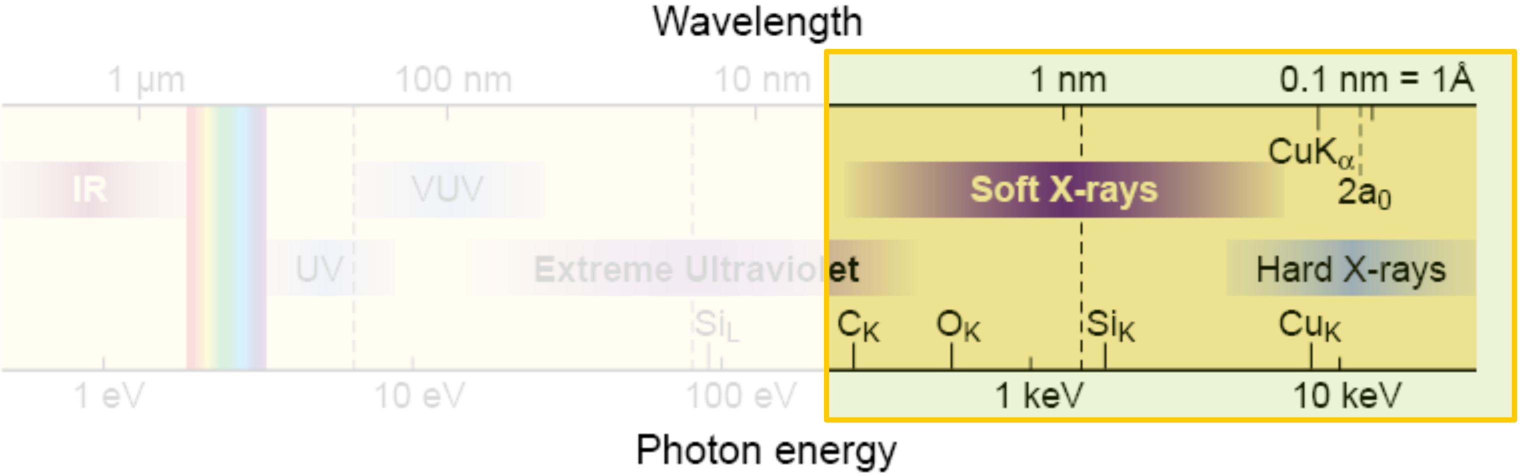
X-ray sources and optics

Dimosthenis Sokaras

SLAC National Accelerator Laboratory

Electromagnetic Waves Spectrum: X-rays



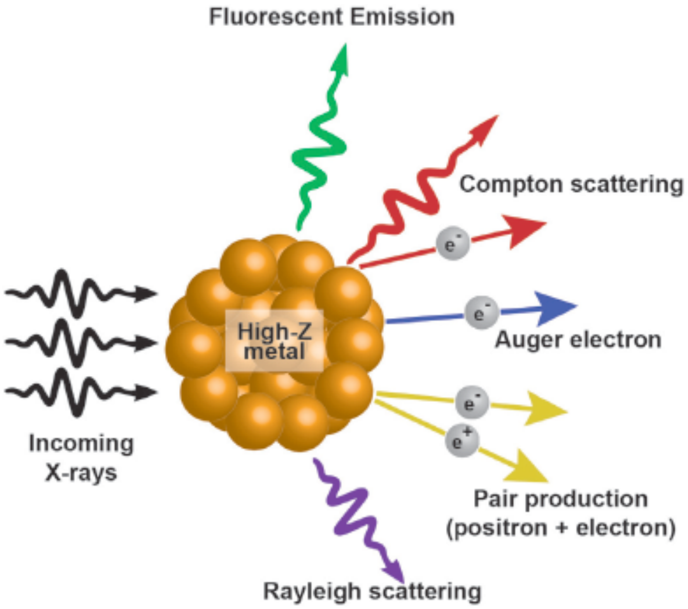
Energy → 0.1-100*keV*

$$\text{Wavelength} \rightarrow \lambda[\mathring{A}] = \frac{12.398}{E[keV]} \rightarrow 0.1 - 60\mathring{A}$$

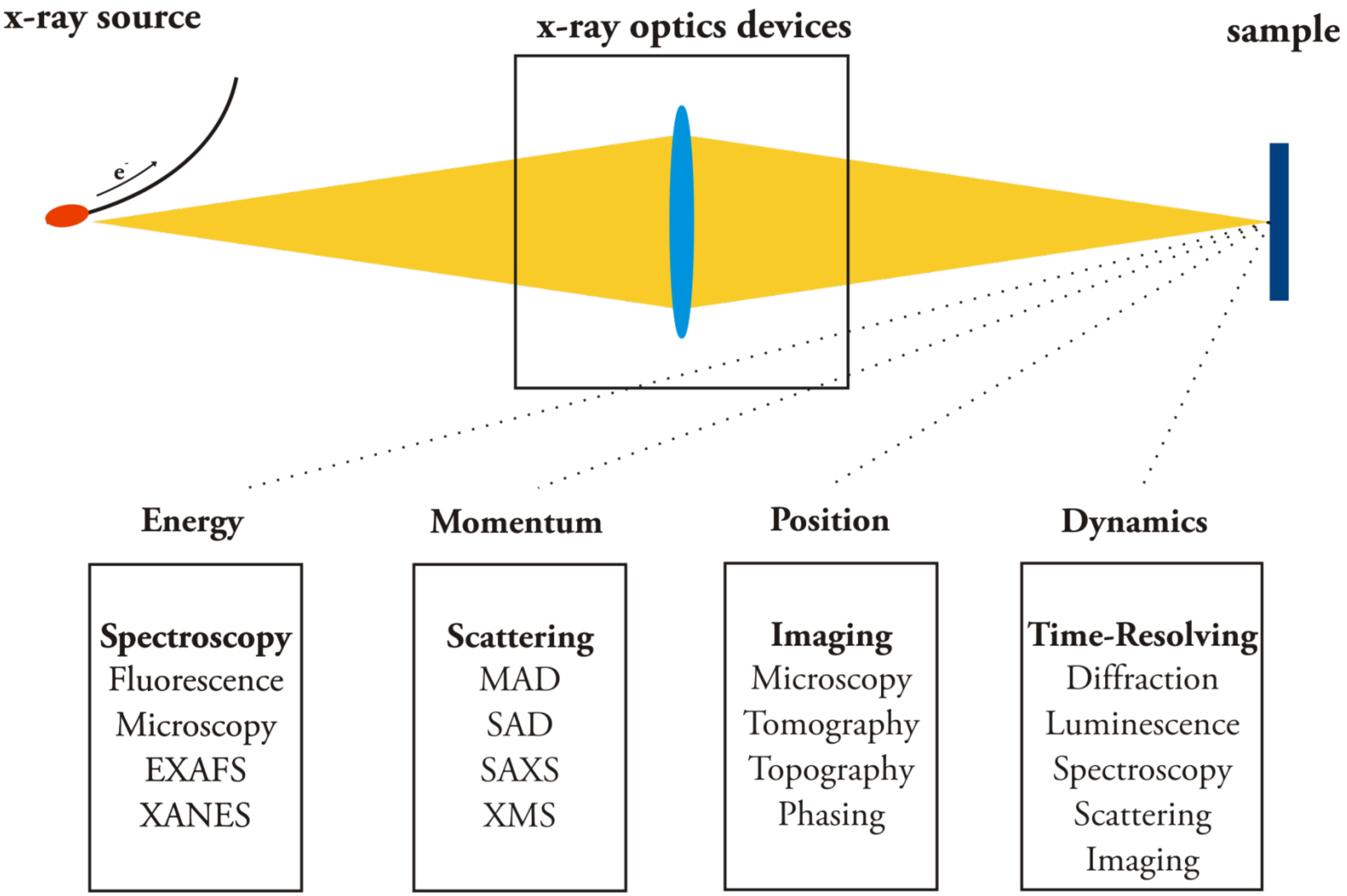
X-rays Interaction with Matter

Properties for the interaction of X-ray with matter are theoretically described with this Hamiltonian interaction

$$H = H_0 - \frac{e}{mc}\underbrace{\mathbf{p}\cdot\mathbf{A}(\mathbf{r})}_{\text{absorption/ emission}} + \frac{1}{2m}\left(\frac{e}{c}\right)^2 \underbrace{\mathbf{A}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})}_{\text{scattering}}$$



X-ray Sources: Motivation – Aim in Research



Energy

Spectroscopy
Fluorescence
Microscopy
EXAFS
XANES

Momentum

Scattering
MAD
SAD
SAXS
XMS

Position

Imaging
Microscopy
Tomography
Topography
Phasing

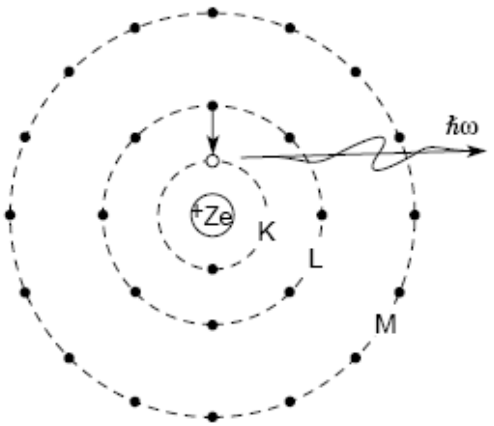
Dynamics

Time-Resolving
Diffraction
Luminescence
Spectroscopy
Scattering
Imaging

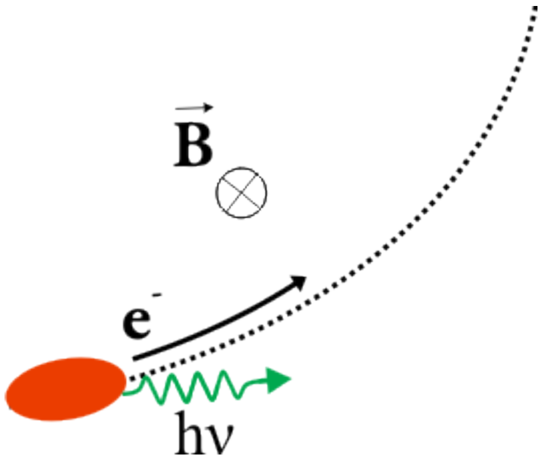
$$E\Psi(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r})$$

X-ray Sources: Principles for X-ray Emission

Main Mechanisms for X-ray Sources



- Characteristic X-rays
  - Relaxation of atomic excited states



- Acceleration of charged particles
  - Synchrotron Radiation
  - Bremsstrahlung Radiation
  - Plasma sources

Properties for an X-ray source

Performance Properties

- ***energy content***
- ***flux***
- ***Beam size***
- *angular convergence*
- ***stability***
- *polarization*
- *time domain*
- *Coherence*

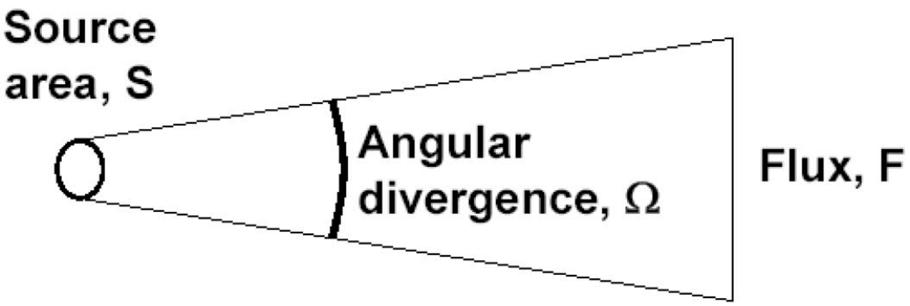
Practical Properties

- ***Cost***
- ***Availability/Access***
- ***Portability ?***

Flux = $\dfrac{\text{\# of photons in given } \Delta\lambda/\lambda}{\text{sec}}$

Brightness = $\dfrac{\text{\# of photons in given } \Delta\lambda/\lambda}{\text{sec, mrad } \theta\text{, mrad } \varphi\text{, mm}^2}$

(a measure of concentration of the radiation)

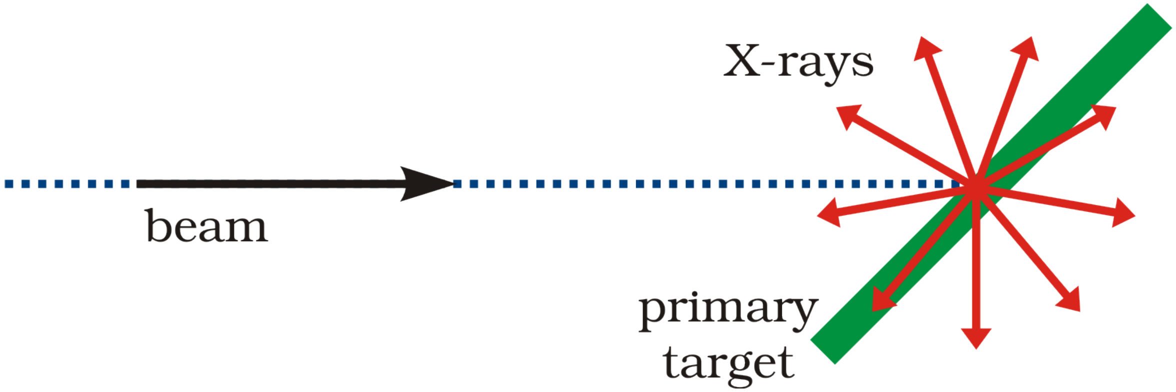


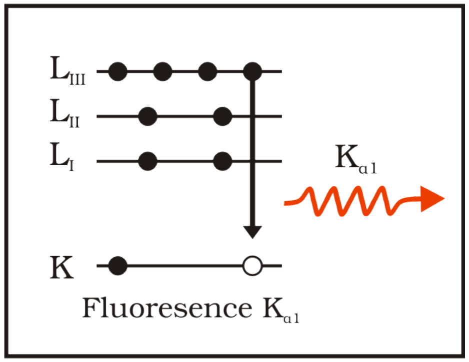
Brightness = constant x $\dfrac{F}{S \times \Omega}$

X-ray Sources: X-ray Tubes

Characteristic X-rays based Sources:

- Ionization of Primary Targets by means of irradiation:
  - Heavy ions (Electrostatic Accelerators)
  - Electrons (X-ray Tubes, e^- accelerators)

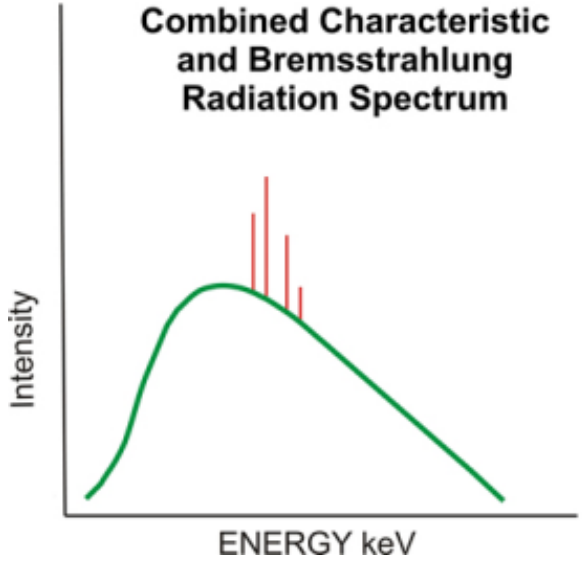


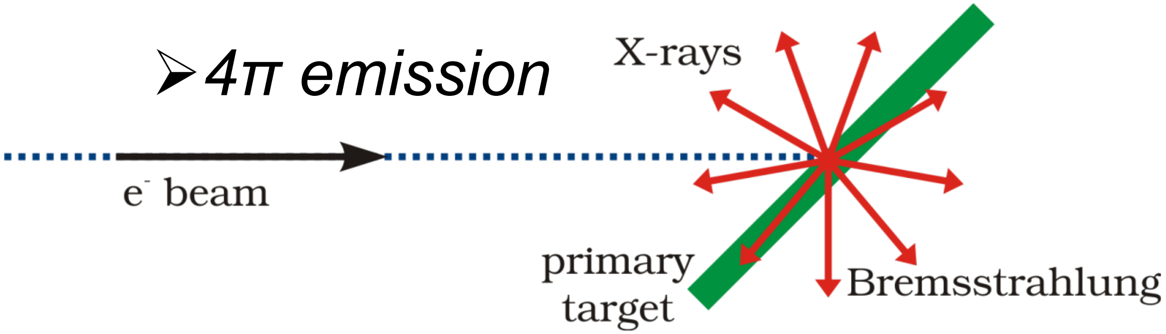


X-ray Sources: X-ray Tubes

Characteristic X-rays based Sources:

