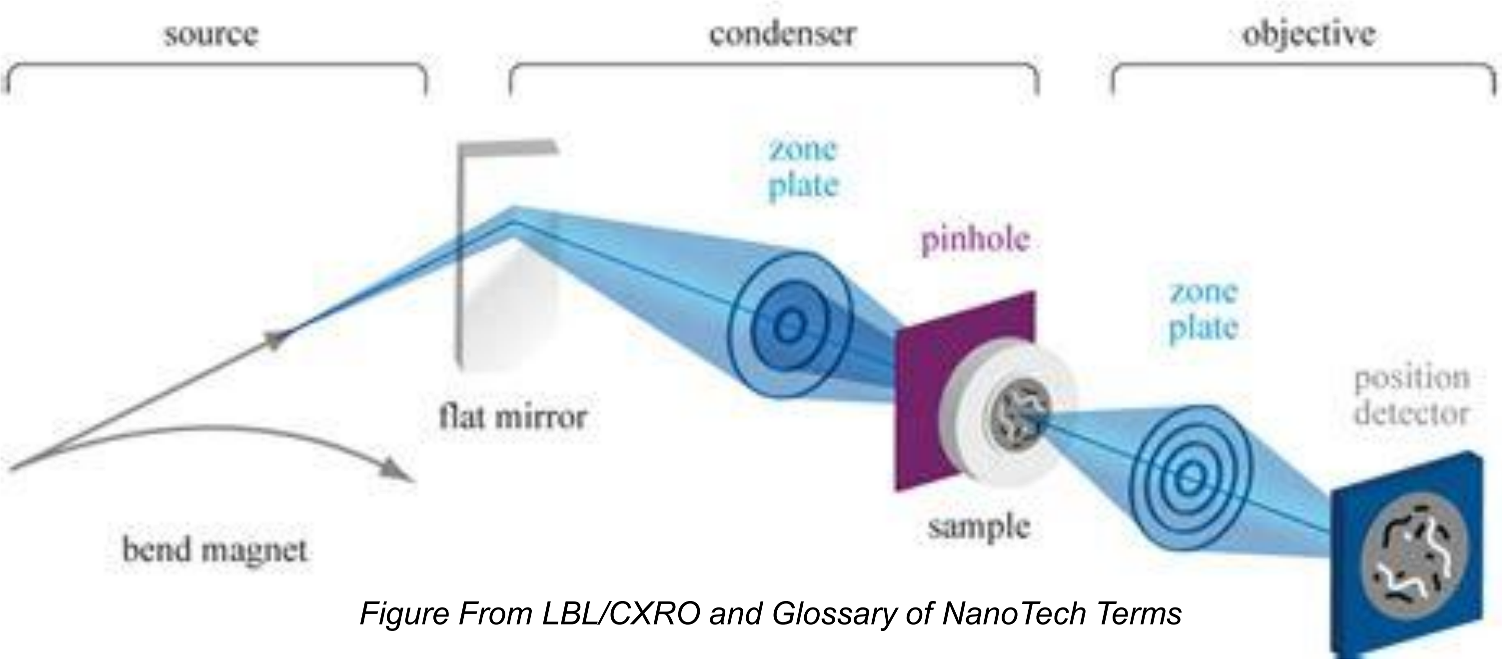
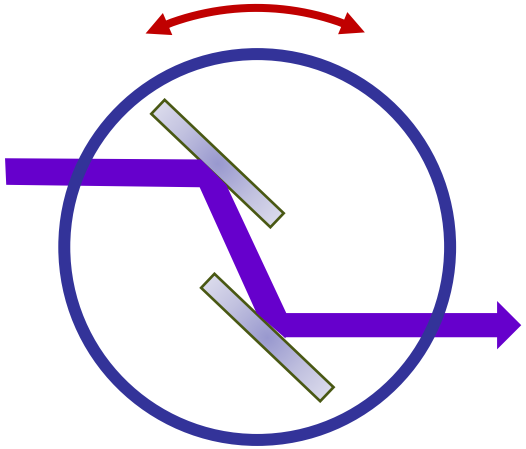


Figure From LBL/CXRO and Glossary of NanoTech Terms

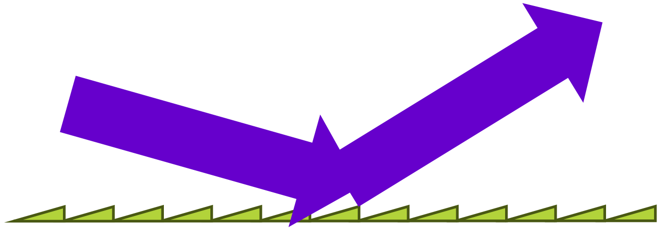
Optics Instruments for Spectroscopy:

