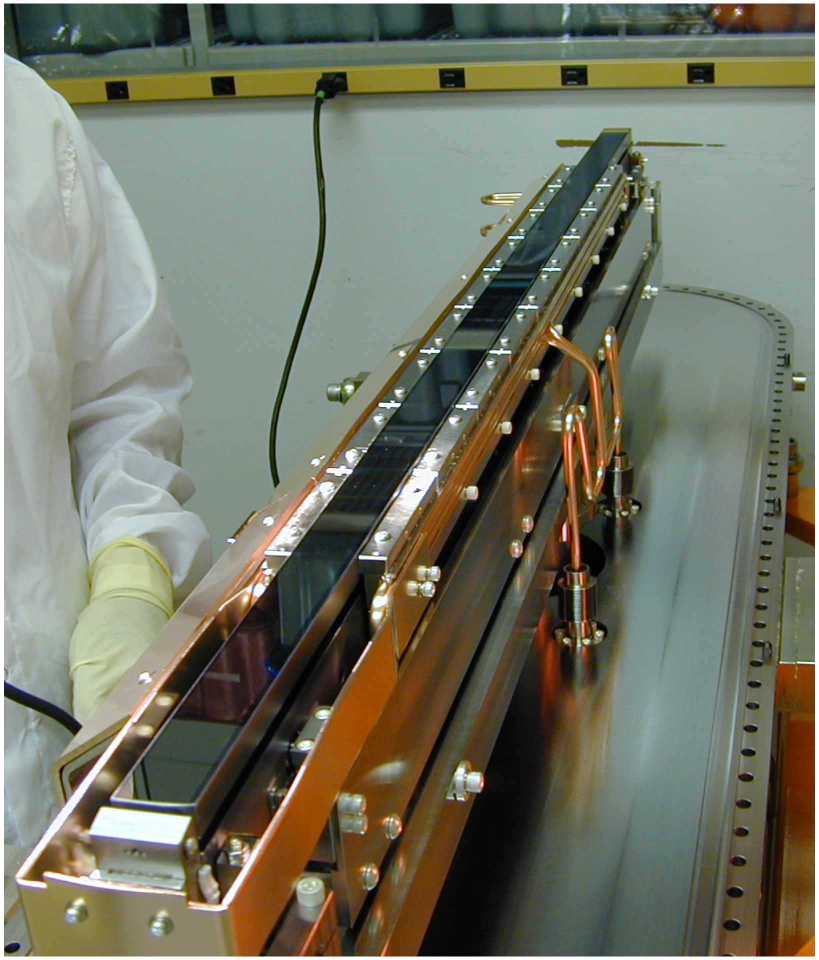
X-ray Optical Components for Hard X-ray Synchrotron Radiation Sources



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Outline

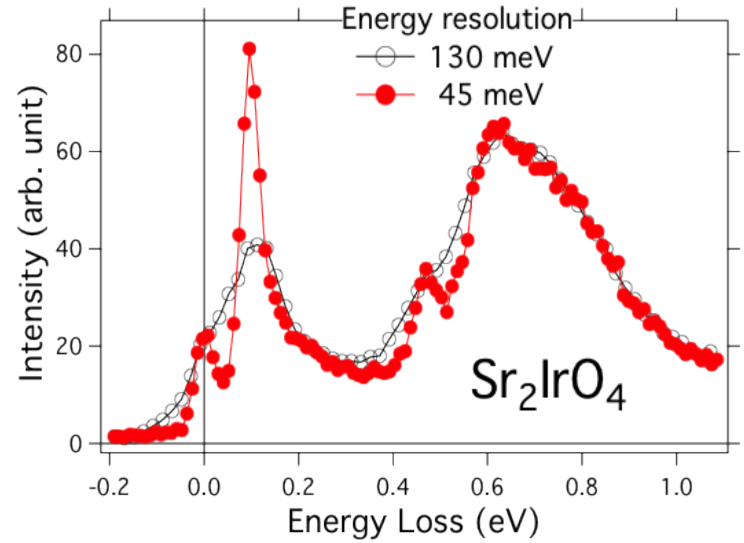
Outline of Presentation

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)

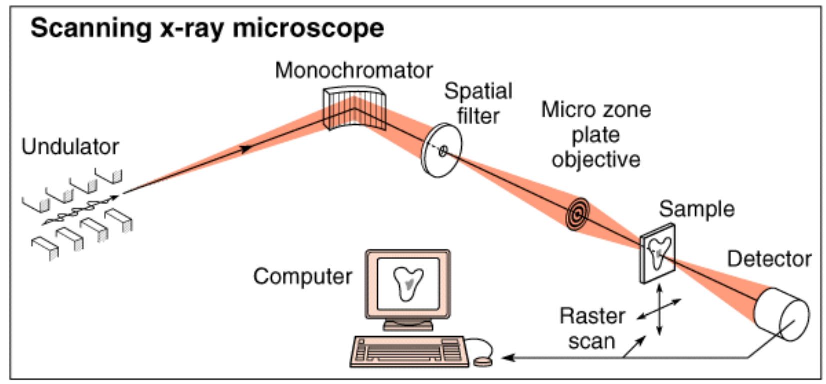
I will not be talking about gratings as they are used in the soft x-ray region of the spectrum and the focus of this talk will be hard x-ray optics.

Why Do We Need Optics

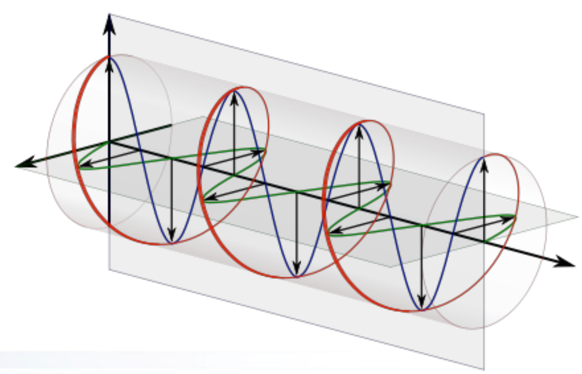
- Control the energy (E) and bandwidth (ΔE) of the beam.
  - ΔE = 1-2 eV @ 10 keV; $\Delta E/E = 10^{-4}$ (typical diffraction exp.)
  - ΔE = 1-2 keV @ 10 keV; $\Delta E/E = 10^{-1}$ (time-resolved studies)
  - ΔE = a few milli-eV @ 10 keV; $\Delta E/E = 10^{-7}$ (inelastic scattering – talk on Thursday)



- 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 (magnetic x-ray scattering or spectroscopy – talk on Tuesday)



Index of Refraction for X-rays: n < 1

See Appendices 1 & 2 for more details

- This expression for the (real part) index of refraction:

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

is usually written as:

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

and $r_e = (e^2/mc^2)$ is the classical radius of the electron (2.82×10^{-13} cm), n_e is the electron density, and λ is the wavelength of the x-ray.

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

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

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

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

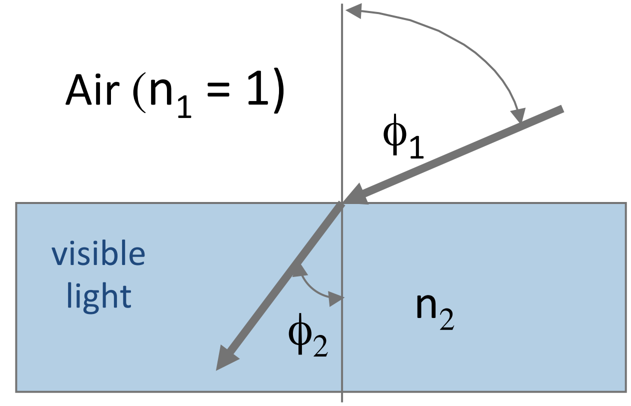
This simple treatment did not include any absorption. A more detailed calculation would result in an expression:

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

Where $\beta = \lambda\mu/4\pi$, with μ the linear absorption coefficient ($I = I_o e^{-\mu t}$).

Snell's (or the Snell-Decartes) 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.

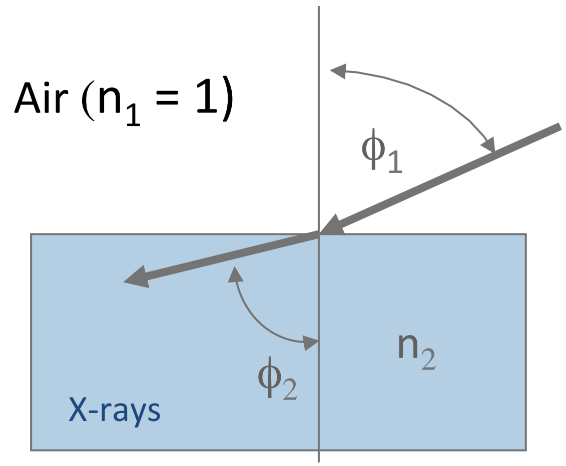


Typical values for n_2 (at 5890Å) are:

water: $n_2 = 1.33$

glass: $n_2 = 1.52$

- 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



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

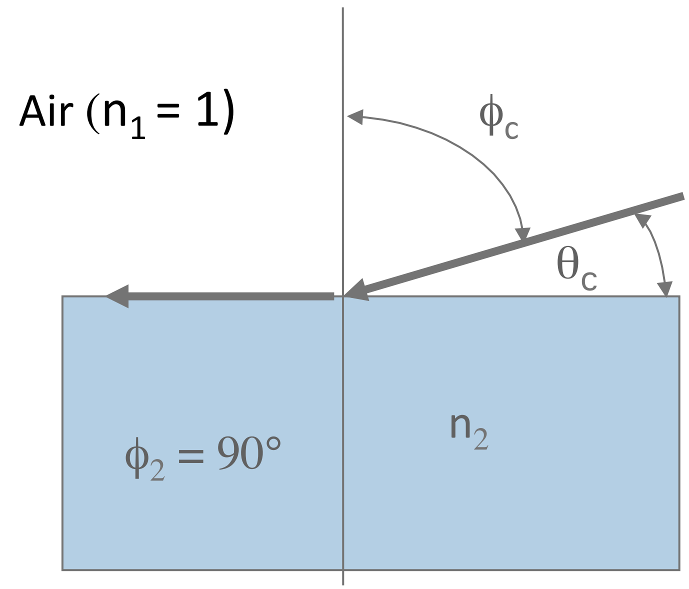
Critical Angle for Total External Reflection

- 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:

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

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

$$\mathbf{\cos(\theta_c) = n_2}$$



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

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

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

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

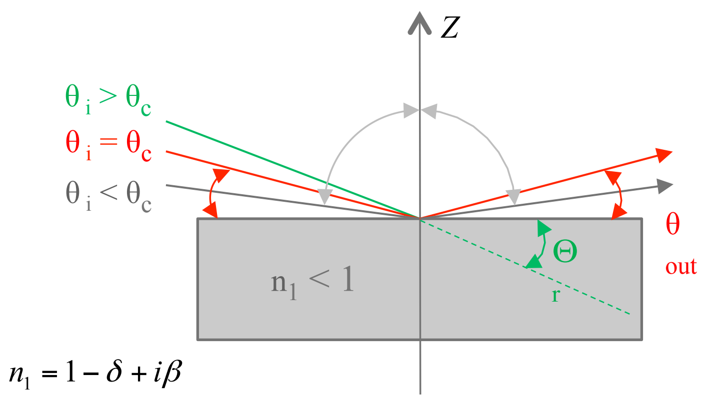
θ_c is the so-called **critical angle**, the angle at which there is total external reflection and the material behaves like a mirror.

