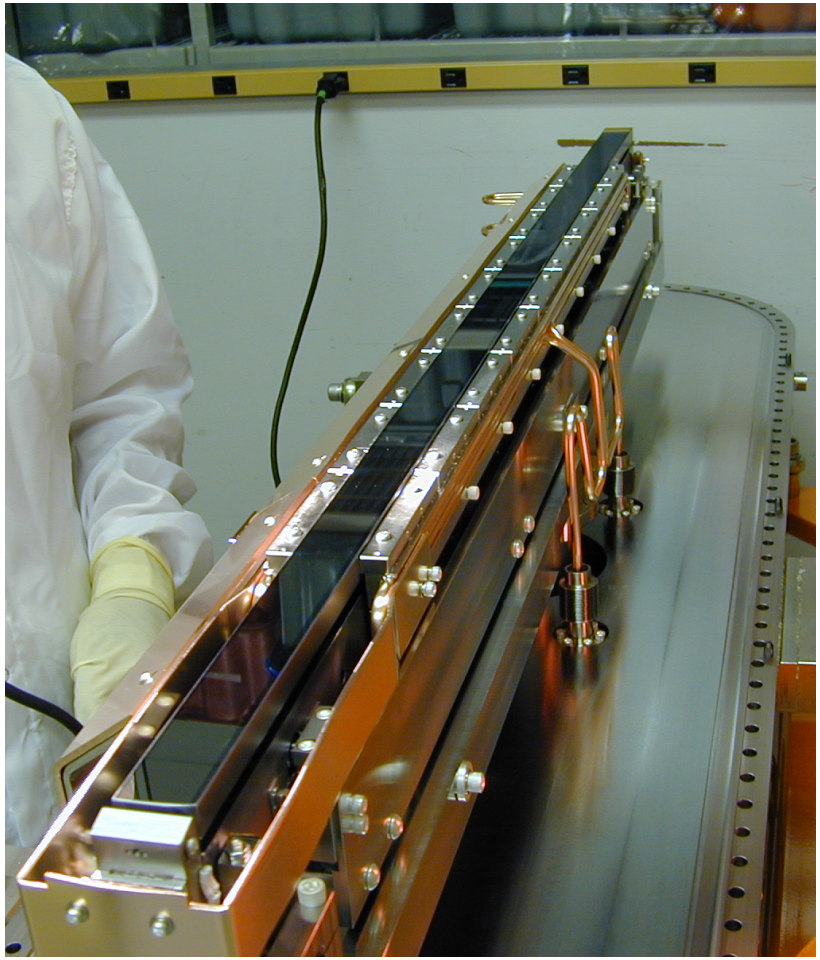
Argonne NATIONAL LABORATORY

X-ray Optical Components for Hard X-ray Synchrotron Radiation Sources



Dennis M. Mills
Deputy Associate Laboratory Director
Advanced Photon Source

National School for Neutron and X-ray Scattering
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U.S. DEPARTMENT OF ENERGY

Outline

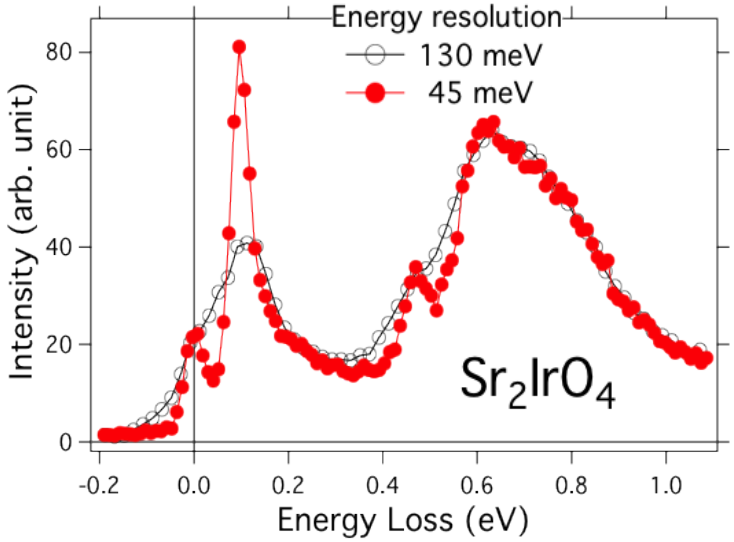
Outline of Presentation

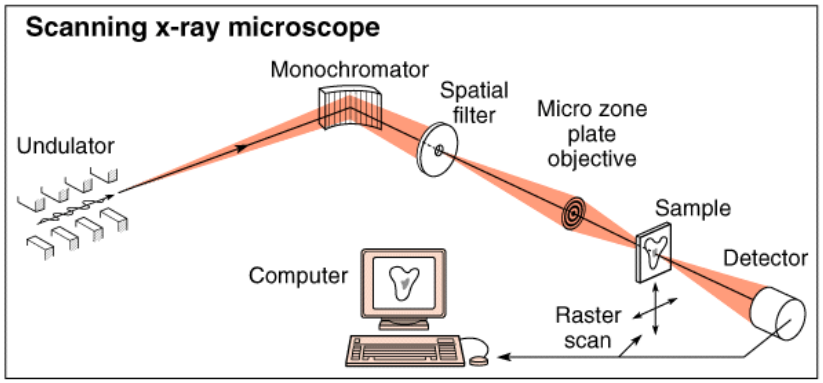
1. **Why Do We Need Optics?**
2. **X-ray Mirrors (Reflective Optics)**
3. **Perfect Crystal X-ray Optics (Diffractive Optics)**
4. **Focusing Optics (Reflective, Diffractive and Refractive)**

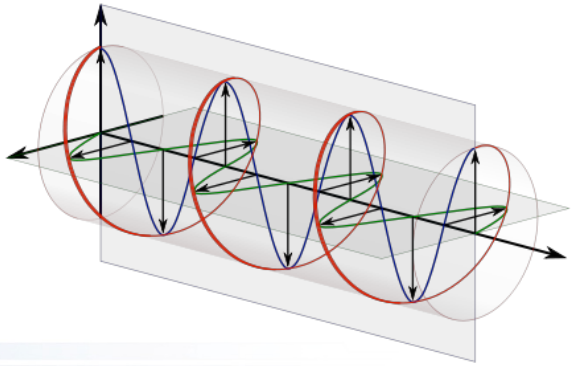
I will not be talking about gratings as they are used in the soft x-ray region of the spectrum and the focus of this talk will be hard x-ray optics.

Why Do We Need Optics

- Control the energy (E) and bandwidth (ΔE) of the beam.
  - Monochromatic beam (ΔE = 1-2 eV @ 10 keV; $\Delta E/E = 10^{-4}$)
  - Polychromatic (ΔE = 1-2 keV @ 10 keV; $\Delta E/E = 10^{-1}$)
  - High-resolution beams (ΔE = a few milli-eV @ 10 keV; $\Delta E/E = 10^{-7}$)
- Control the size/divergence of the beam (often related).
  - Micro or nano beams (spot sizes microns to 10's of nanometers)
  - Highly collimated beams
- Control the polarization of the beam.
  - Linear
  - Circular







Reflective Optics: The Dielectric Constant at X-ray Wavelengths

- Since the reflective properties of a material depends on the index of refraction, we need to know this at x-ray energies/frequencies. It is pretty straight forward to calculate the dielectric constant, κ, for a material using the Drude Theory (simple free electron model) – See Appendix 1:

$$\kappa = 1 + 4\pi(P/E) = 1 + 4\pi\,(e^2/m)n_e\,[1/(\omega_o^2 - \omega^2)]$$

where m is the mass of the electron, e is the charge of the electron, n_e is the electron density, ω the frequency of the x-rays, and ω_o in the Drude model is the frequency of the collective oscillations of the electron gas around the positive ion background or the so-called plasma frequency and equal to:

$$\omega_o = [4\pi n_e e^2/m]^{1/2}$$

- Silicon is often used for monochromators and mirror substrates because large single crystals are readily available at a relatively low cost, so let's calculate this for silicon as an example.

See Appendix 1 for more details

Index of Refraction at X-ray Wavelengths NEW

- For Si, $n_e = 7 \times 10^{23}$ e/cm^3 and so the plasma frequency is:

$$\omega_o = 5 \times 10^{16}/\text{sec}$$

- For a 1 Å x-ray, the angular frequency, $\omega = [2\pi c/\lambda]$, is **$2 \times 10^{19}$/sec which is $>> \omega_o$** and so we can write:

$$\kappa = 1 + 4\pi (e^2/m) n_e [1/(\omega_o^2 - \omega^2)] \approx 1 - 4\pi (e^2/m) n_e [1/(\omega^2)]$$

- The index of refraction, n, is just the square-root of the dielectric constant and can be written as:

$$\mathbf{n} = \kappa^{1/2} = [1 - (n_e (e^2/mc^2) \lambda^2/\pi)]^{1/2} \approx 1 - (n_e r_e/2\pi)\lambda^2$$

where $r_e = (e^2/mc^2)$ is the classical radius of the electron (2.82×10^{-13} cm).

See Appendix 1 for more details

Index of Refraction, n < 1

- This expression for the index of refraction:

$$n = \kappa^{1/2} = [1 - (n_e(e^2/mc^2)\,\lambda^2/\pi)]^{1/2} \approx 1 - (n_e r_e/2\pi)\lambda^2$$

is often written as:

$$n = 1 - \delta \;, \quad \text{where} \quad \delta = (n_e r_e/2\pi)\lambda^2.$$

- When you plug in the numbers for the real part of the index of refraction you get:

$$\delta = 10^{-5} \text{ to } 10^{-6}$$

- So you have:
  - **an index of refraction less than one**
  - **differing from unity by only a few ppm**

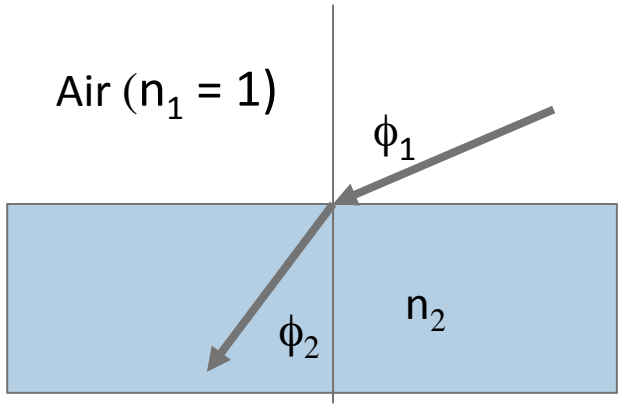
See Appendix 2 for more details

The index of refraction for x-rays was first calculated by Charles Darwin in 1914. More about Darwin a little bit later.

Snell's Law

- The reflection and refraction of x-rays can be treated as any other electromagnetic wave traveling in a medium with index of refraction n_1 encountering a boundary with another material with index of refraction n_2.

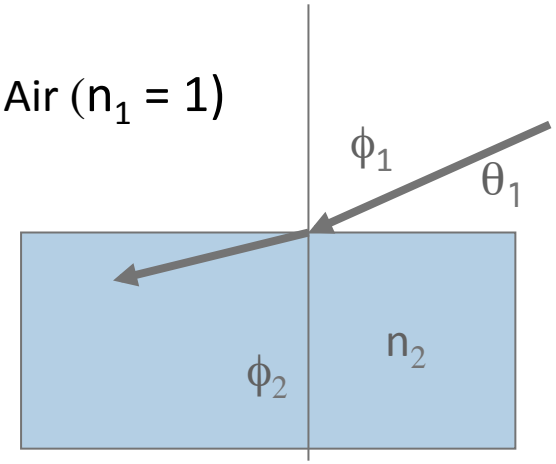
- The resultant kinematic properties (which follow from the wave nature of the radiation at boundaries) are:
  - The angle of incidence equals the angle of reflection
  - **$n_1 \sin(\phi_1) = n_2 \sin(\phi_2)$** (Snell's Law), where the ϕ's are measured with respect to the boundary normal



Typical values for n_2 (at 5890Å) are:

water: $n_2 = 1.33$

glass: $n_2 = 1.52$



For x-rays, the direction of propagation bends away from surface normal.

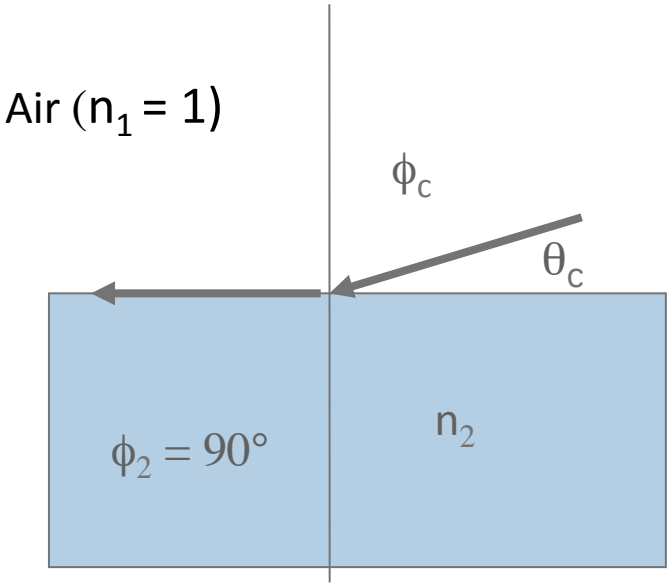
Critical Angle for Total External Reflection

- Let an x-ray (in vacuum, where $n_1 = 1$) impinge on a material with index of refraction n_2. From Snell's Law (when $\phi_2 = 90°$), we have:

$$n_1 \sin(\phi_c) = n_2 \sin(90°) ;$$

$$\cos(\theta_c) = n_2 \cos(0) \quad (\theta = 90° - \phi)$$

$$\cos(\theta_c) = n_2$$



- Expanding the cosine of a small angle and substituting for n_2 gives:

$$1 - (\theta_c)^2/2 = 1 - \delta$$

$$\theta_c = (2\delta)^{1/2}$$

Recall that the typical values for δ at 1 Å is 10^{-5} to 10^{-6} and so the critical angle is going to be about 10^{-3} or a few milliradians

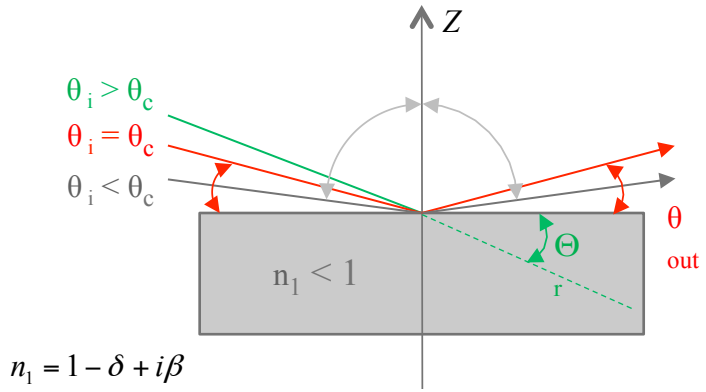
θ_c is the so-called critical angle, the angle at which there is total external reflection and the material behaves like a mirror.