- X-ray Tubes
  - 1% of power becomes x-rays
  - Limitation = heat of the anode
  - Few *W* to several *kW*
  - *Few to tens of keV photons*
  - *4π emission*

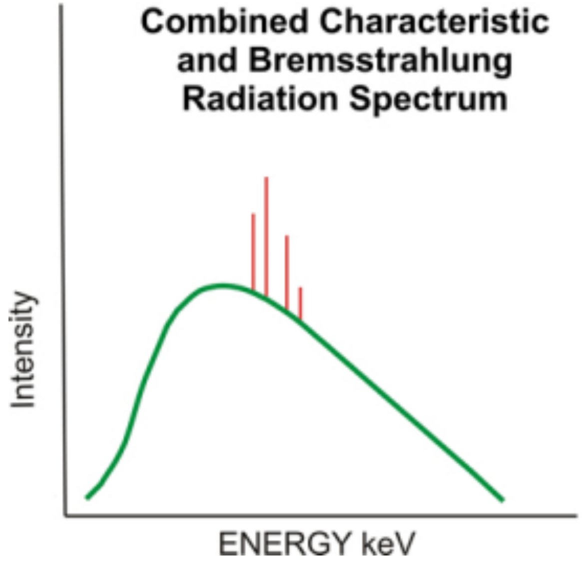


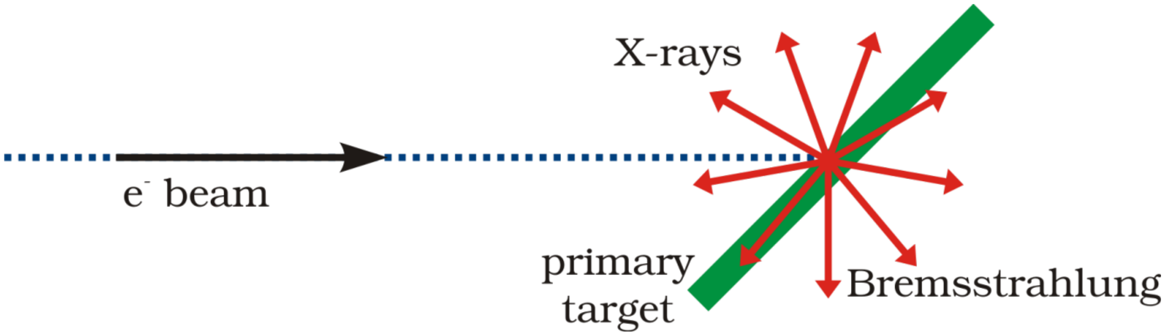


X-ray Sources: X-ray Tubes

Characteristic X-rays based Sources:

- X-ray Tubes
  - Fixed anode tube
  - Rotating Anode
  - Liquid Metal Anode





X-ray Sources: X-ray Tubes

Characteristic X-rays based Sources:

- X-ray Tubes

Combined Characteristic
and Bremsstrahlung
Radiation Spectrum

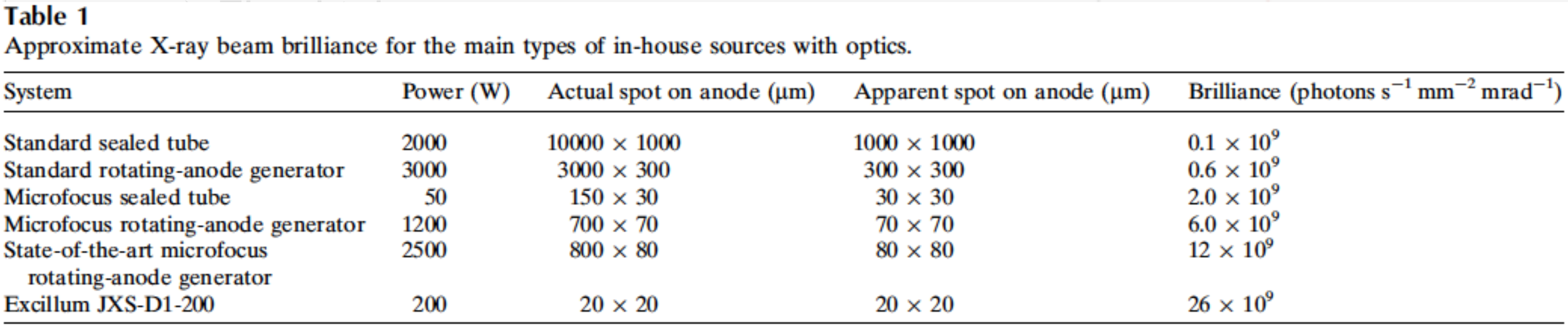


Table 1

Approximate X-ray beam brilliance for the main types of in-house sources with optics.

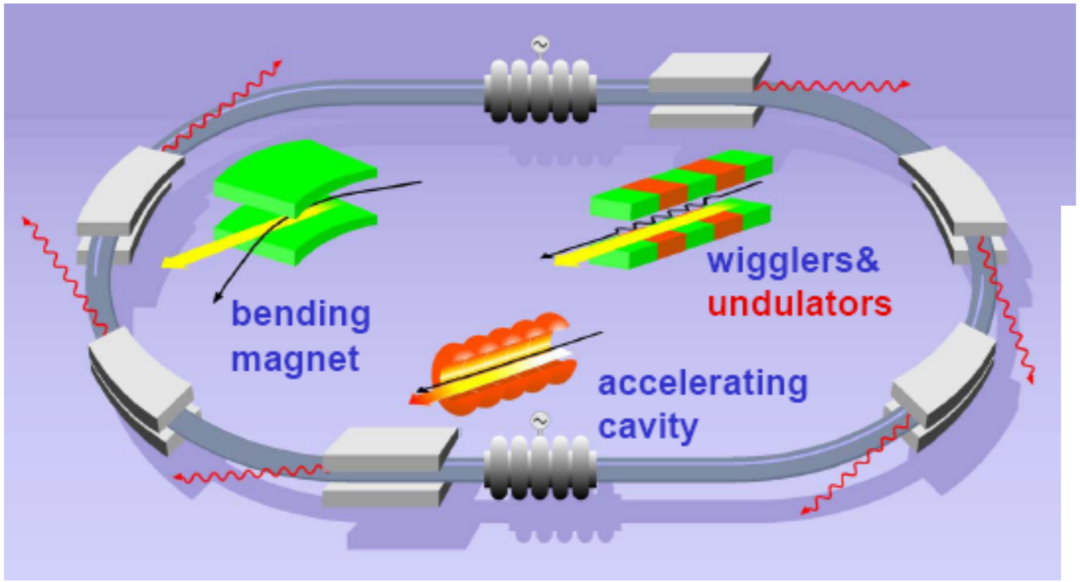
System	Power (W)	Actual spot on anode (μm)	Apparent spot on anode (μm)	Brilliance (photons s^{-1} mm^{-2} $mrad^{-1}$)
Standard sealed tube	2000	10000 × 1000	1000 × 1000	0.1×10^9
Standard rotating-anode generator	3000	3000 × 300	300 × 300	0.6×10^9
Microfocus sealed tube	50	150 × 30	30 × 30	2.0×10^9
Microfocus rotating-anode generator	1200	700 × 70	70 × 70	6.0×10^9
State-of-the-art microfocus rotating-anode generator	2500	800 × 80	80 × 80	12×10^9
Excillum JXS-D1-200	200	20 × 20	20 × 20	26×10^9

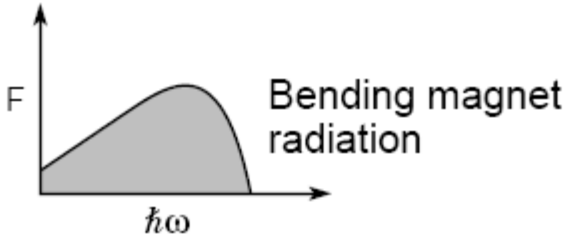
Acta Cryst. (2013). D 69 , 1283–1288

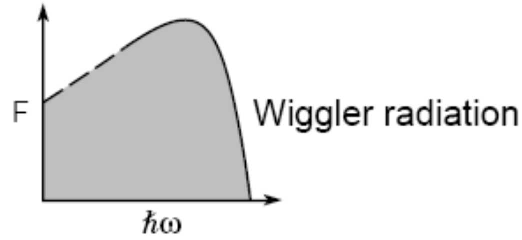
X-ray Sources: Synchrotron Radiation

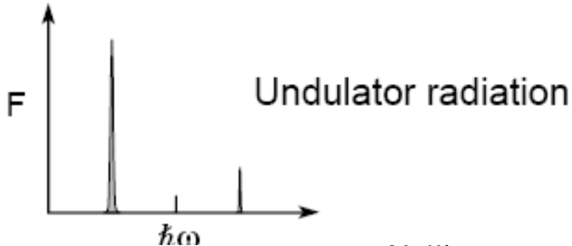
Synchrotron Radiation based Sources

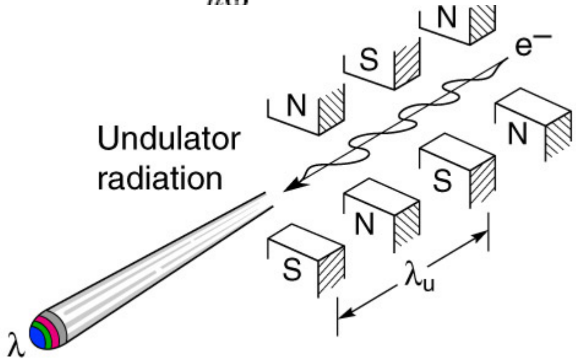
- **Storage Rings**
  - Large Scale Laboratories
  - Relativistic Electrons/Positrons (1-7 GeV)
  - Acceleration Magnetic Field
    - Insertion Devices
  - Emission cone in forward angles









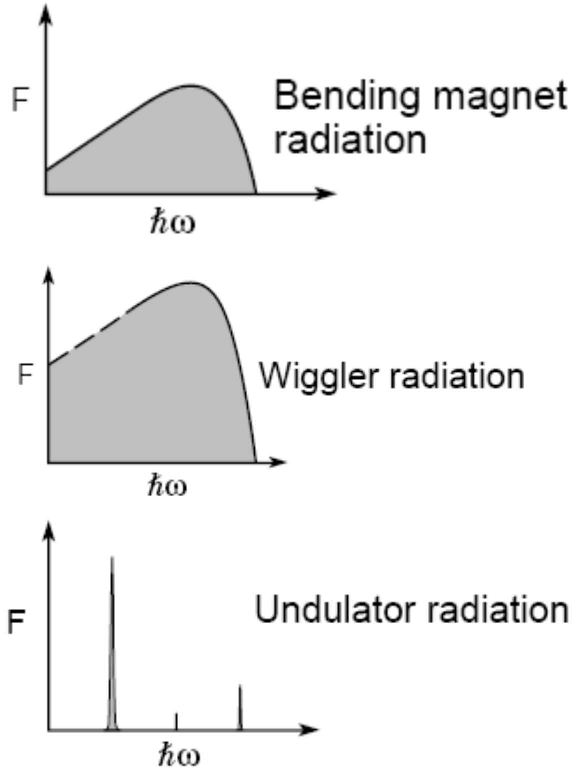


X-ray Sources: Synchrotron Radiation

Synchrotron Radiation based Sources:

- **Storage Rings**
  - Bending Magnets (~10^{11} photons/s)
  - Wigglers (~10^{13} photons/s)
  - Undulators (~10^{14} photons/s)

- **Properties**
  - **Unprecedented flux**
  - **Very broad energy range**
  - **Forward emission / small divergence**
  - **Polarization**



X-ray Sources: Synchrotron Radiation

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- **Pro**
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  - **Polarization**

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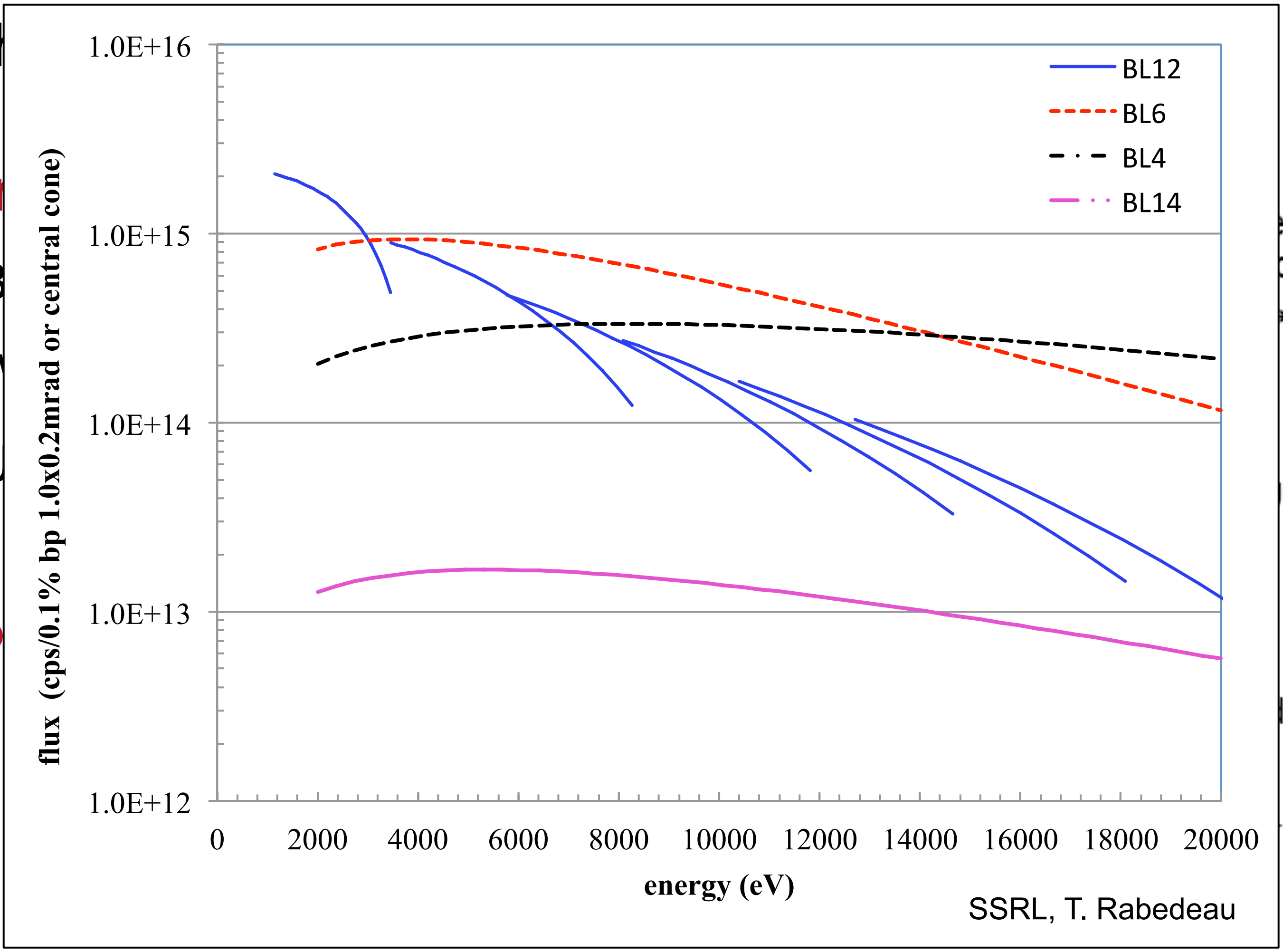
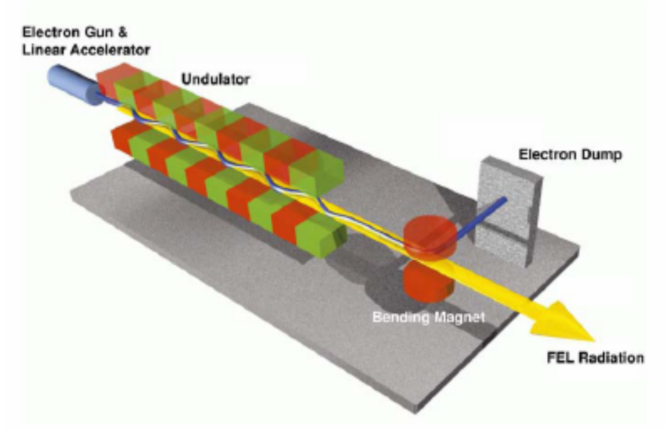
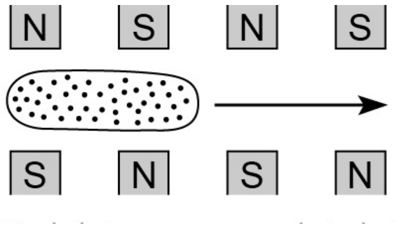


