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X-ray Optical Components for Synchrotron Radiation

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Outline

Outline of Presentation

1. **Why Do We Need Optics?**
2. **X-ray Mirrors**
3. **Perfect Crystal X-ray Optics**
4. **Other Optical Components**

Why Do We Need Optics

- Control the energy (E) and bandwidth (ΔE) of the beam.
  - Monochromatic beam
  - Polychromatic

- Control the size/divergence of the beam (often related).

- Control the polarization of the beam.
  - Linear
  - Circular

Dielectric Constant

- Since the optical properties of a material depends on the index of refraction, we need to calculate that at x-ray energies/frequencies. The dielectric constant, κ, is defined as follows:

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

  where P is the dipole moment (or polarizability), D the displacement field, and *E* is the electric field vector of the incident EM wave (in our case the x-ray beam).

- Using a simple model one can calculate the polarizability of the material:

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

  where n_e is the electron density, ω the frequency of the x-rays, and ω_o some natural frequency of the electrons in the solid, (in the Drude model its the frequency of the collective oscillations of the electrons around the atom or the so-called plasma frequency).

Plasma or Natural Frequency of Electrons

- For Si (my prototypical solid), $n_e = 7 \times 10^{23}$ 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, ω (= $[2\pi c/\lambda]$), is **2×10^{19}/sec** **($>> \omega_o$)** 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:

$$n = \kappa^{1/2} = [1 - 4\pi((e^2/mc^2)\, c^2 n_e\, (\lambda/2\pi c)^2)]^{1/2}$$

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

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

Real and Imaginary Parts of the Index of Refraction

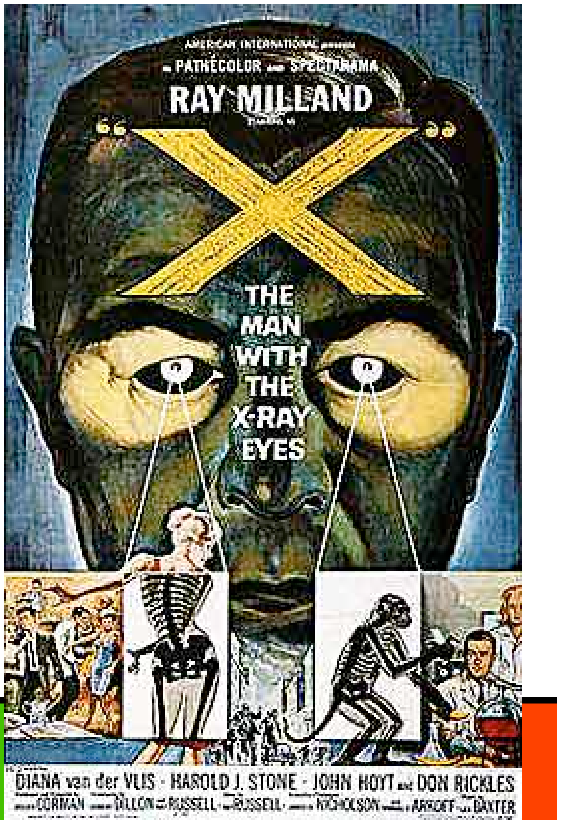
- This simple model did not include any absorption of the incident radiation. A more detailed calculation would result in an expression:

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

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

- When you plug in the numbers for the real part of the index of refraction you et: $\delta = 10^{-5}$ to 10^{-6}

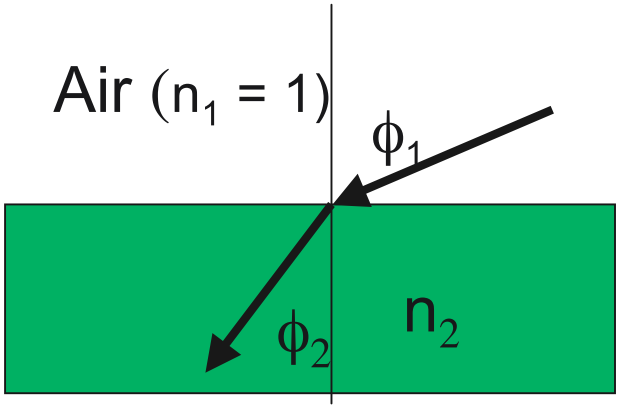
- Consequences of:
  - **an index of refraction less than one**
  - **differing from unity by only a few ppm**



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.

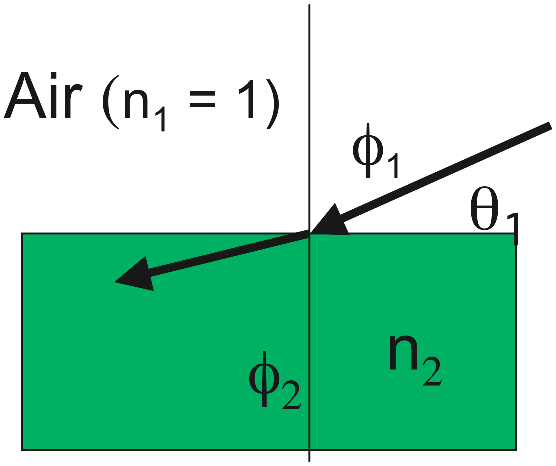
- The resultant kinematic properties (which follow from the wave nature of the radiation at boundaries) are:
  - The angle of incidence equals the angle of reflection
  - $n_1 \sin(\phi_1) = n_2 \sin(\phi_2)$ (Snell's Law), where the ϕ's are measured with respect to the boundary normal



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, it is clear that $\phi_2 > \phi_1$, since $n_2 < 1$. When $\phi_2 = 90°$, we have:

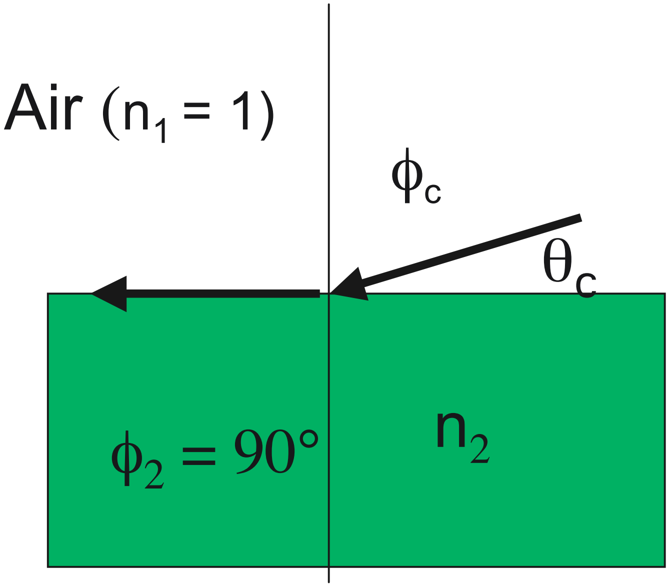
$$\sin(\phi_c) = \cos(\theta_c) = n_2\cos(0); \quad (\theta_c = 90° - \phi_c)$$

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

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

θ_c is the so-called critical angle, the angle at which there is total external reflection.