Spectrometers

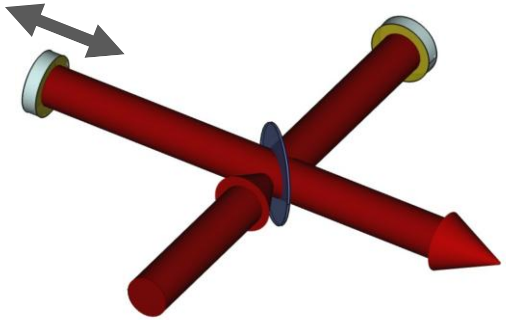
- Medium and hard X-rays: Bragg "scattering" using high quality silicon crystals – "*d*" is accurately known.
  $\lambda = 2d \cdot \sin(\theta)/m$. Tune with θ.
  Do it twice (double crystal monochromator – "DCM") for improved spectral discrimination and output direction control.



- Soft X-rays – use diffraction gratings (reflection type, at grazing incidence) $d \sin(\theta) = n\lambda$.
  Can use variable grating (line) spacing to vary θ and achieve focusing.

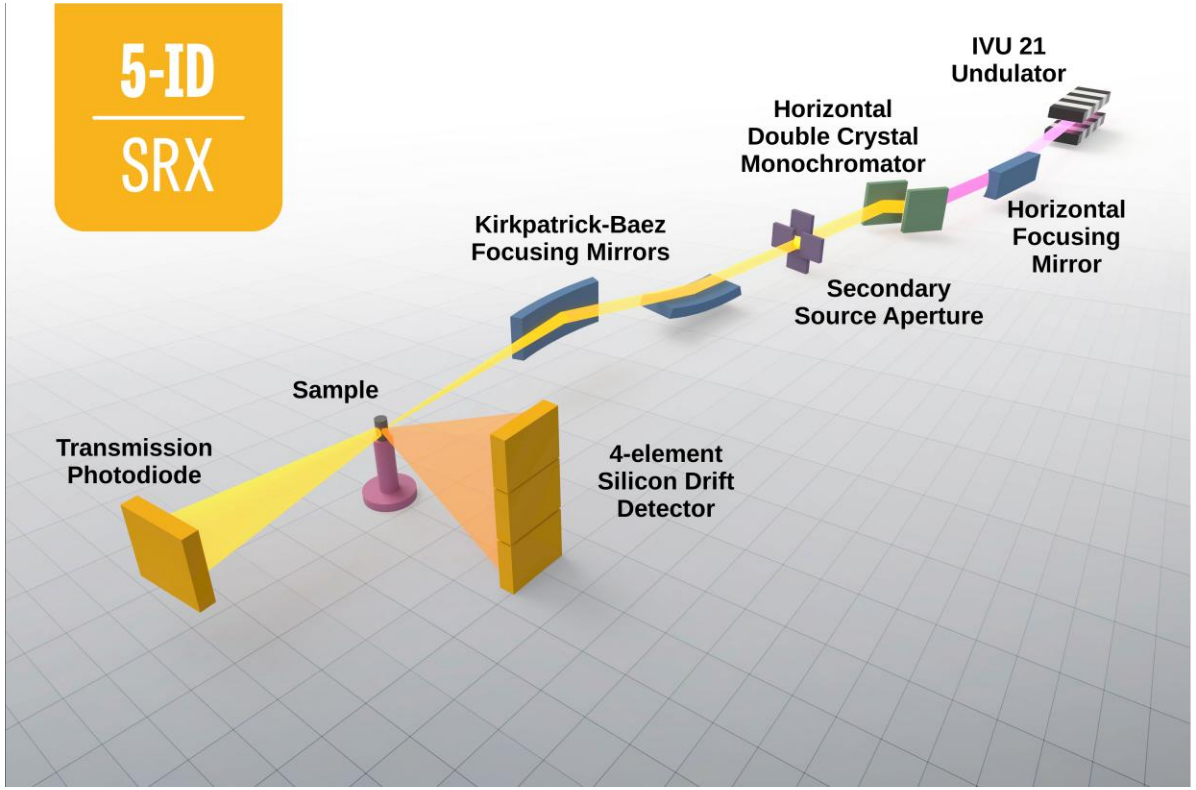


- Infrared – Michelson type interferometers + Fourier Transform

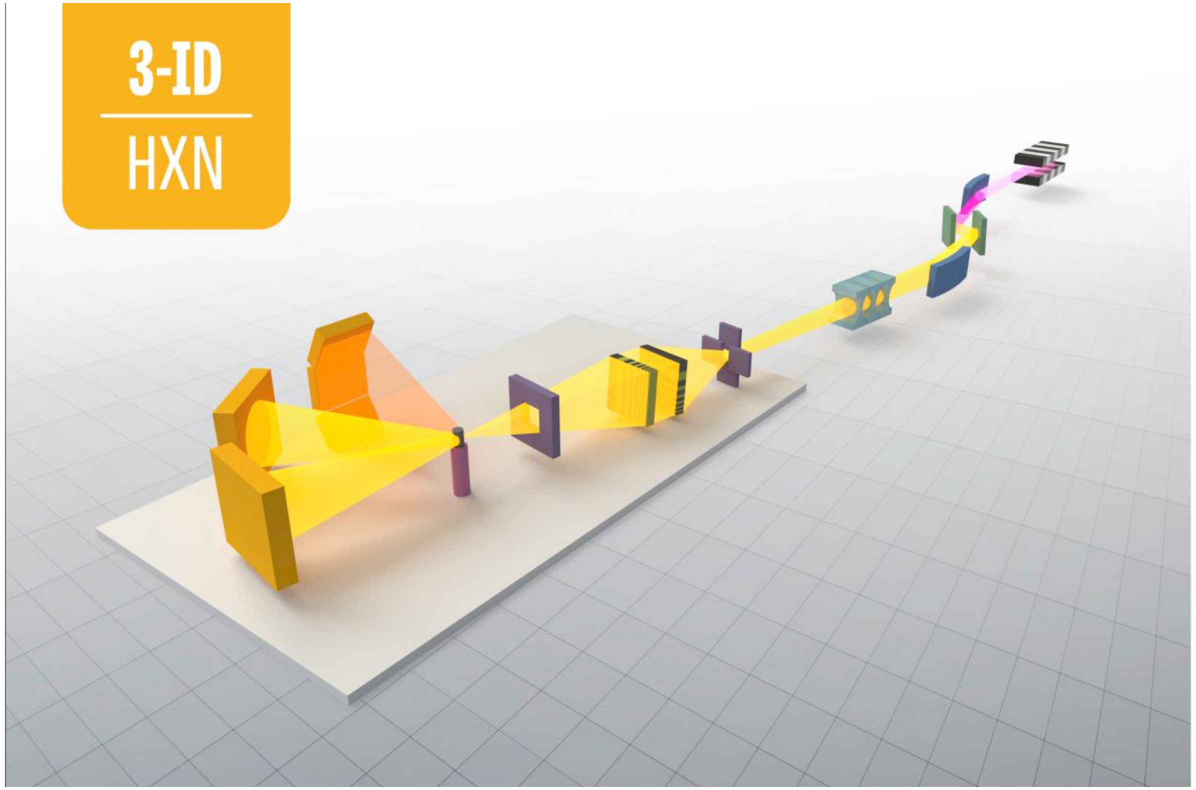


Example Beamlines at NSLS-II for Hard X-ray Energies

Sub-micron Resolution X-ray Spectroscopy



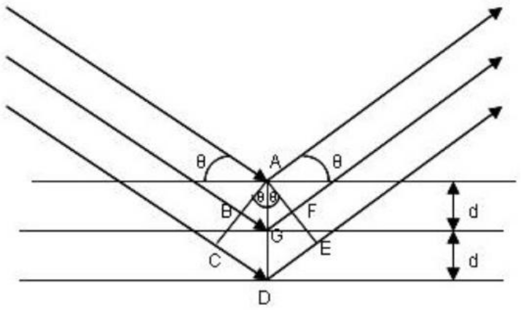