SSRL, T. Rabedeau

X-ray Sources: X-ray Free Electron Laser

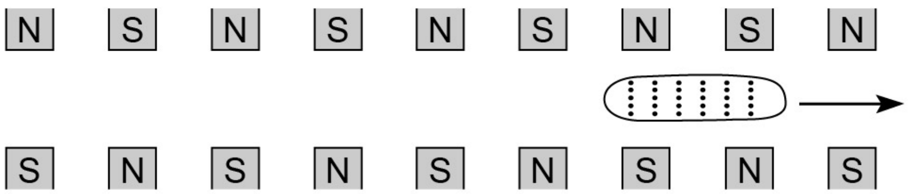


Undulator

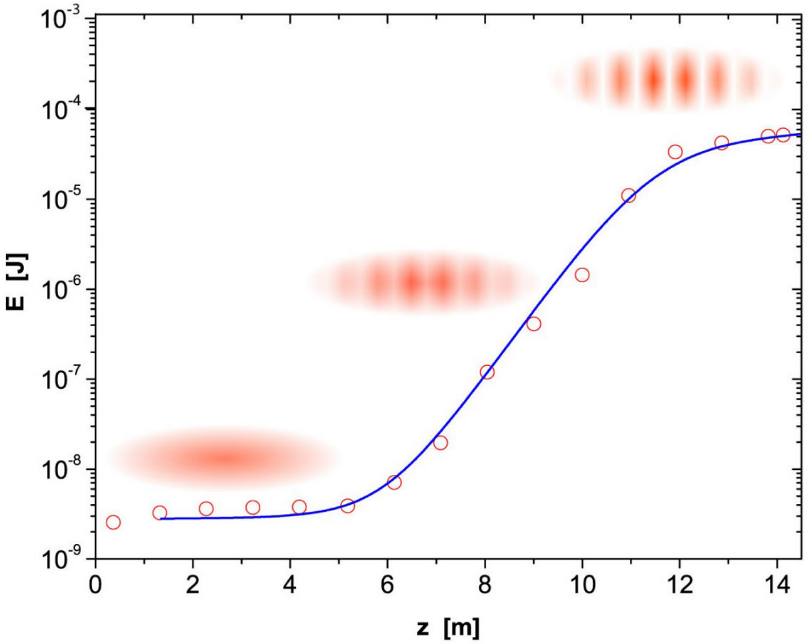


Uncorrelated electron positions / radiated fields

Very long Undulator - XFEL



Microbunching by own radiated fields
strongly correlated waves of electron and fields



Courtesy of K-J. Kim

Gain_Saturation_FEL_graph.ai

X-ray

SLAC

➢X-r

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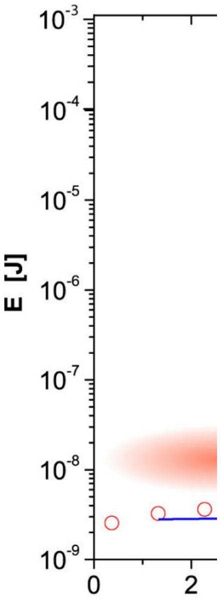

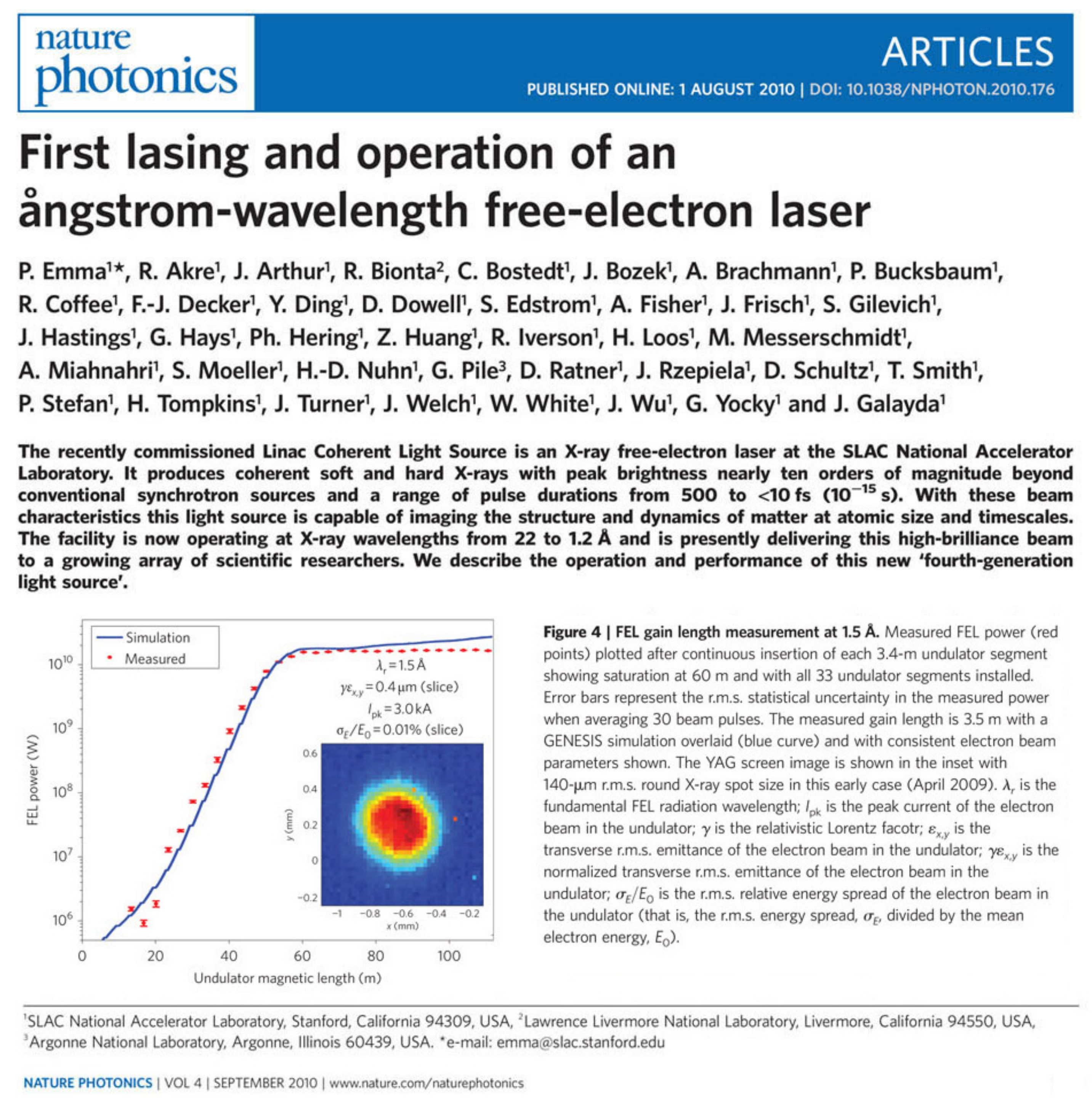

nature photonics | ARTICLES
PUBLISHED ONLINE: 1 AUGUST 2010 | DOI: 10.1038/NPHOTON.2010.176

First lasing and operation of an ångstrom-wavelength free-electron laser

P. Emma[1]*, R. Akre[1], J. Arthur[1], R. Bionta[2], C. Bostedt[1], J. Bozek[1], A. Brachmann[1], P. Bucksbaum[1], R. Coffee[1], F.-J. Decker[1], Y. Ding[1], D. Dowell[1], S. Edstrom[1], A. Fisher[1], J. Frisch[1], S. Gilevich[1], J. Hastings[1], G. Hays[1], Ph. Hering[1], Z. Huang[1], R. Iverson[1], H. Loos[1], M. Messerschmidt[1], A. Miahnahri[1], S. Moeller[1], H.-D. Nuhn[1], G. Pile[3], D. Ratner[1], J. Rzepiela[1], D. Schultz[1], T. Smith[1], P. Stefan[1], H. Tompkins[1], J. Turner[1], J. Welch[1], W. White[1], J. Wu[1], G. Yocky[1] and J. Galayda[1]

The recently commissioned Linac Coherent Light Source is an X-ray free-electron laser at the SLAC National Accelerator Laboratory. It produces coherent soft and hard X-rays with peak brightness nearly ten orders of magnitude beyond conventional synchrotron sources and a range of pulse durations from 500 to <10 fs (10^{-15} s). With these beam characteristics this light source is capable of imaging the structure and dynamics of matter at atomic size and timescales. The facility is now operating at X-ray wavelengths from 22 to 1.2 Å and is presently delivering this high-brilliance beam to a growing array of scientific researchers. We describe the operation and performance of this new 'fourth-generation light source'.

Figure 4 | FEL gain length measurement at 1.5 Å. Measured FEL power (red points) plotted after continuous insertion of each 3.4-m undulator segment showing saturation at 60 m and with all 33 undulator segments installed. Error bars represent the r.m.s. statistical uncertainty in the measured power when averaging 30 beam pulses. The measured gain length is 3.5 m with a GENESIS simulation overlaid (blue curve) and with consistent electron beam parameters shown. The YAG screen image is shown in the inset with 140-μm r.m.s. round X-ray spot size in this early case (April 2009). λ_r is the fundamental FEL radiation wavelength; I_{pk} is the peak current of the electron beam in the undulator; γ is the relativistic Lorentz facotr; $\varepsilon_{x,y}$ is the transverse r.m.s. emittance of the electron beam in the undulator; $\gamma\varepsilon_{x,y}$ is the normalized transverse r.m.s. emittance of the electron beam in the undulator; σ_E/E_0 is the r.m.s. relative energy spread of the electron beam in the undulator (that is, the r.m.s. energy spread, σ_E, divided by the mean electron energy, E_0).

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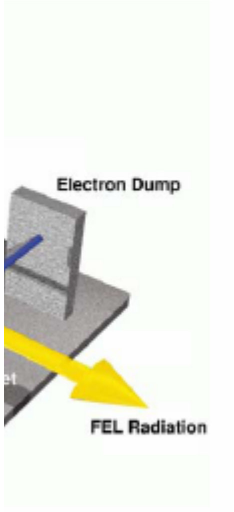
[1]SLAC National Accelerator Laboratory, Stanford, California 94309, USA, [2]Lawrence Livermore National Laboratory, Livermore, California 94550, USA, [3]Argonne National Laboratory, Argonne, Illinois 60439, USA. *e-mail: emma@slac.stanford.edu



X-ray Sources: Brilliance

Quality Factor for X-ray Sources

Brilliance = Radiated power per unit area per unit solid angle per unit spectral bandwidth

Unit → *photons/s/mrad*^{2}*/mm*^{2}*/0.1%bandwith*

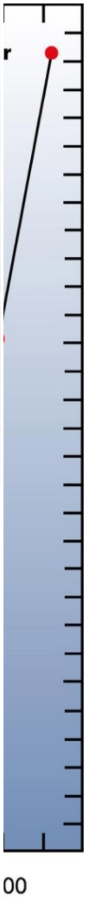
Brilliance → Invariant quantity

X-ray Sources: Brilliance

X-ray tubes

Synchrotron Radiation sources

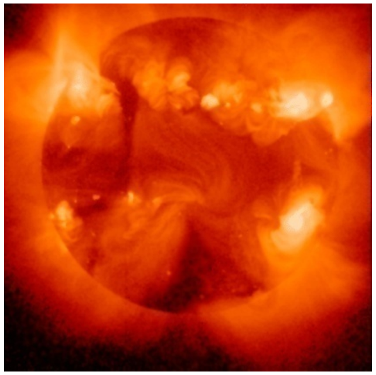
X-ray FELs



X-ray Sources: Natural Sources

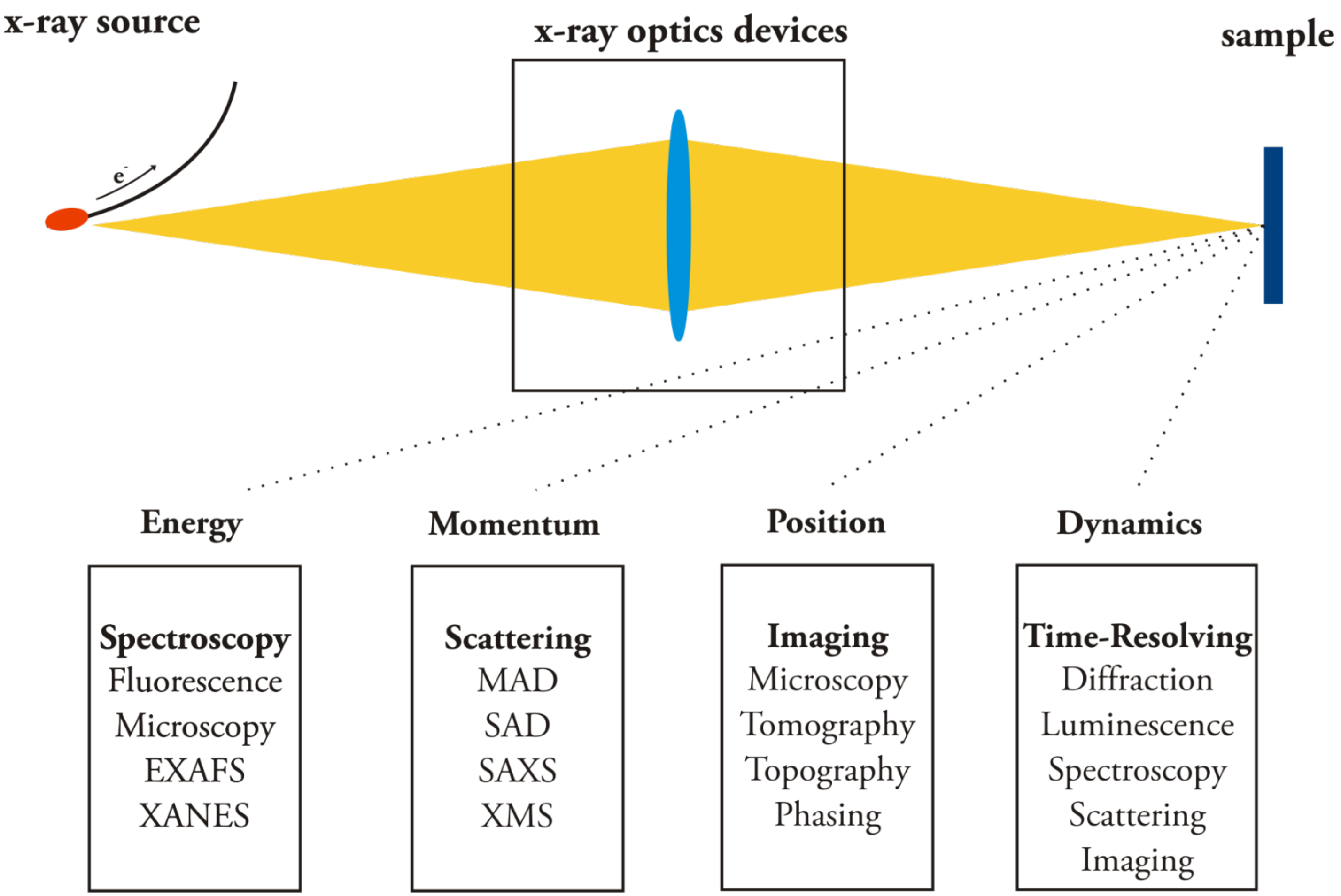
Natural X-ray Sources:

- *Radioisotopes (^{241}Am, ^{55}Fe, ^{109}Cd, etc.)*
- *Stars, Super Novas, Cosmic Background*