- 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.

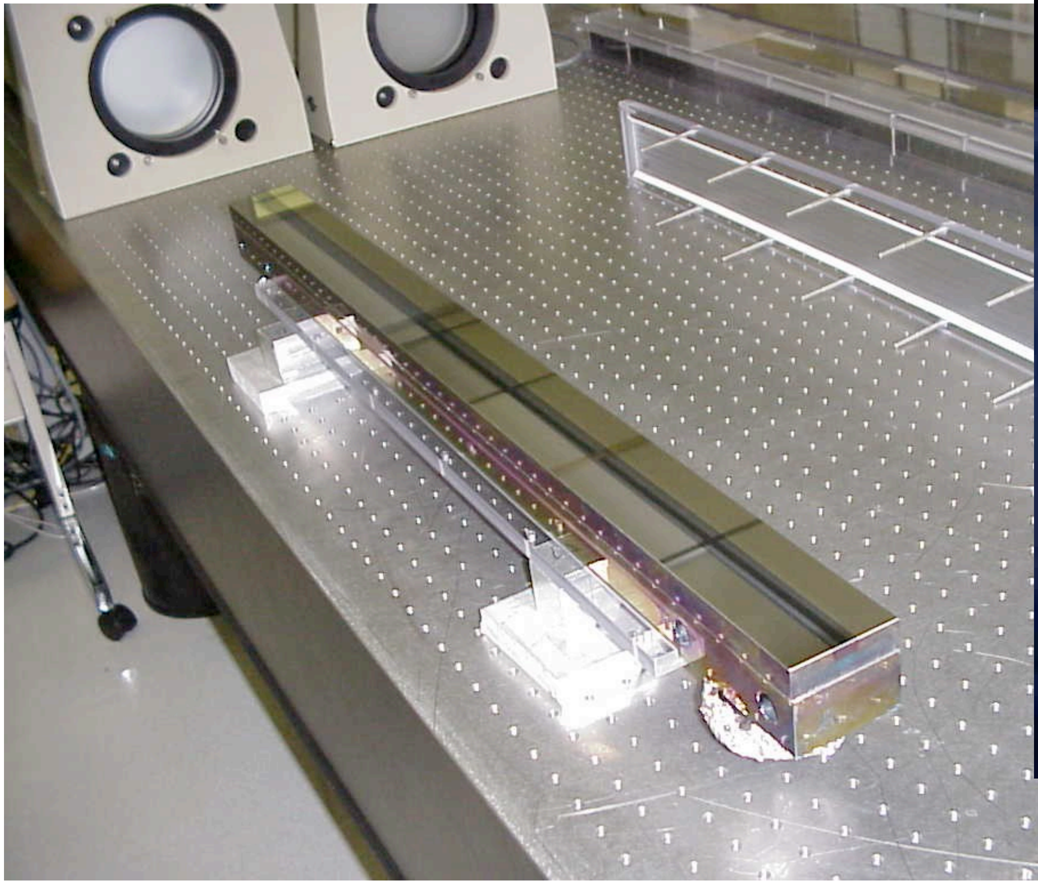


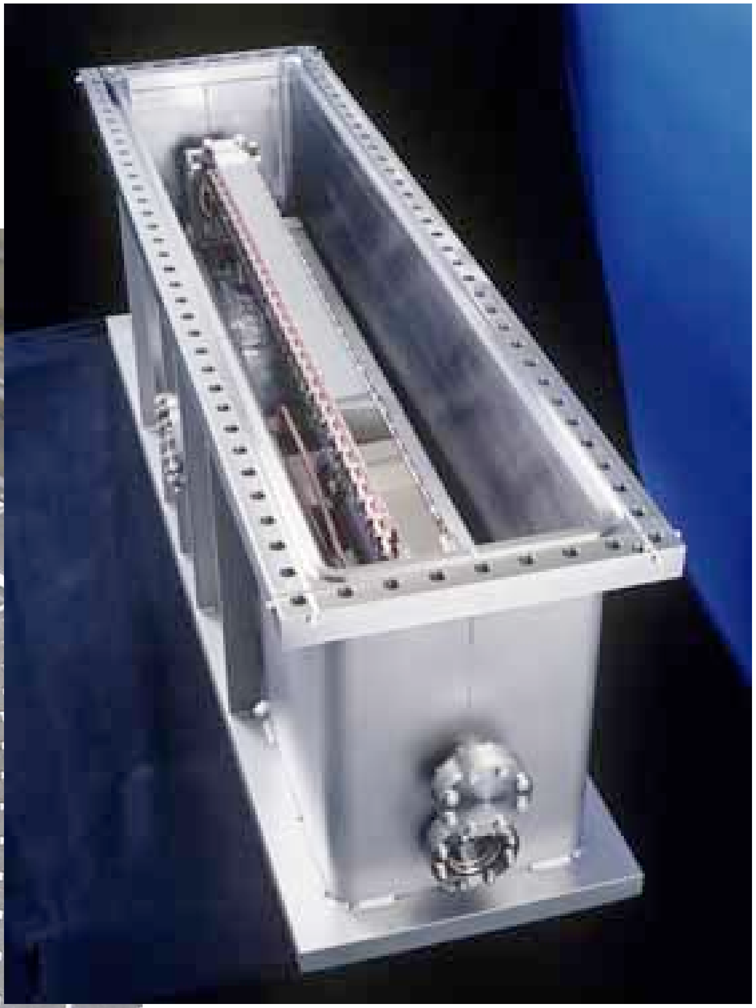
For x-rays typical values for n_2 are $(1 - 10^{-5})$ to $(1 - 10^{-6})$

Values of the Critical Angle for X-rays

In practical units, (assuming Z/A = 2):

$$\theta_c[\text{mrad}] = 1.6\ \lambda[\text{Å}]\ (\rho\ [\text{g/cm}^3])^{1/2}$$