Hard X-ray Nanoprobe

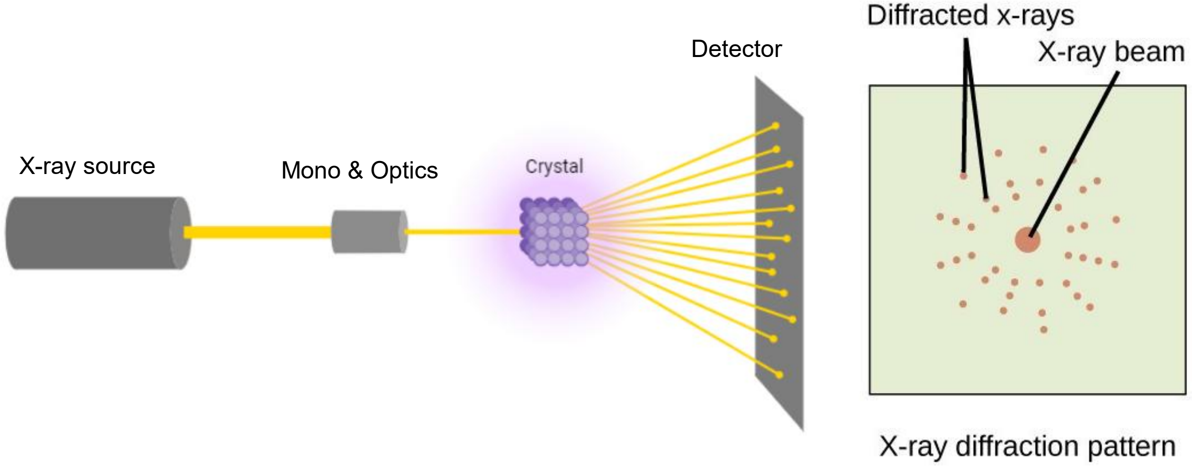


Diffraction Examples: Crystallography

Bragg's Law: X-rays are diffracted at an angle given by

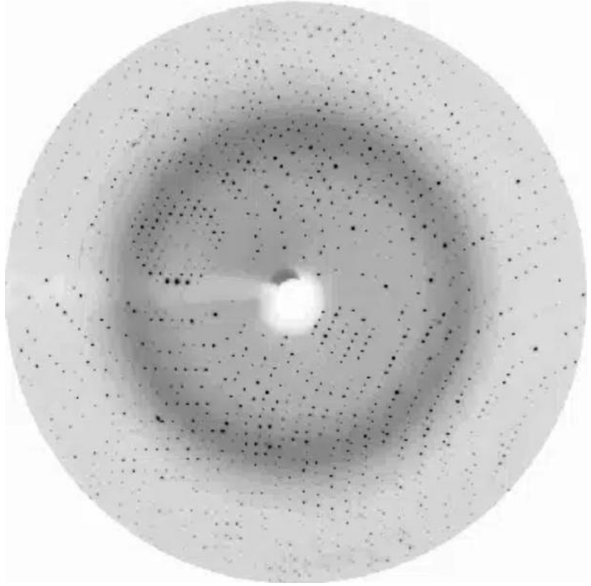
$\sin\theta = \frac{n\lambda}{2d}$ where d is the (atomic) layer spacing

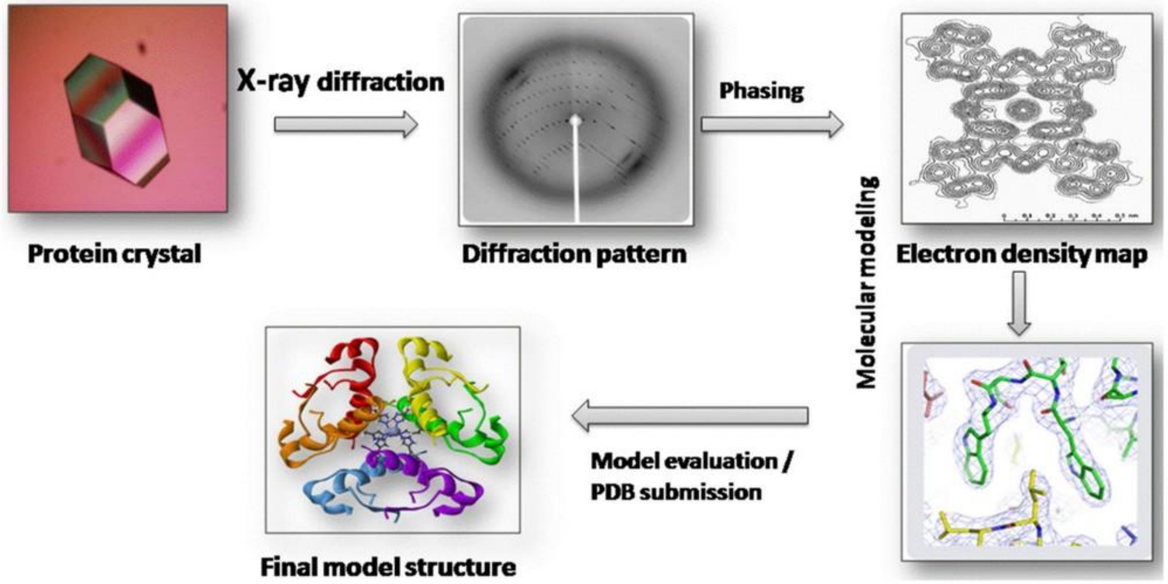




https://sciencevivid.com/x-ray-crystallography-introduction-workflow-braggs-law-applications/