An X-ray image of the Sun, T~2·10^6K

X-ray Sources: Motivation – Aim in Research



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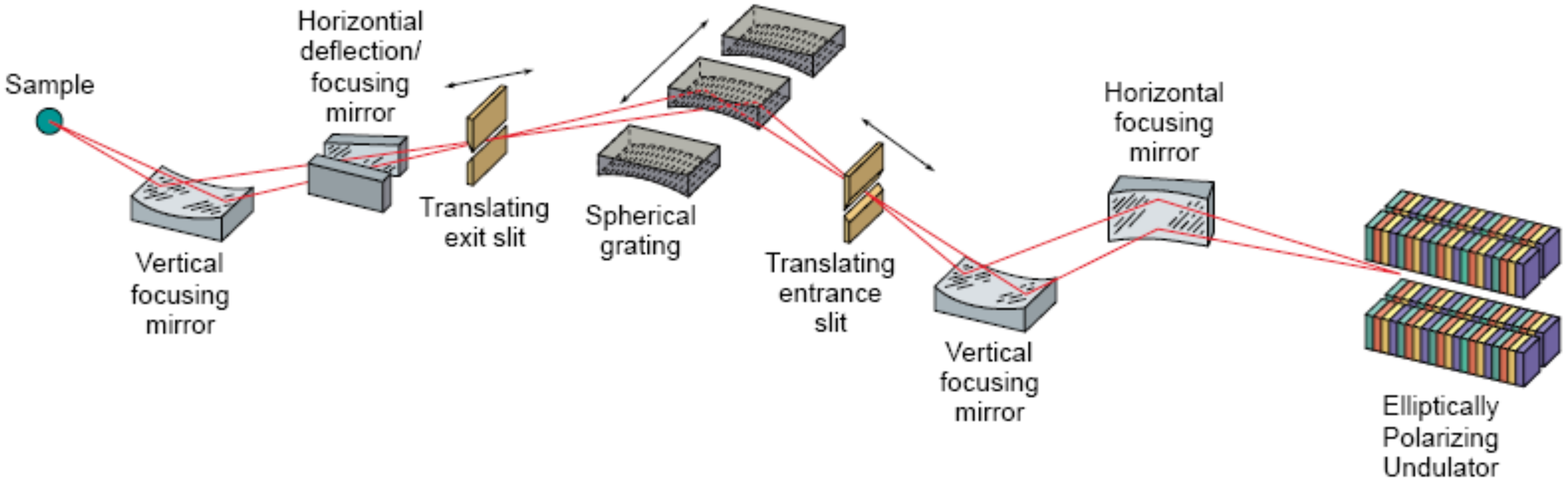
$$E\Psi(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r})$$

X-ray Optics: Delivering X-rays for Experiments

Transferring x-ray photons (beam) to the sample:

- *focus size*
- ***energy content***
- *angular convergence*
- *stability*
- *polarization*

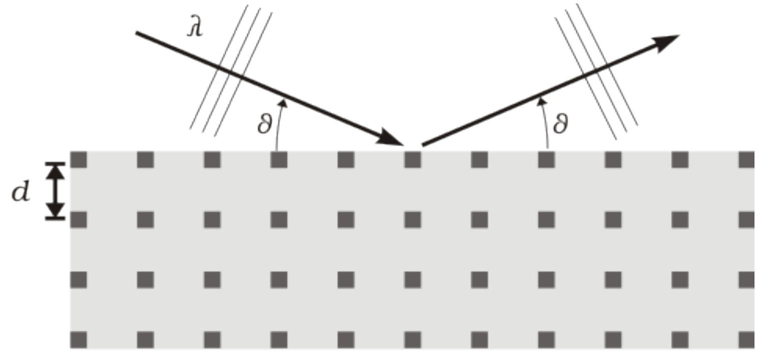
The job of x-ray optics is to transform the source beam characteristics to provide the best possible match to the sample requirements.

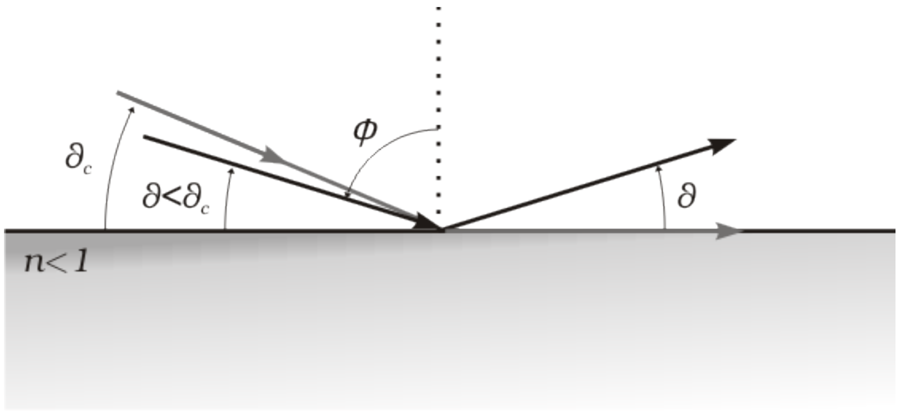


X-ray Optics: Principles

X-rays Interaction Mechanisms for Optics:

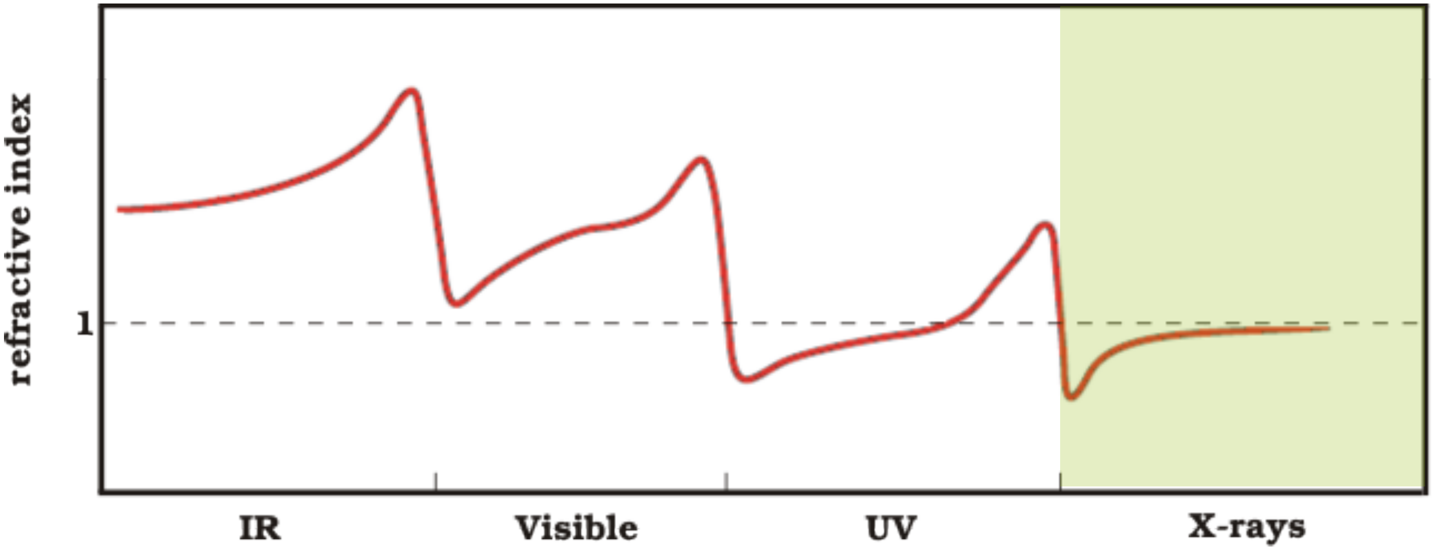
- X-ray Diffraction (monochromatizing x-rays)
- X-ray Refraction/Reflection (guiding/collimating)





X-ray Optics: Refractive Index

Refractive index $\Rightarrow \quad n = \dfrac{c}{u_p}$



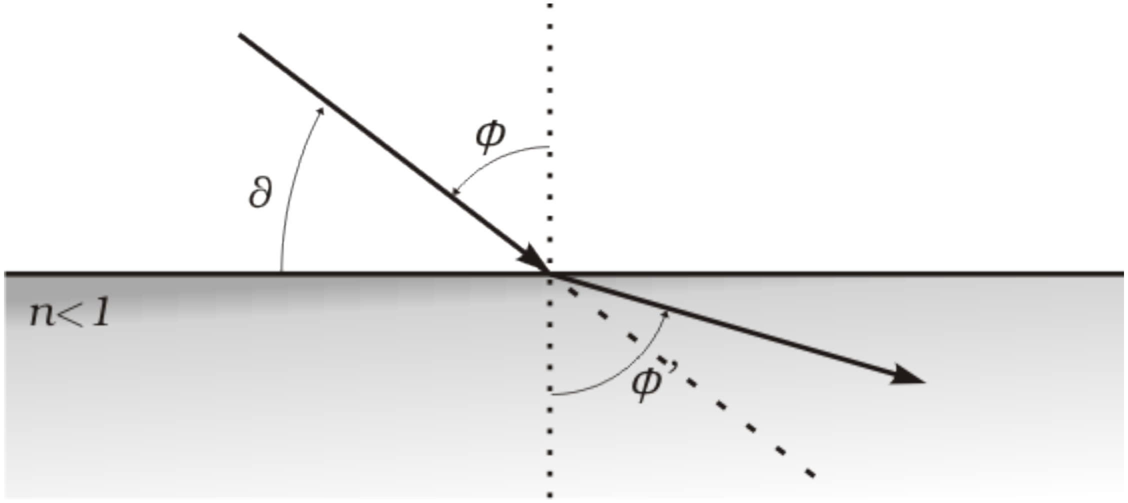
$$n = 1 - \boxed{\delta} + \boxed{i\beta}$$

attenuation term

phase term

X-ray Optics: Refraction

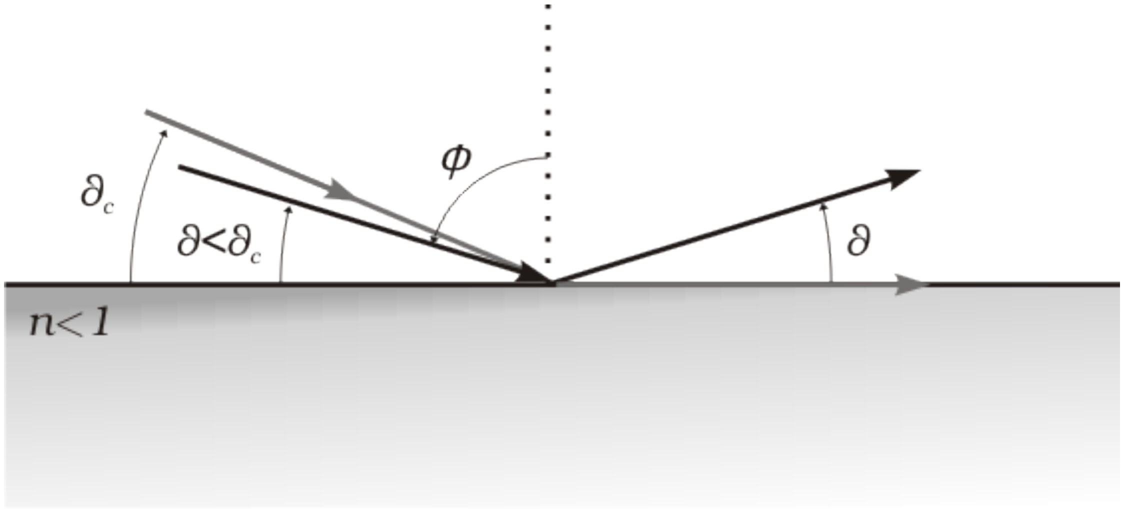
Refraction



Snell Law: $\sin\phi' = \dfrac{\sin\phi}{n} \overset{n<1}{\Longrightarrow} \boxed{\phi' > \phi}$

X-ray Optics: Total External Reflection

Total external reflection



$$n \approx 1 - \delta \;\Rightarrow\; \cos\partial_c = 1 - \delta \;\overset{\delta\ll 1}{\Rightarrow}\; \boxed{\partial_c = \sqrt{2\delta}} \;\Rightarrow \partial_c \propto \lambda\sqrt{Z}$$

$$\delta \sim 10^{-5}\text{-}10^{-6} \quad\Rightarrow\quad \theta_c < 3^{\circ}\text{-}4^{\circ}$$

X-ray Optics: X-ray Mirrors

Focusing

condense beam to source dimensions on sample demagnify source image to better couple photons on small sample at the expense of greater angular convergence on sample)

Collimation

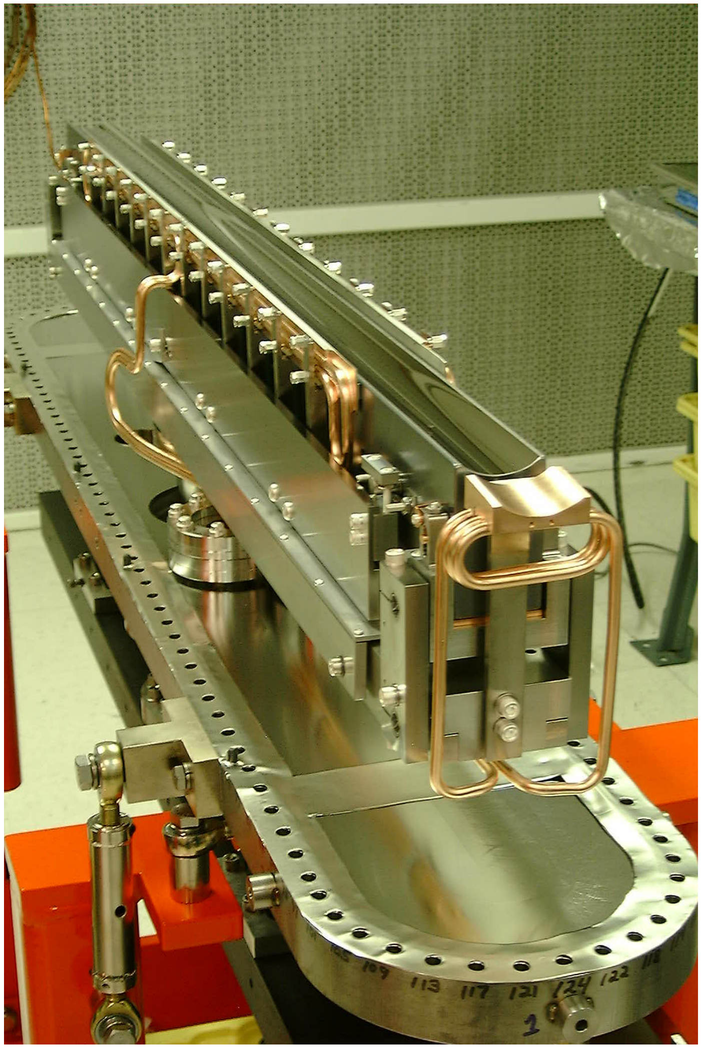
collimate divergent beam to improve energy resolution of a monochromator

Power filter

absorb waste power at low power density on grazing incident optic

Harmonic filter

suppress higher energy contamination of beam (low pass filter)