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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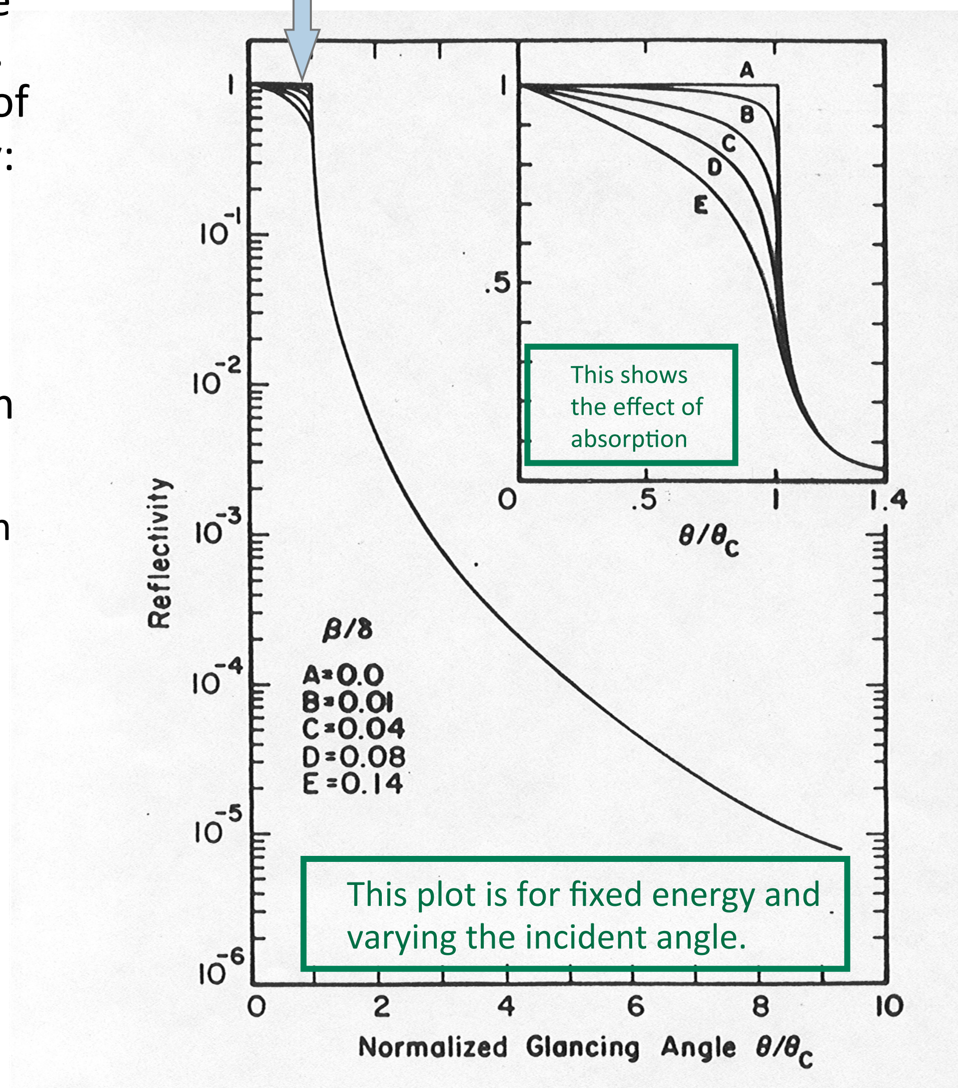


PHYSICAL REVIEW VOLUME 95, NUMBER 2 JULY 15, 1954

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

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

Energy Cutoff for a Fixed Angle of Incidence Mirror

- 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 re-written in terms of a critical energy, E_c, for a fixed angle of incidence θ. Since $E = hc/\lambda$, I can re-write this for a fixed θ, and determine the maximum energy, E_c, that will be totally reflected by the mirror.

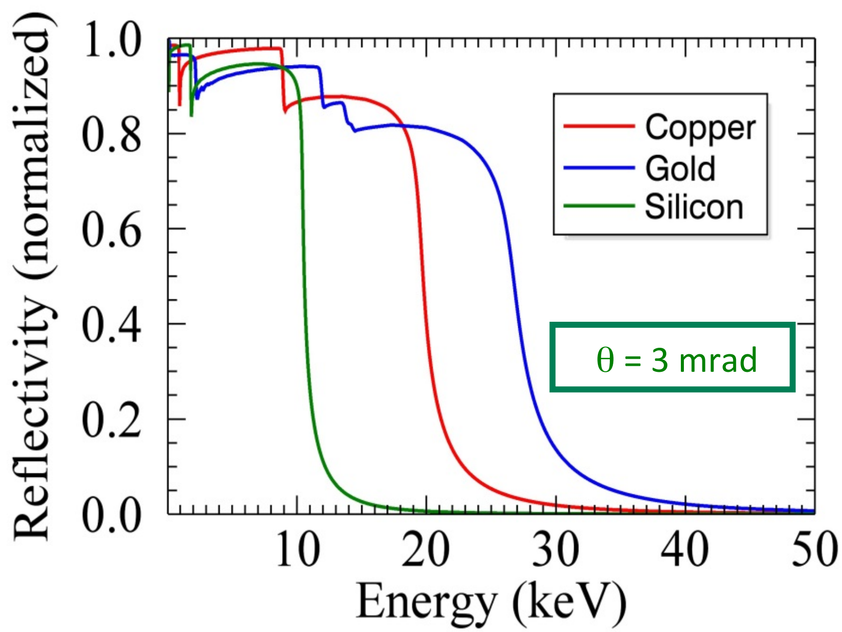
Reflectivity(θ) $\theta_c = (2\delta)^{1/2} = \lambda(n_e r_e/\pi)^{1/2}$

Critical angle, θ_c, for fixed wavelength λ

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

Critical energy, E_c for fixed angle θ

For a fixed angle of incidence, you can vary the critical (cut-off) energy by coating the mirror with materials of different electron densities, n_e.

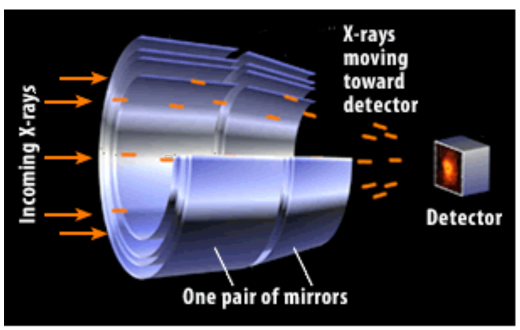


X-ray Mirrors

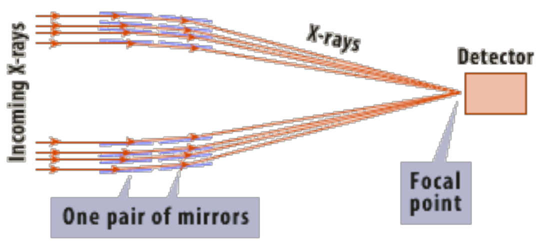
- Because the incidence angle are small (a few milliradians) to capture the full extent of the beam (say 1 mm or so), x-ray mirrors tend to be very long (sometimes over a meter).

- Low-pass filters
  - mirrors can be used to effectively suppress high energies
  - mirrors are designed so that the cutoff energy, E_c, can be varied by having several different coatings deposited on the mirror substrate

- Mirrors can effectively remove a considerable amount of the heat in the raw (incident) beam and reduce the thermal loading on downstream optics.



Courtesy Chandra mission website: http://chandra.harvard.edu

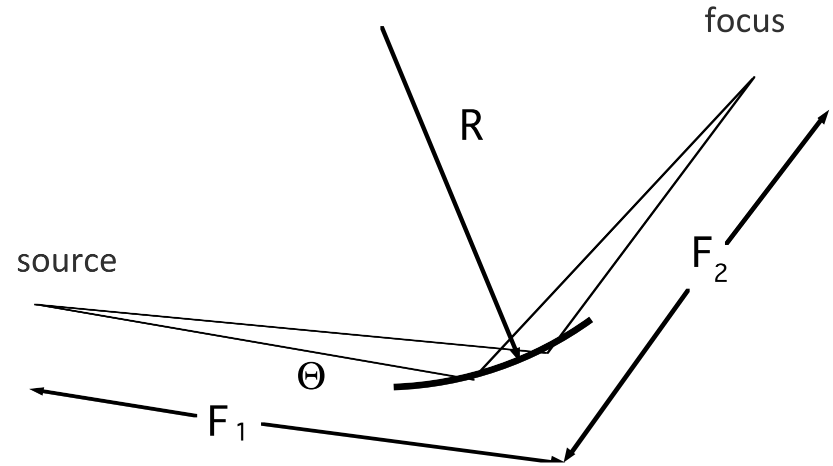


Chandra's mirrors are positioned so they're almost parallel to the entering X-rays. The mirrors look like open cylinders, or barrels. The X-rays skip across the mirrors much like stones skip across the surface of a pond.

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.



Focal length, $f = [R_m \sin\theta]/2$. When we plug this into the so-called lens formula:

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

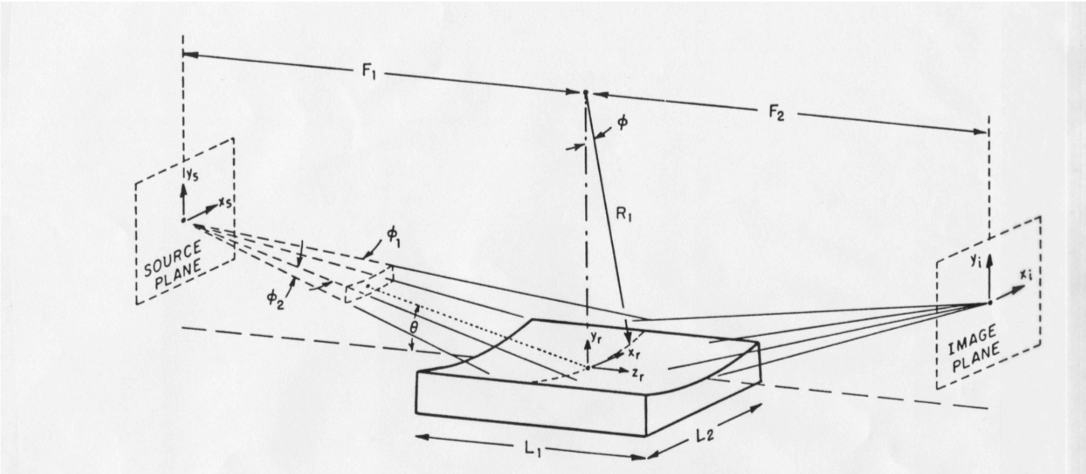
and solve for the radius of curvature, we get $R_m = [2/\sin\theta]\,[F_1 F_2/(F_1 + F_2)]$.