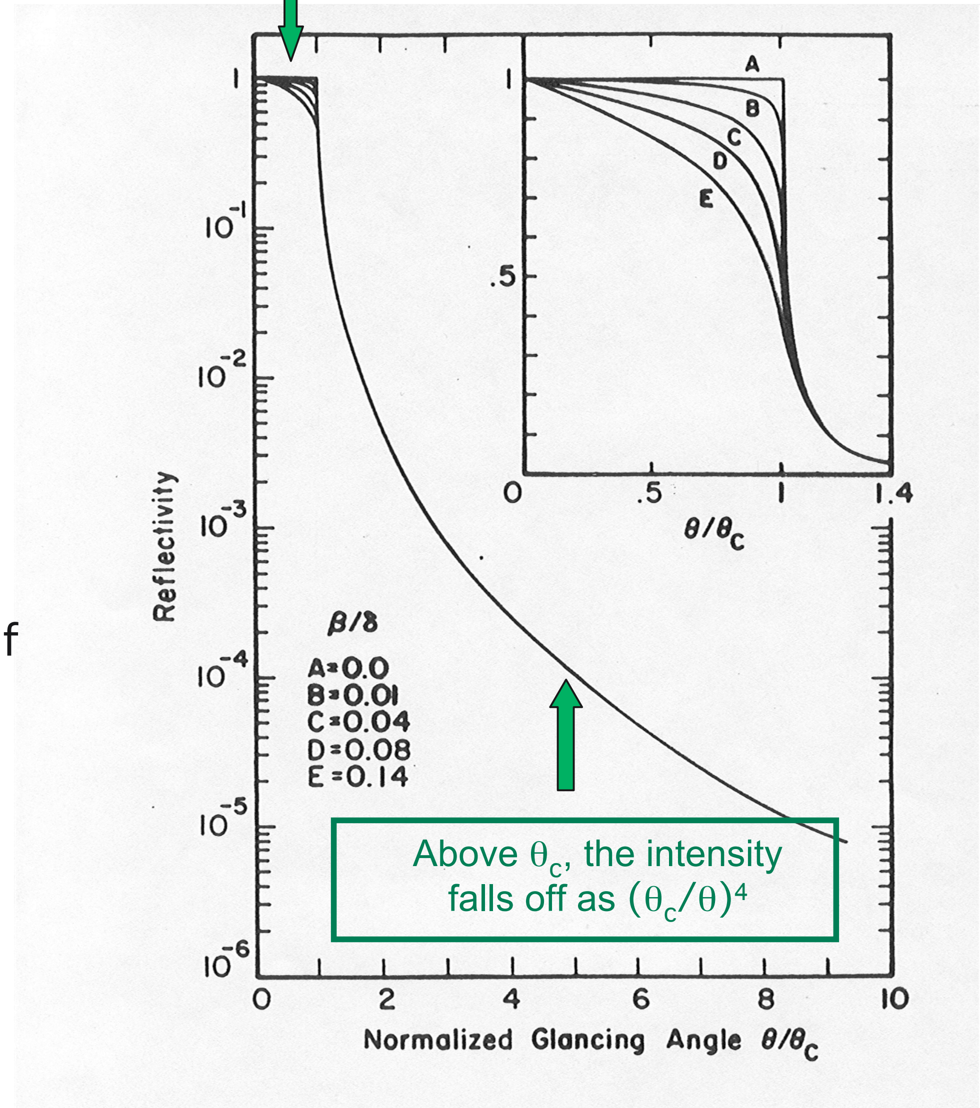


X-ray Reflectivity

- The amplitude of the reflected wave can also be determined (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 these relations it can be shown that:
  - Below θ_c, there is unit reflectivity (if $\beta = 0$)
  - Above θ_c, the intensity falls off as $(^1/_{16})(\theta_c/\theta)^4$



Below θ_c, there is unit reflectivity (if $\beta = 0$)

Above θ_c, the intensity falls off as $(\theta_c/\theta)^4$

Energy Cut-off for a Fixed Angle of Incidence

- All the above was developed assuming a monochromatic incident beam and a variable angle of incidence. Often mirrors are used as first optical components. This means polychromatic incident radiation and fixed angle. The relationship for the angle and wavelength (or energy) can be rewritten in terms of a cut-off energy, E_{cut},

$$E_{cut} = hc/\lambda_{cut} = (hc/\theta)\,(n_e r_e/\pi)^{1/2}$$

Since $E[\mathrm{keV}] = 12.4/\lambda[\text{Å}]$ and $\theta[\mathrm{mrad}] \approx 1.6\,\lambda[\text{Å}]\,(\rho\,[\mathrm{g/cm^3}])^{1/2}$, we can write the above eq'n in practical units as:

$$E_{cut}\,[\mathrm{keV}] \approx 20\,(\rho\,[\mathrm{g/cm^3}])^{1/2} / \theta[\mathrm{mrad}]$$

- For energies below the cutoff energy ($E < E_{cut}$), there is near total reflection, while for those energies above the cutoff energy, the reflection coefficient is considerably reduced.

Uses of X-ray Mirrors

- Low-pass filters
  - Since there is an 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 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_{cut}, can be varied by having several different coatings deposited on the mirror substrate.

Fix the angle of incidence and vary the material properties (density).

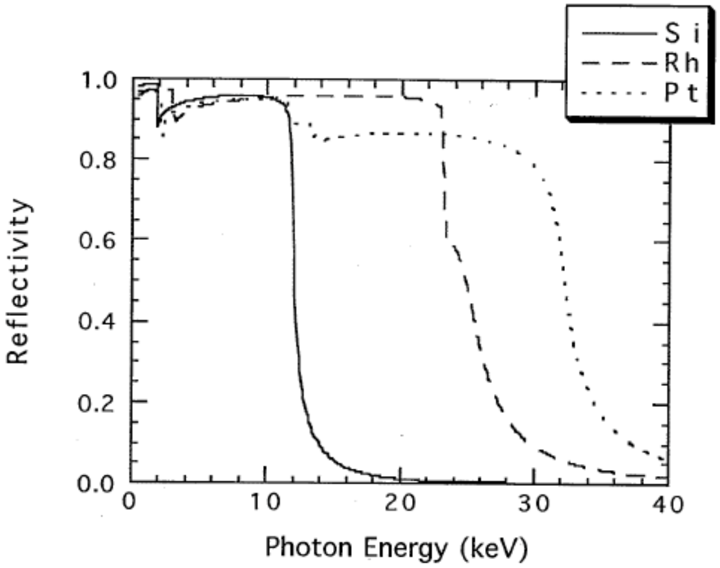
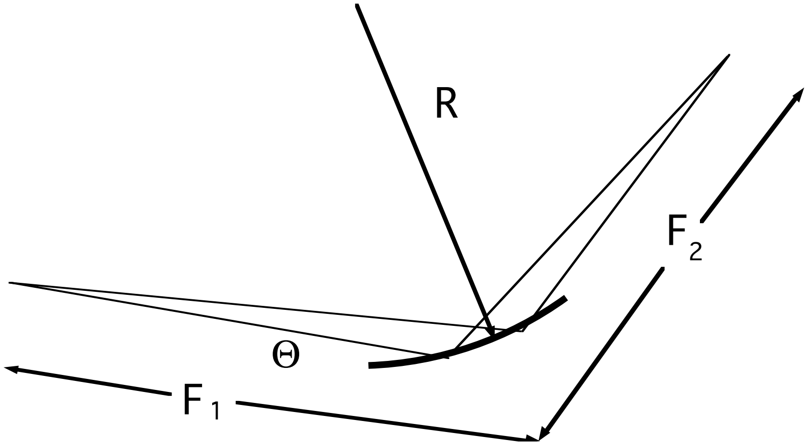


Fig. 2ID-4 X-ray reflectivity as a function of x-ray energy for Si, Rh, and Pt mirrors at 0.15° of incidence angle. Note the cut-off energy for a Pt mirror is about 34 keV.

Focusing with Mirrors

- Production of small beams is important for research for use in micro-diffraction, microspectroscopy, microtomography and a host of micro-imaging techniques.

- 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.