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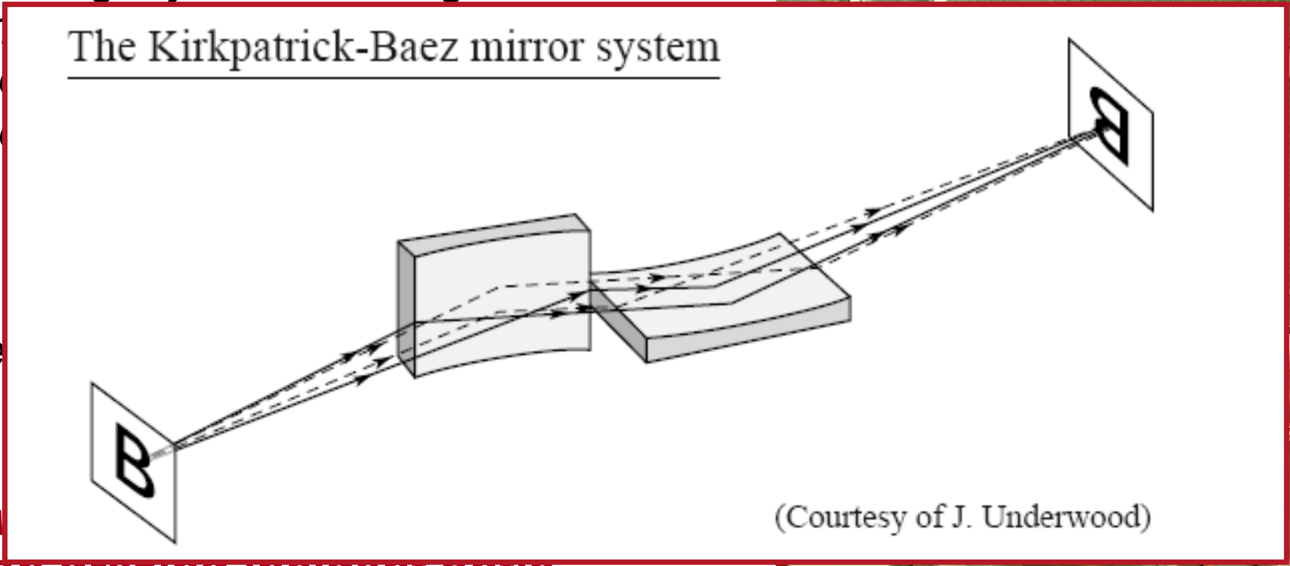
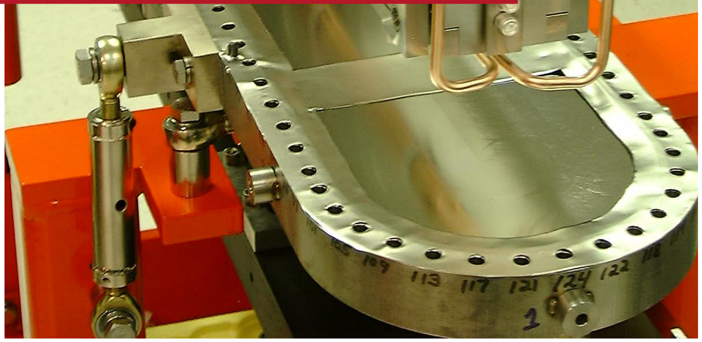

The Kirkpatrick-Baez mirror system

(Courtesy of J. Underwood)



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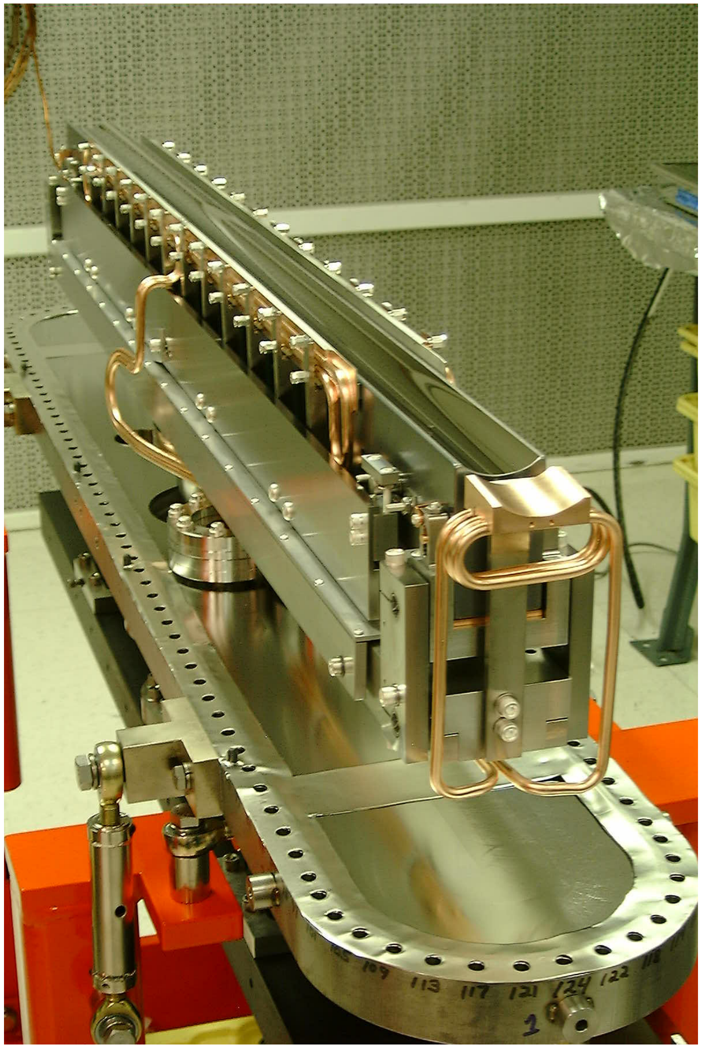

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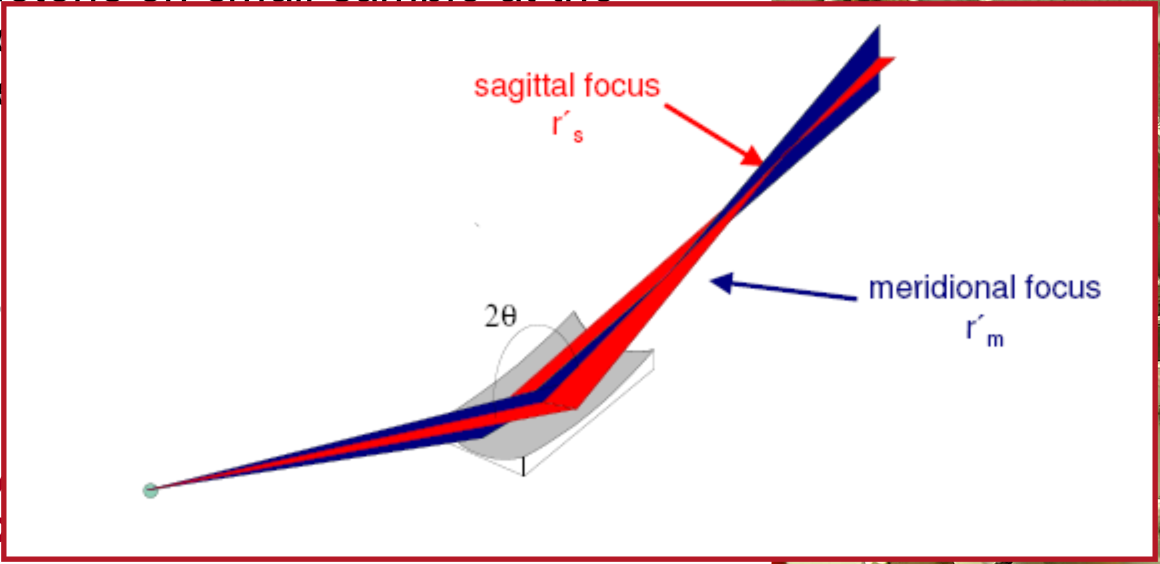

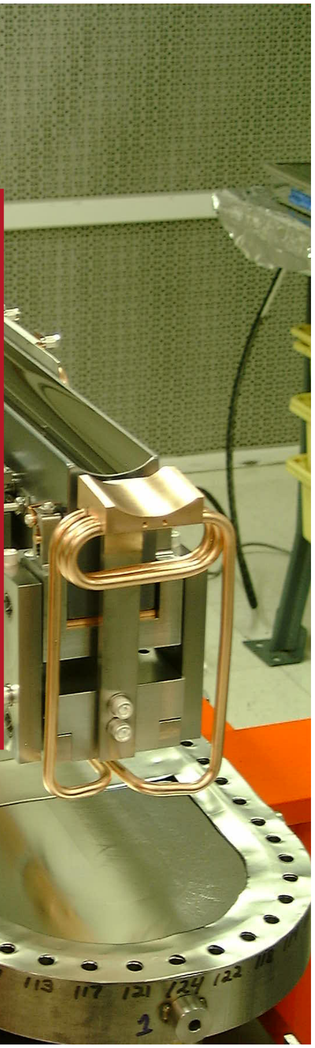

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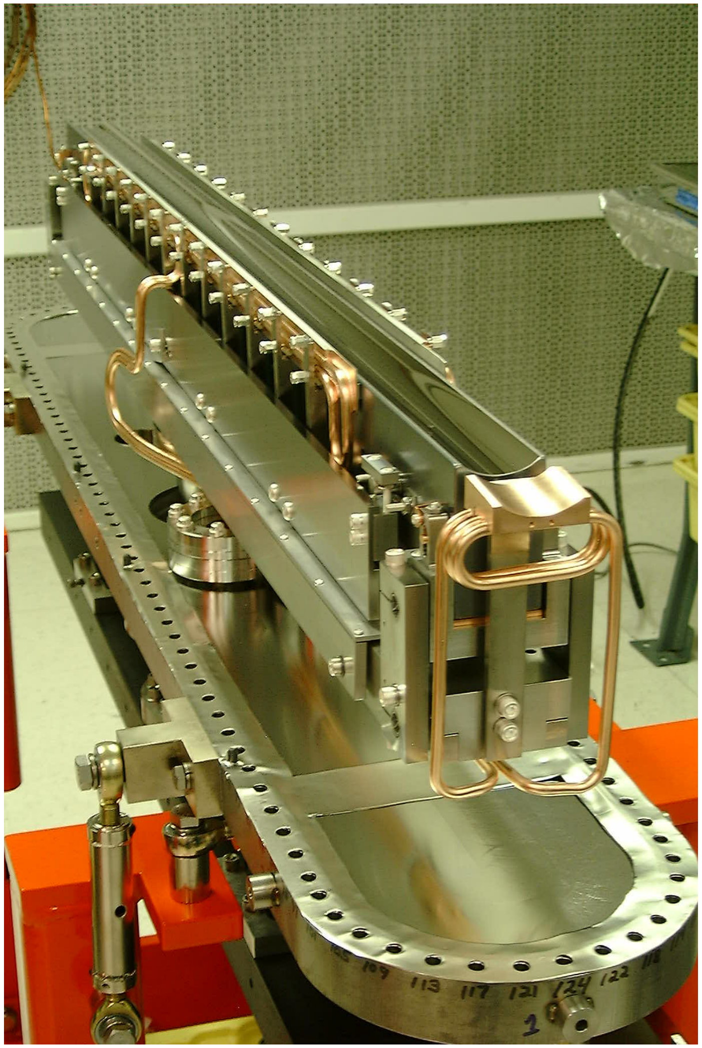
Harmonic filter

suppress higher energy contamination of beam (low pass filter)



X-ray Optics: X-ray Mirrors

Focusing

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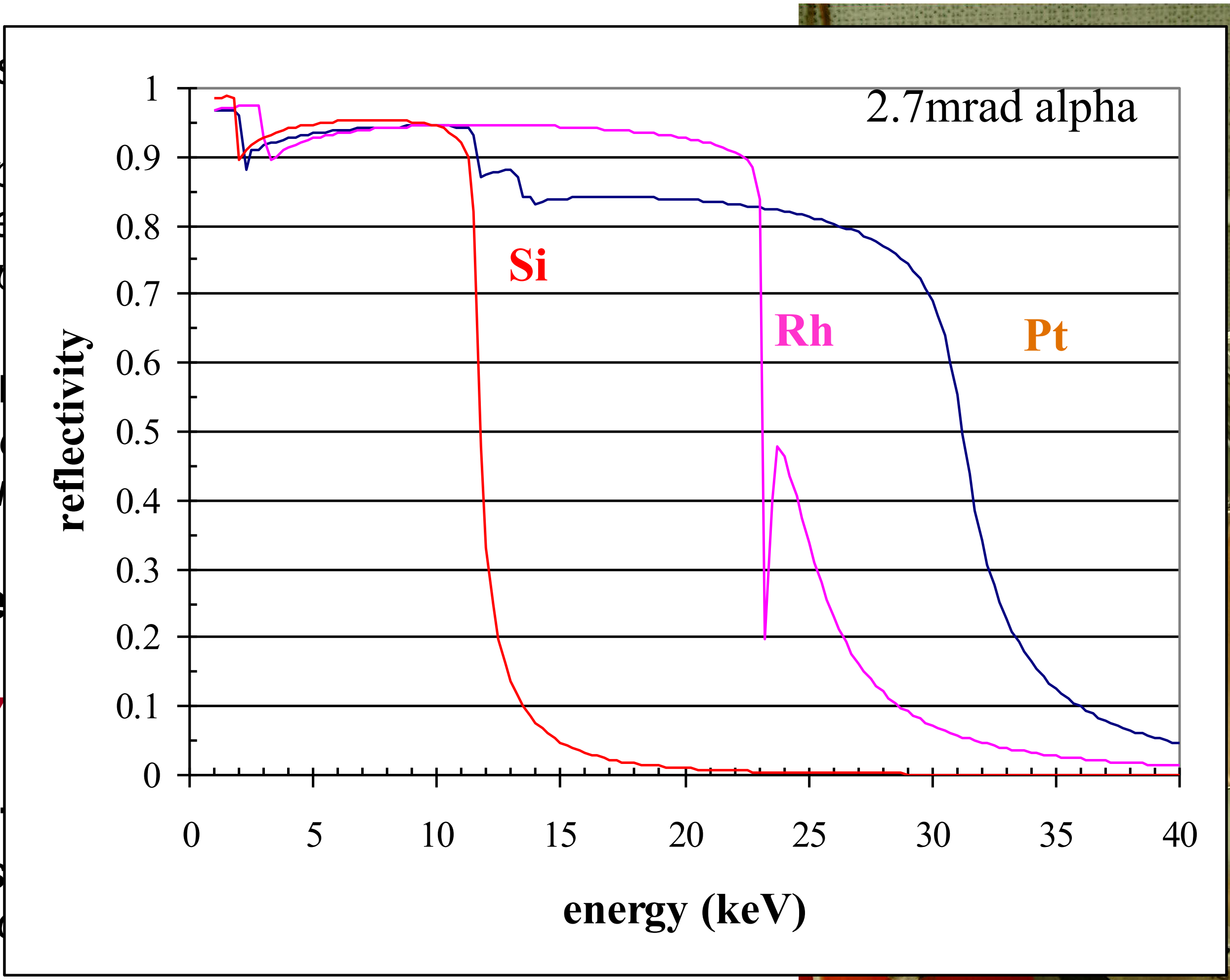
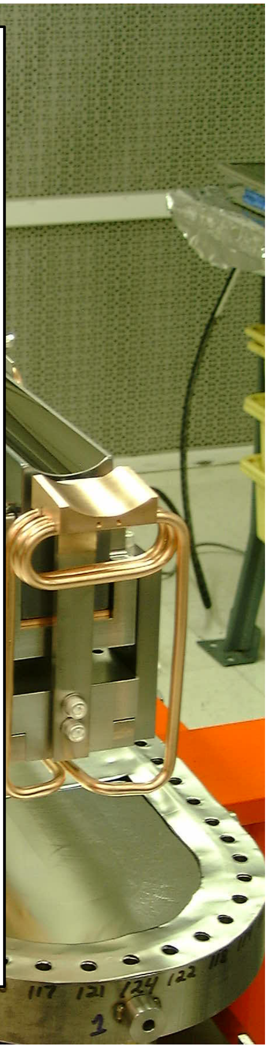
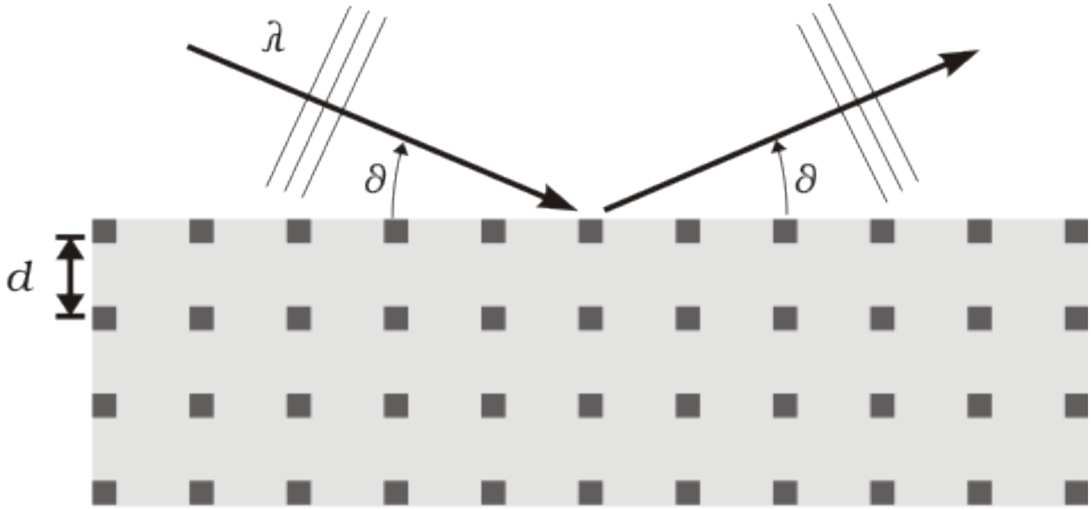