Typically θ is a few milliradians, $\sin\theta \approx \theta$ and so if $F_1 = F_2 = 30$ m, then the radius of curvature, R_m, is around 10 kilometers.

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:

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



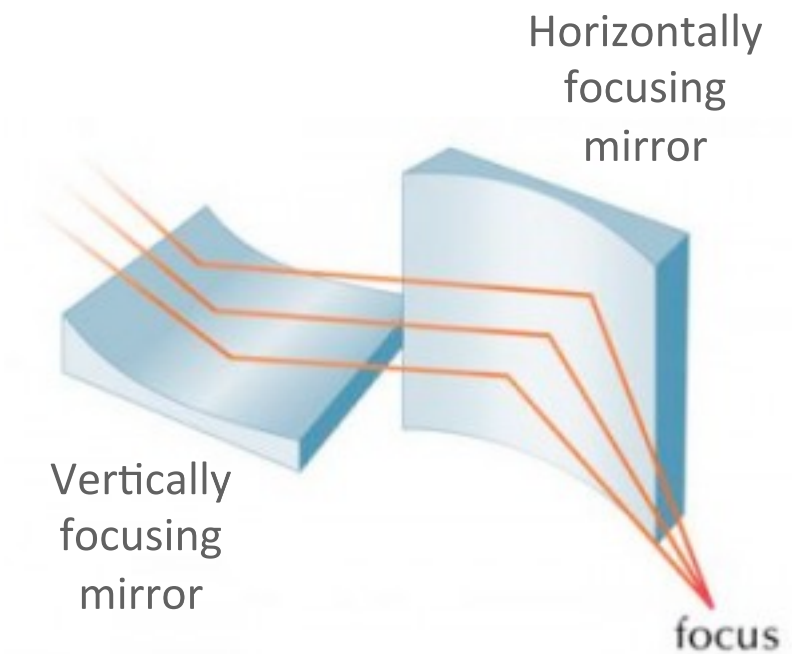
- In our example, from the last slide, θ = 3 mrad and R_m = 10 km so the sagittal radius would be:

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

Focusing in Two Dimensions - KB Systems

- Another system that 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.



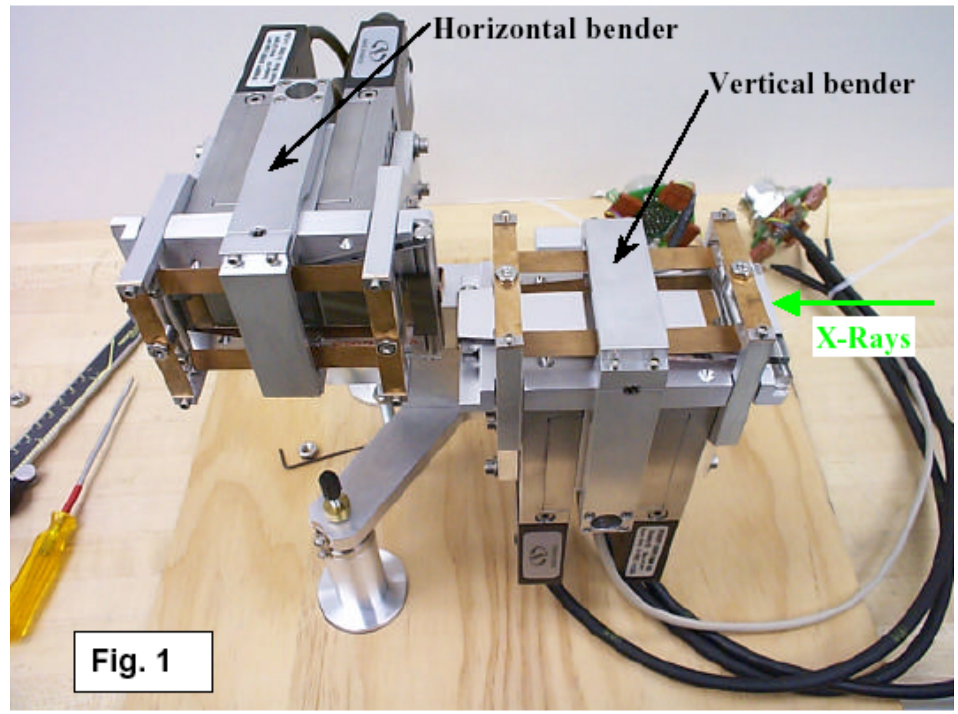
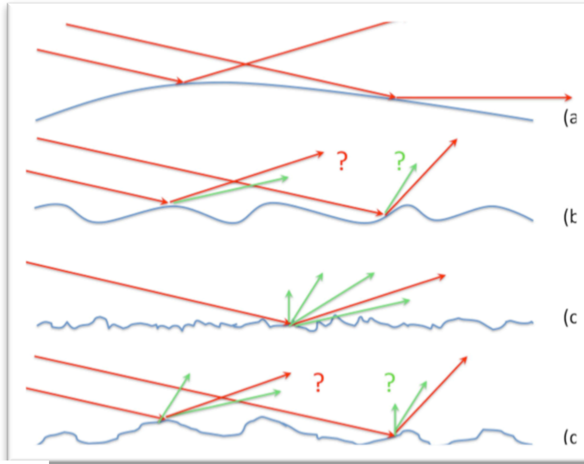


Fig. 1

These are achromatic, i.e. the focal length is not dependent on x-ray wavelength.

High-Brightness Sources Put Stringent Demands on Mirror Quality

- The mirrors requirements are very stringent if you want to use them for focusing or to preserve the x-ray beam brightness.



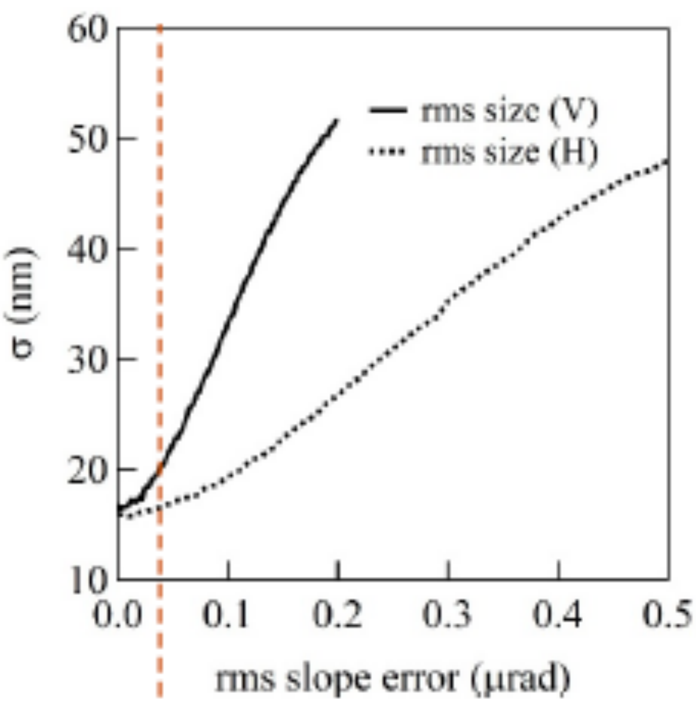
Sources of errors in mirrors

(a) long range slope errors

(b) medium range slope errors

(c) surface roughness

(d) sum of all three errors



If we hope to focus the x-ray beam to 20 nm, the specifications required are:

- slope error must be < 0.03 microradians (rms)
- surface roughness < 1 nm (rms)

over the length of the mirror.

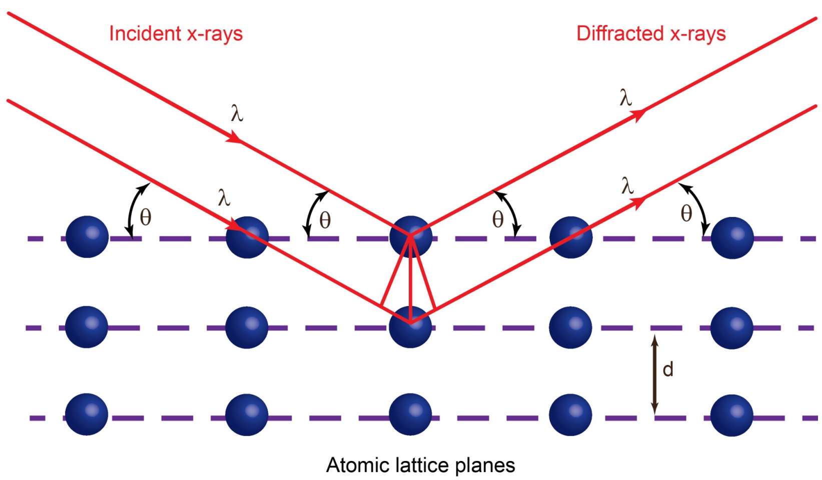
Diffractive Optics

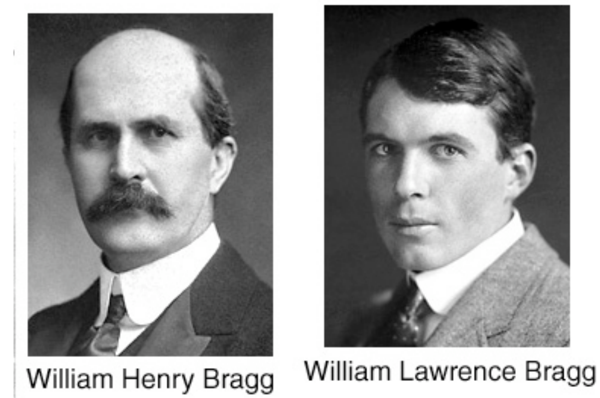
- By far, the most commonly used optical component for x-rays are crystals satisfying Bragg's law, i.e.,

Constructive interference when

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

Bragg's Law





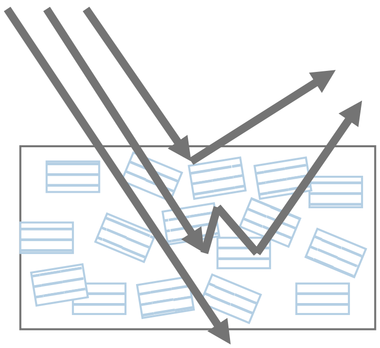
The Braggs shared the 1915 Nobel Prize in Physics.