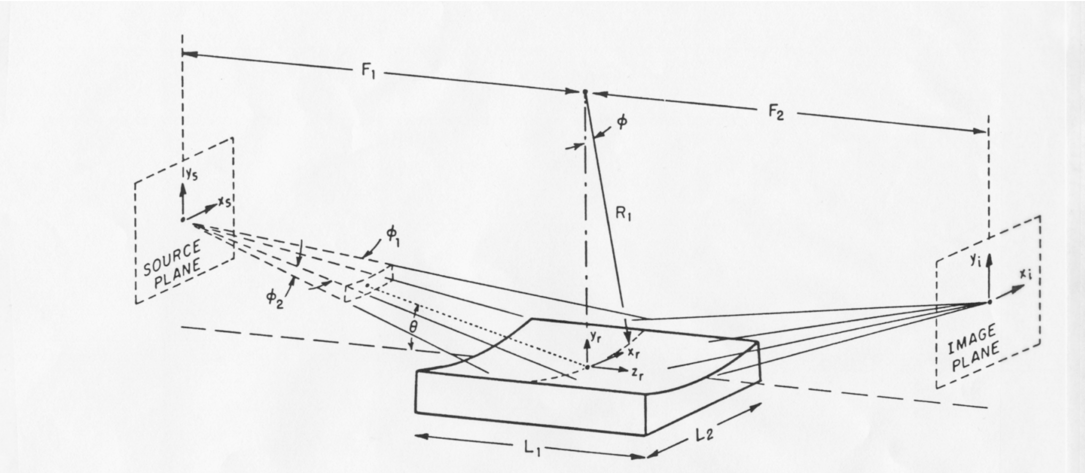
$R_m = [2/\sin\theta]\,[F_1 F_2/(F_1 + F_2)]$

Typically, $\theta = 3$ mrad, $F_1 = 30$m, $F_2 = 30$m and so $R_m = 10$ kilometers

Focusing in Two Dimensions

- Two-dimensional focusing (toroids and ellipses)
  - 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:

$$\mathbf{R_s = R_m \sin^2 \theta}$$



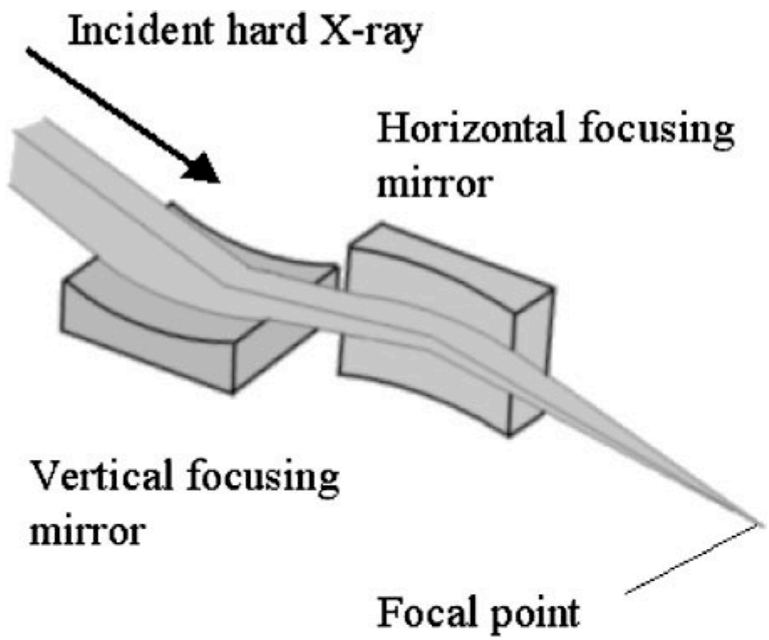
- In our example, from the last slide, q = 3 mrad and Rm = 10 km so the sagittal radius would be:

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

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.

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



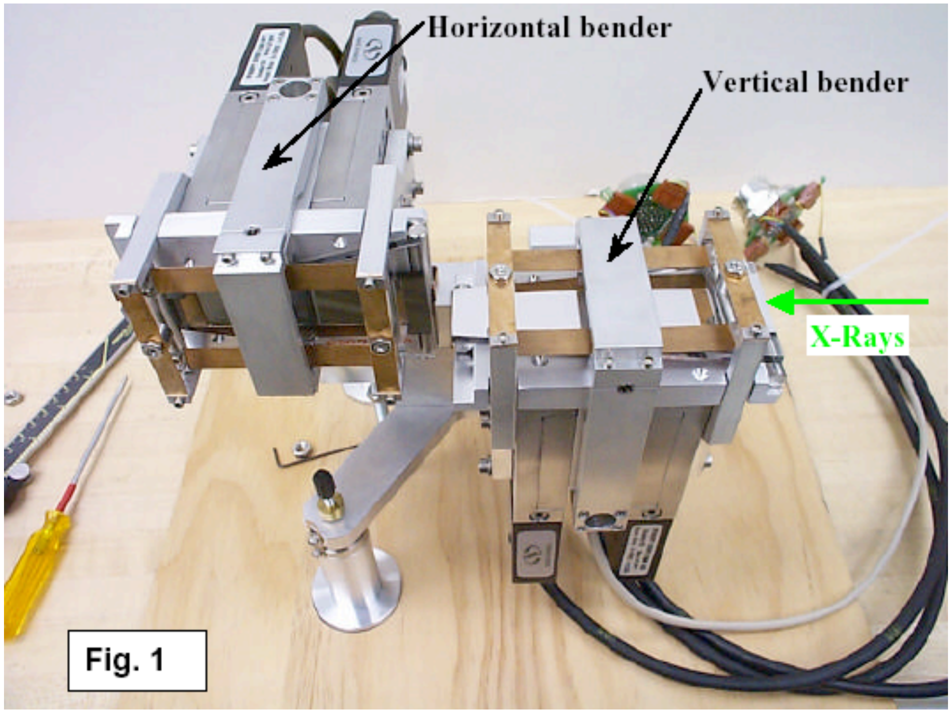
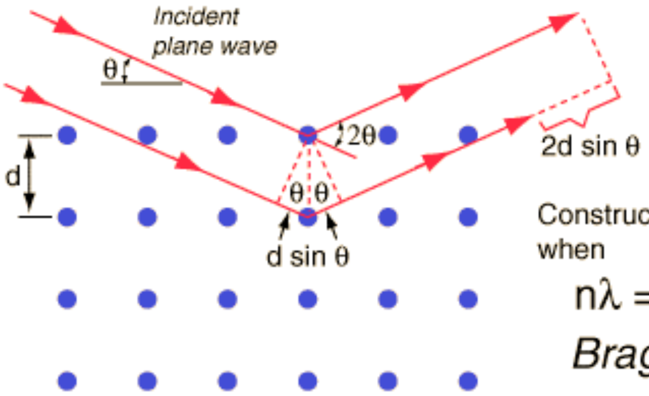


Fig. 1

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
  - they preserve the beam brilliance

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).

- The name comes from 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".)