X-ray Reflectivity

- The amplitude of the reflected wave can be determined through the Fresnel equations. Sparing you the details, the intensity ratio of the reflected and incident beam is given by:

$$I^R / I = |E^R/E|^2$$

- From the Fresnel equations it can be shown that:
  - Below θ_c, there is unit reflectivity (when β, the absorption equals 0)



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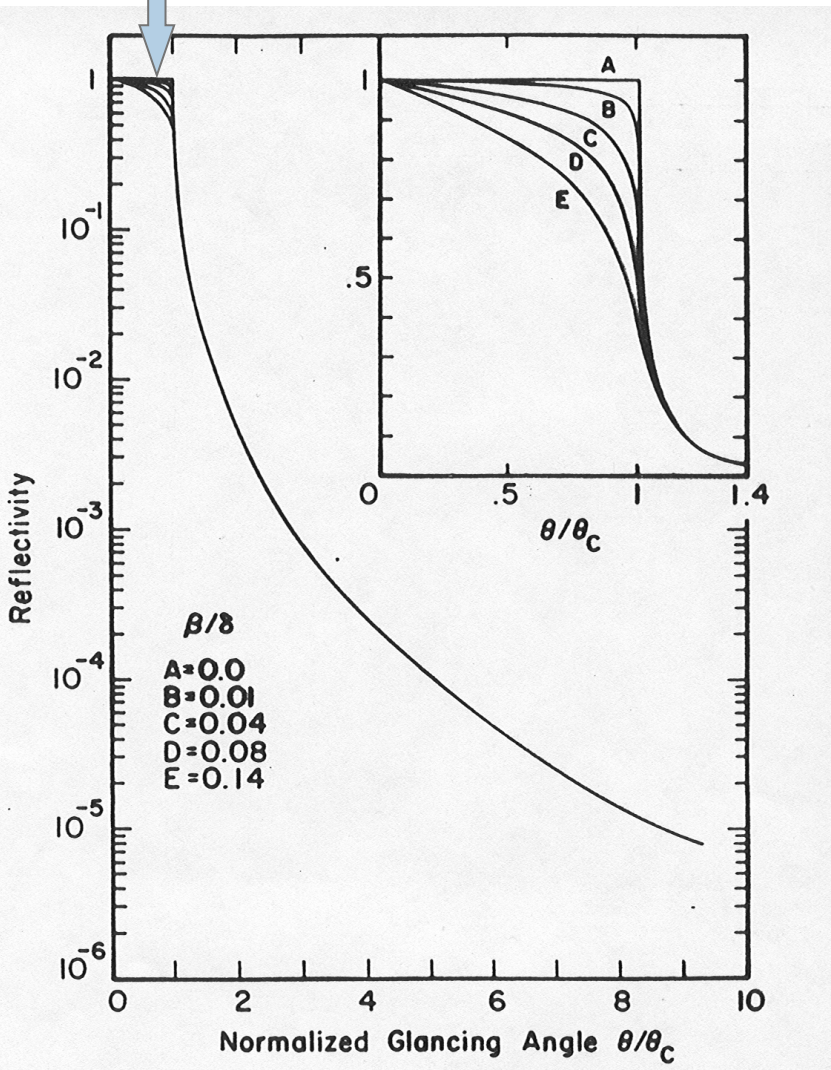


PHYSICAL REVIEW VOLUME 95, NUMBER 2 JULY 15, 1954

Surface Studies of Solids by Total Reflection of X-Rays*

L. G. Parratt
Cornell University, Ithaca, New York
(Received March 22, 1954)

Energy Cut-off for a Fixed Angle of Incidence Mirror

- All the above was developed assuming a single wavelength (monochromatic) incident beam and a variable angle of incidence.

- Often mirrors are used as first optical components. This means a polychromatic incident beam strikes the mirror at some fixed angle.

- The relationship for the critical angle and wavelength can be rewritten in terms of a cut-off energy, E_c.

- So for a mirror at a fixed angle θ, energies below E_c will be totally reflected (since the reflectivity is nearly 1) and energies above E_c will be reduced because of the fall-off of reflectivity:

$$\theta_c = (2\delta)^{1/2} = \lambda(n_e r_e/\pi)^{1/2}$$

- Since $E = hc/\lambda$, I can re-write this for a fixed θ, and determine the maximum energy, E_c, (or minimum wavelength, λ_c) that will be totally reflected by the mirror.

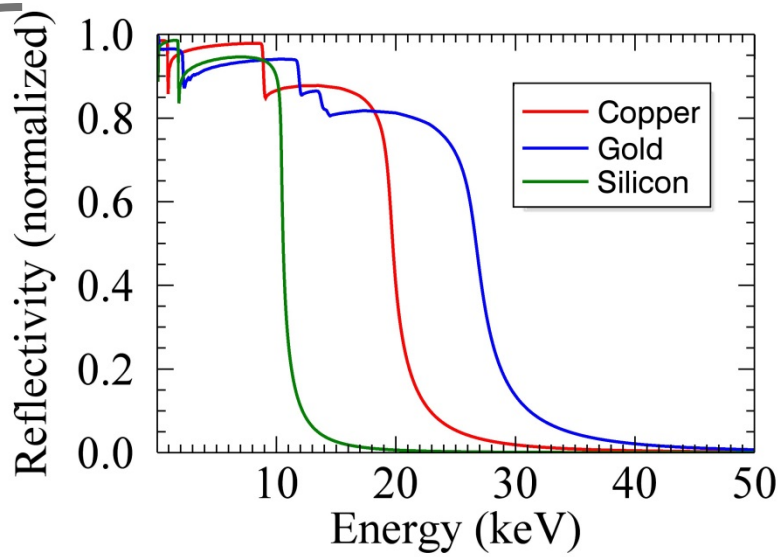
$$E_c = hc/\lambda_c = (hc/\theta)\,(n_e r_e/\pi)^{1/2}$$

Uses of Reflective Optics: X-ray Mirrors

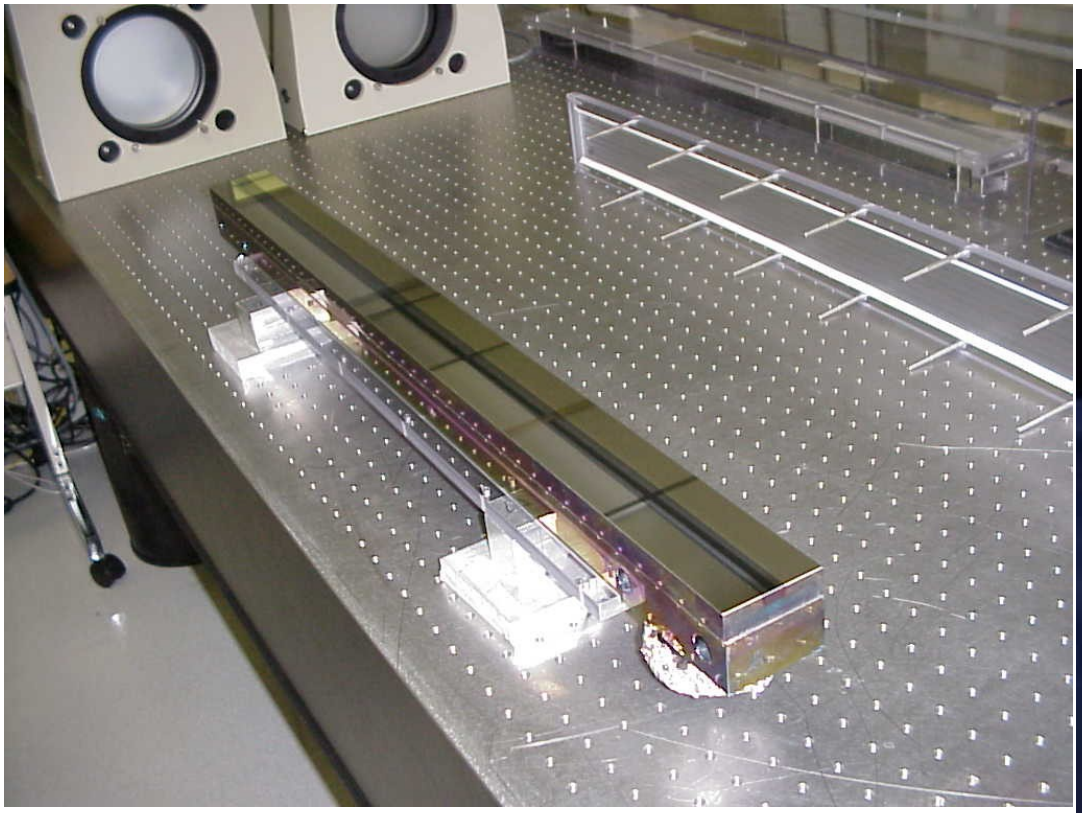
- Low-pass filters
  - Since there is an high energy cut-off above which radiation is reflected with low efficiency; this means that mirrors can be used to effectively suppress high energies.
  - Depending on the critical energy of the source, mirrors can effectively remove a considerable amount of the heat and reduce the thermal loading on downstream optics.
  - Since in many cases the angle of incidence is fixed (due to the various beamline components downstream), mirrors are designed so that the cut-off energy, E_c can be varied by having several different coatings deposited on the mirror substrate.

Fix the angle of incidence and vary the material density, i.e., n_e).

Typically, the mirror is set at a fixed angle, resulting in an energy cutoff, E_c; energies below E_c are reflected and those above are not. In the lower figure, the reflectivity curves as a function of x-ray energy for three different materials; copper, gold, and silicon are shown. The incident angle is fixed at 3 milliradians.

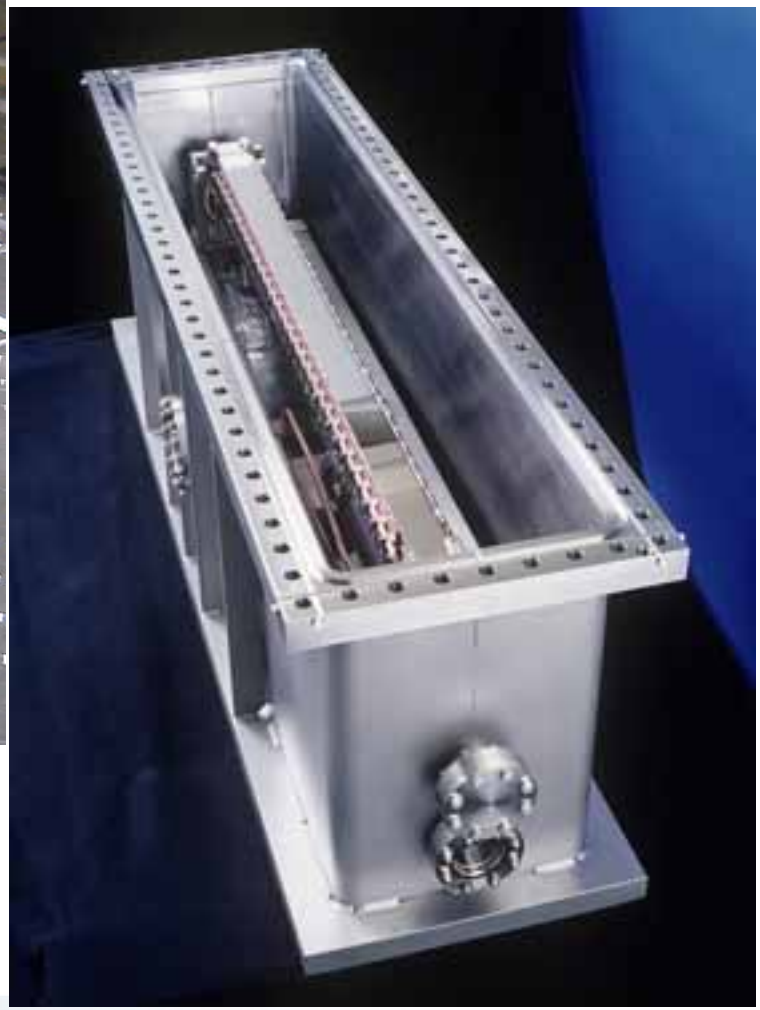


Consequence of Small Critical Angles - Long Mirrors to Capture Full Beam



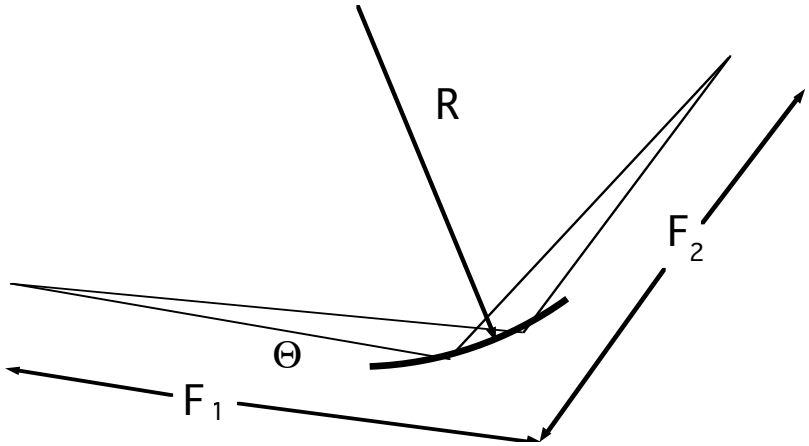
An x-ray mirror that had been in the x-ray beam (you can see the black stripe where the beam hit) being measured for surface roughness off-line.

