Synchrotron Radiation Sources and Optics

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topics

- sources
- monochromators
- mirrors
- focussing

Requirements for Diffraction

- Precise details depend on nature of sample
- Collimated beam is needed to define Θ
  - ΔΘ should be < reflection width of sample
- Monochromatic beam is needed to define λ
  - $\Delta E/E = - \Delta\lambda/\lambda$ for photons
- MAD requires tunable beam, $\Delta E/E < 10^{-4}$
- Powders may benefit from larger ΔΘ
- Laue may require bandwidth of ~ 1KeV

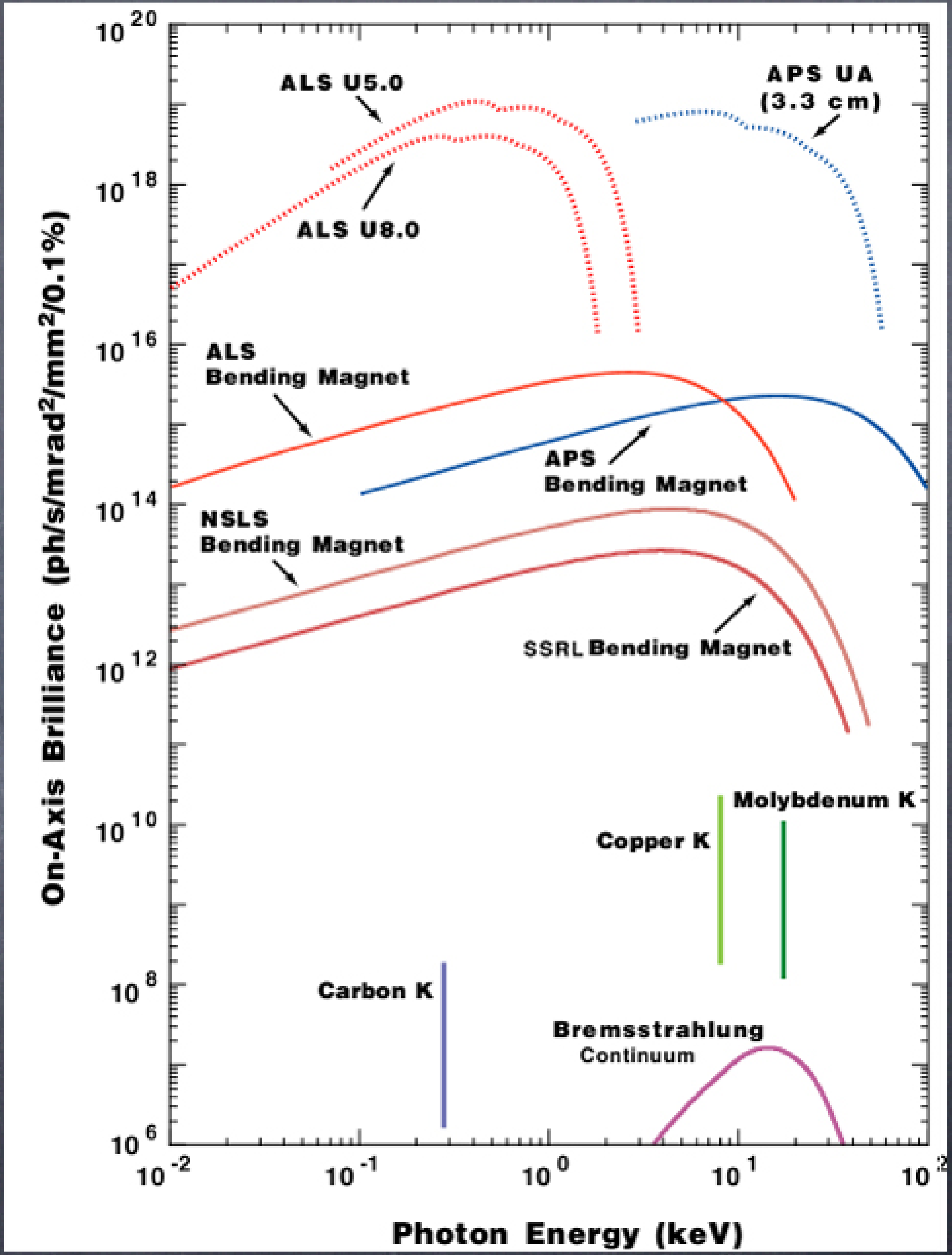
What's the problem with Lab Sources?

- Fluorescence emission from anode that is induced by high energy electron impact produces mostly monochromatic x-rays
  - not (continuously) tunable
- x-rays are emitted in all directions
  - need special optics to collect the X-rays and redirect them into roughly collimated beam

Why Synchrotron Radiation?

- It's far more intense (>10^6) than lab sources
- Tunable energy
- Naturally collimated in vertical plane - clean
  - well-matched to crystal monochromators
  - undulators produce pencil beam of x-rays
- Brilliance is much greater than other sources
  - photons/sec/source size/angular divergence
- Light comes in rapid pulses - useful for time resolution

Brilliance of X-ray Sources



graphic courtesy of APS

Light Emission

- Accelerating charged particles emit light
  - radio, microwave, infrared, visible, UV, X-rays
  - These are emitted in a dipole pattern
  - Not collimated - frequency is same as oscillation frequency - radio waves?