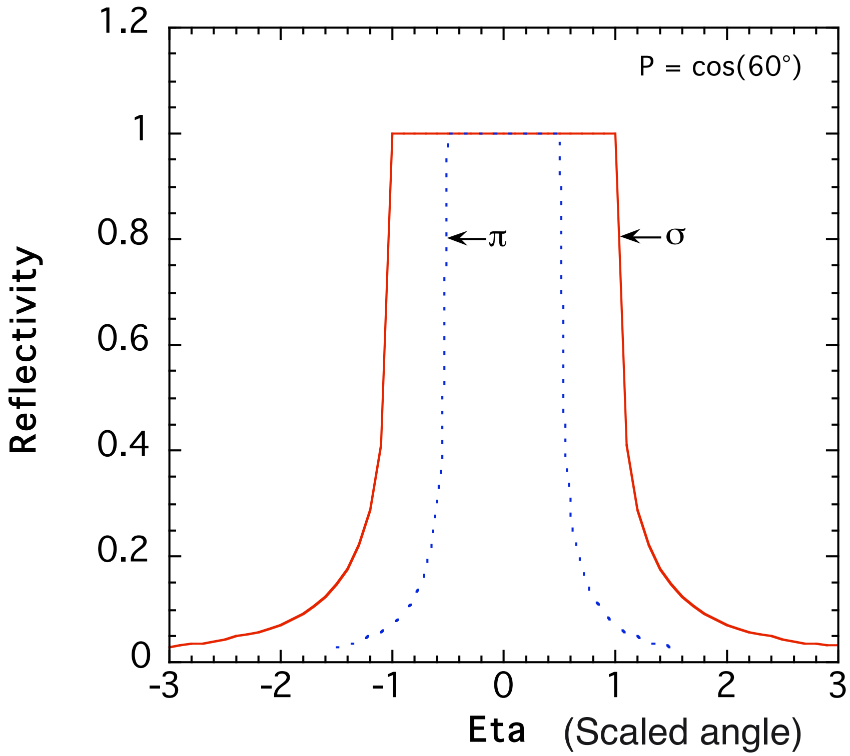
Darwin Width

- The limited penetration means:
  - the beam only interacts with a limited number of atomic planes
  - the scattered beam gets in and out of the crystal with little loss of amplitude from (photoelectric) absorption.

- A consequence of the first item:
  - There is a finite angular width over which the diffraction occurs. This is is often called the ***Darwin width*** , ω_D, for the reflection (hkl) at some specified wavelength.

- A consequence of the second item is:

  The reflectivity over this narrow Darwin width is nearly unity.



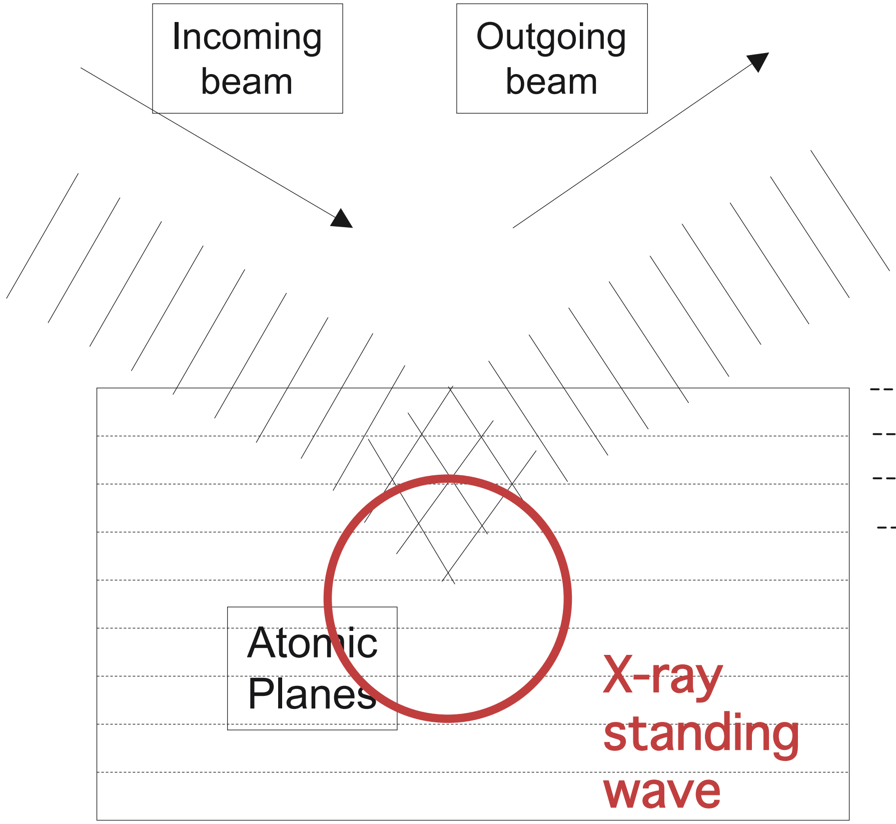
The Darwin width for π-polarization (E || to diffraction plane) is equal to cos(2θ) times the width for σ polarized x-rays (E ⊥ to diffraction plane).