Water cooled mirror in its vacuum tank.



Mirrors as Focusing Optics

- One-dimensional focusing, collimating, etc.
  - An ellipse is the ideal shape for a reflecting surface for point-to-point focusing. (A source at one foci will be imaged at the other foci.)
  - Collimation can be achieved by a parabola if the source is placed at the focal point. (This is simply an ellipse with the second focal point at infinity.)
  - In many cases cylindrically shaped mirrors are used rather than ellipses and parabolas since they are considerably easier to fabricate.



Typically, $\theta = 3$ mrad, $F_1 = 30$m, $F_2 = 30$m and so

$R_m = 10$ kilometers

Focal length, $f = [R_m \sin \theta]/2$

The "lensmaker" equation is:

$$\frac{1}{f} = \frac{1}{F_1} + \frac{1}{F_2}$$

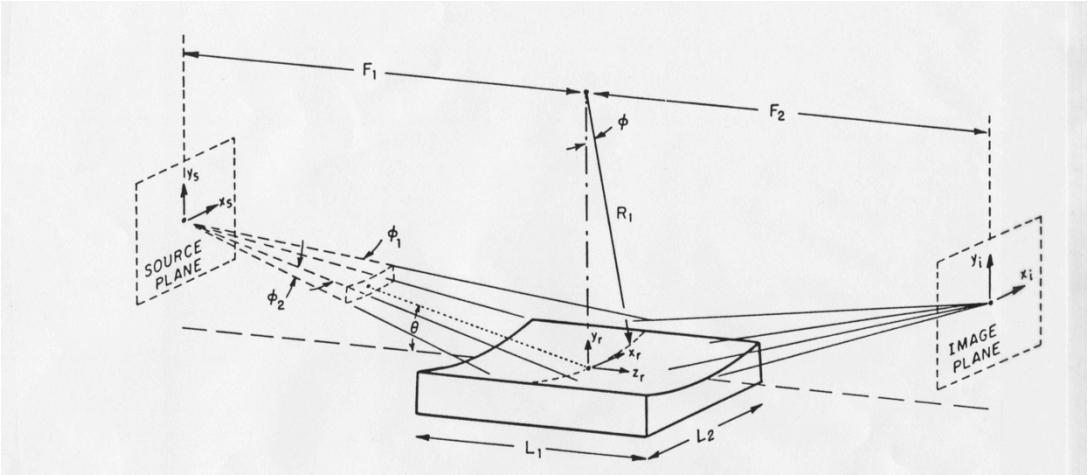
So:

$R_m = [2/\sin \theta]\,[F_1 F_2/(F_1 + F_2)]$

Focusing in Two Dimensions with Mirrors

- Two-dimensional focusing (toroids and ellipsoids)
  - An ellipsoid is the ideal shape for a reflecting surface for point-to-point focusing.
  - Bent cylinders are often used in place of an ellipsoid.
  - The sagittal radius, R_s, is given by:

$$R_s = R_m \sin^2 \theta$$



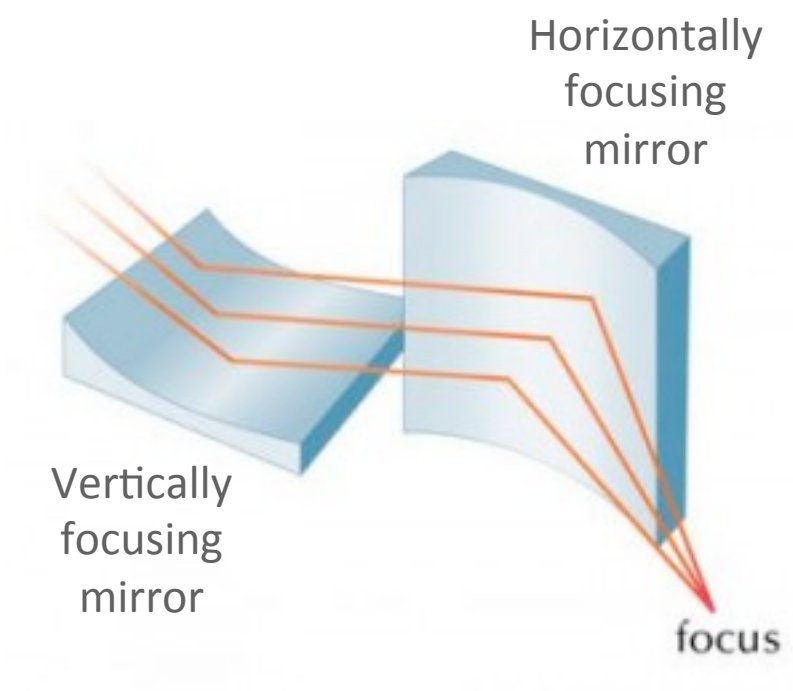
- In our example, from the last slide, q = 3 mrad and R_m = 10 km so the sagittal radius would be:

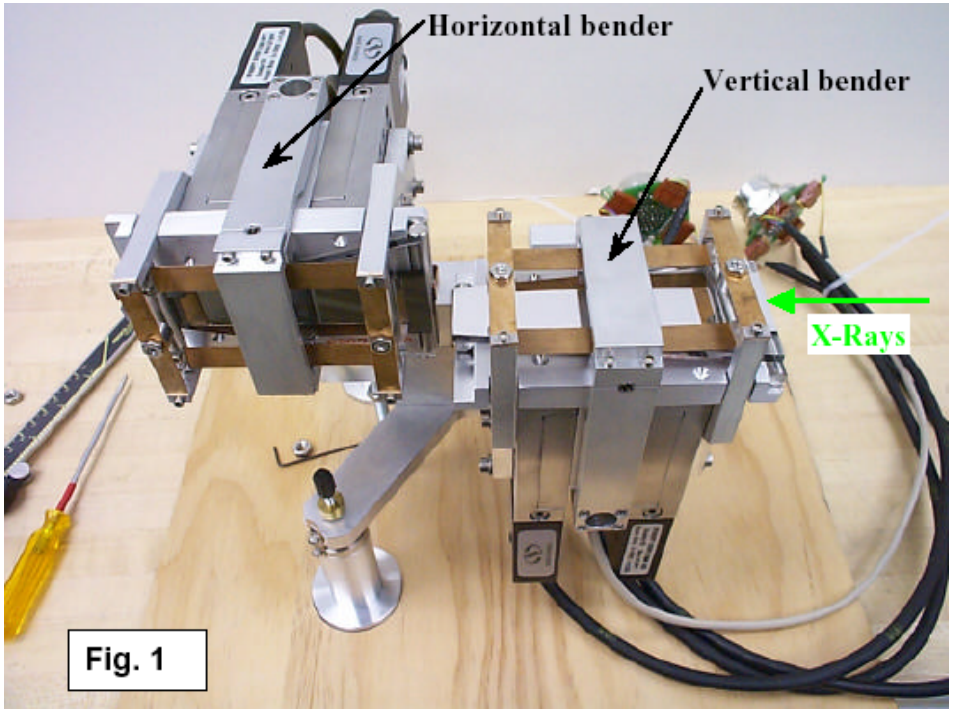
$$R_s = 9 \text{ cm}$$

Focusing in Two Dimensions - KB Systems

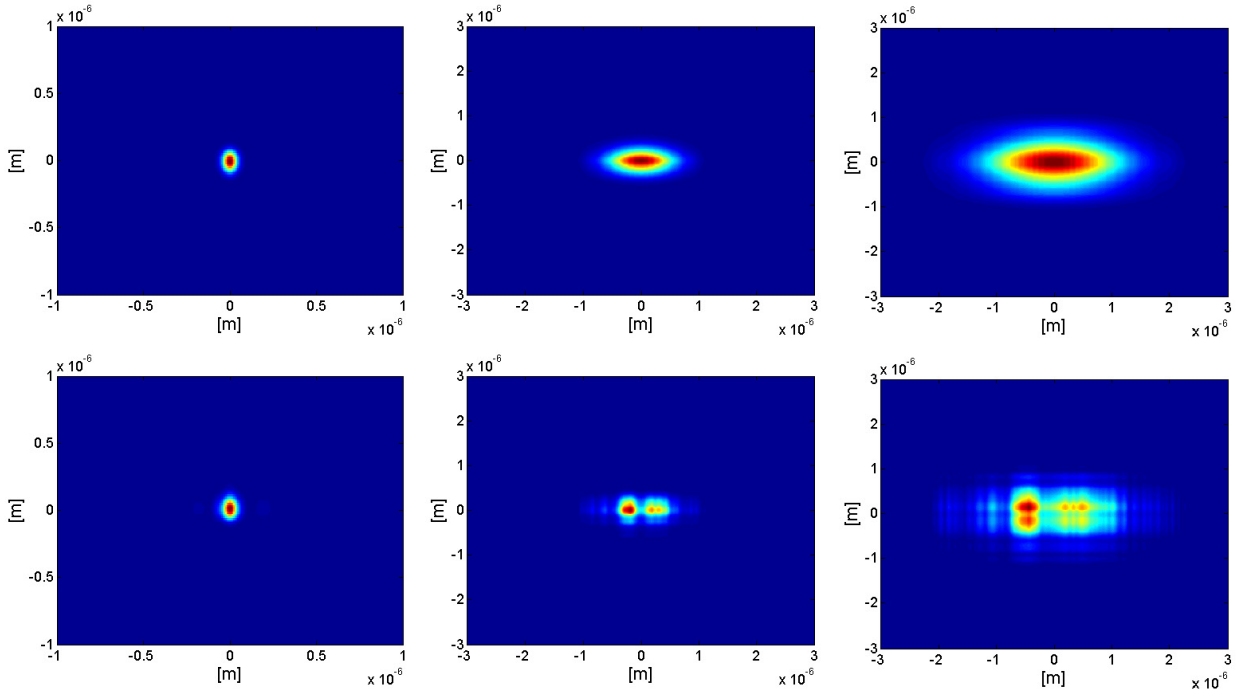
- Another system which focuses in two dimensions consists of a set of two orthogonal singly focusing mirrors, off which incident X-rays reflect successively, as first proposed in 1948 by Kirkpatrick and Baez (KB).

- This system allows for easier fabrication of the mirrors and is used frequently at synchrotron sources.





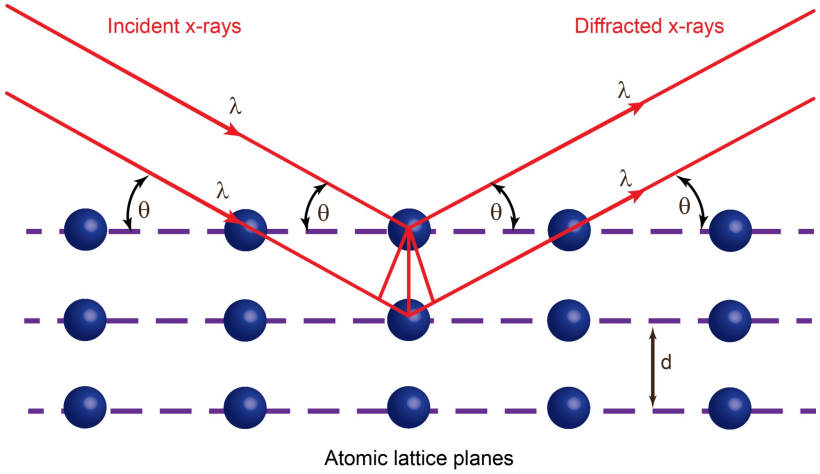
High Brightness Sources Put Stringent Demands on Mirror Quality



- False-color simulated intensity profiles for the 10-keV diffraction-limited example calculated at the focus (left), 1 mm from the focus (middle), and 2 mm from the focus (right). The upper row simulates the effect of 0.3-nm rms figure height error while the lower row depicts that of 1-nm rms figure height error. The resultant wave-front error has limited impact on the focus spot size, but even slightly off the focus the beam structure introduced by 1-nm rms figure height error is profound. (Simulation results courtesy of Jacek Krzywinski – LCLS using measured LCLS mirror height error data.)