Protein or Macromolecular Crystallography

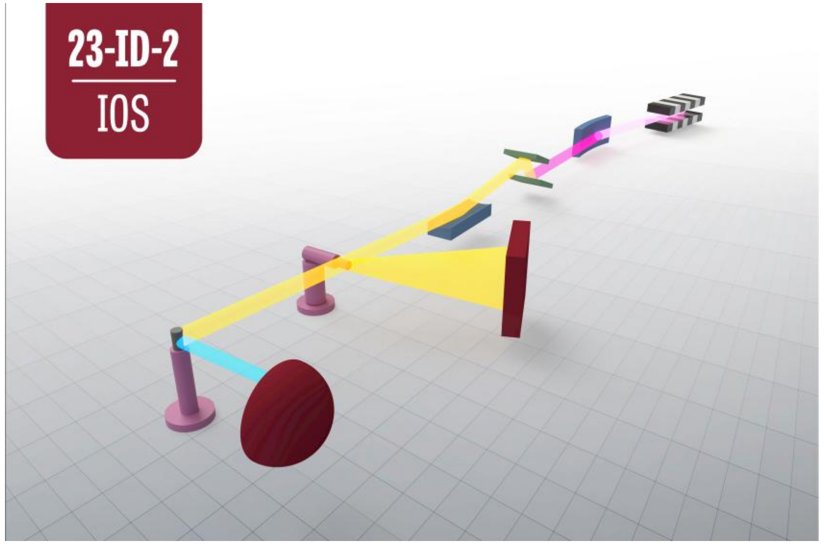


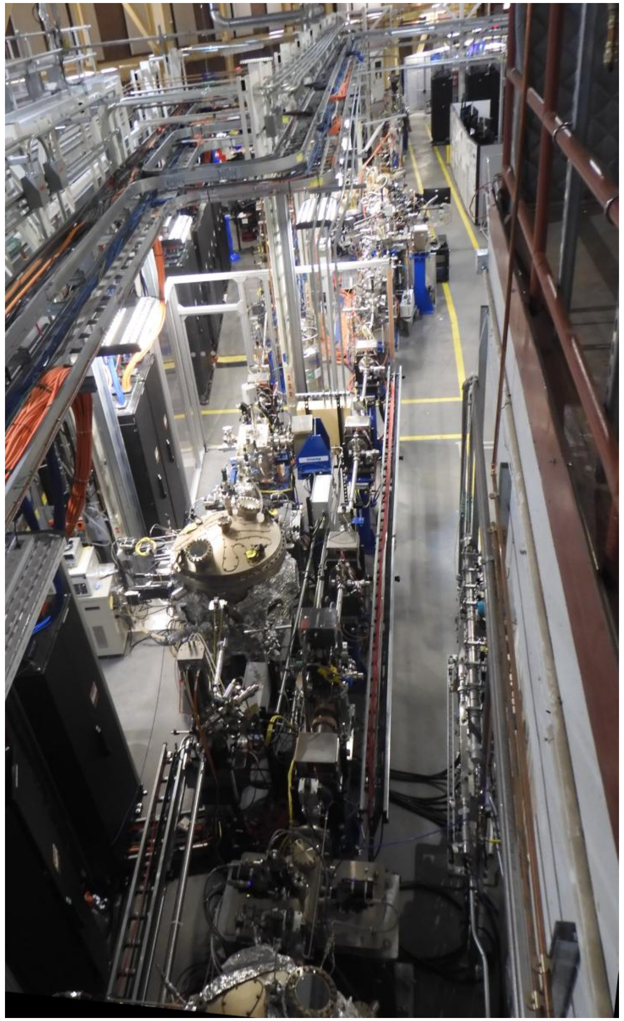


https://www.creative-biostructure.com/protein-crystallography-452.htm

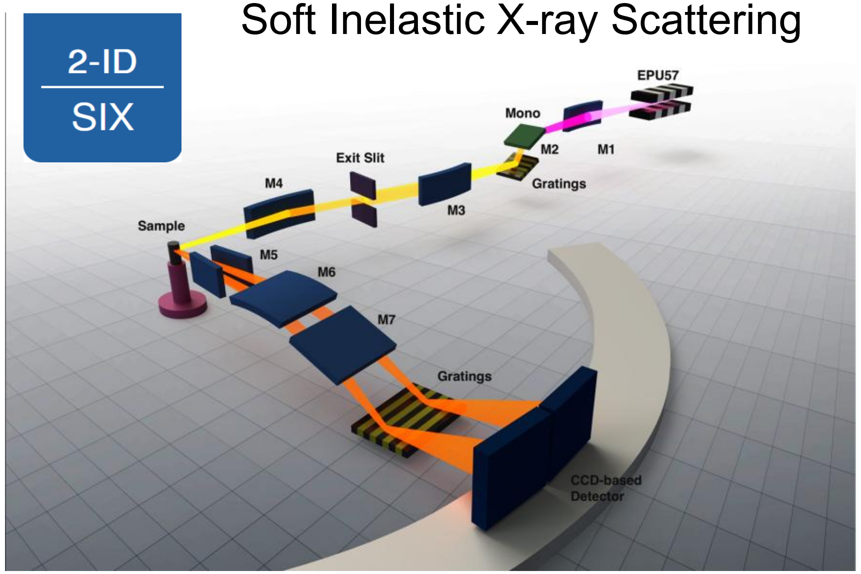
Example Beamlines at NSLS-II for Soft X-ray Energies