- 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

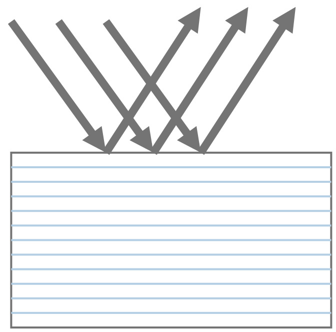
Images from: http://www4.nau.edu/microanalysis/Microprobe-SEM/History.html

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

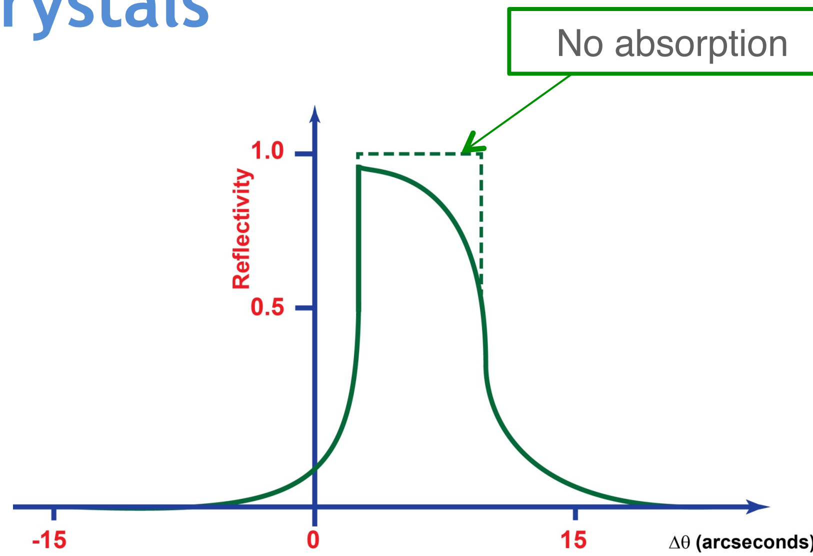
http://www.eoht.info/page/C.G.+Darwin

- The name "dynamical diffraction" was coined due to the fact that, during the diffraction process from perfect single crystals, there is a dynamic 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.

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

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

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

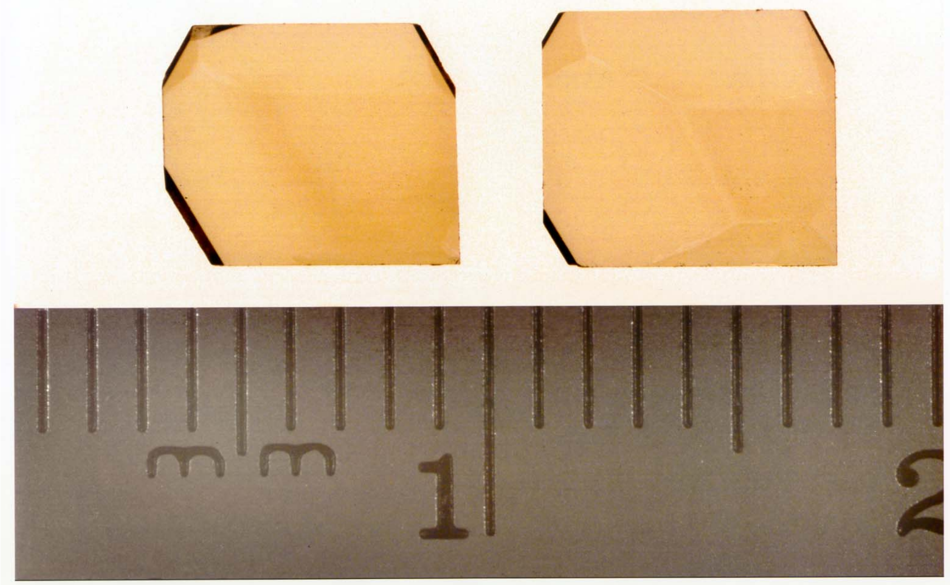
F(hkl) = structure factor
V = volume of unit cell

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, <u>**silicon and germanium**</u>, 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) <u>diamonds</u> 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 $\lambda = hc/E$):

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

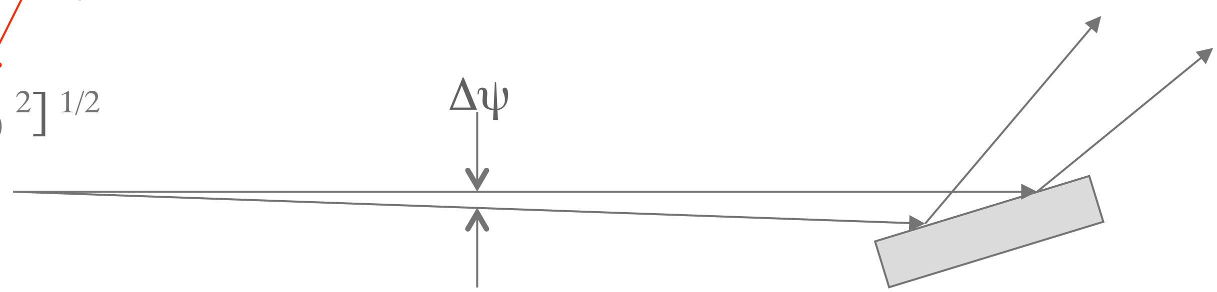
- If we differentiate Bragg's Law, we can determine the energy resolution of the monochromator.

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

X-ray divergence (source)

Darwin width (optic)

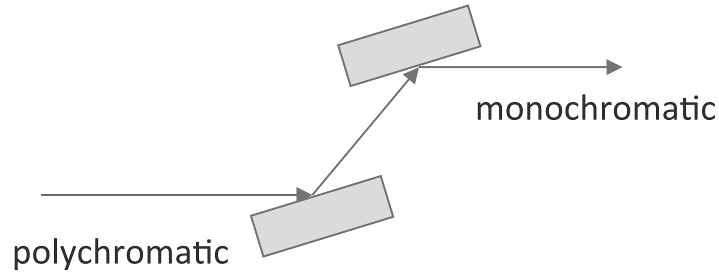
$$\Delta\theta = [\Delta\psi^2 + \omega_D^2]^{1/2}$$



- 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 microradians at the APS. Here the energy resolution of the mono is determined by the crystal.

Real Monochromators

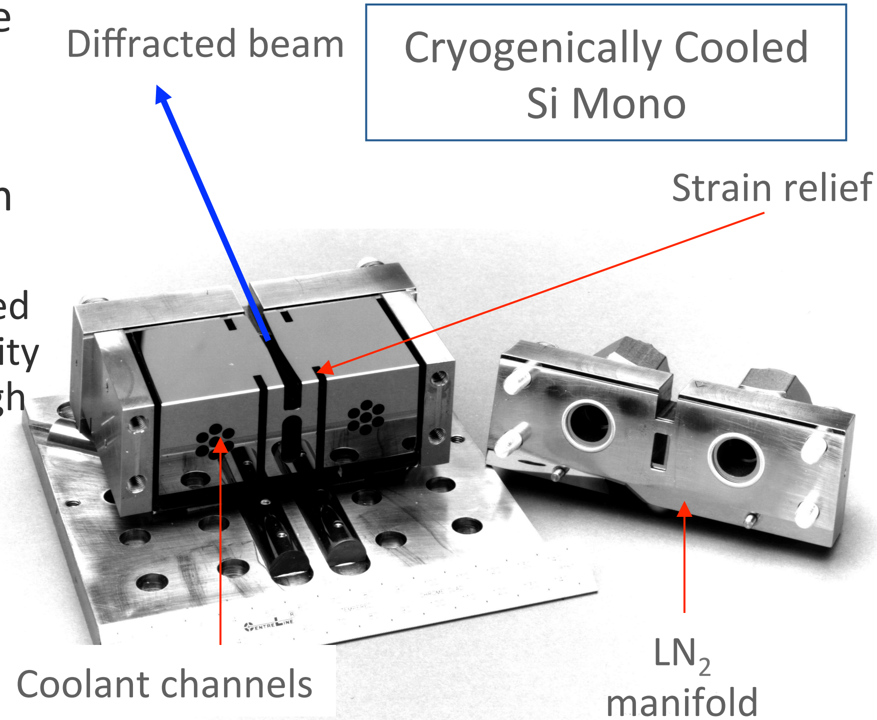
- The most common arrangement is the double-crystal monochromator. It:
  - is non-dispersive, that is all rays that diffract from the first crystal simultaneously diffract from the second crystal (if same crystals with same hkl's are used)
  - keeps the beam fixed in space as the energy is changed.



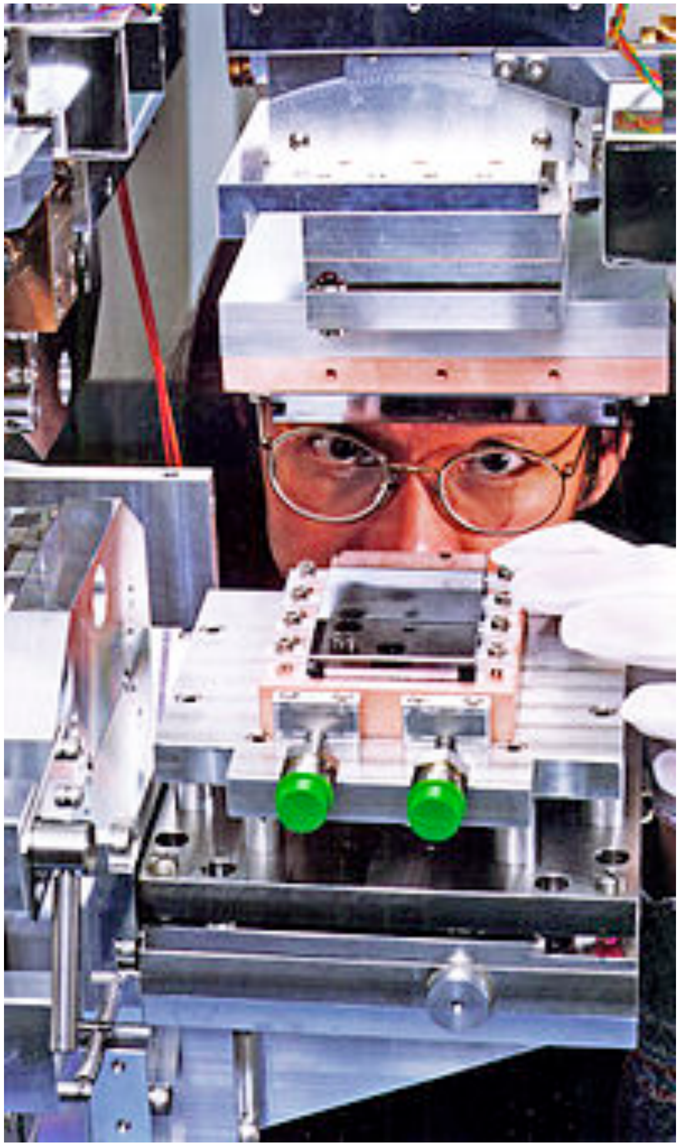
- There is little loss in the throughput because the reflectivity is near unity over the Darwin width.