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

$$\omega_D^\pi = \omega_D^\sigma \cos(2\theta)$$

F = structure factor & V = volume of unit cell

X-ray Standing Waves at the Bragg Condition

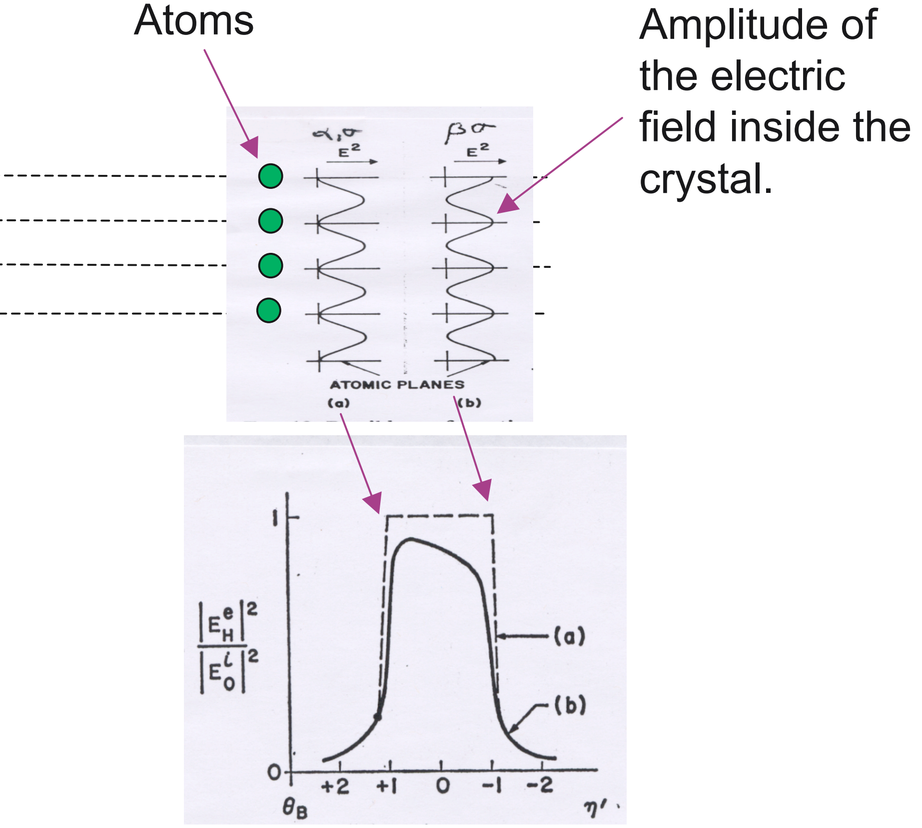


Incoming beam

Outgoing beam

Atomic Planes

X-ray standing wave

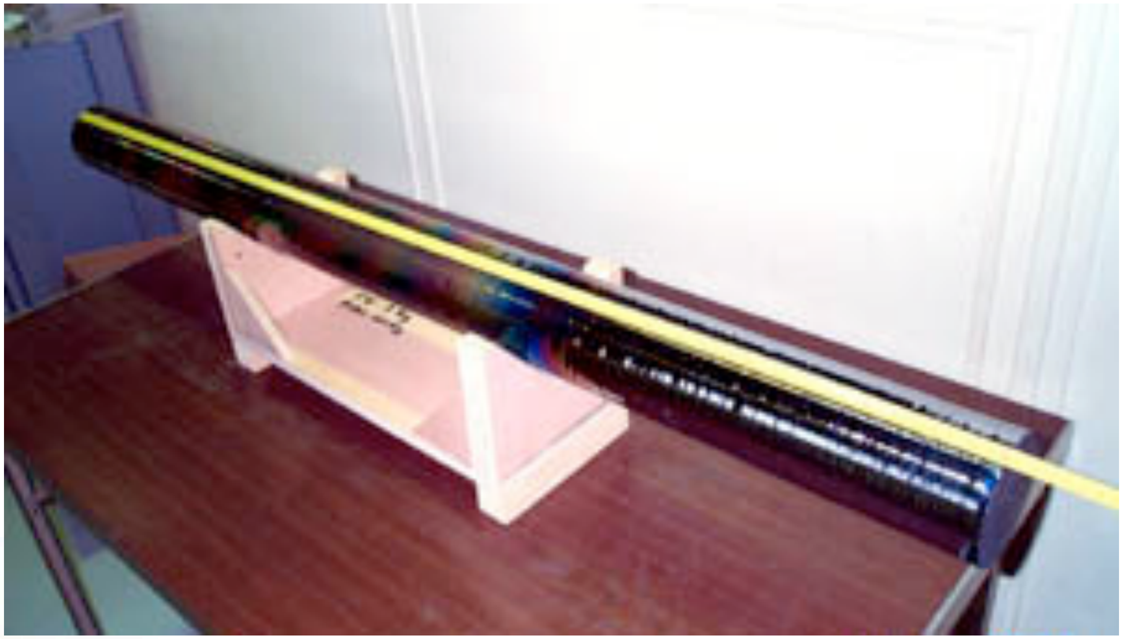


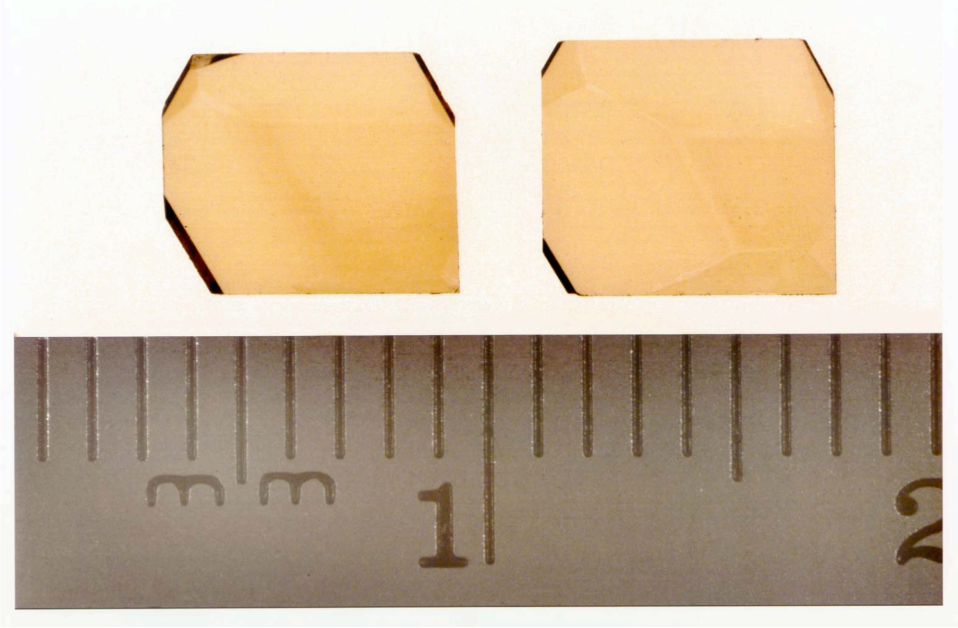
Atoms

Amplitude of the electric field inside the crystal.

Real World Perfect Crystals

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 $\lambda = hc/E$), namely:

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

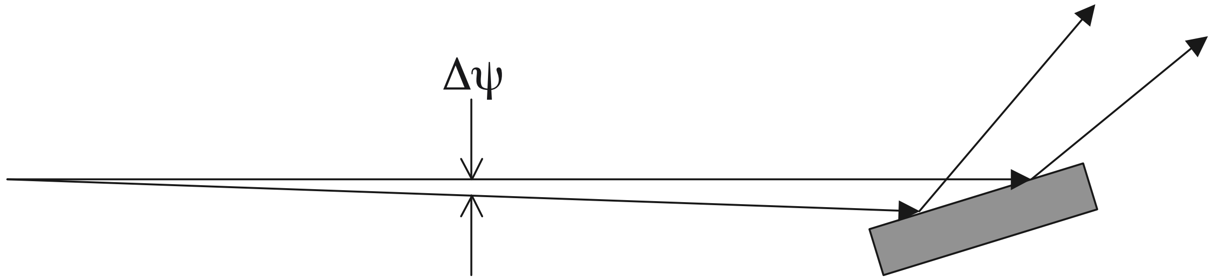
- If we differentiate Bragg's Law, we can determine the energy resolution of the monochromator.

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

- Because of the small angular divergence of the x-ray beam in the vertical direction (and the polarization of the beam - in the plane of the orbit), synchrotron radiation monochromators normally diffract in the vertical plane.

Energy Resolution in Monochromators

- Contributions to $\Delta\theta$ come from the angular divergence of the incident beam ($\Delta\psi$) and the natural width of the reflection (ω_D).