Relativity changes everything

- When particles move at speeds close to the speed of light
  - dipole pattern in their rest frame
  - in lab frame, radiation pattern tilts sharply into the forward direction "headlight effect"
- Frequency of emitted light measured in lab frame is dramatically higher -> x-rays

Our Neighborhood Synchrotron Source

Advanced
Photon
Source
Argonne, IL

Inside the APS:

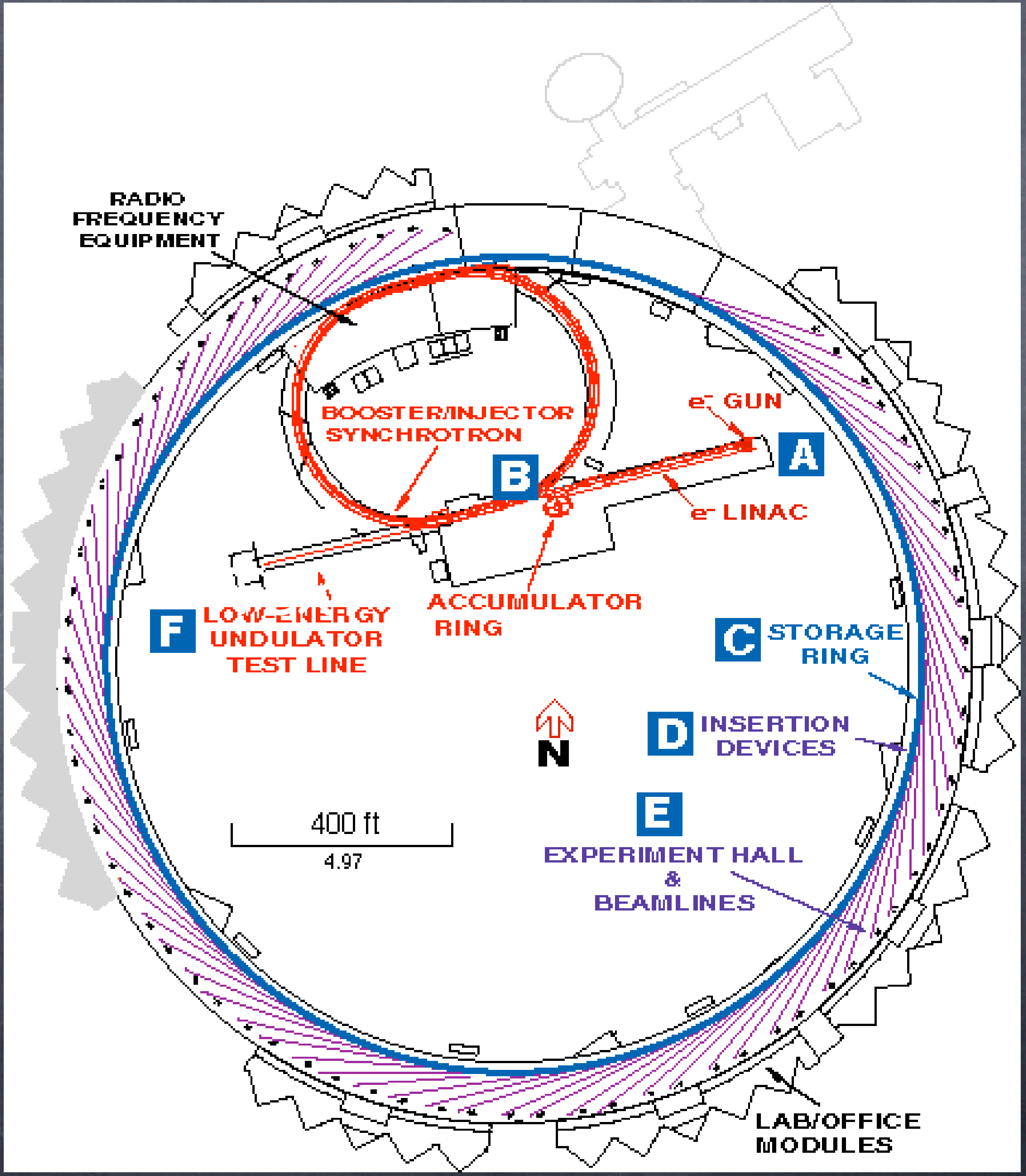
Linac

Synchrotron

Storage Ring

Insertion Devices

Beamlines!