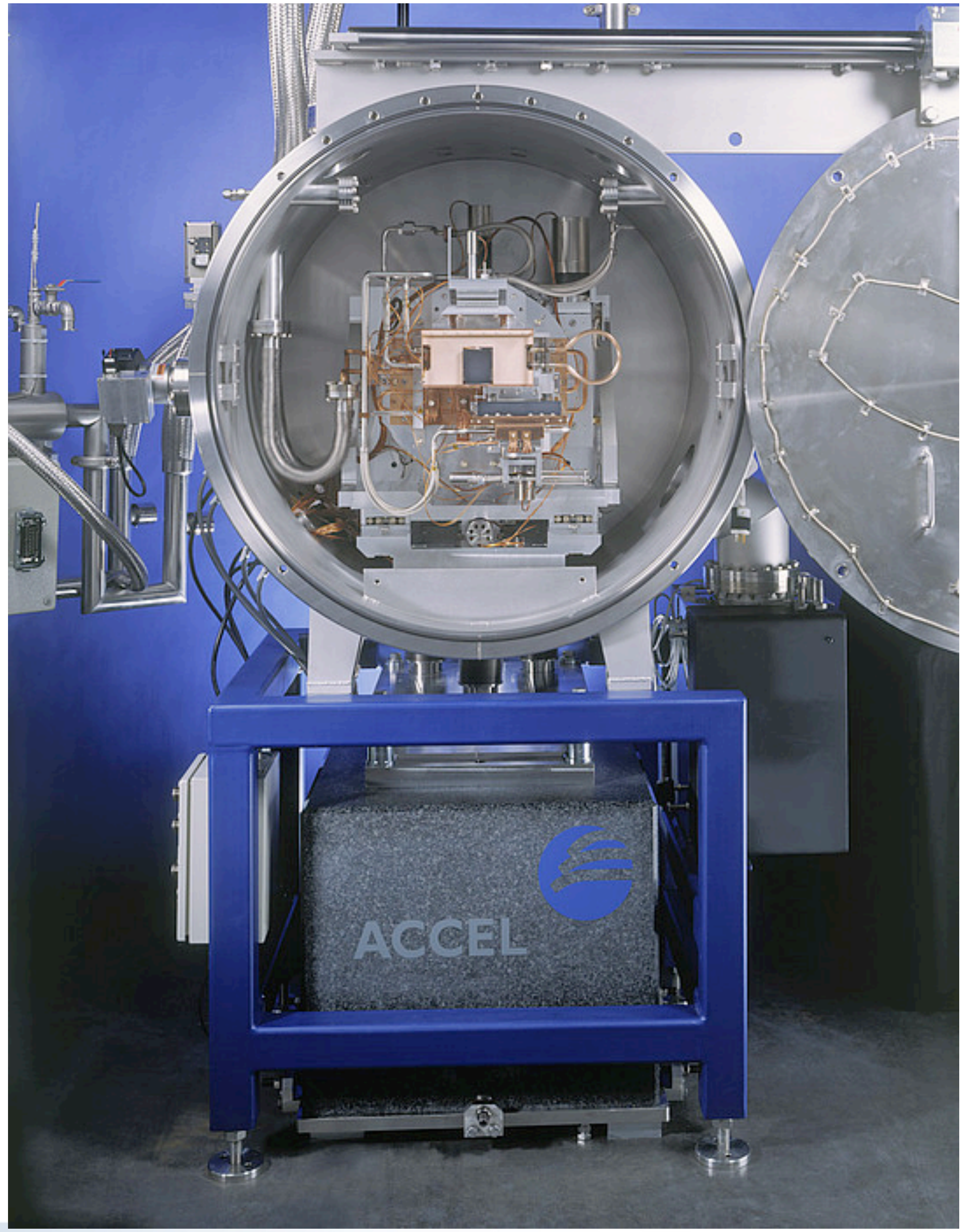
- Monochromators need to be cooled to maintain the desired properties.
  - Silicon monochromators are often liquid N_2 cooled to enhance thermal properties (higher conductivity and coefficient of thermal expansion goes through a zero at about 120°K.

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



Crystal Monochromators



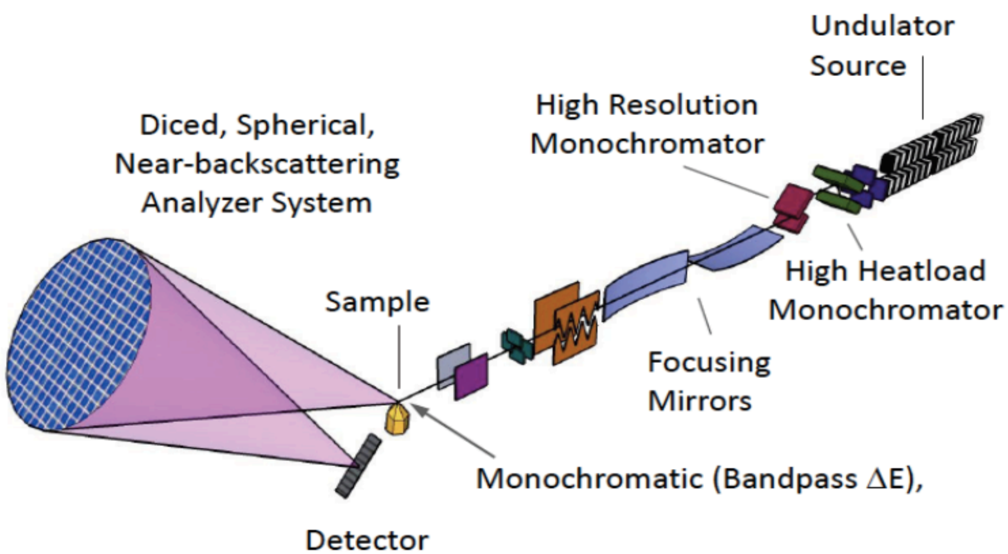


High-Energy Resolution Optics

- 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 $\theta \to 90°$



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.

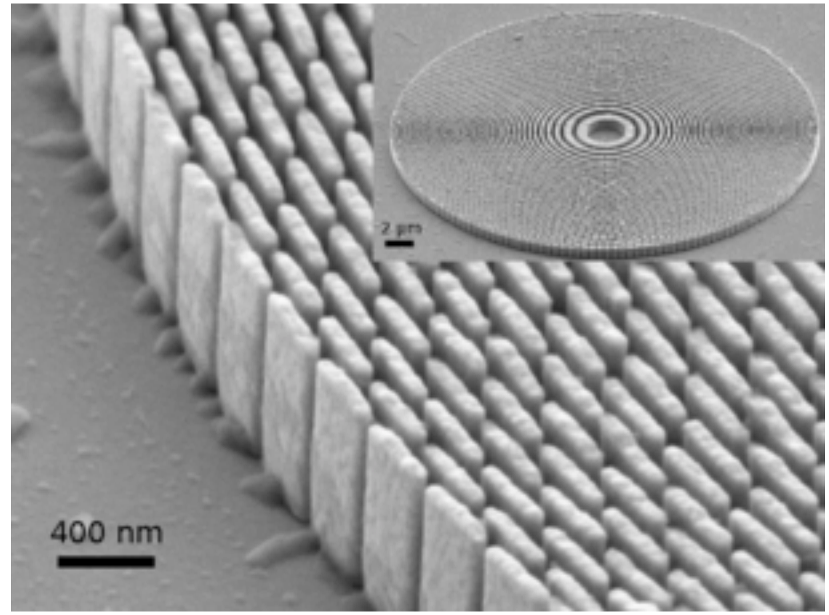
After being inelastically scattered by the sample, the x-rays of the desired energy are sorted out and focused onto a detector by a spherically bent analyzer. The monochromators, high-resolution monochromators, and analyzer are all fabricated from perfect single crystals of silicon.

See Thursday's lecture on Inelastic X-ray Scattering

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

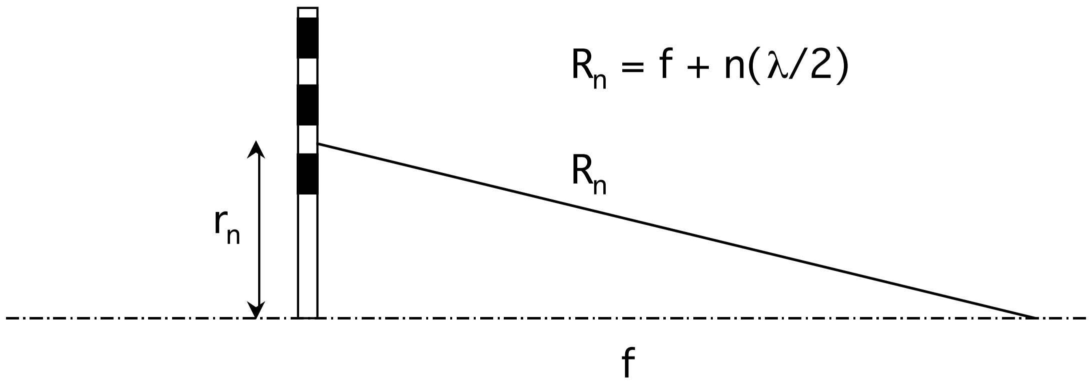
Fresnel Zone Plate for Optical Image Formation Using Extreme Ultraviolet and Soft X Radiation

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:

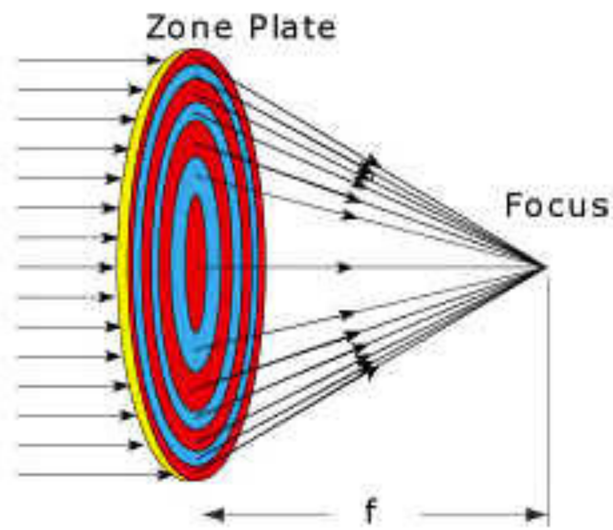
$$r_n = (R_n^2 - f^2)^{1/2} = [(f + n(\lambda/2))^2 - f^2]^{1/2}$$