Diffractive Optics

- By far, the most commonly used optical component for x-rays are crystals satisfying Bragg's law, i.e.,



Constructive interference when

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

Bragg's Law

- In nearly all cases **perfect single crystals** are used as the diffractive elements since:
  - they have a reflectivity near unity (more later)
  - the physics is well understood and components can be fabricated with predicted characteristics
  - If designed properly, they preserve the beam brightness

Some History: Laue and the Braggs

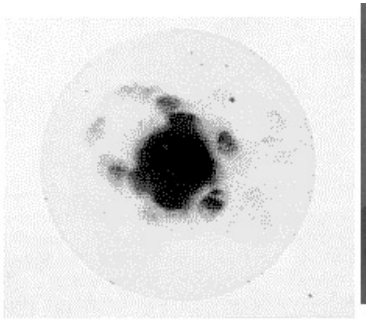
- Max von Laue (1879-1960) realized that short wavelength electromagnetic rays, such as X-rays, should cause diffraction or interference phenomena in crystals and had worked out the positions of of the x-ray interference maxima (reflections) but not the intensity. (M. Laue, Kon. Bay. Ak. 1912, p. 303) based on the work by Friedrich and Knipping (W. Friedrich & P. Knipping, Kon. Bay. Ak. 1912, p. 311).

- Von Laue received Nobel Prize in 1914 for his work.

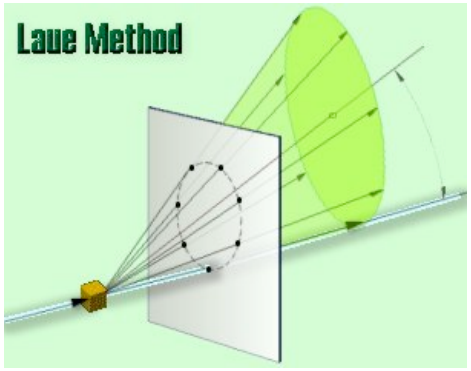
- William L. Bragg (the son), using his father's spectrometer, reported in 1913 that the scattering phenomena in crystals as the reflection of x-rays from sets of parallel planes of atoms in the crystal. ("*The diffraction of short electromagnetic waves*", W. L. Bragg. Proc. Camb. Phil. Soc., Vol. XVII, p. 43, 1913) and first wrote down what we now call Bragg's Law.

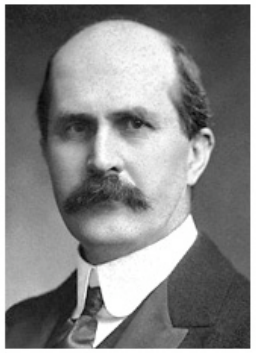
- The Braggs shared the 1915 Nobel Prize in Physics.

Images from: http://www4.nau.edu/microanalysis/Microprobe-SEM/History.html

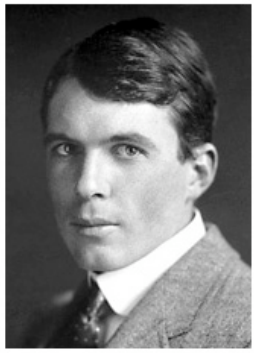


Max von Laue





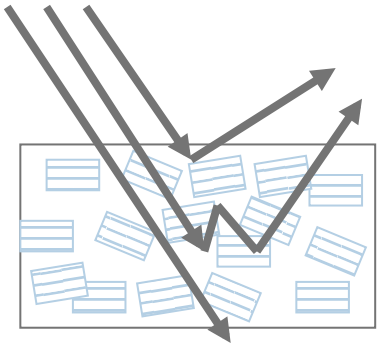
William Henry Bragg



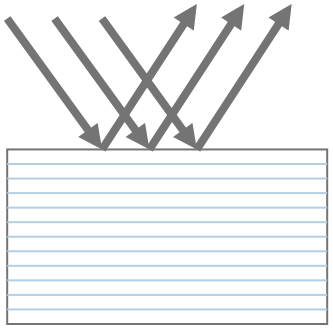
William Lawrence Bragg

Diffraction from Perfect Crystals

- The theory that describes diffraction from perfect crystals is called dynamical diffraction theory (as compared with kinematical theory, which describes diffraction from imperfect or mosaic crystals) first proposed in 1914 by Charles Darwin in two seminal papers.



Mosaic crystal model



Perfect crystal model

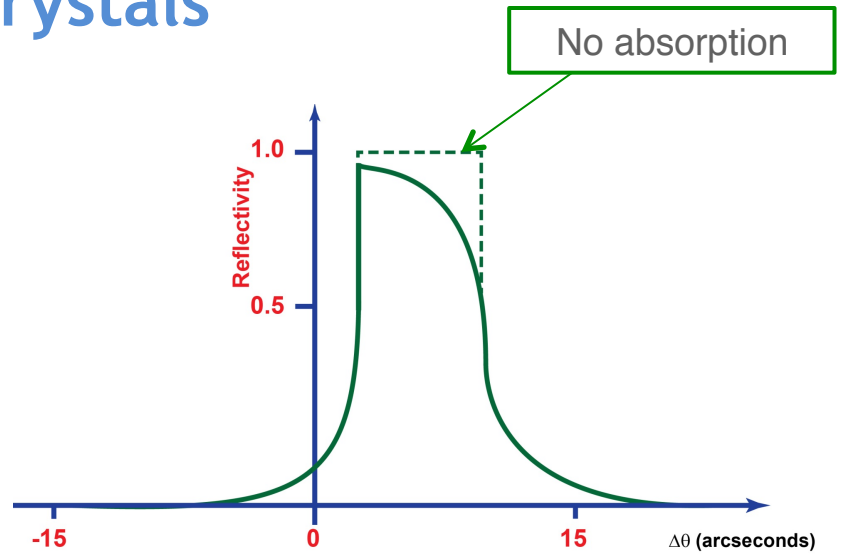
http://www.eoht.info/page/C.G.+Darwin

- The name "dynamical diffraction" was coined due to the fact that, during the diffraction process from perfect single crystals, there is a dynamical interplay between the incident and scattered beam, which can be comparable in strength.
- In the case of a strong reflection from a perfect crystal of a monochromatic x-ray beam, the penetration of the x-rays in to the crystal is not limited by the (photoelectric) absorption, but the beam is attenuated due to the reflecting power of the atomic planes. (This type of attenuation is called "extinction".)

> *" if the crystal is perfect all the radiation that can be reflected is so, long before the depth at which the rays at a different angle are appreciably absorbed."*

Two Important Consequences of Limited Penetration in Diffraction from Perfect Crystals

- The limited penetration due to extinction (reflection by the atomic planes) means:
  - At the Bragg condition, the x-ray beam is limited in the amount of materials it "sees"
  - and hence the scattered beam can get in and out of the crystal with little loss of amplitude from (photoelectric) absorption.



- Consequence #1:
  - There is a finite angular width over which the diffraction occurs. This is is often called the ***Darwin width***, ω_D (after Darwin)
  - Depends on the strength of the reflection (hkl) and wavelength.

Using modern notation, Darwin width, ω_D, can be written as:

$$\omega_D = 2r_e F(hkl)\lambda^2/\pi V \sin(2\theta)$$

F(hkl) = structure factor
V = volume of unit cell

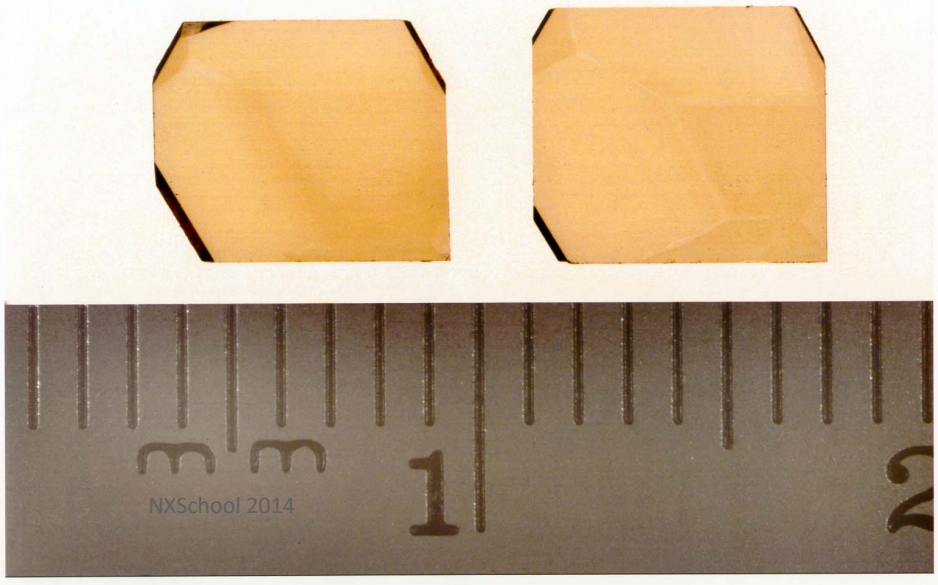
- Consequence #2:
  - The reflectivity over this narrow Darwin width is nearly unity, even in crystals with a finite absorption.

Real World Perfect Crystals

Perfect single crystal optics are used as the diffractive elements since:

- they have a reflectivity near unity
- the physics is well understood and components can be fabricated with predicted characteristics
- If designed properly, they preserve the beam brightness

At first glance, requiring the use of only perfect crystals for x-ray optical components may seem very limiting. However, **silicon and germanium**, are readily available (due to their use in the semiconductor industry) and are grown in large boules that are relatively inexpensive.



Nearly perfect single crystals of synthetic (grown) diamonds are also desirable, primarily for their mechanical properties which are extremely important when used as first optical components.

Perfect Crystal Monochromators

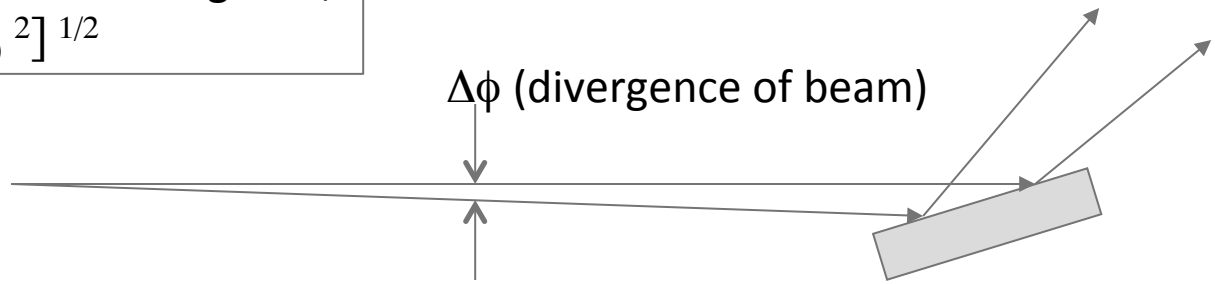
- The most frequent use of perfect crystal optics are for x-ray monochromators. They simply use Bragg's Law to select a particular wavelength (or energy, since $\lambda = hc/E$):

$$\lambda = 2d \sin(\theta).$$

- If we differentiate Bragg's Law ($\Delta\lambda = \cot(\theta)\ \Delta\theta$) , we can determine the energy resolution ($\Delta\lambda / \lambda$ or $\Delta E/E$) of the monochromator.

$$\Delta\lambda / \lambda = \Delta E/E = \cot(\theta)\ \Delta\theta$$

$\Delta\theta$ has contributions, the Darwin width, ω_D, and x-ray beam divergence, $\Delta\phi$. $\Delta\theta = [\Delta\phi^{2} + \omega_D^{2}]^{1/2}$

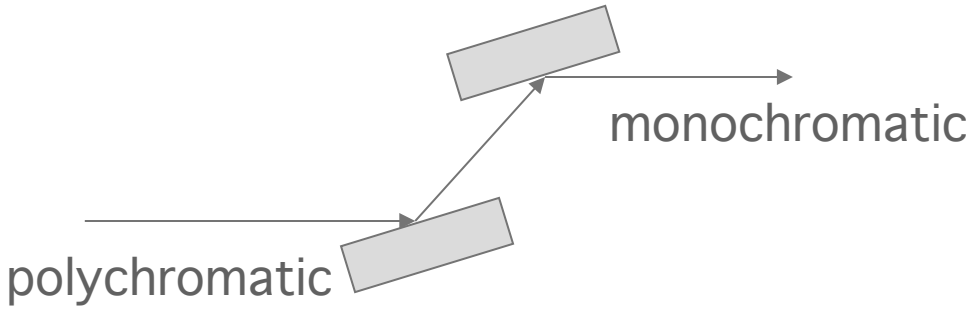


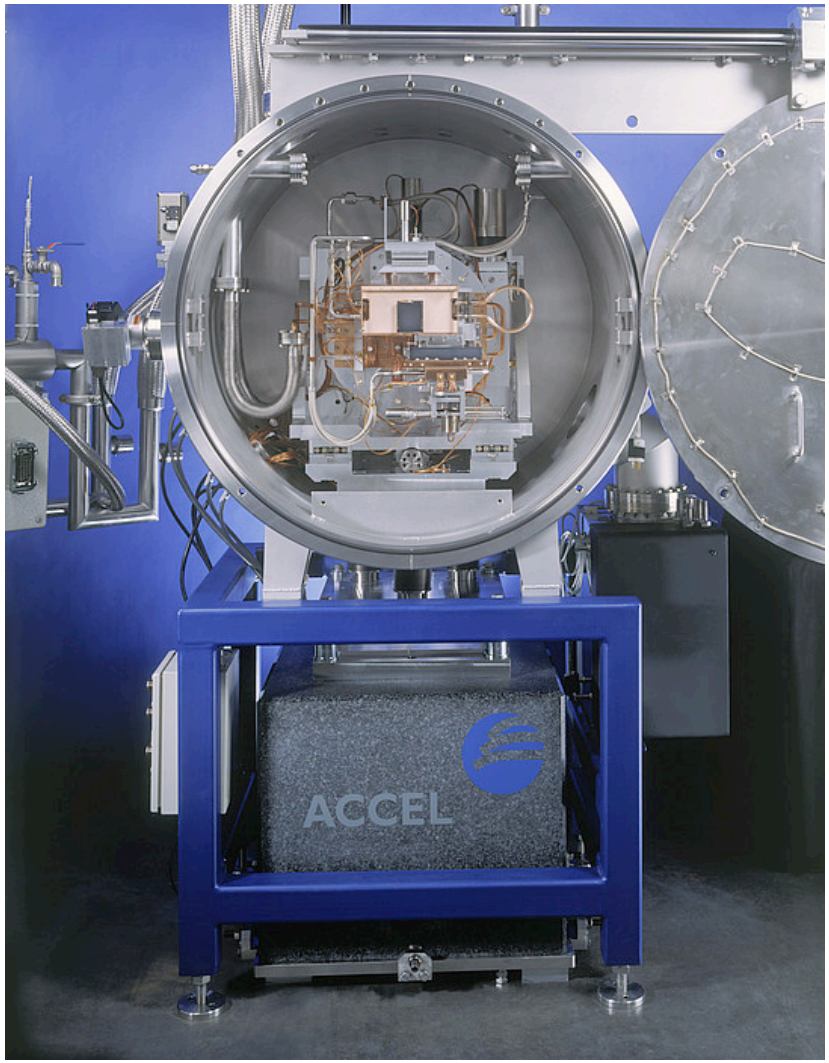
- A value of ω_D for the (111) reflection in silicon at 8 keV (1.5Å) is about 8 sec of arc or 40 microradians. Recall that, for an undulator, the opening angle is about 10 - 15 microradians. Here the energy resolution of the mono is determined by the crystal.