In situ and Operando Soft X-ray Spectroscopy





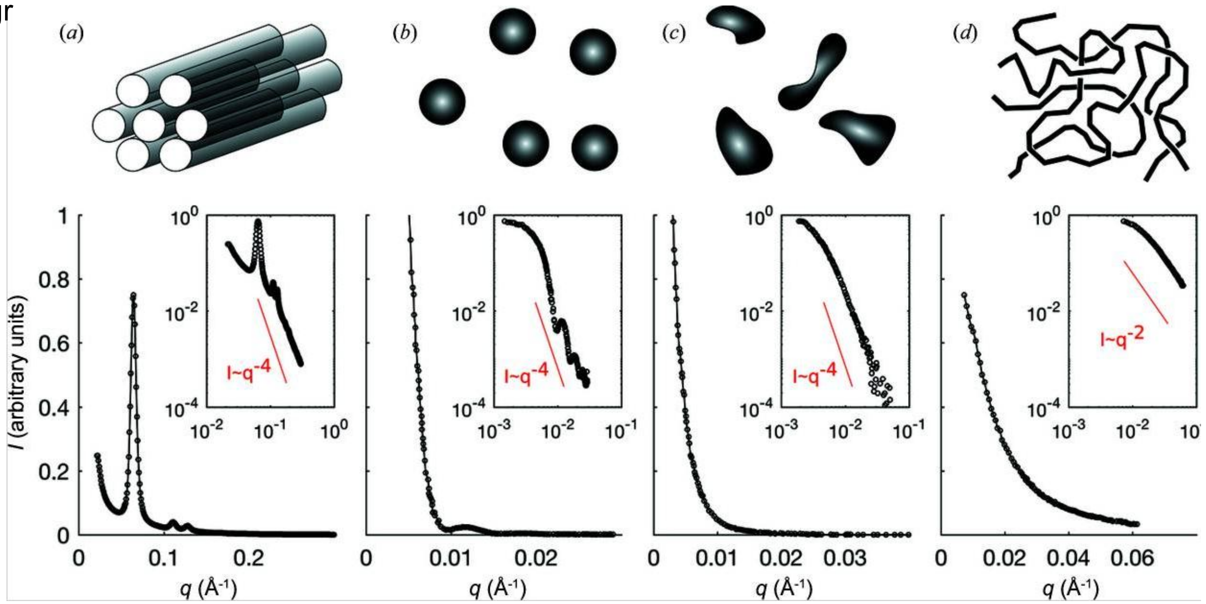
Soft Inelastic X-ray Scattering



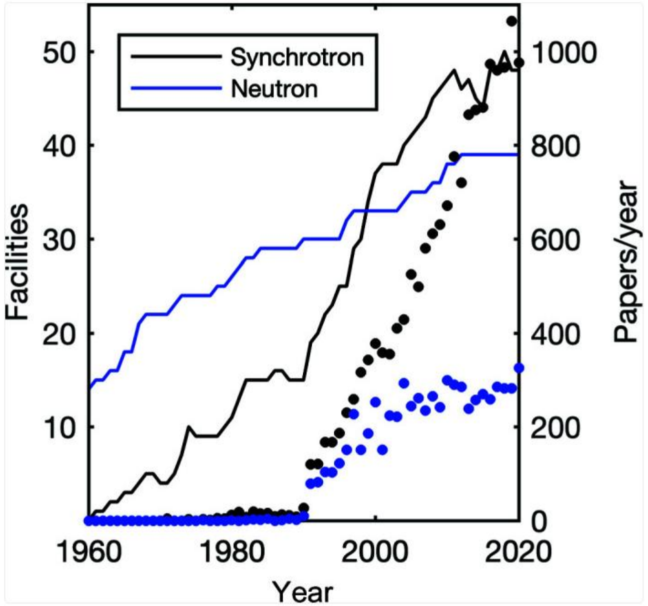
Scattering Examples: Structure and Interactions

- Materials can have structures on scales larger than atomic and crystalline
  - e.g. polymers, geological, biological …
  - Can provide useful information on protein shapes when crystallography fails.