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

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

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

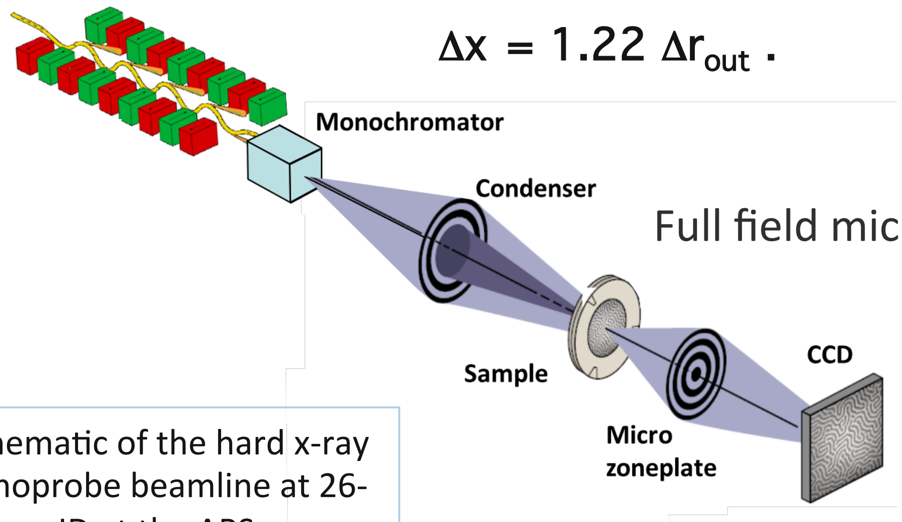
These are chromatic, i.e. the focal length is dependent on x-ray wavelength.



Zone Plane Focal Spot Size

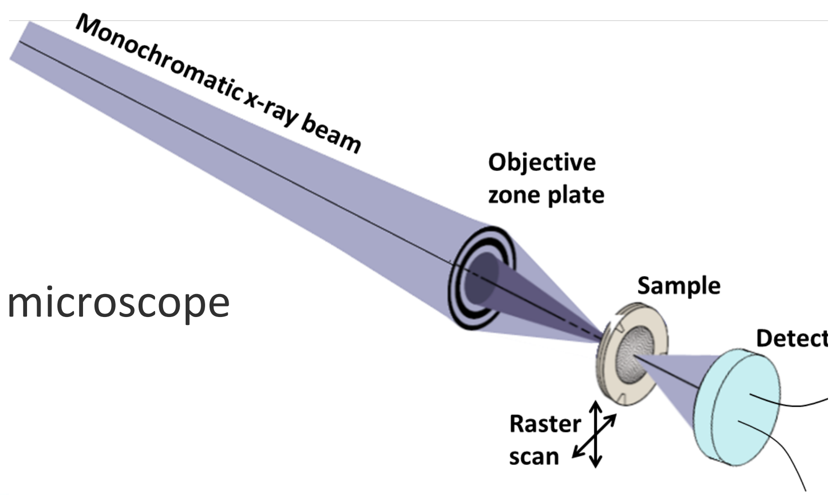
- In general, the size of the focal spot from the zone plate is determined by the width of the outermost ring, Δr_{out} , and is given by:

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



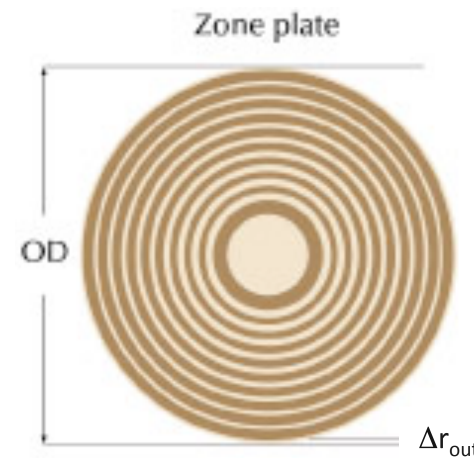
Full field microscope

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



Scanning microscope

See lecture Monday on X-ray Imaging

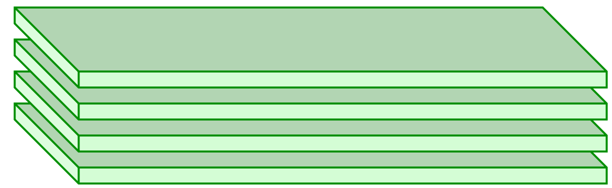


Zones plates with outermost ring widths of less than 20 nanometers can currently be fabricated.

Hard X-ray Phase Zone Plates

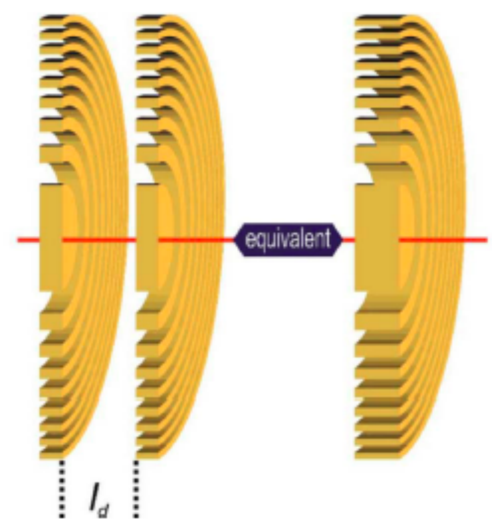
- The difficulty with making zone plates at hard x-ray energies is one of fabrication. You need:
  - small width outermost zone for focusing (less than 50 nms)
  - but it has to be thick (high) to totally absorb the unwanted waves
  - i.e. the aspect ratio (height/width) is very large – 10^2 - and therefore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

At 8 keV, a tantalum ZP with outer most zone of 50 nm would need an aspect ration of 30:1



- 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.
- Multiple zone plates can be "stacked" to increase the effective thickness, but alignment is critical.

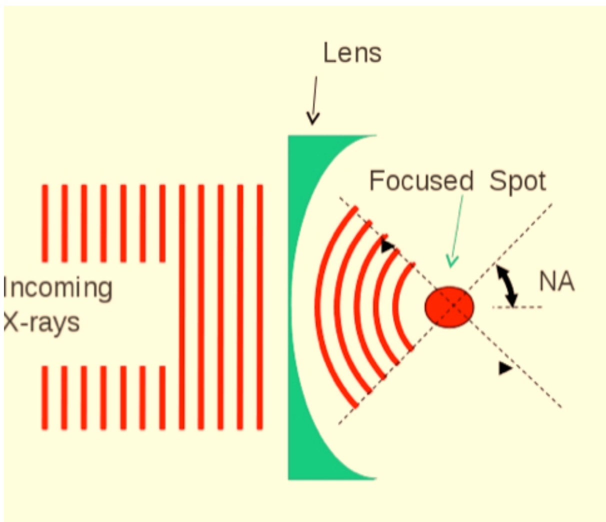
Stacking for high efficiency



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 δ are also strong absorbers, because the absorption coefficient increases much more rapidly than δ with increasing atomic number. Therefore, an element of low atomic number, such as beryllium, is typically used.

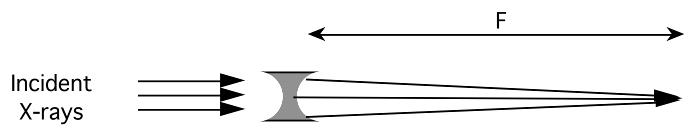
- For a single concave lens: $1/F = \delta(1/R)$

- Plugging in some numbers, suppose that:

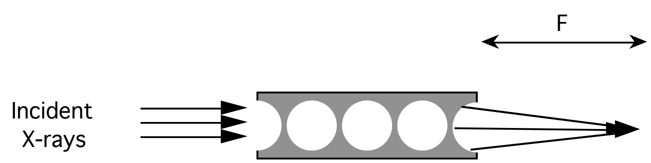
$$R = 1 \text{ mm} \quad \delta \approx 10^{-5}$$

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

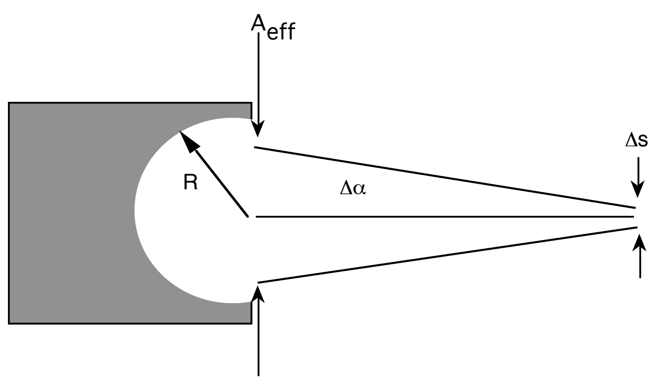
Compound Refractive Lenses



Single Refractive Lens



Compound Refractive Lens



These are chromatic, i.e. the focal length is dependent on x-ray wavelength.

- 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:

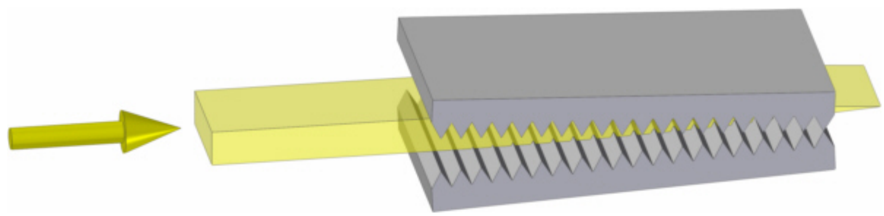
$$F = R/2N\delta$$

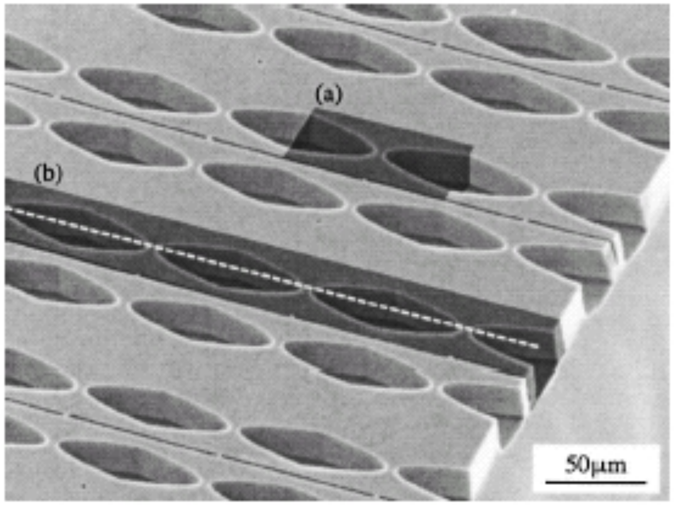
- Using the same numbers as before but with 50 lenses, i.e.:
  $R = 1$ mm $\delta \approx 10^{-6}$ $N = 50$
- Then the focal length, F, would be at 10 m.
- These lenses focus at rather larger distances and are well adapted to the scale of synchrotron radiation beamlines.