Double Crystal Monochromators

- The most common arrangement for a monochromator is the double-crystal monochromator. It:
  - is non-dispersive, that is all rays that diffract from the first crystal simultaneously diffract from the second crystal (if same crystals with same hkl's are used)
  - keeps the beam fixed in space as the energy is changed.

- There is little loss in the throughput because the reflectivity is near unity over the Darwin width.

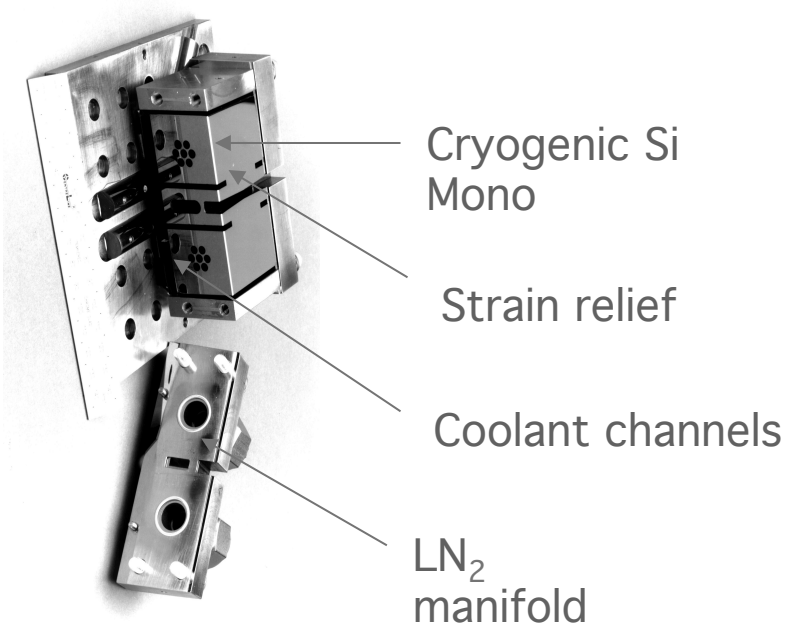




http://www.bruker-est.com/monochromator.html

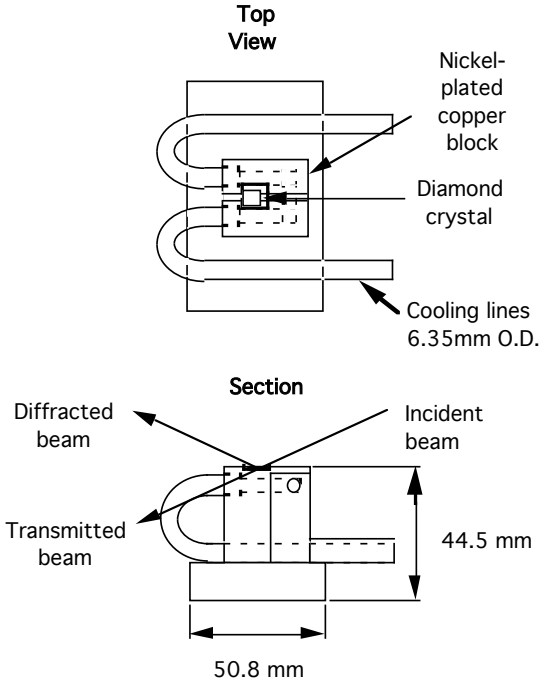
Cooled Monochromators

- One solution to this problem is to cool the Si crystals to liquid nitrogen temperatures for that increases the thermal conductivity and reduces the coefficient of thermal expansion.



Cryogenically Cooled Si Mono

Water Cooled Diamond Mono



Another solution to this thermal problem is to go to other materials (i.e. , diamond) that have better thermal and mechanical properties than Si at room temperature.

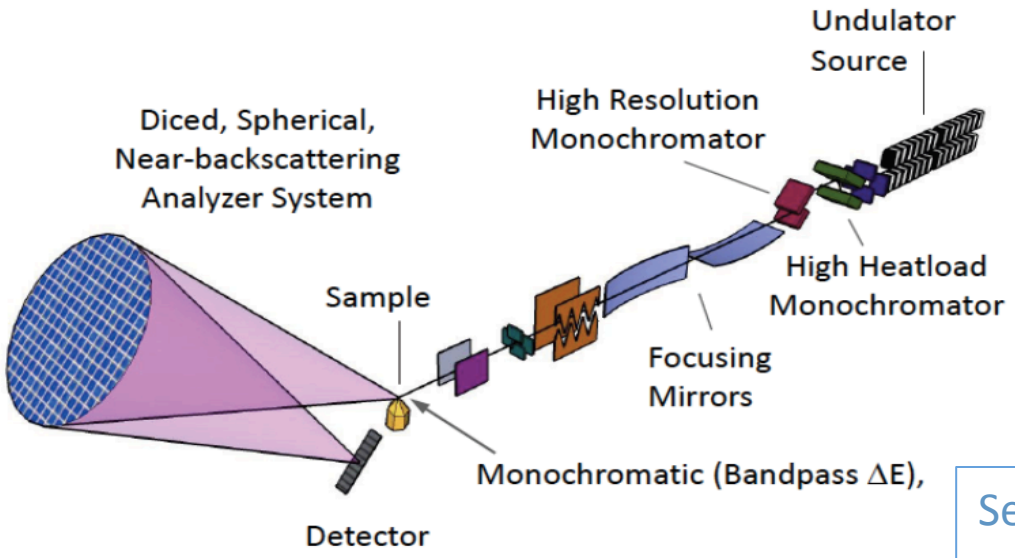
See Appendix 3 for more information regarding thermal issues for monochromators.

High-Energy Resolution Optics

- For techniques such as inelastic x-ray scattering, additional spectral filtering for higher energy resolution ($\Delta E/E \sim 10^{-5} - 10^{-6}$) is required for both the x-rays impinging on the sample as well as for those that scatter from it.

- To achieve energy resolution at this level requires special geometries for the optical components, often Bragg scattering with the angle of incidence near 90°.

- Recall that: $\Delta\lambda / \lambda = \Delta E/E = \cot(\theta)\ \Delta\theta$, so this can be made small by θ -> 90°



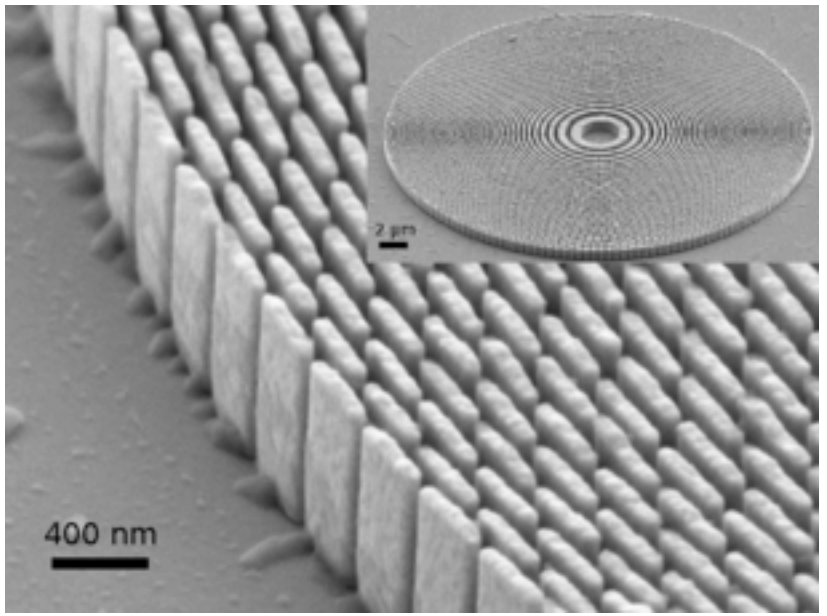
The x-rays from an undulator are monochromated by the high heat load monochromator ($\Delta E/E \approx 10^{-4}$) and then the bandpass is further reduced ($\Delta E/E \approx 10^{-5}$ to 10^{-6}) by a high resolution monochromator.

After being inelastically scattered by the sample, the x-rays of the desired energy are sorted out and focused onto a detector by a spherically bent analyzer. The monochromators, high resolution monochromators, and analyzer are all fabricated from perfect single crystals of silicon.

See Appendix 4 for more information regarding high resolution optics

Diffractive Focusing Optics: X-ray Zone Plates

- Zone plates are diffraction gratings, that is, structures composed of alternating concentric zones of two materials with different (complex) refractive indices.
- The focusing capability is based on constructive interference of the wavefront modified by passage through the zone plate.
- The wave that emerges from the zone plate is the superposition of spherical waves, one from each of the zones.
- The wavefront modification is obtained through the introduction of a relative change in amplitude or phase in the beams emerging from two neighboring zones.



http://www.psi.ch/lmn/electron-beam-lithography

JOURNAL OF THE OPTICAL SOCIETY OF AMERICA VOLUME 51, NUMBER 4 APRIL, 1961

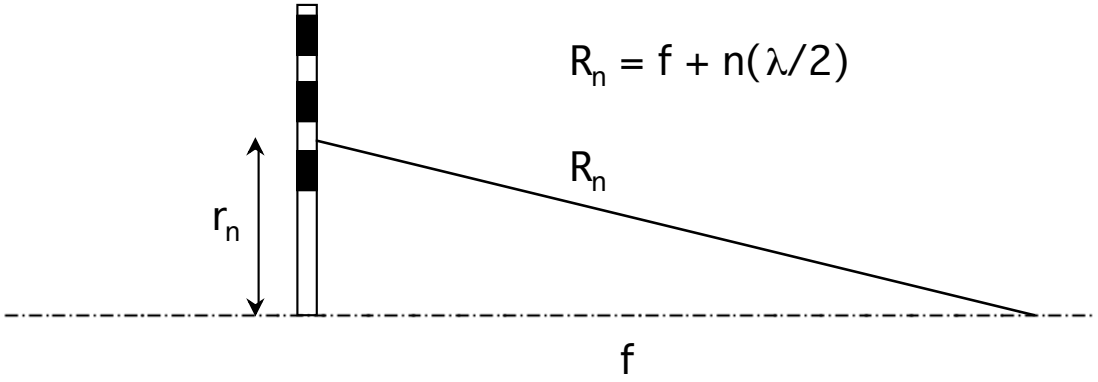
Fresnel Zone Plate for Optical Image Formation Using Extreme Ultraviolet and Soft X Radiation

ALBERT V. BAEZ
Smithsonian Astrophysical Observatory, Cambridge, Massachusetts
(Received April 25, 1960)

Zone Plate Physics

Condition so the pathlength varies by $\lambda/2$ for each ring.