X-ray Optics: X-ray Diffraction

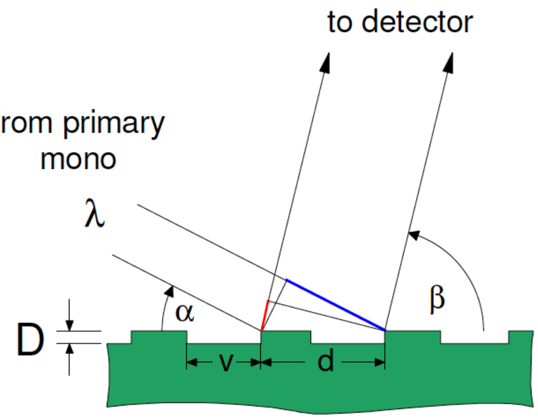
Bragg Diffraction: Constructive interference of radiation reflections from sequential planes.



$$\boxed{m\lambda = 2d\sin(\vartheta)}$$

X-ray Optics: X-ray Diffraction

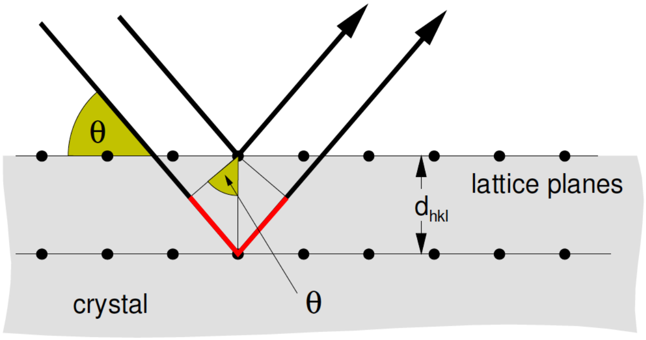
- Diffraction Gratings



$$m\frac{\lambda}{d} = (\sin\alpha + \sin\beta)$$

soft x-rays

- Bragg-type x-ray crystal optics

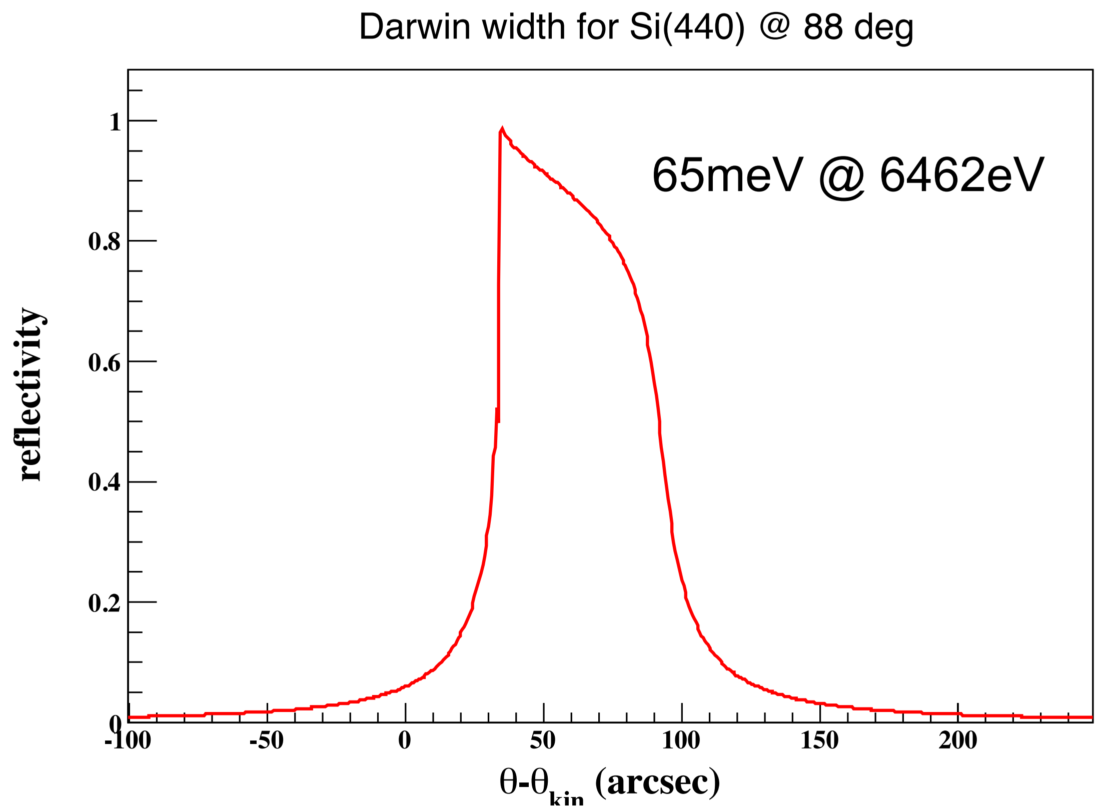


$$2d_{hkl}\sin\theta = \lambda$$

hard x-rays

X-ray Optics: X-ray Diffraction - Darwin Width

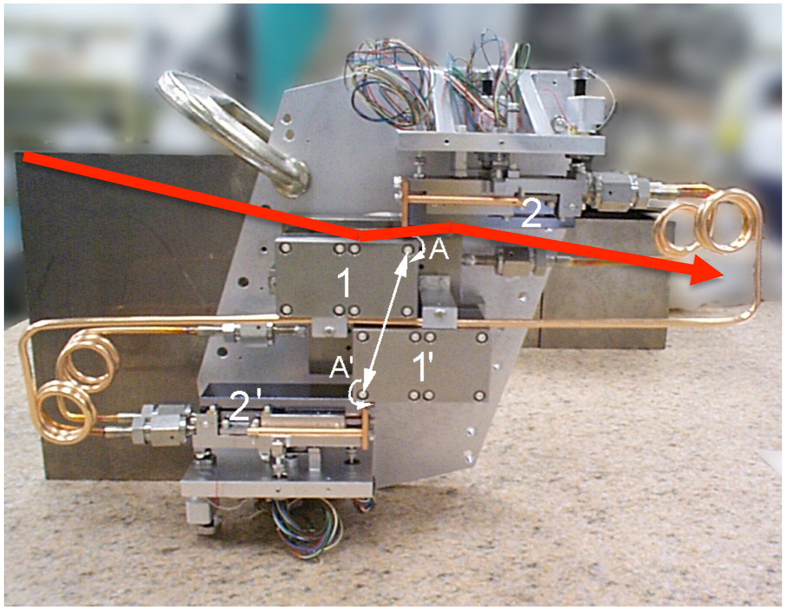
- Energy Resolution- Darwin width (dynamical diffraction theory) and geometrical factors