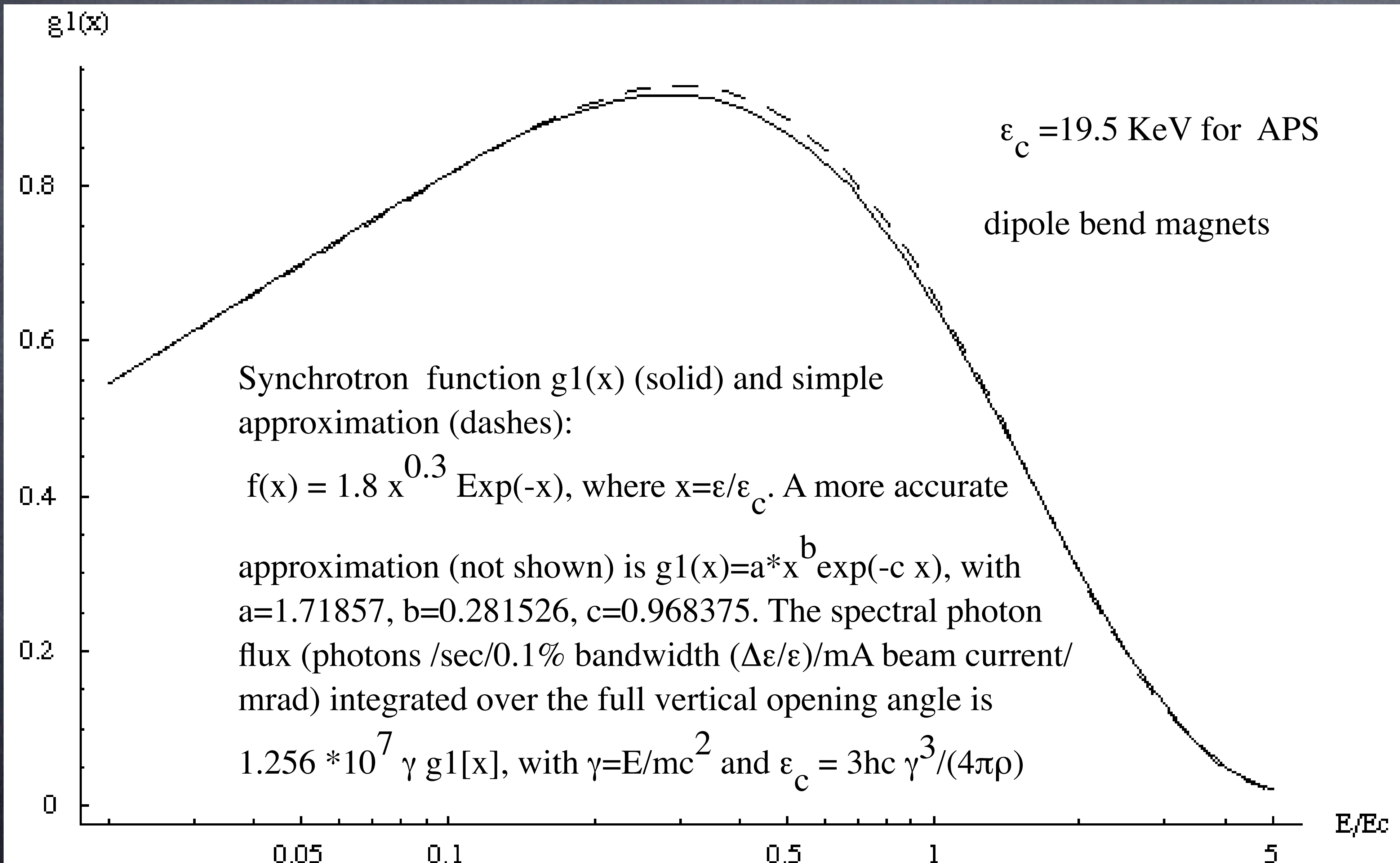
Inside the ring

- Electrons circulate very nearly at the speed of light (at the APS, only 0.75 m/s slower than c!).
- Relativistic parameter $\gamma = E/mc^2$
- Their paths are made to bend using dipole bend magnets. The beams are focussed with quadrupole and sextupole magnets
- “insertion devices” (wigglers and undulators) can be placed in straight sections between dipole bend magnets