Focusing in One Dimensions with Refractive Lenses

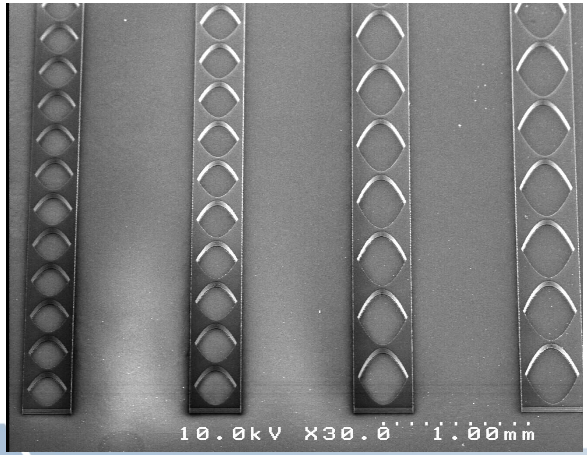
- Planar technologies
  - Leverage planar technologies from micro-electronics industry
  - Fabricate compound lens systems in a small space
  - Small radius means moderate focal spots with a single lens or nano-focusing with a moderate number of lenses

Sawtooth lens - Vary opening angle to keep focal length fixed as energy is changed or to vary the focal length





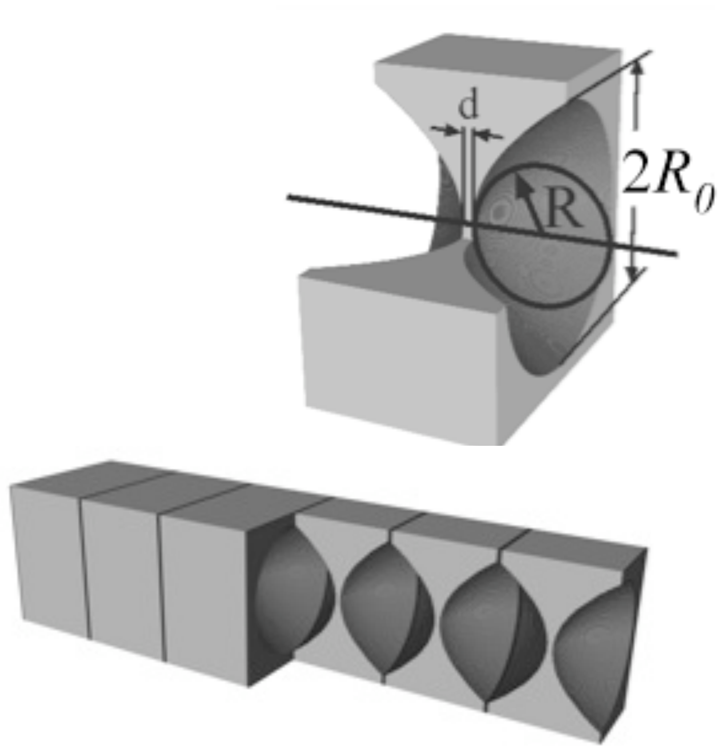
Parabolic refractive x-ray lenses made of silicon. The shaded areas a) and b) delineate an individual and a compound Nano-Focusing Lens. Source: Schroer et. al. APL.(2003)

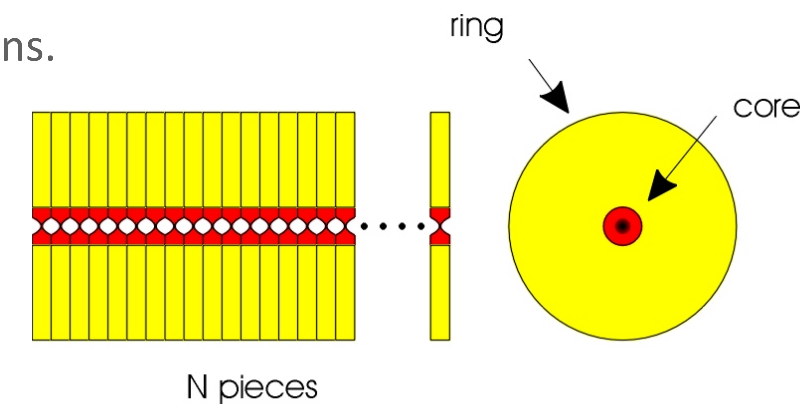


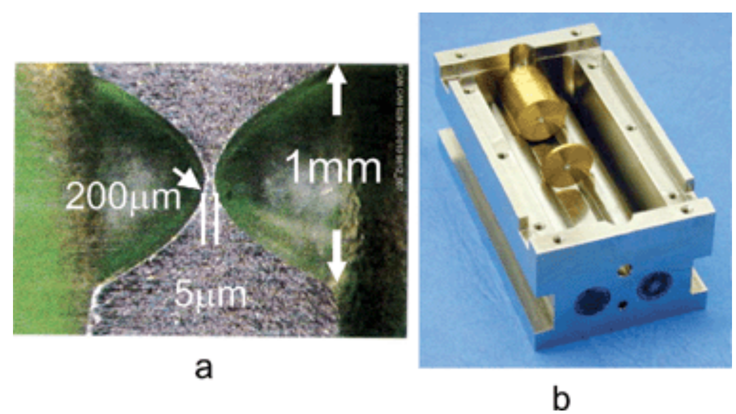
Compound lens array of nano-crystalline diamond lenses. Alianelli et. al., J. of Appl. Phys., 108, 123107 (2010)

Focusing in Two Dimensions with Refractive Lenses

- 2-D lenses typically "embossed" and typically made from Be, Al or Nickel
- 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=&content=crl#Focusingmethods

http://pubs.rsc.org/is/content/articlehtml/2006/em/b511446m

Current Optics R&D Activities

- X-ray optics is still an active area of research at both universities and national laboratories (in particular here at the APS).
  - Adaptive mirrors
  - Nanodiffractive optics
  - Simulation tools.

Optics EXPRESS

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)

Synchrotron JSR

A hybrid method for X-ray optics simulation: combining geometric ray-tracing and wavefront propagation

Xianbo Shi,[a*] Ruben Reininger,[a] Manuel Sanchez del Rio[b] and Lahsen Assoufid[a]

SCIENTIFIC REPORTS

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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]

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journal homepage: www.elsevier.com/locate/nima
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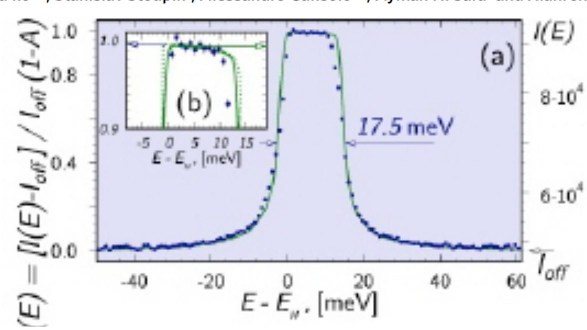
X-ray nanofocusing using a piezoelectric deformable mirror and at-wavelength metrology methods

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]

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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*, Dennis Mills and Howard Padmore, Co-Chairs, 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:

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

For a single electron:

$$P = -ex$$

and for multiple electrons:

$$P = -exn_e \qquad (n_e \text{ is the number of electrons/unit volume})$$

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:

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

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:

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

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

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 $\mathbf{2 \times 10^{19}/sec}$ **(>>** $\boldsymbol{\omega_o}$**)** and so we can write:

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

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

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

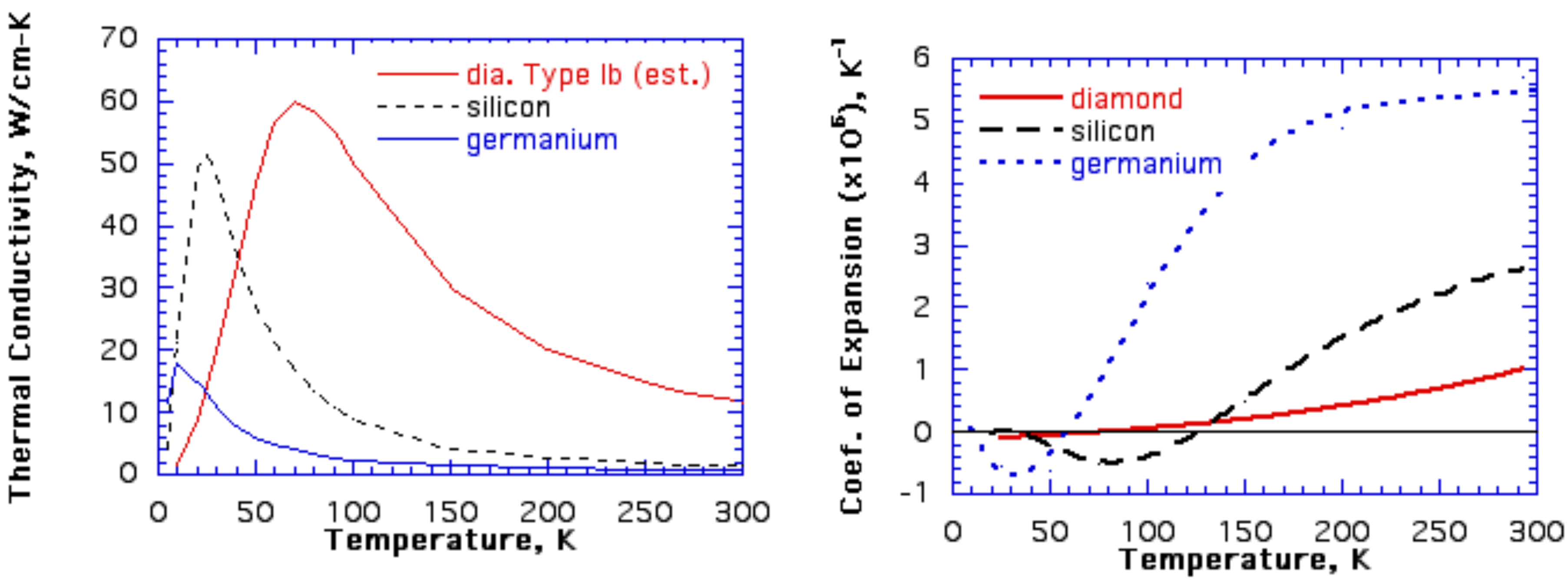
- Along with the enormous increase in x-ray beam brilliance from insertion devices comes unprecedented powers and power densities that must be effectively handled so that thermal distortions in optical components are minimized and the full beam brilliance can be delivered to the sample.