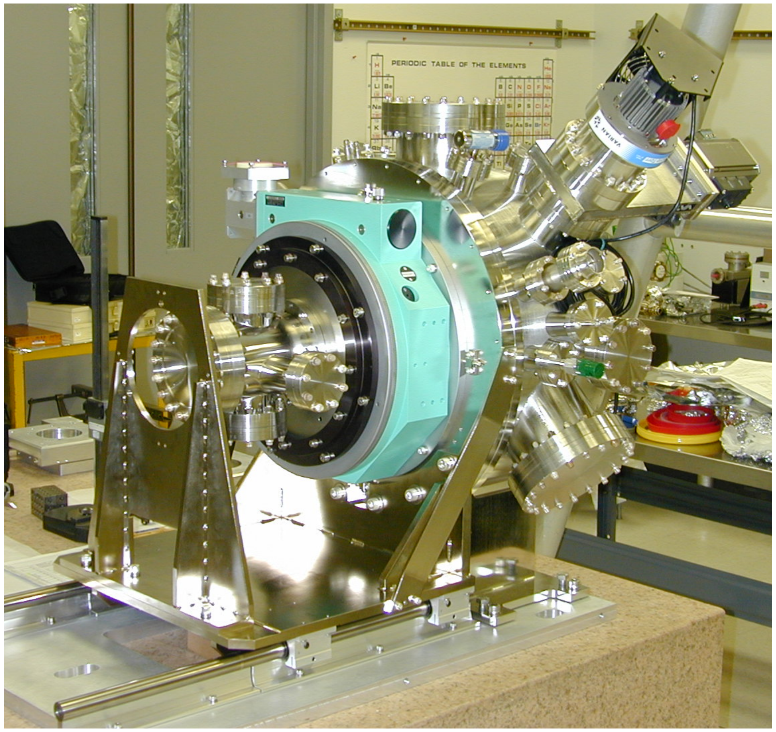


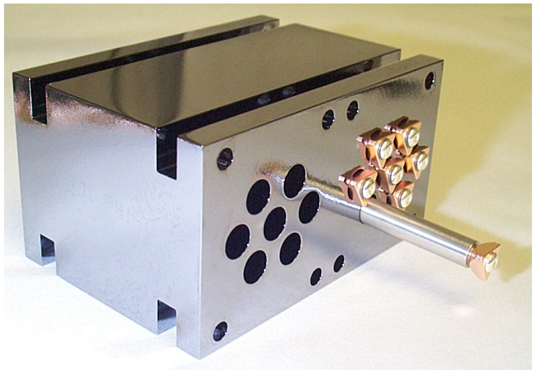
$$2d \sin\theta = \lambda$$

$$\frac{\lambda}{\Delta\lambda} = \frac{\tan\theta}{\Delta\theta}$$

X-ray Optics: Double Crystal monochromators



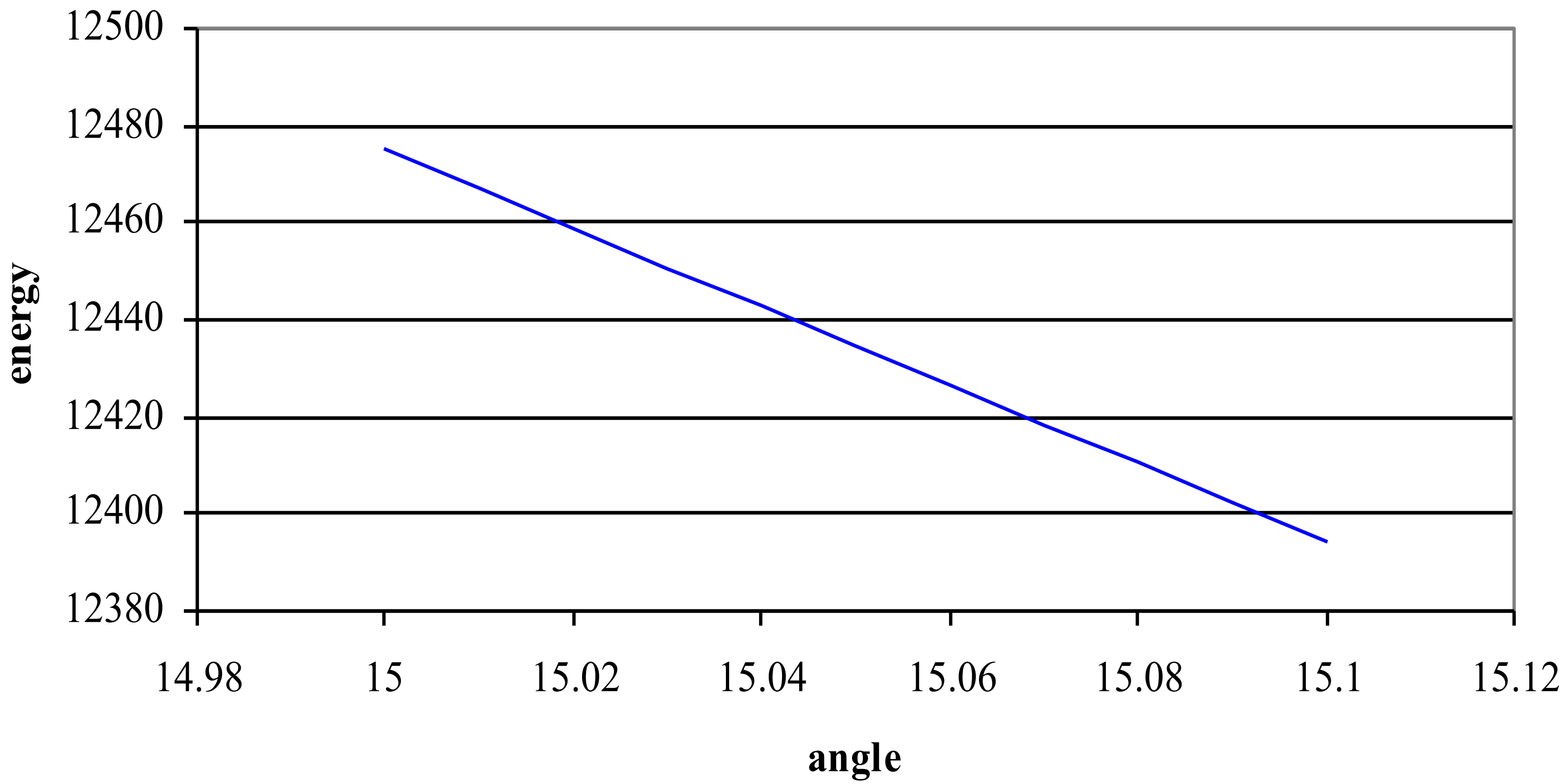




cooling channel bundle

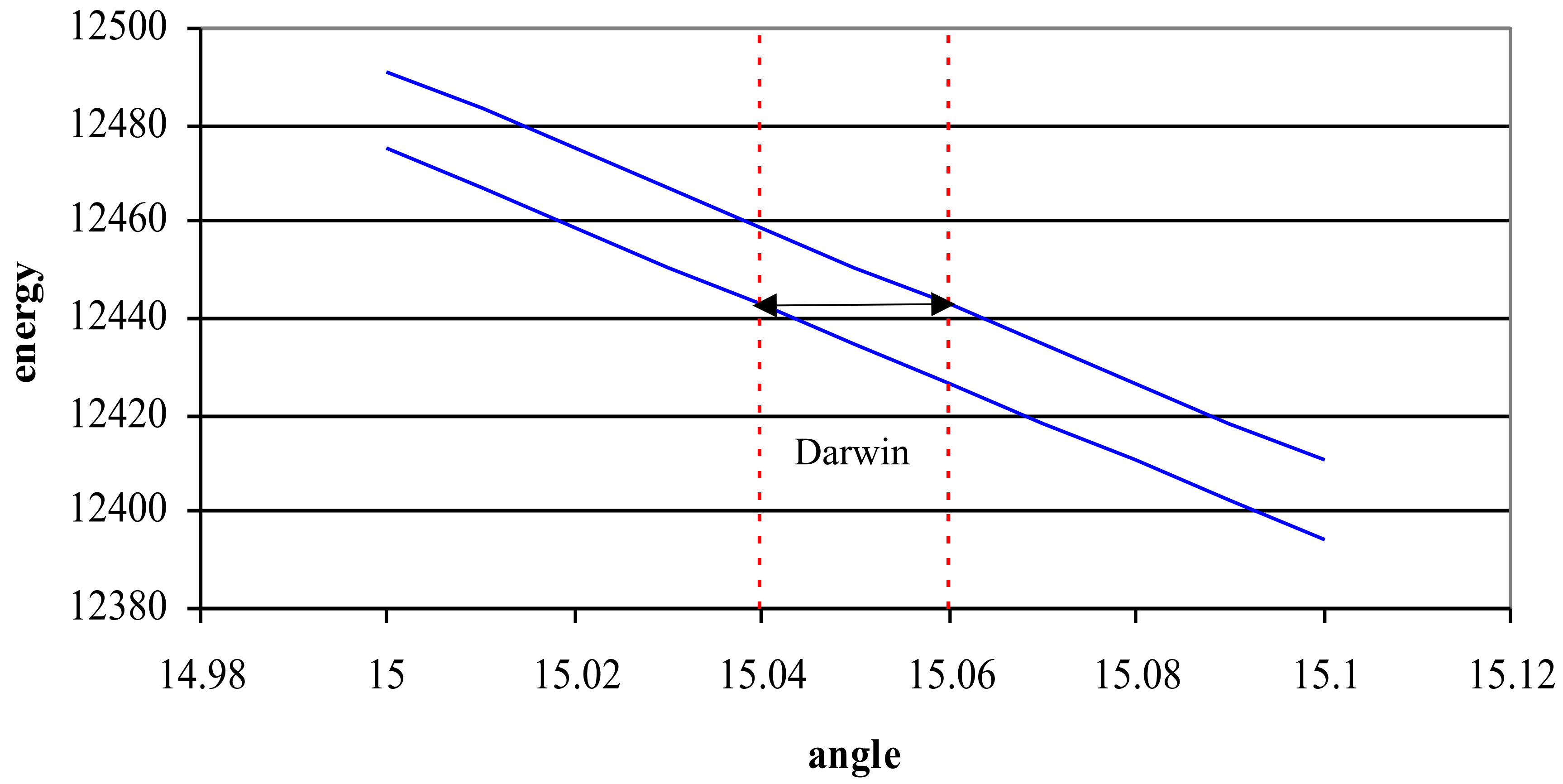
Liquid Nitrogen Cooled Monochromators

X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram



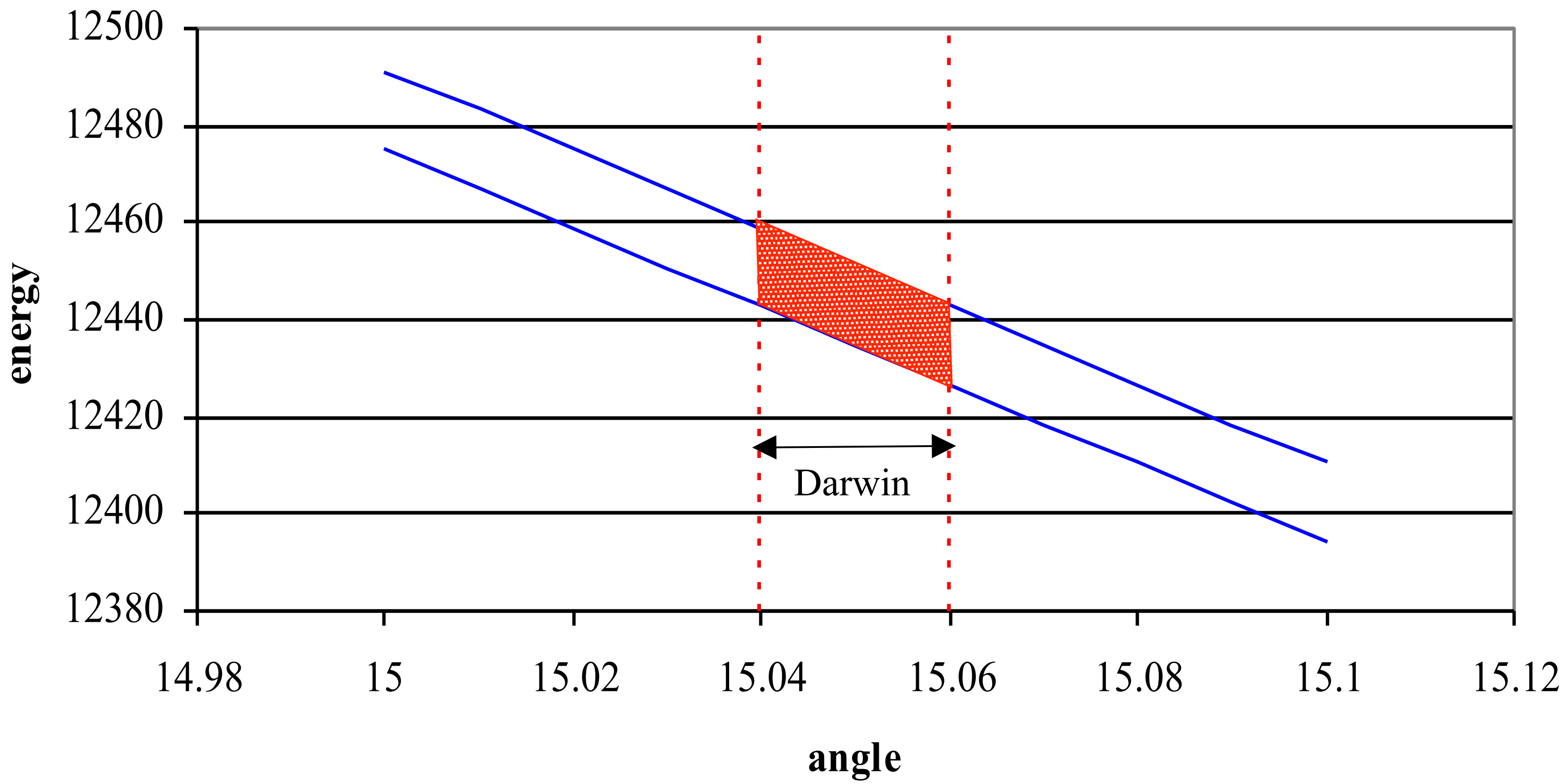
T. Rabedeau, SSRL

X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram



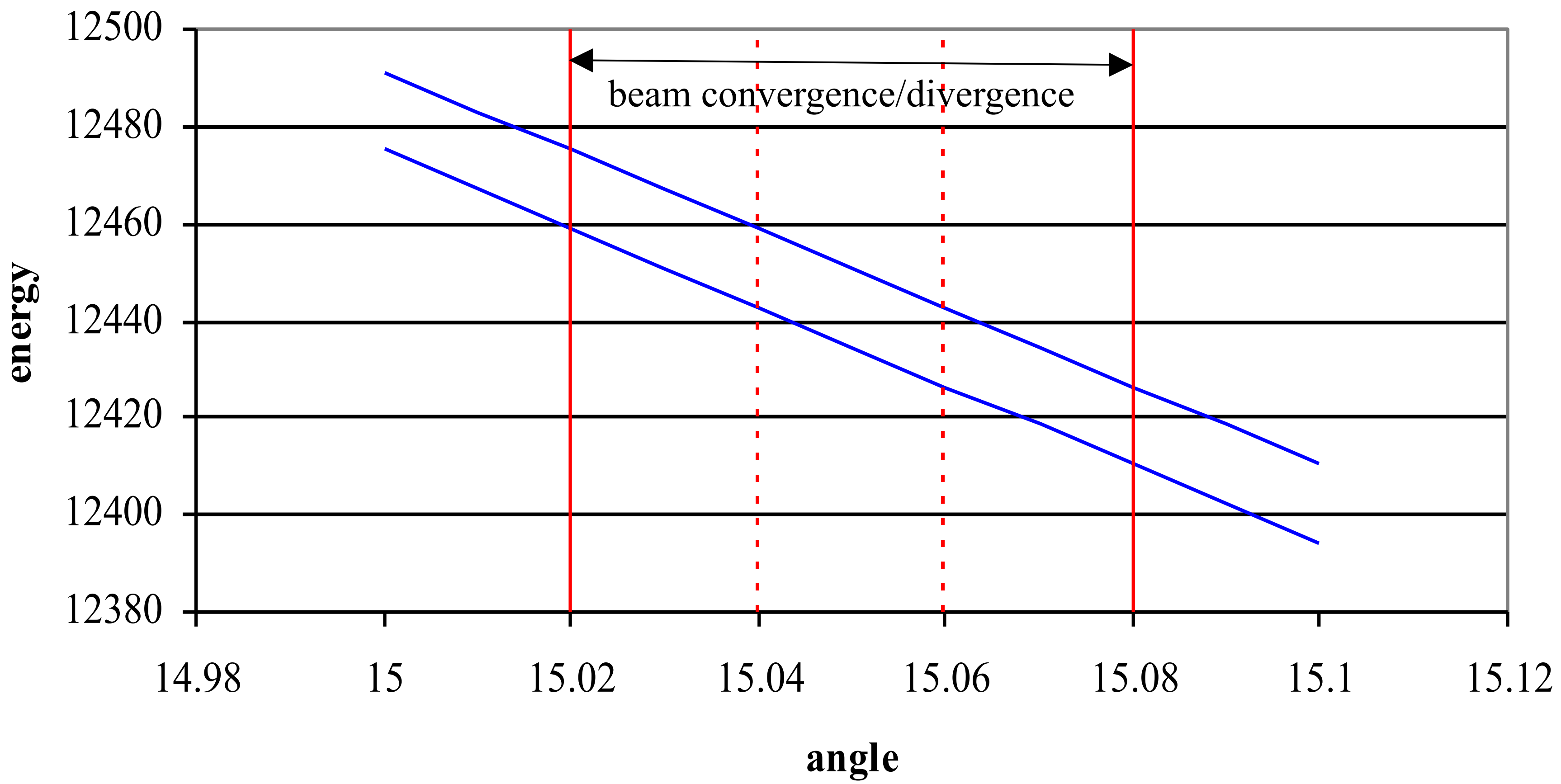
T. Rabedeau, SSRL

X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram



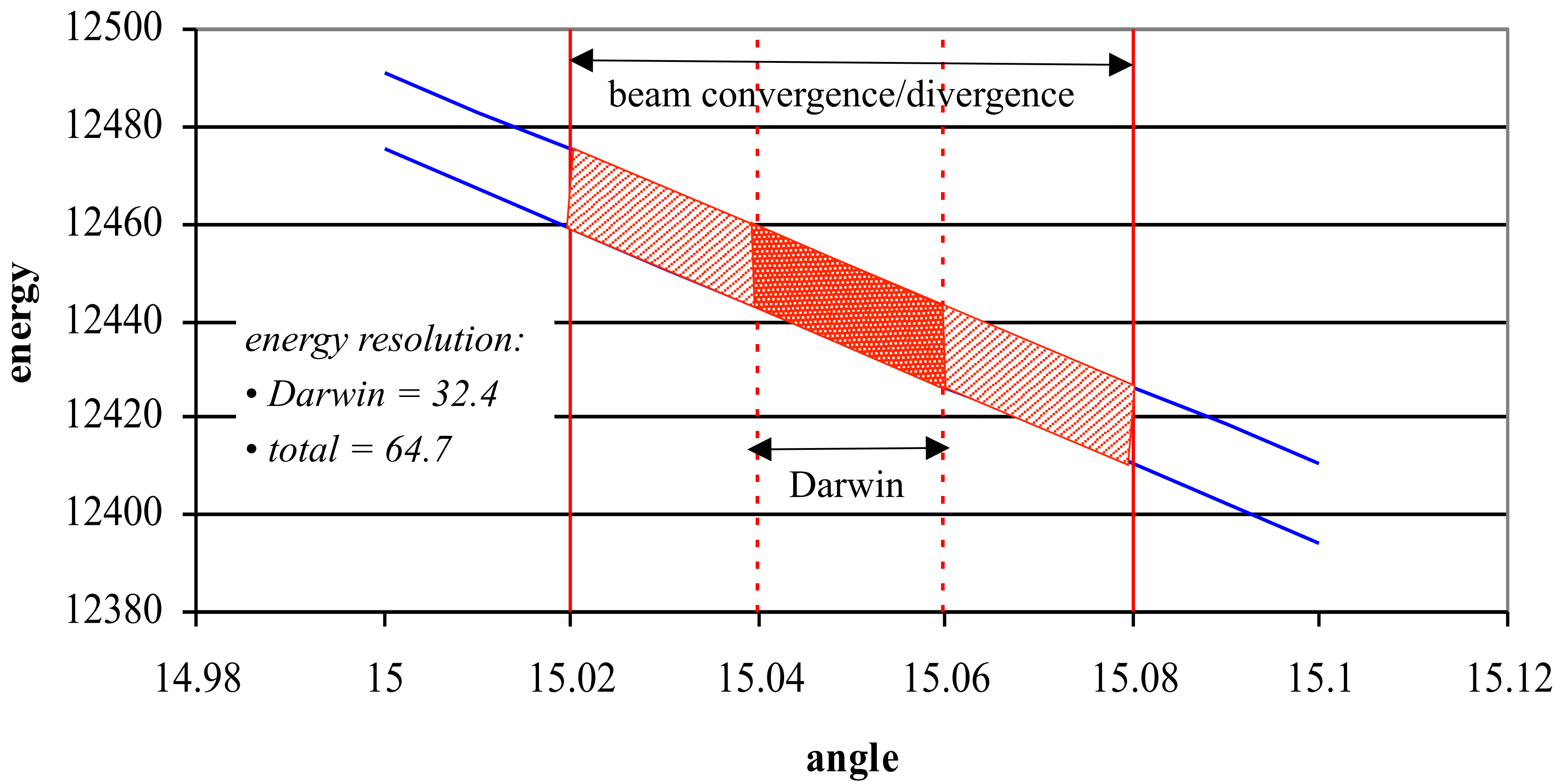
T. Rabedeau, SSRL

X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram



T. Rabedeau, SSRL

X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram



energy resolution:
- *Darwin = 32.4*
- *total = 64.7*

T. Rabedeau, SSRL

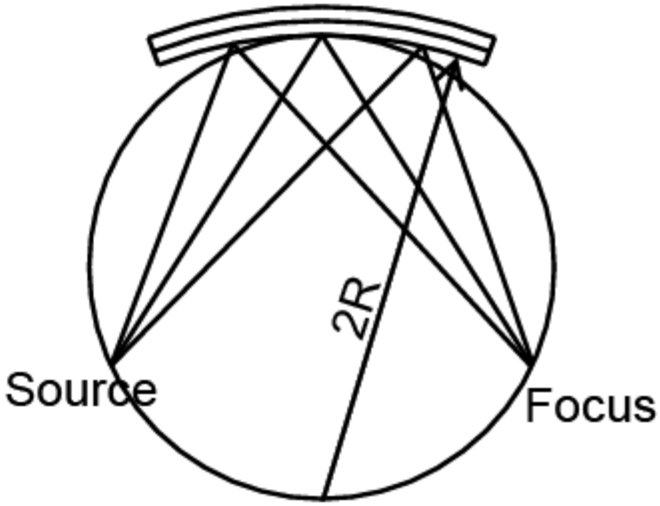
X-ray Optics: Monochromatizing Divergent Sources

Doubly Curved Crystals

- *Based on Bragg Diffraction*
- *Monochromator & Focusing*

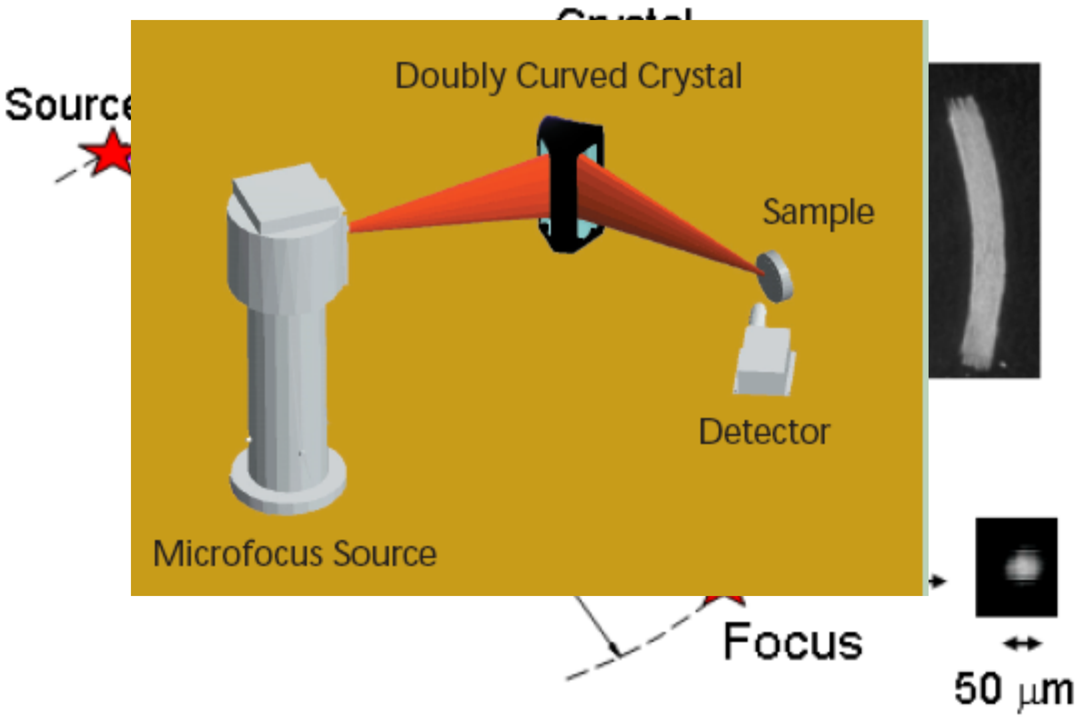
Curved vs. Plate Crystal

- Increased beam area that meets Bragg condition.
- Improve Energy resolution
- Focusing Effect