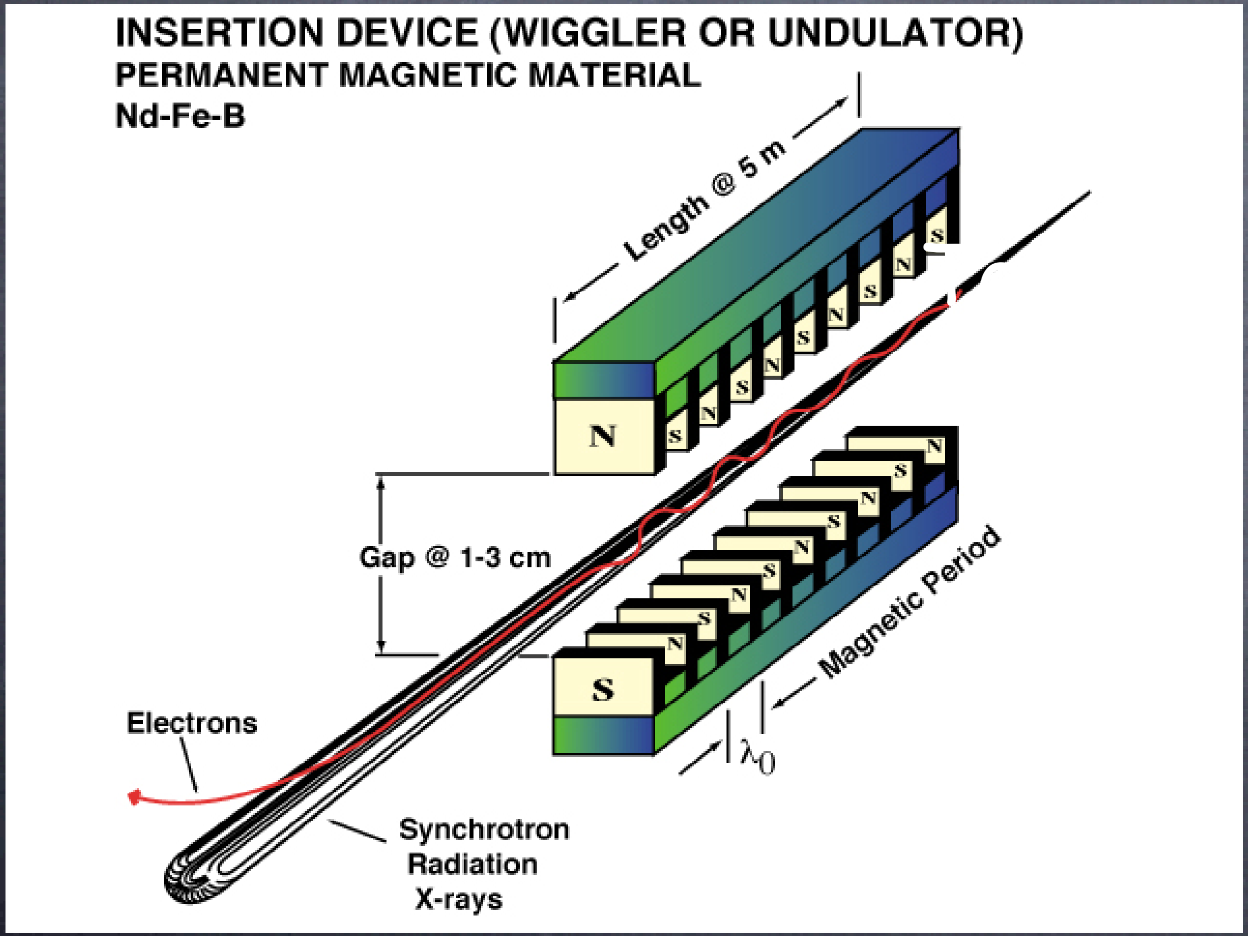
Synchrotron Radiation

- Wherever the path of the electrons bends, their velocity vector changes
- This acceleration causes them to produce electromagnetic radiation
- In the lab rest frame, this produces a horizontal fan of x-rays that is highly collimated (to $\Delta\Theta \approx 1/\gamma$) in the vertical direction and extends to high energies
- Energy is put back into electron beam by “surfing” through radio frequency (RF) cavities

Universal Flux Curve



Insertion Devices



- arrays of magnets of alternating polarity between which beam travels
- The alternating magnetic field causes the path of the electrons to wiggle back and forth
- Acceleration causes emission of radiation at each pole (typically 50 -100 poles)
- Unlike bend magnets, ID properties can be chosen to optimize beam specifically for experiments
- Two main types: Wigglers and Undulators

ID Characteristics

- Wigglers cause the electron beam to oscillate with angular deviation that is large compared to $1/\gamma$
  - Wiggler spectrum follows universal curve (like bend magnet), scaled by number of poles
- Undulators use small deflections
  - Light emitted at each pole interferes with that emitted from others
  - Energy spectrum is bunched up into harmonics
  - Radiation pattern is a pencil of light in forward direction

x-ray energy from undulator

We will take the average speed of the electron through the undulator as essentially c, with relativistic parameter $\gamma = \frac{1}{\sqrt{1-v^2/c^2}}$.

The undulator period λ_0 in the lab frame appears to the electron as λ_0/γ, i.e. very much shortened by the Lorentz contraction.

The electron oscillates back and forth and emits radiation with frequency $\omega \approx \frac{c}{(\lambda_0/\gamma)} = \gamma c/\lambda_0$ in the rest frame of its average motion through the undulator.

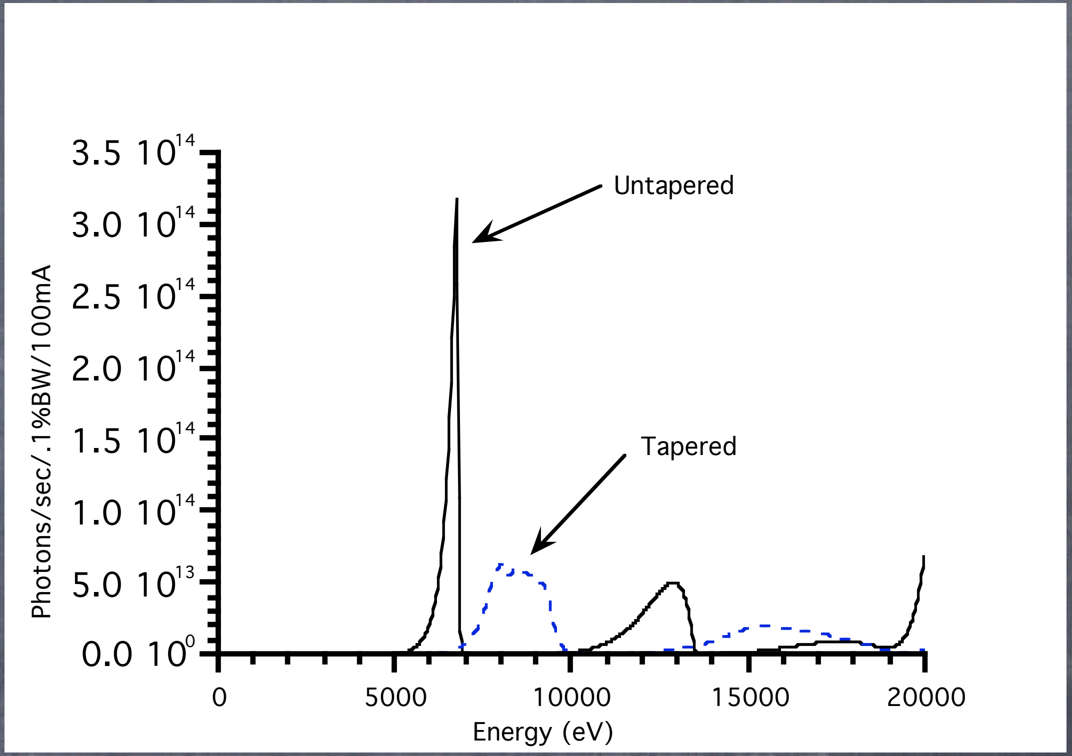
In the lab frame, the frequency of the light is increased by the relativistic doppler shift $\sqrt{\frac{1+v/c}{1-v/c}} = \gamma(1+v/c) \approx 2\gamma$.