- Larger structure => scattering into smaller angles: Small Angle X-ray Scattering (SAXS)
  - Scattered intensity analyzed in terms of "q" where $q = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right)$

From Gommes et al, J Appl Crystallogr 2021 Nov 25;54(Pt 6):1832–1843. doi: 10.1107/S1600576721010293

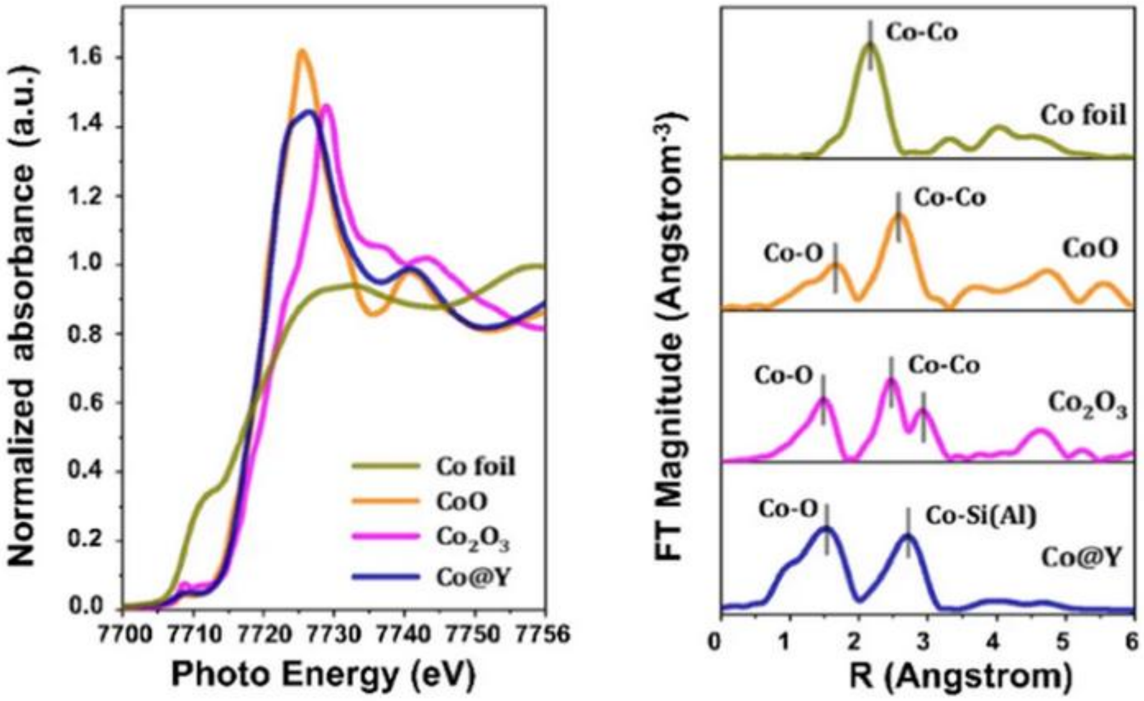


Note rapid growth of technique with availability of synchrotron facilities, large area detectors and computational facilities