$$R_n = f + n(\lambda/2)$$



Cape Meares Lighthouse (Oregon); first-order Fresnel lens

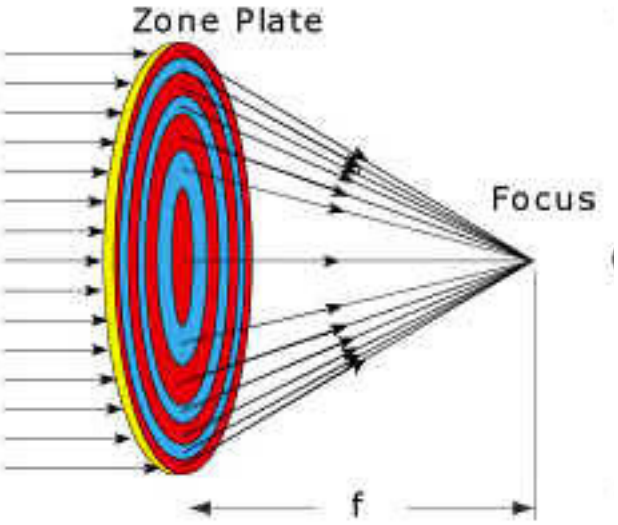
The radius of the nth zone is therefore:

$$r_n = (R_n^2 - f^2)^{1/2} = [(f + n(\lambda/2))^2 - f^2]^{1/2}$$

$$= [nf\lambda + n^2(\lambda^2/4)]^{1/2}$$

If $f >> n\lambda$, as is usually the case with hard x-rays, then:

$$r_n = (nf\lambda)^{1/2}$$

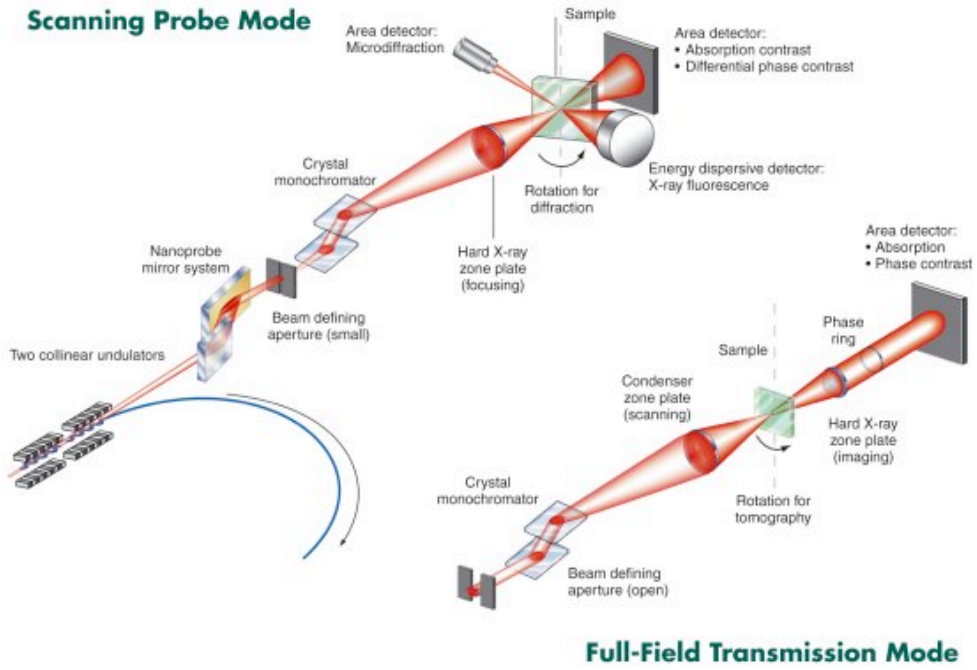


Zone Plane Focal Spot Size

- In general, the size of the focal spot from the zone plate is determined by the width of the outermost ring, Δr_{out} , and is given by:

$$\Delta x = 1.22\ \Delta r_{out}\ .$$

- Zones plates with outermost ring widths of less than 20 nanometers can currently be fabricated.



The hard x-ray nanoprobe beamline at 26-ID at the APS.

Hard X-ray Phase Zone Plates

- The difficulty with making zone plates at hard x-ray energies is one of fabrication. You need:
  - small width outermost zone for focusing (less than 50 nms)
  - but it has to be thick (high) to totally absorb the unwanted waves
  - i.e. the aspect ratio (height/width) is very large - 10^2 to 10^3 and therefore difficult to fabricate

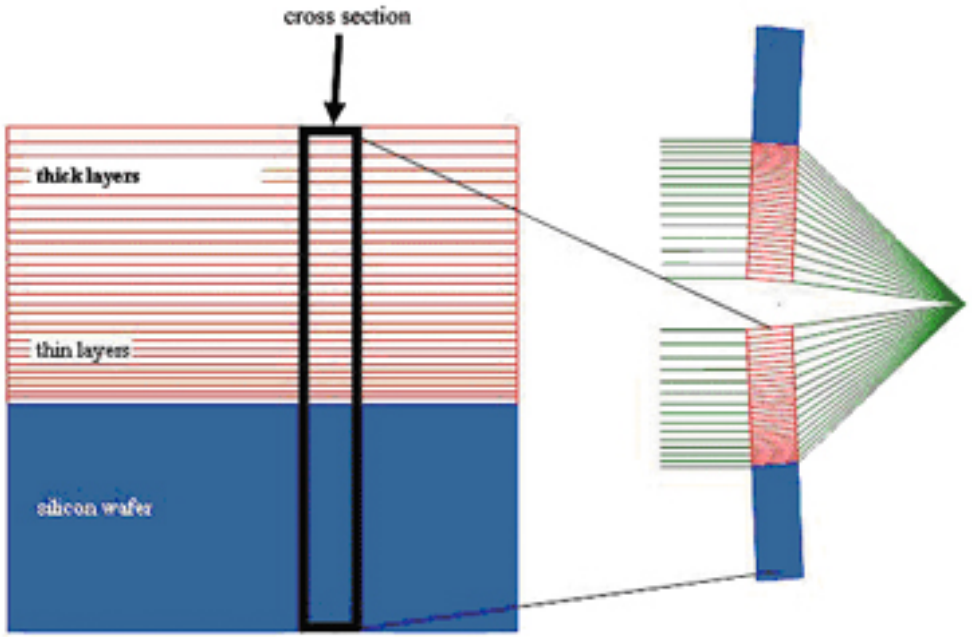
- An alternative to "blocking" out those rays that are out of phase (as in an amplitude zone plate), the thickness of the material can be adjusted so that the wave experiences a phase shift of π.

- Phase zone plates have a much better efficiency than amplitude zone plates (10% efficiency for amplitude zone plates vs 40% for phase zone plates).

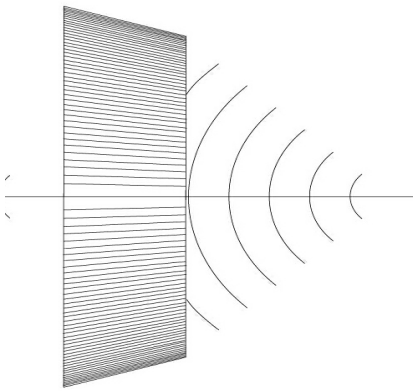
- The phase zone plates ease the thickness requirement (as compared to the amplitude zone plates) but the aspect ratio is still an issue.

A New Approach to Fabricating Zone Plates

- Start with a linear zone plate geometry and then use a Kirkpatrick-Baez configuration to get focusing in both directions.



- Using state-of-the-art deposition techniques, start with the thinnest layer first and fabricate a multilayer structure with the layer spacing following the Fresnel zone plate rule.
- Slice and polish the multilayer structure to get a linear zone plate.



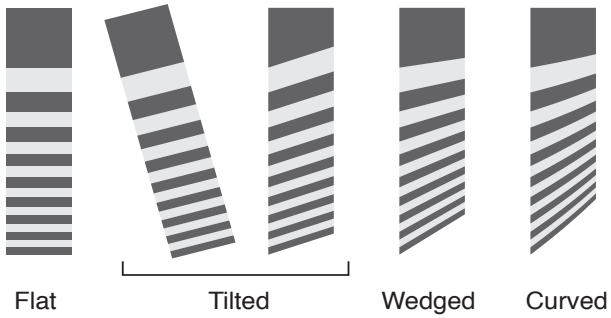
Wedged MLL

- Each MLL comprises 1,588 layers (lines)
- The thinnest layer (line) is 5 nanometers thick
- The MLL has a current focus of 11 nanometers at 12 keV and 16 nanometers @ 19 keV!

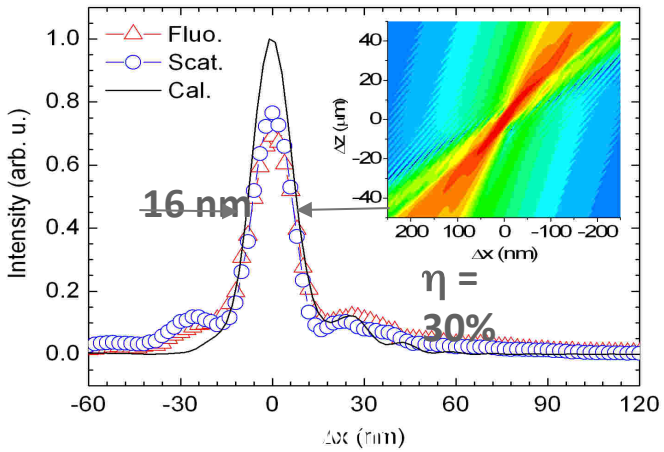
H. C. Kang, J. Maser, G. B. Stephenson, C. Liu, R. Conley, A. T. Macrander, and S. Vogt, "Nanometer Linear Focusing of Hard X Rays by a Multilayer Laue Lens," Phys. Rev. Lett. 96, 127401 (2006).

Multilayer Laue Lenses

- **Technical approach**
  - Crossed multilayer-based linear zone plate structure

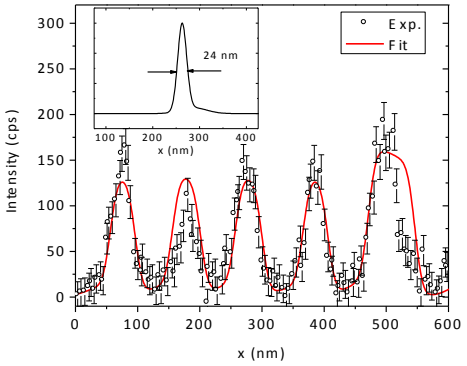


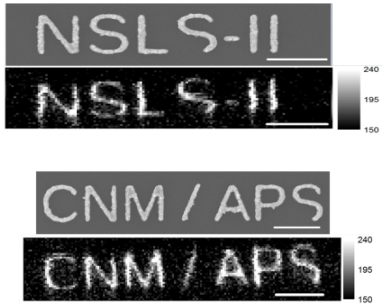
1-D focus: 16 nm (half MLL) **@ 19.5 keV**



Kang et al, APL 92, 221114 (2008)

2-D focus: 25 x 40 nm^2 (2D, crossed MLL) **@ 20 keV**





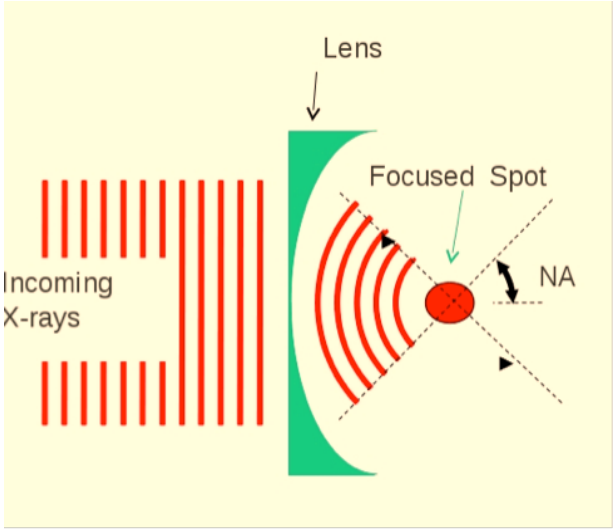
2-D imaging with crossed MLL (ANL/BNL collaboration)

Yan et al, H. Yan et al, Opt. Exp. 2011

Refractive Focusing Optics: X-ray Lenses

- Roentgen's first experiments convinced him that x-rays could not be concentrated by lenses; many years later his successors understood why (index of refraction is very close to 1).

- Refractive lenses were considered by Kirkpatrick and Baez in 1948 for focusing but were abandoned for crossed mirrors.



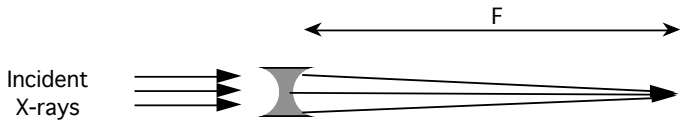
- Unfortunately materials of large d are also strong absorbers, the absorption coefficient increasing much more rapidly than δ with increasing atomic number. An element of low atomic number, such as beryllium, is indicated.

- For a single concave lens: $1/F = \delta(1/R)$

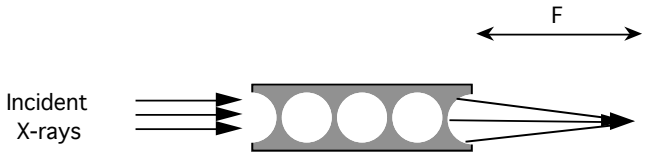
- Plugging in some numbers, suppose that:
  $R = 1$ mm $\delta \approx 10^{-5}$

- Then the focal length, F, would be at 100 m!

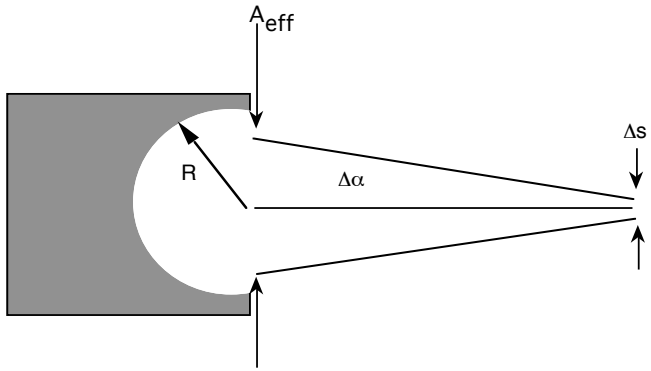
Compound Refractive Lenses



Single Refractive Lens



Compound Refractive Lens



- The Lens Maker's Equation:

$$1/F = \delta\,(1/R_1 + 1/R_2 + \text{etc.})$$

- For a single lens:

$$1/F = \delta(1/R + 1/R)$$

or

$$F = R / 2\delta$$

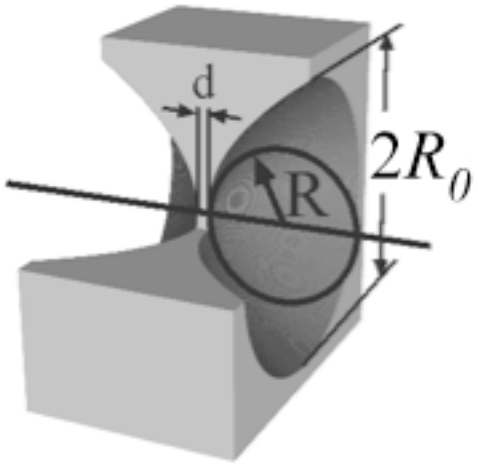
- If we have N surfaces, all with radius r:

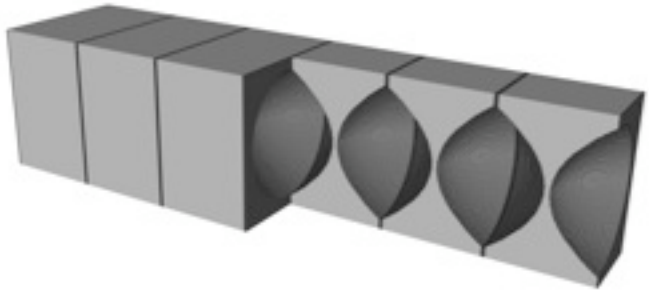
$$F = R/2N\delta$$

- Using the same numbers as before but with 50 lenses, i.e.:
  R = 1 mm $\delta \approx 10^{-6}$ N = 50
- Then the focal length, F, would be at 10 m.
- These lenses focus at rather larger distances and are well adapted to the scale of synchrotron radiation beamlines.