Therefore the frequency of radiation observed in the lab frame is then $2\gamma^2 c/\lambda_0$. At the APS, $\gamma^2 \approx 2 \times 10^8$.

Calculated Flux from Undulator A

The position of undulator peaks can be tuned by adjusting the undulator gap, which varies the strength of the magnetic field felt by the electrons.

Decreasing the gap increases the field, causing a larger deflection, and slightly slowing down the electron's average speed through the undulator. This shifts the spectrum to lower energy.



The x-ray frequency of the fundamental is given approximately by $2\,\gamma^2\ \Omega_w/(1+K^2/2+\gamma^2\,\theta_0{}^2)$. Here $K=\gamma\delta_w$, where $\delta_w=\lambda_0/2\pi\rho_0$, λ_0 is the undulator period, and ρ_0 is the bend radius corresponding to the peak magnetic field.

X-ray Polarization

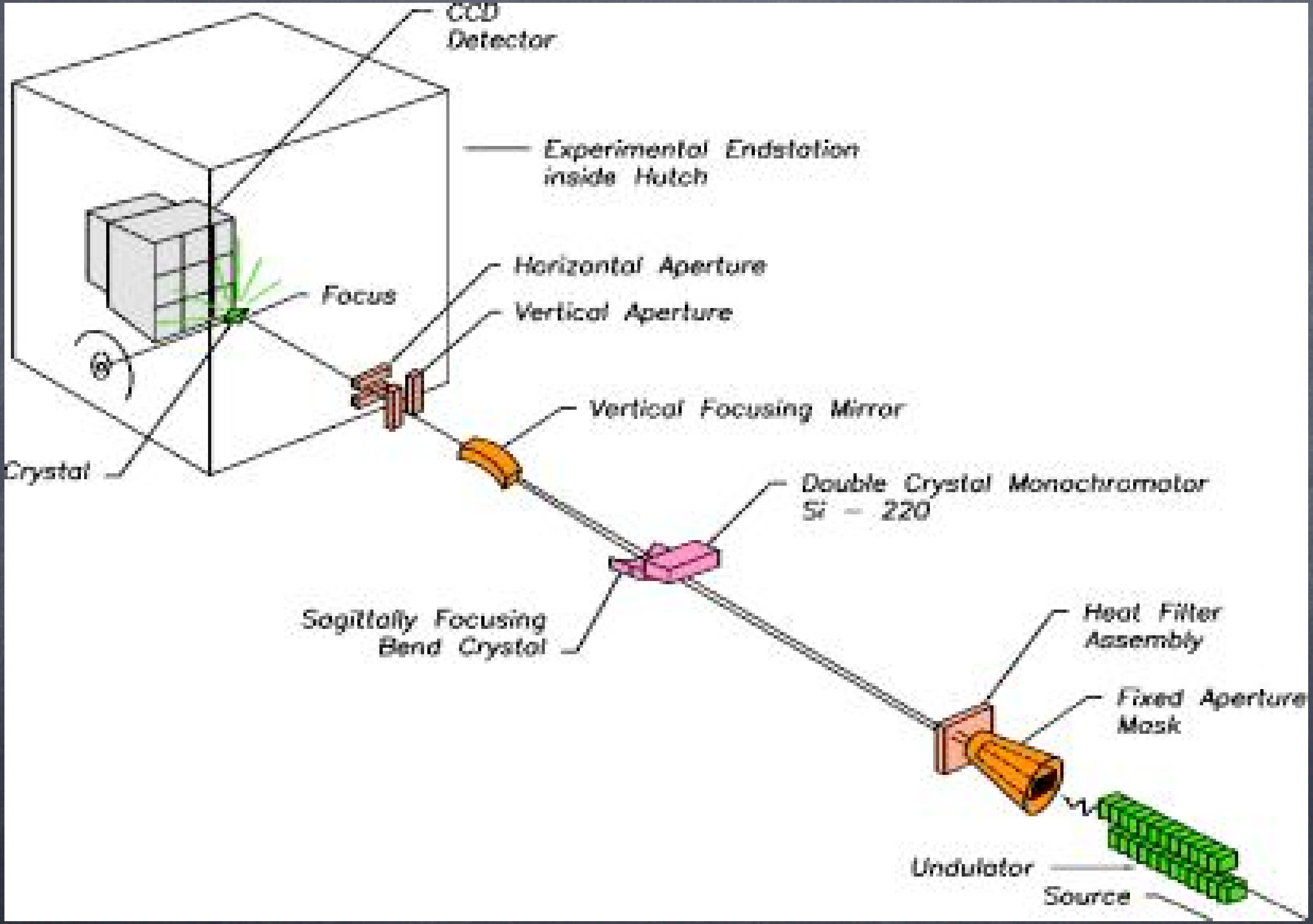
- In the orbital plane, the radiation is nearly 100% linearly polarized
- This can be used for polarized XAFS (x-ray linear dichroism) experiments on oriented specimens
- Out of the orbital plane, bend magnet radiation has some degree of left/right circular polarization
- Wiggler/undulator radiation is not circularly polarized (planar devices)

Beamlines

- Beamlines prepare the beam for experiments, and protect the users against radiation exposure. They combine x-ray optics, detector systems, computer interface electronics, and computer hardware and software.
- Typical functions:
  - Radiation shielding and safety interlock
  - Select specific energies/wavelengths using monochromators
  - Focus the beams with x-ray mirrors, bent crystals, fresnel zone plates, or refractive optics
  - Define the beams with x-ray slits
  - Detectors measure beam intensity and record diffraction pattern
  - Electronics amplify signal and interface to the computers
  - Computer control and data acquisition system orchestrates motion of the monochromator and other optics, and reads detectors, and helps remote control alignment of samples.