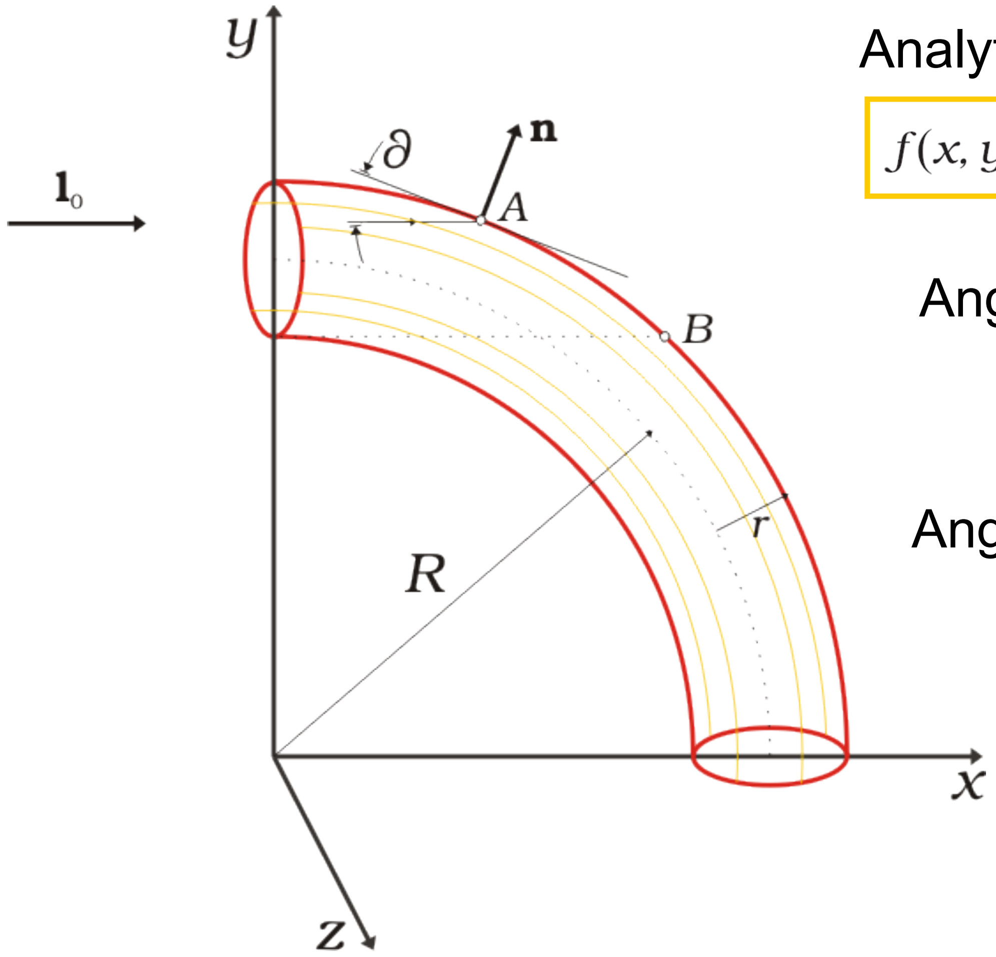


Rowland circle

X-ray Optics: Monochromatizing Divergent Sources



X-ray Optics: X-rays transmission in waveguides



Analytical description of waveguide

$$\boxed{f(x, y, z) = \left(\sqrt{x^2 + y^2} - R\right)^2 + z^2 - r^2 = 0}$$

Angle of incidence at point A(x,y,z)

$$\boxed{\partial = \sin^{-1}\left(\mathbf{l}_0 \cdot \mathbf{n}\right)}$$

Angle of incidence at $B(2\sqrt{rR}, R - r, 0)$

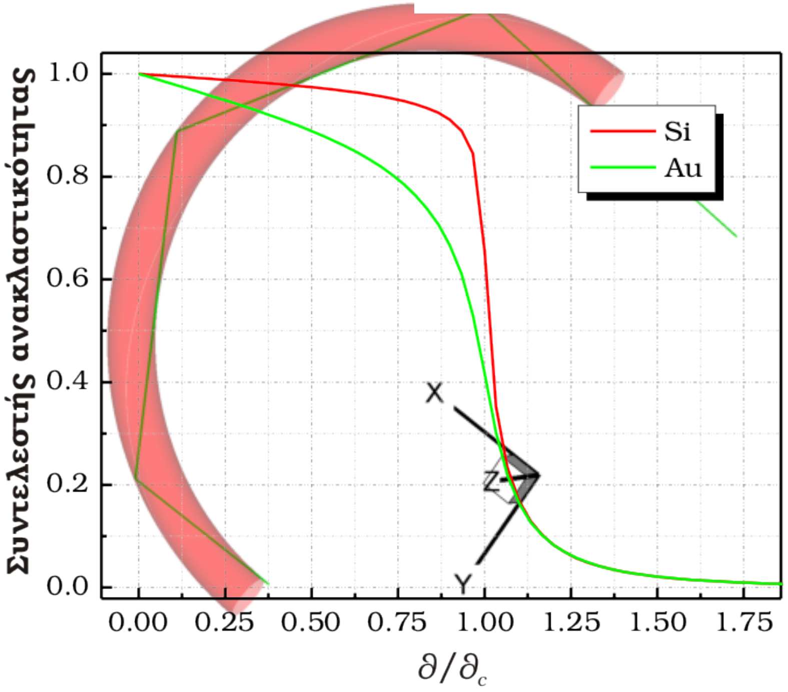
$$\boxed{\sin \partial_{\max} = \frac{2\sqrt{rR}}{R + r}}$$

Geometrical Parameters constrain

$$\boxed{\frac{R\,\partial_c^2}{4\,r} > 1}$$

X-ray Optics: X-rays transmission in waveguides

Reflectivity $I_1 = I_{\hat{}} - \Longrightarrow R_\partial = \frac{\left|\partial - \sqrt{(\partial^2 - \partial_c^2) + 2i\beta}\right|^2}{\left|\partial + \sqrt{(\partial^2 - \partial_c^2) + 2i\beta}\right|^2}$

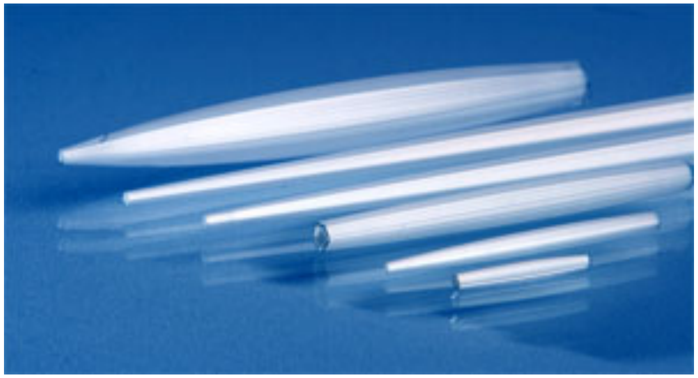


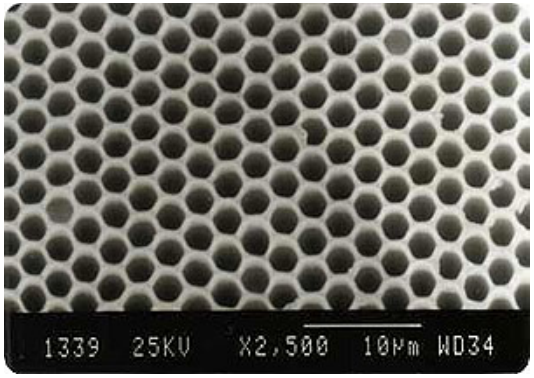
Photon energy: 8 *keV*

X-ray Optics: Polycapillary X-ray lenses

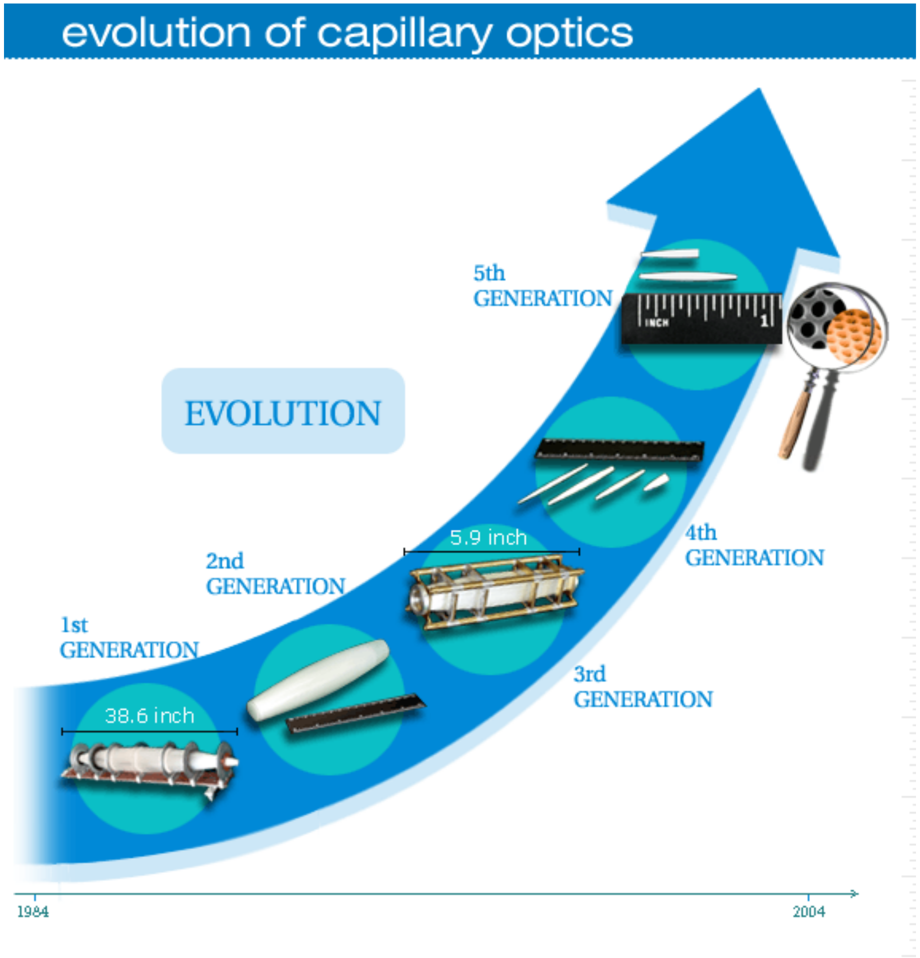
Bundles of thousands glass mono-capillaries in certain arrangements can be used for:

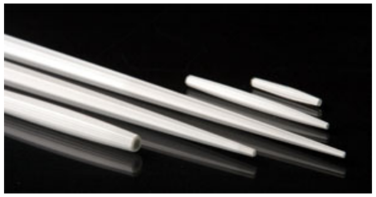
- **Directing**
- **Focusing**
- **Parallelizing**

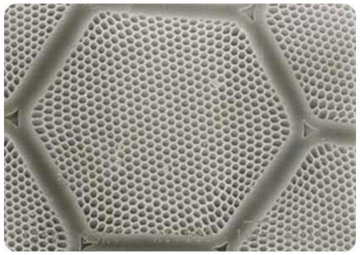


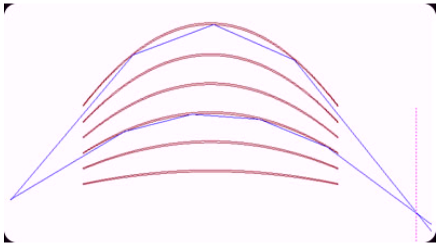


X-ray Optics: Polycapillary X-ray lenses









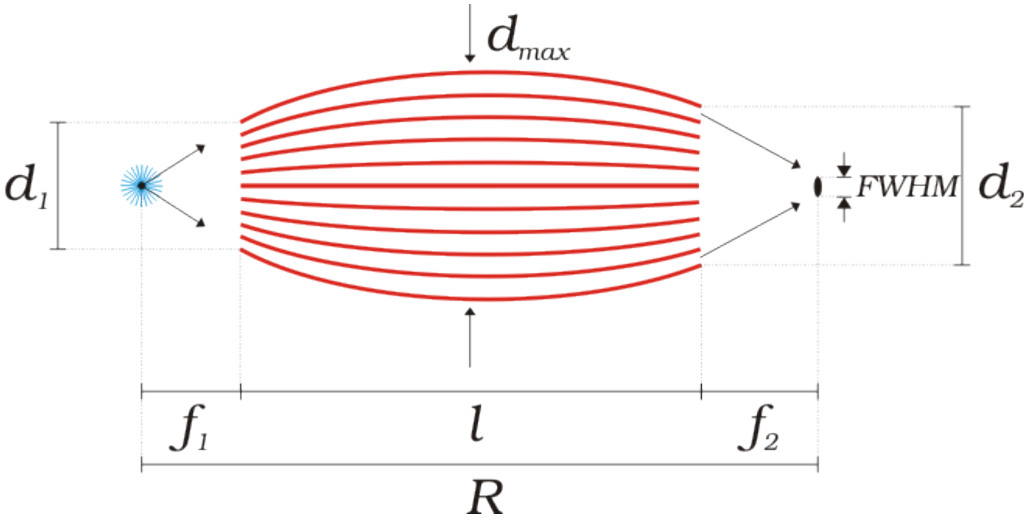
X-ray Optics: Polycapillary X-ray lenses

Polycapillary lens

Functionality: Spot focusing of diverging x-ray beam.

Main Applications: Focusing x-ray tubes beams .

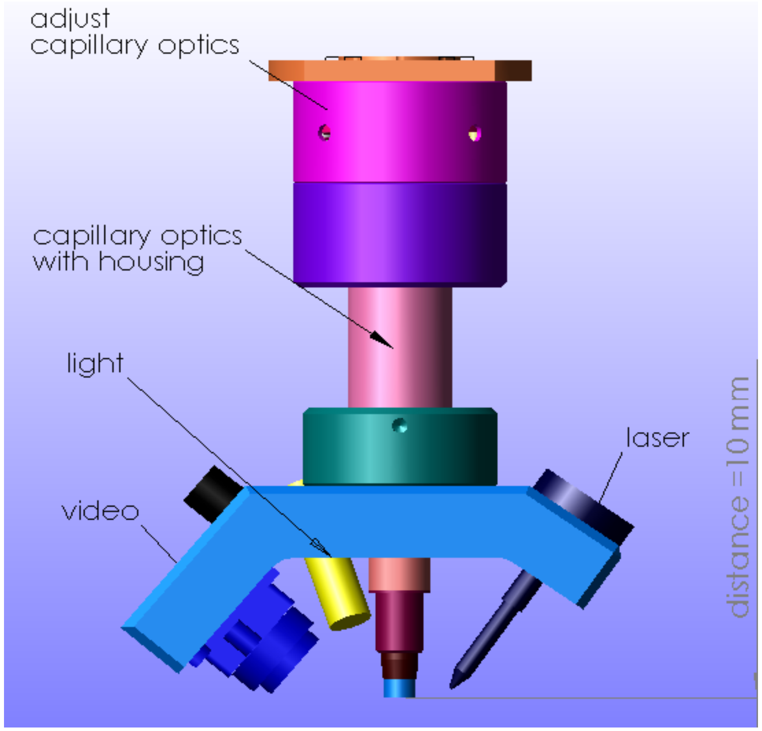
d_1, d_2	0.3…1 *mm*
d_{max}	1…2 *mm*
l	40…50 *mm*
f_1,f_2	15…100 *mm*
FWHM	15…100 *μm*



X-ray Optics: Polycapillary-based XRF

X-ray tube based Micro-XRF setup

sample



Summary

X-ray Sources

- X-ray Tubes
- Synchrotron Radiation Beamlines

X-ray Optics

- Mirrors
- Monochromators

- Double Curved Crystals
- Polycapillary lenses

Thank you !