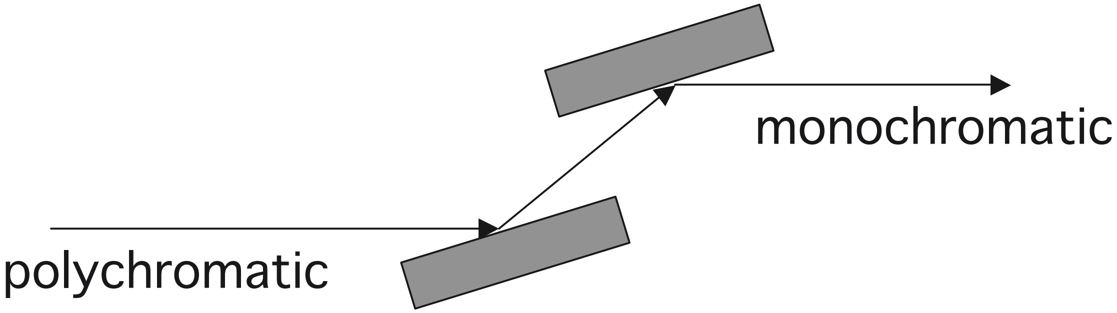
i.e. $$\Delta\theta = [\Delta\psi^{2} + \omega_D{}^{2}]^{1/2}$$

- A value for the Darwin width (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, $\Delta\psi$, is about 10 - 15 microradians. In this case, the energy resolution of the mono is determined by the crystal, and you can't get any better than that!

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.



Thermal Loading on Optics

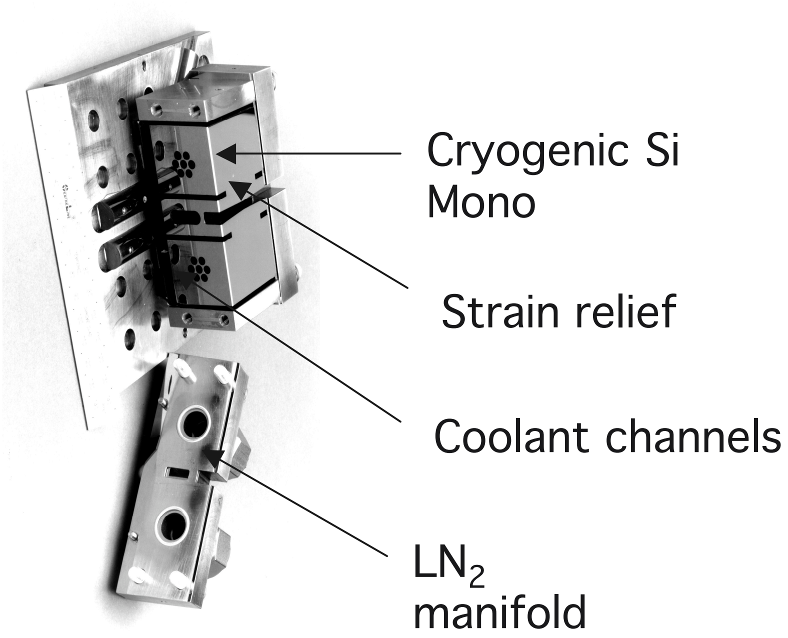
- Along with the enormous increase in x-ray beam brilliance from insertion devices comes unprecedented powers and power densities that must be effectively handled so that thermal distortions in optical components are minimized and the full beam brilliance can be delivered to the sample.

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. (See Appendix 2 for details.)

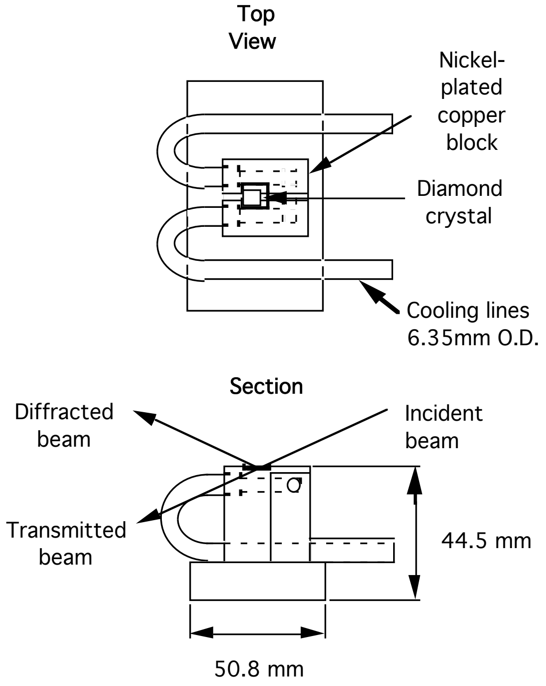
Cooled Monochromators

- 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.

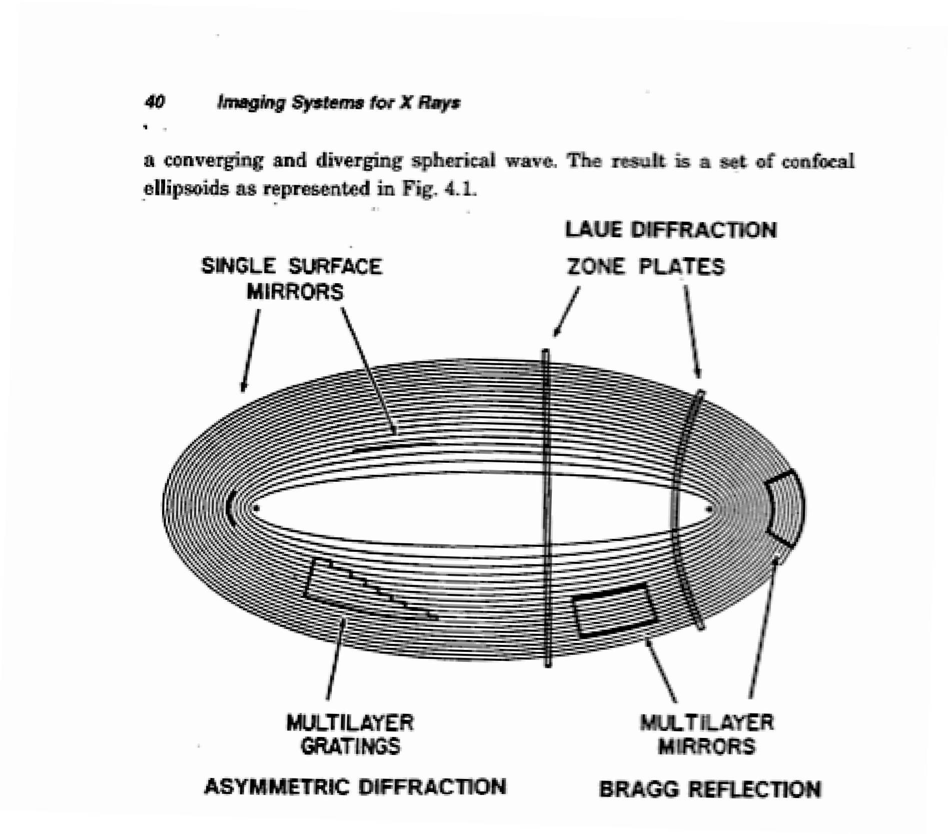
More Focusing X-ray Optics

- There is considerable interest in focused x-ray beams from 100's of microns to sub-micron in size.

- We have already seen that
  - mirrors can be configured for
  - focusing.

- Bent single crystals can also
  - be used to focus x-ray beams.