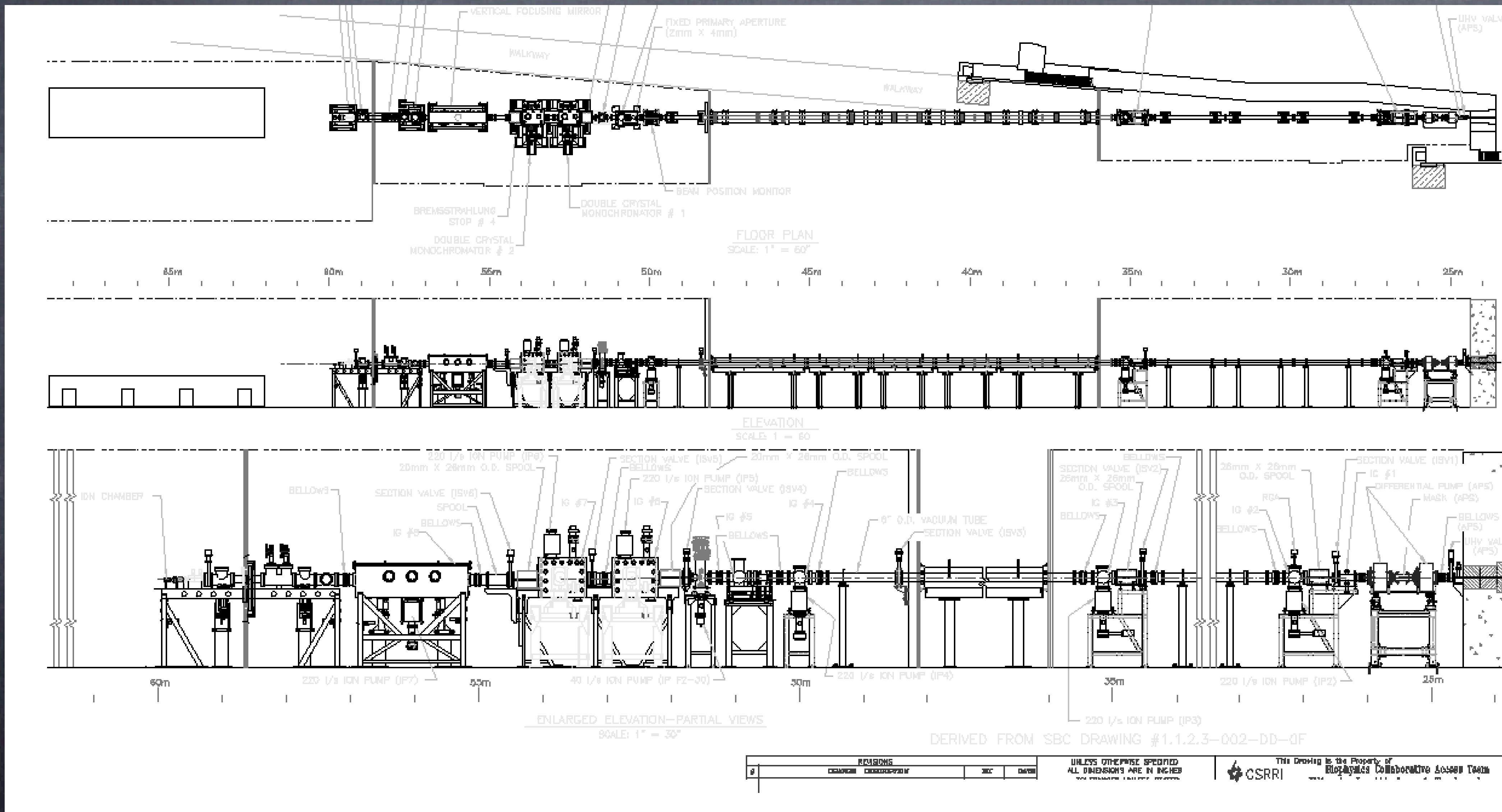
BioCAT beamline panorama

Crystallography Beamline Layout



graphic courtesy of SER-CAT

ID-18/19 Layout



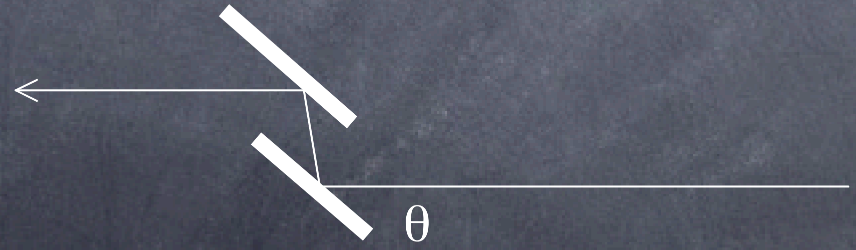
Monochromators

BioCAT
ID-18

Design by
Gerd Rosenbaum
& Larry Rock

Double-crystal monochromators

The “white” x-ray beam impinges on a perfect single crystal of silicon at a specified orientation. Those X-ray photons that are of the correct wavelength and angle of incidence θ to meet the Bragg diffraction condition $n\lambda=2\, d_{hkl} \sin(\theta)$ are diffracted through an angle 2θ; the rest are absorbed by the crystal. Here λ is the x-ray wavelength; the photon energy $\varepsilon=hc/\lambda$; and n is the harmonic number.
The spacing between diffracting atomic planes in the crystal for "reflection" hkl is $d_{hkl} =a_0/(h^2+k^2+l^2)^{1/2}$, where a_0 is the lattice constant (0.5431 nm for Si).