Spectroscopy Examples: Absorption, Photoemission

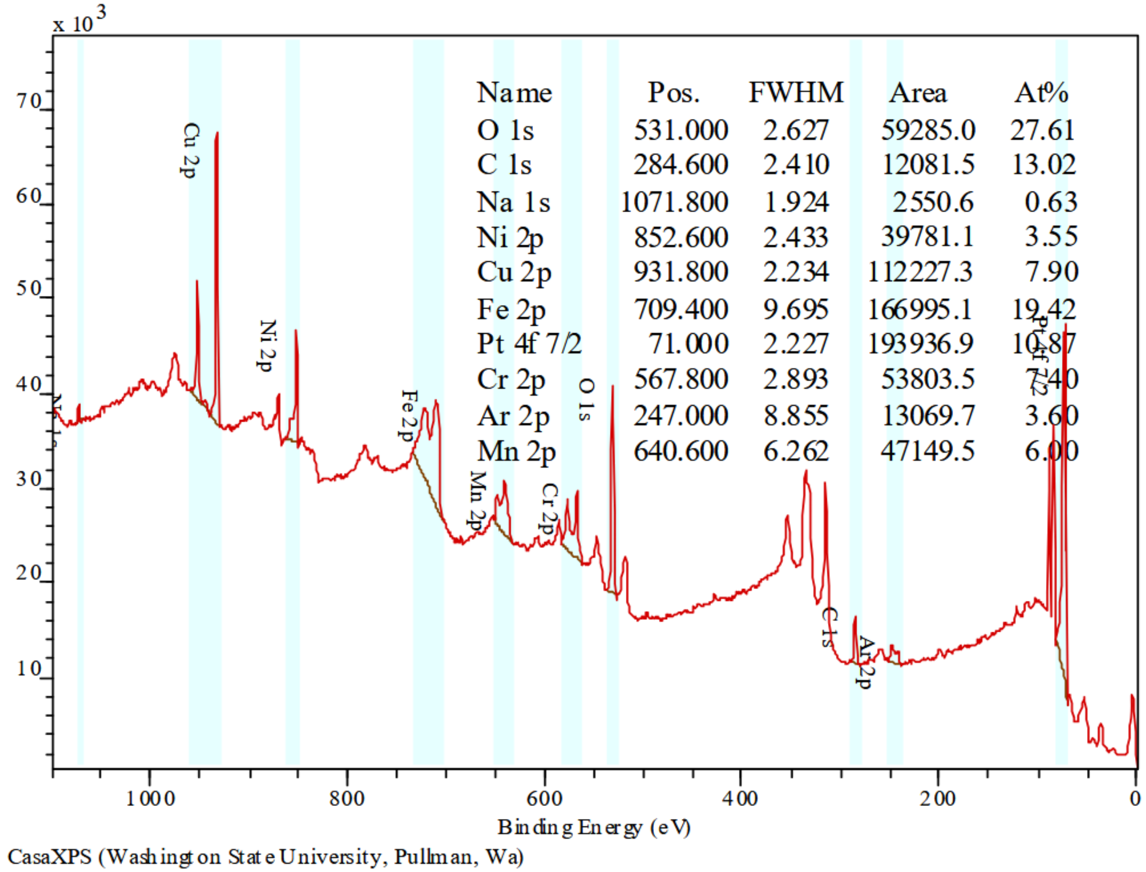
X-ray absorption spectra (XAS) showing XANES and EXAFS



M. Liu et al, Industrial Chemistry & Materials (2023)

DOI:10.1039/D3IM00074E

X-ray Photoemission Spectroscopy (XPS)



https://public.archive.wsu.edu/scudiero/public_html/documents/Examples.pdf

Summary

- Synchrotron Light Sources serve a wide and diverse range of measurement methods that are used by scientists from almost all disciplines.
- National Synchrotron Light Source II is one of four DOE synchrotron light sources
  - Advanced Photon Source @ Argonne NL, Advanced Light Source @ Berkeley Lab, Stanford Synchrotron Light Source @ SLAC
  - Others (non-DOE): Cornell High Energy Synchrotron Source (CHESS @ Cornell), Center for Advanced Microelectronic Devices (CAMD at LSU), Synchrotron Ultraviolet Radiation Facility (SURF III at NIST).
- Next Generation of synchrotron light sources (APS-U, ALS-U, NSLS-IIU)
  - Will have even smaller electron beams to yield diffraction-limited performance => Advanced scattering methods that utilize transverse coherence, e.g. X-ray speckle imaging, dynamics, …