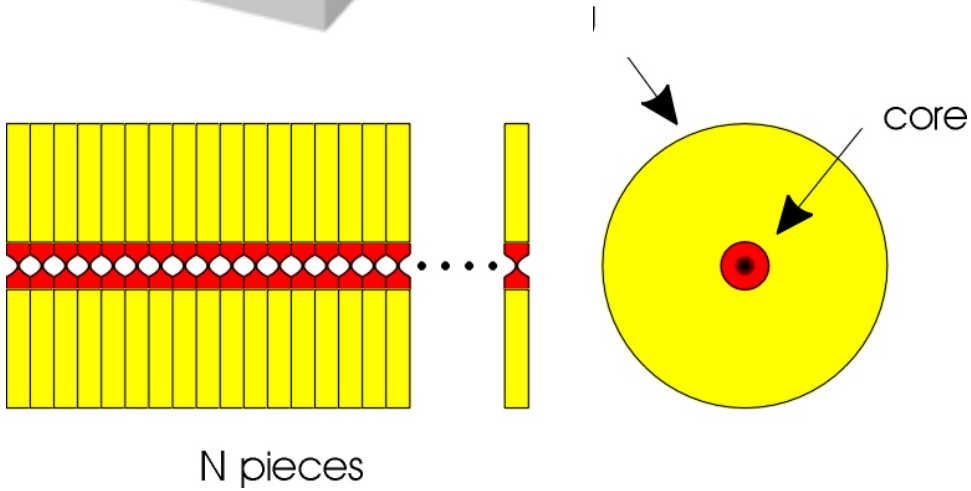
Focusing in Two Dimensions with Refractive Lenses

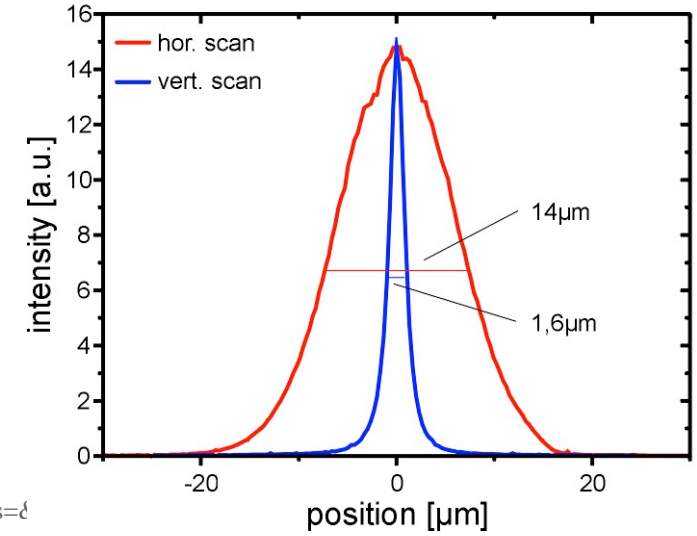
- Spherical lenses are easy to make but suffer from spherical aberrations.
- Paraboloids eliminate spherical aberrations.





tu-dresden.de/.../isp/skm/research/xray_lenses

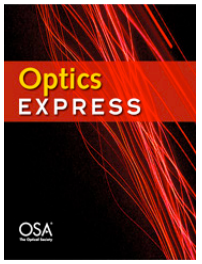




Figures from:
http://2b.physik.rwth-aachen.de/xray/imaging/main.php?language=en&frames=

Current Optics R&D Activities

- X-ray optics is still an active area of research at both universities and national laboratories.
- **New nano-fabrication capabilities** are opening up new possibilities for novel x-ray optical components.
- Also, availability of **high quality materials** (other than silicon) have opened up new opportunities.



Coherent x-ray zoom condenser lens for diffractive and scanning microscopy
Takashi Kimura, Satoshi Matsuyama, Kazuto Yamauchi, and Yoshinori Nishino
Optics Express, Vol. 21, Issue 8, pp. 9267-9276 (2013)

SCIENTIFIC REPORTS

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Accepted 28 November 2013
Published 20 December 2013

11 nm hard X-ray focus from a large-aperture multilayer Laue lens

Xiaojing Huang[1], Hanfei Yan[1], Evgeny Nazaretski[1], Raymond Conley[1,2], Nathalie Bouet[1], Juan Zhou[1], Kenneth Lauer[1], Li Li[1], Daejin Eom[1]*, Daniel Legnini[2], Ross Harder[2], Ian K. Robinson[3,4] & Yong S. Chu[1]

Contents lists available at SciVerse ScienceDirect
Nuclear Instruments and Methods in Physics Research A
journal homepage: www.elsevier.com/locate/nima

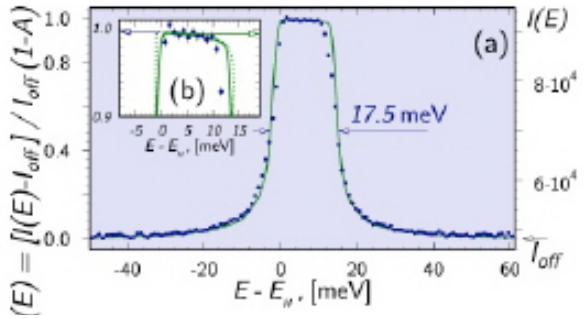
X-ray nanofocusing using a piezoelectric deformable mirror and at-wavelength metrology methods

Hiroki Nakamori[a], Satoshi Matsuyama[a,*], Shota Imai[a], Takashi Kimura[b], Yasuhisa Sano[a], Yoshiki Kohmura[c], Kenji Tamasaku[c], Makina Yabashi[c], Tetsuya Ishikawa[c], Kazuto Yamauchi[a,d]

LETTERS
PUBLISHED ONLINE: 17 JANUARY 2010 | DOI: 10.1038/NPHYS1506
nature physics

High-reflectivity high-resolution X-ray crystal optics with diamonds

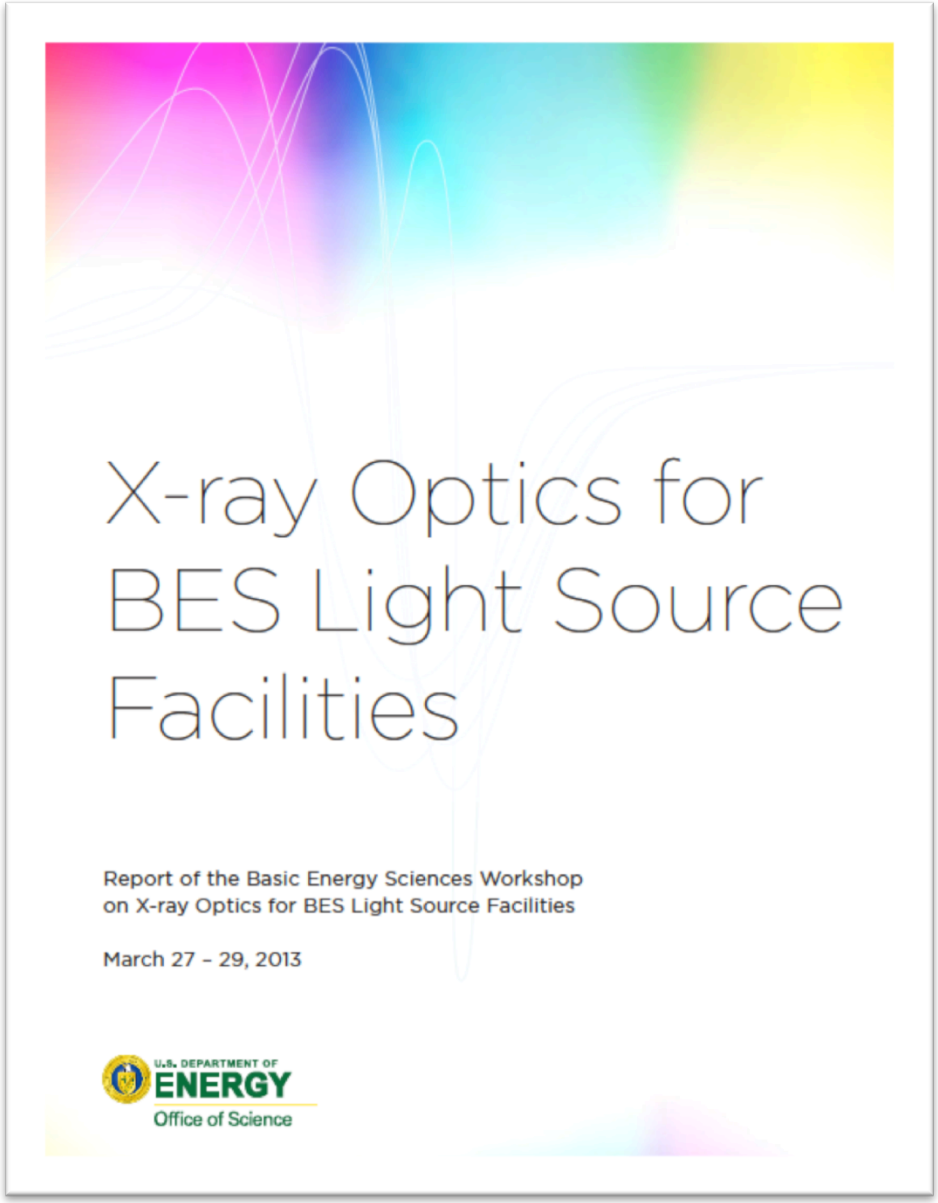
Yuri V. Shvyd'ko[1]*, Stanislav Stoupin[1], Alessandro Cunsolo[1,2], Ayman H. Said[1] and Xianrong Huang[2]



LETTERS
PUBLISHED ONLINE: 22 NOVEMBER 2009 | DOI: 10.1038/NPHYS1457
nature physics

Breaking the 10 nm barrier in hard-X-ray focusing

Hidekazu Mimura[1]*, Soichiro Handa[1], Takashi Kimura[1], Hirokatsu Yumoto[2], Daisuke Yamakawa[1], Hikaru Yokoyama[1], Satoshi Matsuyama[1], Kouji Inagaki[1], Kazuya Yamamura[3], Yasuhisa Sano[1], Kenji Tamasaku[4], Yoshinori Nishino[4], Makina Yabashi[4], Tetsuya Ishikawa[4] and Kazuto Yamauchi[1,3]



http://science.energy.gov/~/media/bes/pdf/reports/files/BES_XRay_Optics_rpt.pdf

The Department of Energy (DOE), Office of Basic Energy Sciences (BES) is sponsoring this workshop to identify opportunities and needs for X-ray optics developments at the existing and future BES facilities.

This workshop will assess the state of the art and future developments, with emphasis on the underlying engineering, science, and technology necessary to realize the next generation of X-ray optics instruments to advance photon-based science. The scope will include adaptive optics, nanodiffractive optics, mirrors, and simulation tools.

The workshop will explore opportunities for discovery enabled by advanced X-ray optics, and identify processes to enhance interactions and collaborations among DOE laboratories to most effectively use their resources and skills to advance scientific frontiers in energy-relevant areas, as well as the challenges anticipated by advances in source brightness. Consequently, the workshop has the opportunity to influence BES strategic investment in X-ray optics research.

Co-chairs
Dennis Mills
Argonne National Laboratory
Howard Padmore
Lawrence Berkeley National Laboratory

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Hard X-ray Optics

- *Elements of Modern X-ray Physics*, Jens Als-Nielsen and Des McMorrow, John Wiley and Sons (2001).

- *Third Generation Hard X-ray Synchrotron Radiation Sources*, Dennis Mills, Editor, John Wiley and Sons (2002).

- *Dynamical Theory of X-ray Diffraction*, Andre Authier, IUCr Oxford Science Publications (2001).

- *Report of the Basic Energy Sciences Workshop on X-ray Optics for BES Light Source Facilities*, Potomac, MD / March 27-29, 2013. (http://science.energy.gov/~/media/bes/pdf/reports/files/BES_XRay_Optics_rpt.pdf)

- *The Optical Principles of the Diffraction of X-rays*, R. W. James, Cornell University Press (1965)

Soft X-ray Optics

- *Soft X-ray Optics*, Eberhard Spiller, SPIE Optical Engineering Press (1994)

Appendix 1a: Dielectric Constant and the Drude Model

The dielectric constant, κ, is defined as follows:

$$\kappa = D/E = (E + 4\pi P)/E = 1 + 4\pi(P/E)$$

For a single electron:

$$p = -ex$$

and for multiple electrons:

$P = -exn_e$ (n_e is the number of electrons/unit volume)

In the Drude model, the frequency of the collective oscillations of the electron gas around the positive ion background is the so-called plasma frequency and equal to:

$$\omega_o = [4\pi n_e e^2/m]^{1/2} .$$

If we assume a simple harmonic approximation then:

$$F = ma = mx'' = -eE - kx$$

where k is the "spring constant" associated with ω_o (= $[k/m]^{1/2}$).