Si double crystal monochromator

The second crystal simply redirects the diffracted beam parallel to the incident beam. If bent, it can be used for horizontal “sagittal” focussing.

Heat load issues

- Undulators pose special challenges for optics
  - high power density makes silicon at room temperature unsuitable (mostly): need higher thermal conductivity or lower thermal expansion coefficient
  - Cooling silicon to ~100K improves both properties
  - Diamonds are excellent thermal conductors and synthetic diamonds are suitable monochromator crystals

Mirrors

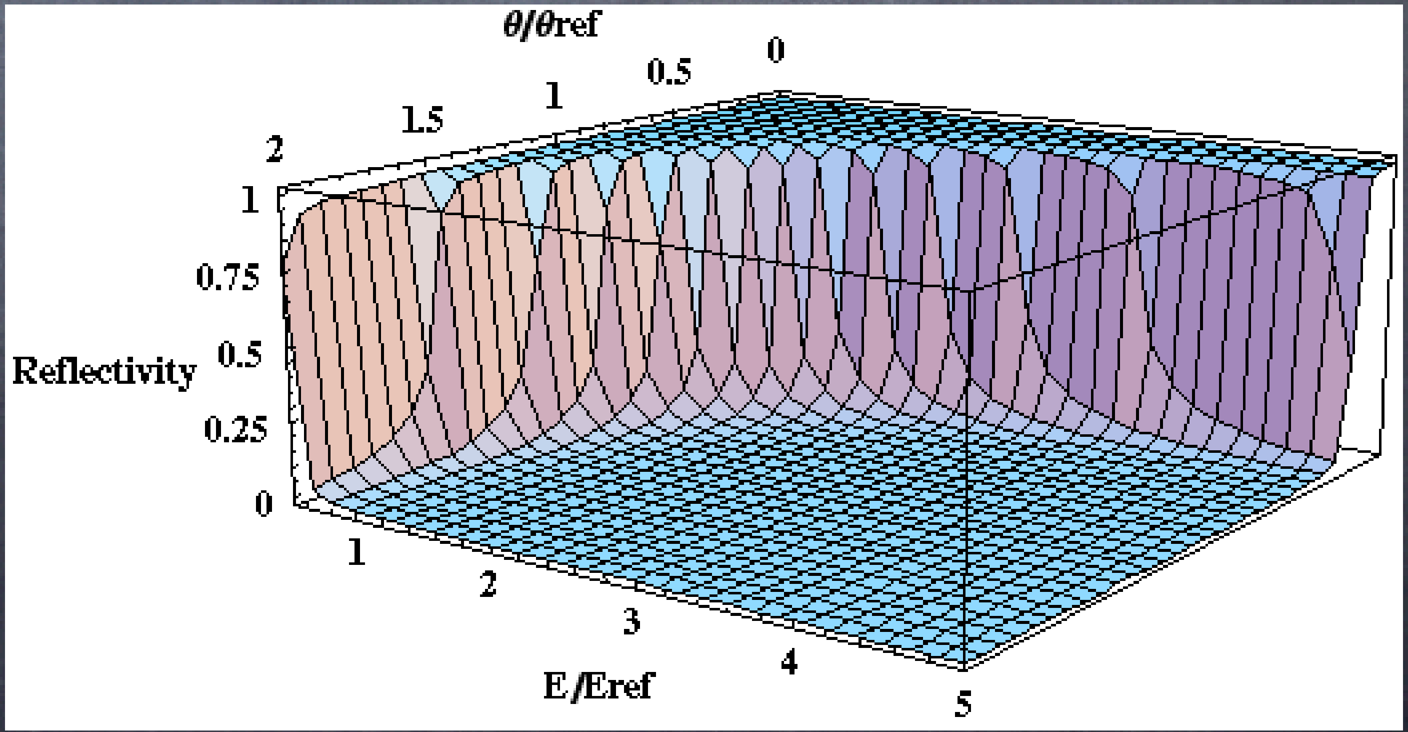
This is a one meter long ULE titanium silicate. It is polished to ~ 2Å RMS roughness; it was measured at ~1 microradian RMS slope error before bending. It is has Pt, Rh, and uncoated stripes to allow the user to choose the coating.

The mirror is dynamically bent and positioned.
Design by Gerd Rosenbaum and Larry Rock Automation.