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

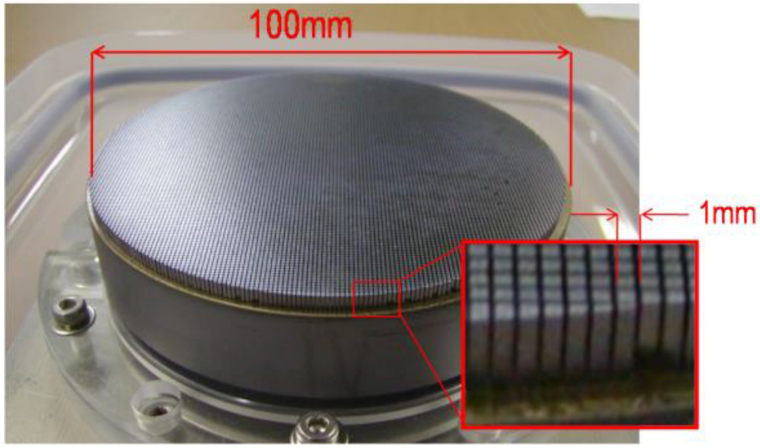
material	k - thermal conductivity	α - coef. of thermal expansion	k/α FOM
Si (300°K)	1.2 W/cm-°C	2.3×10^{-6} /°K	0.5
Si (78°K)	14 W/cm-°C	-0.5×10^{-6} /°K	28
Dia. (300°K)	20 W/cm-°C	0.8×10^{-6} /°K	25

Appendix 4: High Energy-Resolution Optics

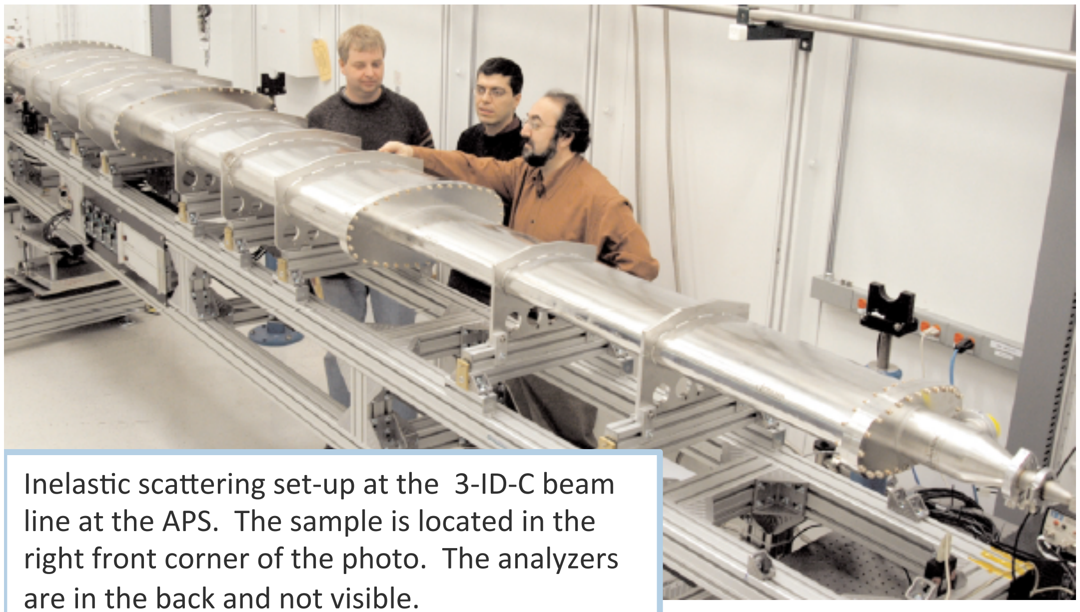
- At θ = 89°, $\cot(\theta)$= 1.7 x 10^{-2}. For E = 20 keV (0.64Å), then:

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

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

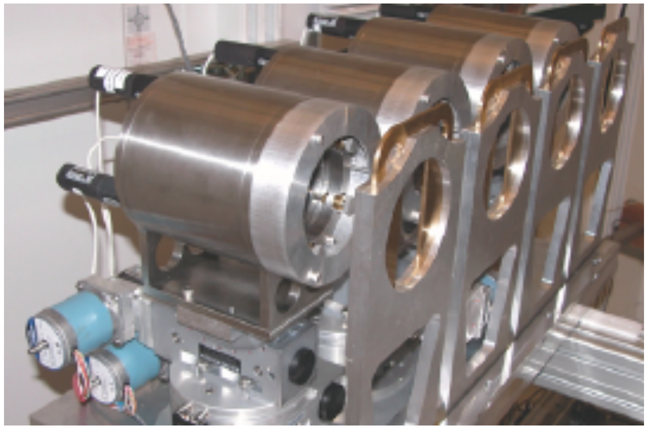


A diced, high energy resolution inelastic x-ray spherical analyzer.



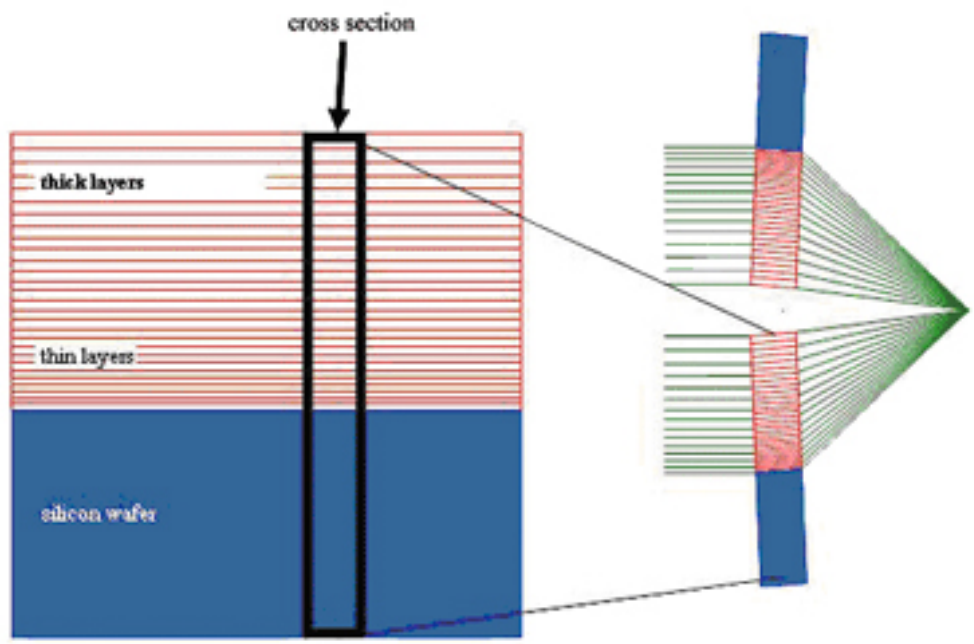
Inelastic scattering set-up at the 3-ID-C beam line at the APS. The sample is located in the right front corner of the photo. The analyzers are in the back and not visible.

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

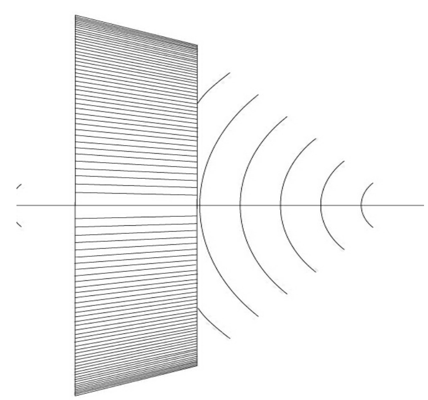


A New Approach to Fabricating Zone Plates - Multilayer Laue Lenses (MLLs)

- 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.



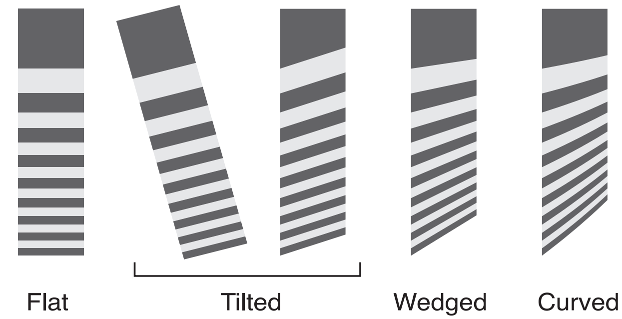
Wedged MLL

- 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!

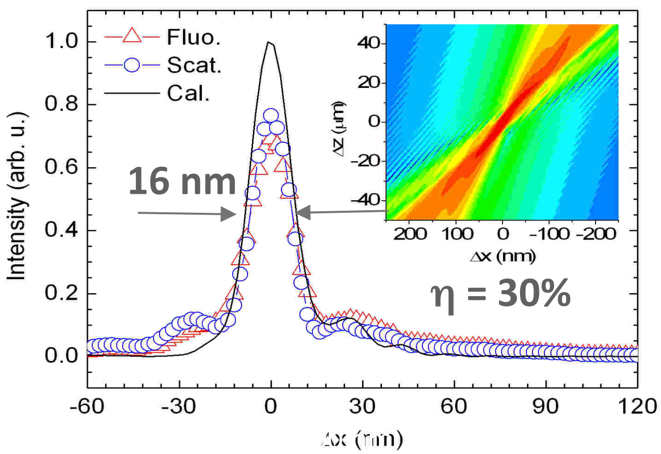
H. C. Kang, J. Maser, G. B. Stephenson, C. Liu, R. Conley, A. T. Macrander, and S. Vogt, "Nanometer Linear Focusing of Hard X Rays by a Multilayer Laue Lens," Phys. Rev. Lett. 96, 127401 (2006).

Multilayer Laue Lenses

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

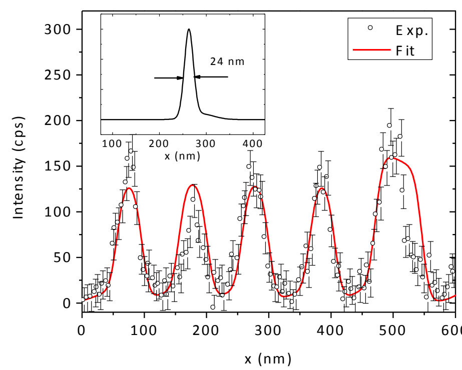


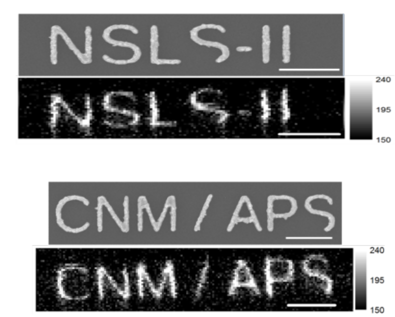
1-D focus: 16 nm (half MLL) **@ 19.5 keV**



Kang et al, APL 92, 221114 (2008)

2-D focus: 25 x 40 nm² (2D, crossed MLL) **@ 20 keV**





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

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