Appendix 1b: X-ray Index of Refraction

If x has the form $x = Ae^{i\omega t}$, solving for x we get:

$$x = (e/m)E/(\omega_o^2 - \omega^2) \quad \text{and}$$

$$P = -(e^2/m)n_e E/(\omega_o^2 - \omega^2)$$

Using this simple model, one can then calculate the polarizability of the material:

$$\kappa = 1 + 4\pi(P/E) = 1 + 4\pi (e^2/m)n_e [1/(\omega_o^2 - \omega^2)]$$

For Si, $n_e = 7 \times 10^{23}$ e/cm^3 and so the plasma frequency is:

$$\omega_o = \mathbf{5 \times 10^{16}/sec}$$

For a 1 Å x-ray, the angular frequency, ω (= $[2\pi c/\lambda]$), is **2×10^{19}/sec (>> ω_o)** and so we can write:

$$\kappa = 1 + 4\pi (e^2/m)n_e [1/(\omega_o^2 - \omega^2)] \approx 1 - 4\pi (e^2/m)n_e [1/(\omega^2)]$$

$$n = \kappa^{1/2} = [1 - (n_e(e^2/mc^2)\lambda^2/\pi)]^{1/2} \approx 1 - (n_e r_e/2\pi)\lambda^2$$

Appendix 2a: Inclusions of Absorption in the (Complex) Index of Refraction

- This simple model did not include any absorption of the incident radiation. A more detailed calculation would result in an expression:

$$n = 1 - \delta - i\beta$$

where $\delta = (n_e r_e/2\pi)\lambda^2$ and $\beta = \lambda\mu/4\pi$, with μ the linear absorption coefficient ($I = I_o e^{-\mu t}$).

Appendix 2b: Index of Refraction for X-rays is <1

- OK, isn't $V_{group} = (c/n)$? If $n < 1$, doesn't that mean the x-rays are traveling faster than the speed of light? **NO!**

$$V_{group} = \frac{d\omega}{dk} \quad \text{and} \quad \omega = \frac{ck}{n} \quad \text{so} \quad V_{group} = \frac{d}{dk}\left(\frac{ck}{n}\right); \quad k = \frac{2\pi}{\lambda} \quad n = 1 - \frac{2\pi n_e r_e}{k^2}$$

$$V_{group} = \frac{d}{dk}\left[\frac{ck}{1 - \frac{2\pi n_e r_e}{k^2}}\right] \approx \frac{d}{dk}\left[ck\left(1 + \frac{2\pi n_e r_e}{k^2}\right)\right] = c\frac{d}{dk}\left[\left(k + \frac{2\pi n_e r_e}{k}\right)\right] = c\left(1 - \frac{2\pi n_e r_e}{k^2}\right)$$

Appendix 3a: Thermal Loading on Optics

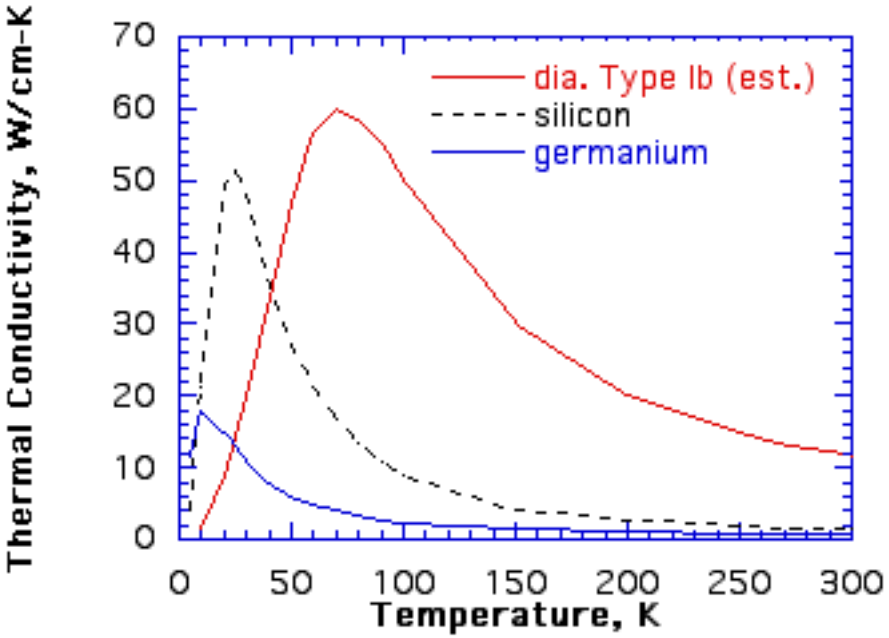
- Along with the enormous increase in x-ray beam brilliance from insertion devices comes unprecedented powers and power densities that must be effectively handled so that thermal distortions in optical components are minimized and the full beam brilliance can be delivered to the sample.

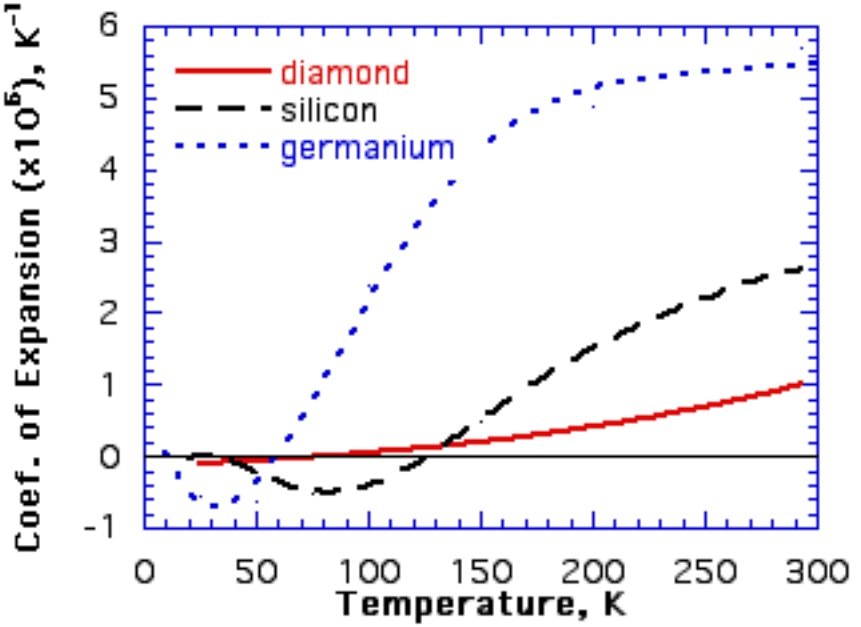
Process	Approx. Heat Flux (W/mm^2)
Fission reactor cores	1 to 2
Interior of rocket nozzle	10
Commercial plasma jet	20
Sun's surface	60
Fusion reactor components	0.05 to 80
Meteor entry into atmosphere	100 to 500
APS insertion devices (2.4 m and 100 mA)	**10 to 160**

- In order to maintain the beam intensity and collimation (i.e., brilliance) through the optics, special attention must be paid to the issue of thermal management.

Appendix 3b: Properties of Si, Ge, and C(diamond)

- Thermal gradients, ΔT, and coefficient of thermal expansion, α, contribute to crystal distortions:
  - $\alpha\Delta T = \Delta d/d = \cot(\theta)\,\Delta\theta = \cot(\theta)\,\omega_D$.
- We therefore need to look for materials that have a very low coefficient of thermal expansion, α, and/or have a very high thermal conductivity, k, so that the material cannot support large ΔT's.





Appendix 3c: Figure of Merit (FOM) for Various Materials and Temperatures

- These conditions motivate us to use cryogenically cooled silicon or room temperature diamond as high heat load monochromators.

FOM of various materials

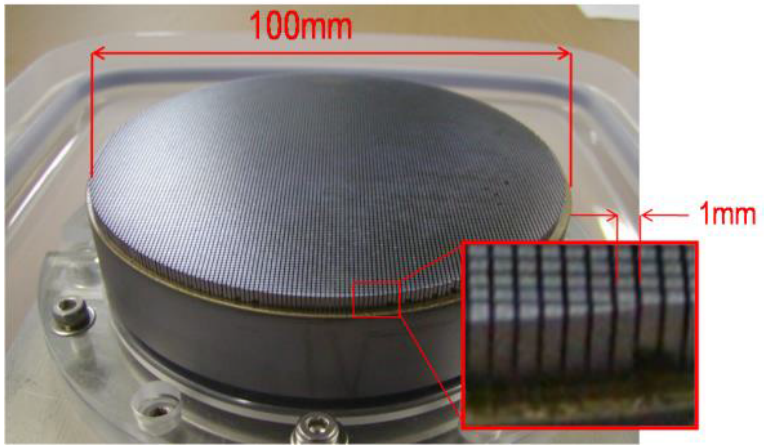
material	k - thermal conductivity	α - coef. of thermal expansion	k/α FOM
Si (300°K)	1.2 W/cm-°C	2.3×10^{-6} /°K	0.5
Si (78°K)	14 W/cm-°C	-0.5×10^{-6} /°K	28
Dia. (300°K)	20 W/cm-°C	0.8×10^{-6} /°K	25

Appendix 4: High Energy-Resolution Optics

- At $\theta = 89°$, $\cot(\theta) = 1.7 \times 10^{-2}$. For E = 20 keV (0.64Å), then:

$$\Delta E = E \cot(\theta)\Delta\theta = (2 \times 10^4 \text{ keV})(1.7 \times 10^{-2})(10^{-5}\text{rad}) = 3 \times 10^{-3} \text{ eV}.$$

- Note: For Si (111) at a Bragg angle of $\theta = 89°$, the wavelength is 6.2Å (2 keV) and so to get near 20 keV at $\theta = 89°$, we need to use a very high d-spacing such as Si (11 11 11).



A diced, high energy resolution inelastic x-ray spherical analyzer.

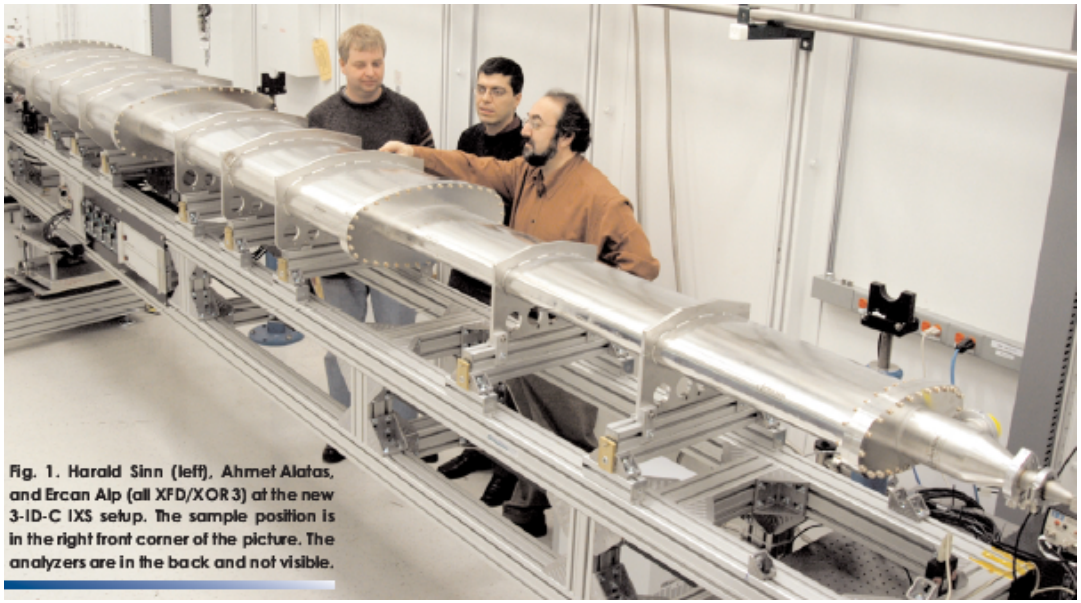
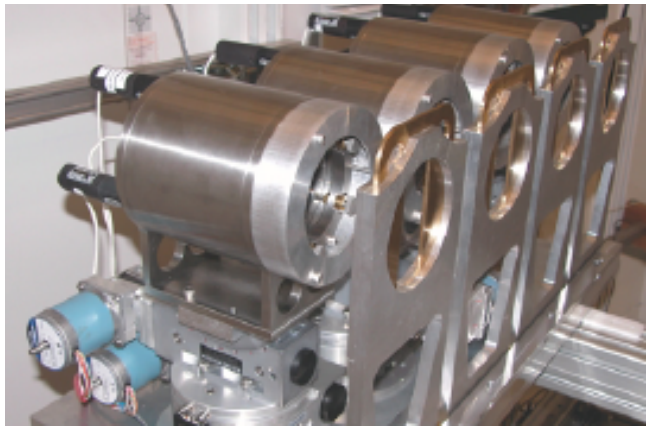


Fig. 1. Harald Sinn (left), Ahmet Alatas, and Ercan Alp (all XFD/XOR 3) at the new 3-ID-C IXS setup. The sample position is in the right front corner of the picture. The analyzers are in the back and not visible.

The high energy resolution inelastic x-ray (HERIX) beamline at the APS with an array of analyzers.