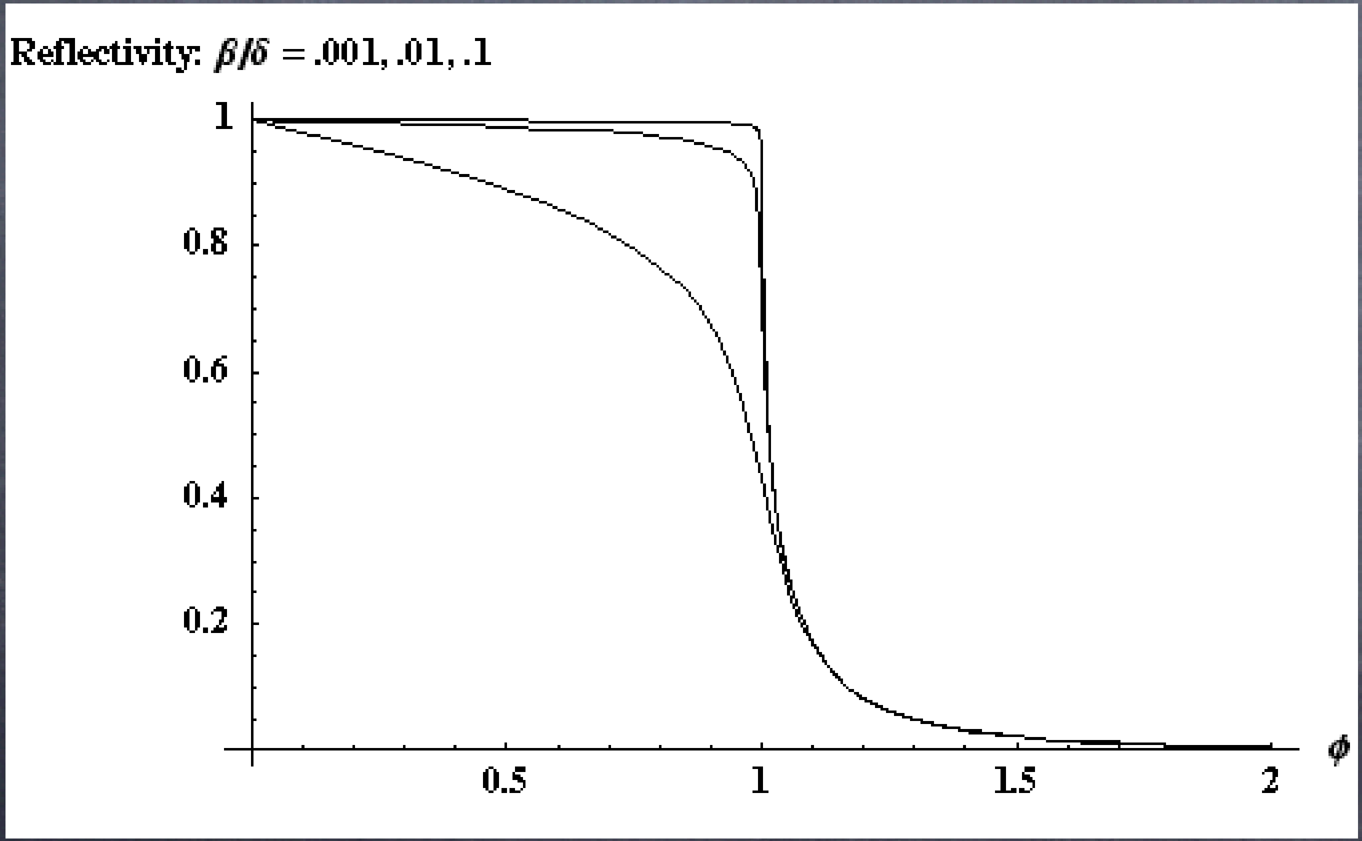
Grazing incidence mirrors

For most materials, the index of refraction at x-ray energies is a complex number $n=1-\delta - i\beta$. The real and imaginary parts describe dispersion and absorption. Total external reflection occurs at angles $\theta < \theta_c$, where the "critical angle" $\theta_c = (2\delta)^{1/2}$, which is typically 5-10 milliradians, i.e. grazing incidence. Higher atomic number coatings (e.g. Pt, Pd, Rh) allow the mirror to reflect at greater angles and higher energies, at the cost of higher absorption. To a good approximation $E_c\,\theta_c$ = constant for a given coating. For ULE ~30 KeV mrad; Pd, Rh ~ 60 KeV mrad; Pt ~ 80 KeV mrad.

Surface plot of reflectivity vs angle and photon energy



Mirror reflectivity vs absorptivity of surface coating



$\Phi = \Theta / \Theta_c$

Harmonics

- Monochromators transmit not only the desired fundamental energy, but also some harmonics of that energy. Allowed harmonics for Si(111) include 333, 444, 555, 777…
- These can be reduced by slightly misaligning "detuning" the second crystal using a piezoelectric transducer ("piezo"). Detuning reduces the harmonic content much more than the fundamental.
- If a mirror follows the monochromator, its angle can be adjusted so that it reflects the fundamental, but does not reflect the harmonics.
- We have developed devices called "Beam Cleaners" can be made to select particular energies

Focussing equations

- Meridional focussing (typically, vertical mirror)
  - optic curved along beam direction
  - $2/(R\,\mathrm{Sin}(\Theta)) = 1/u + 1/v$
- Sagittal focussing (typically, horizontal crystal or mirror)
  - optic curved perpendicular to beam direction
  - $2\,\mathrm{Sin}(\Theta)/R = 1/u + 1/v$
- u,v are source to optic distance, optic to focus distance
- R is local radius of curvature of optic
- Kirkpatrick-Baez mirror or Toroidal mirror

Conclusion

- We have covered sources, monochromators, mirrors, and focussing
- In single crystal diffraction experiments, once a monochromatic beam is delivered to the sample, the goniometer and detector do most of the work.
- In MAD experiments, it is necessary to measure the diffraction patterns at several relatively close energies, but the principles are the same
- Other variants of diffraction (e.g. DAFS) require more sophisticated control system, but the principles are the same