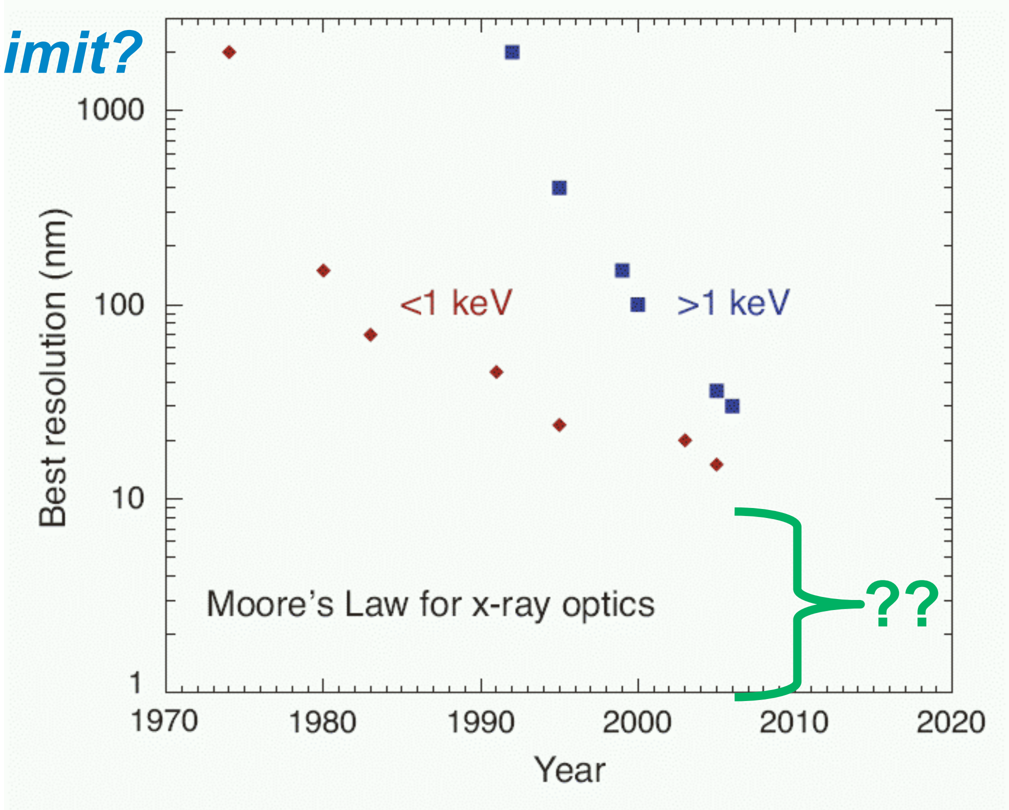
- As an example of non-diffraction
  - based optical components, we will
  - look at two focusing elements:
    - zone plates
    - compound refractive lenses



40 *Imaging Systems for X Rays*

a converging and diverging spherical wave. The result is a set of confocal ellipsoids as represented in Fig. 4.1.

What is the Spatial Resolution Limit?

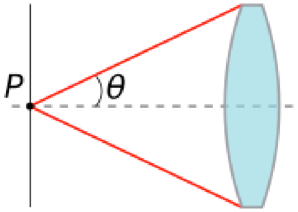


- 1912: Friedrich, Knipping, Laue:
  X-rays are electromagnetic waves

  → Spatial resolution limit:

  $\Delta r = 0.6\,\lambda / NA$ ($\approx \lambda$ visible light)

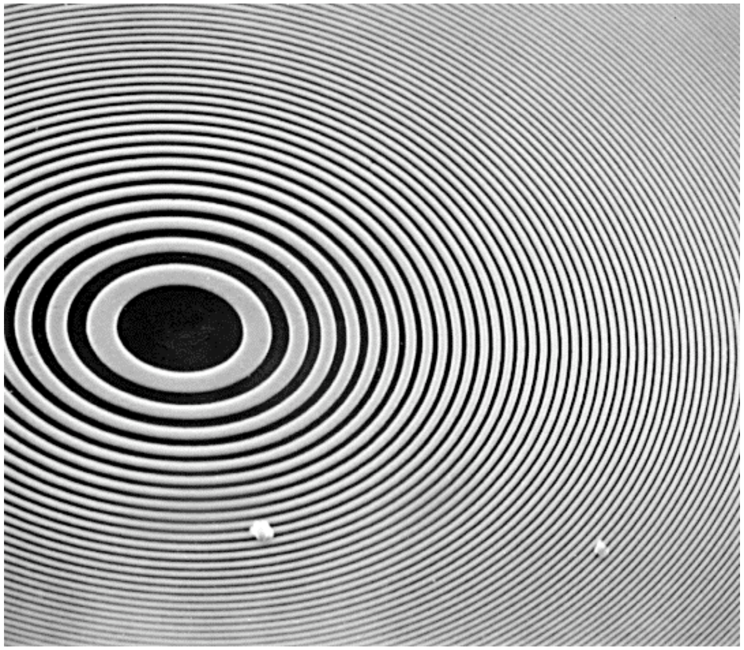
  where the numerical aperture,
  $NA = n \sin(\theta)$



- 95 years later (2D resolution):
  - Refractive Optics: d ~ 50 nm (E = 21 keV) (*Schroer, APL, 2005*)
  - Reflective Optics: d ~ 25 nm (E ~ 15 keV) (*Mimura, APL, 2007)*
  - Diffractive Optics: d ~ 15 nm, (E = 0.8 keV) (*Chao, Nature, 2005*)

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.

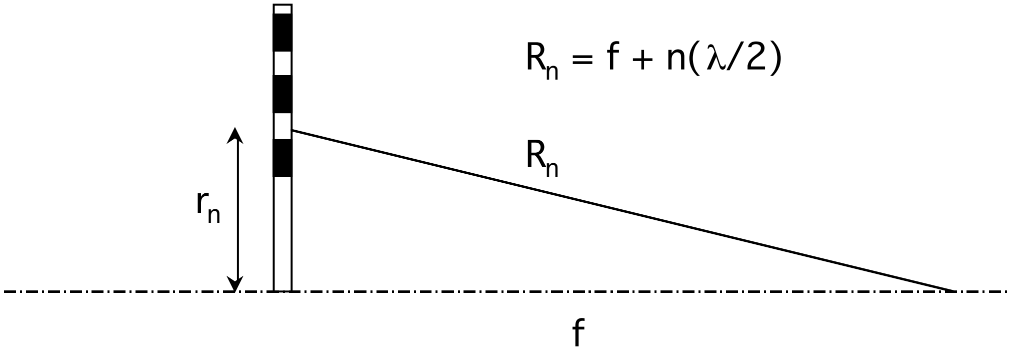


- The wave that emerges from the zone plate is the superposition of spherical waves, one from each of the zones.
- The wavefront modification is obtained through the introduction of a relative change in amplitude or phase in the beams emerging from two neighboring zones.

Zone Plate Physics

Condition so the pathlength varies by λ/2 for each ring.

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



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:

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

Focal Length and Focus Spot Size

- The focal length for the m^th^ order can be written as:

$$f_m = r_n^2 / m\lambda n$$

- 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:

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

- Zones plates with outermost ring widths of less than 30 nanometers can currently be fabricated for soft x-rays.

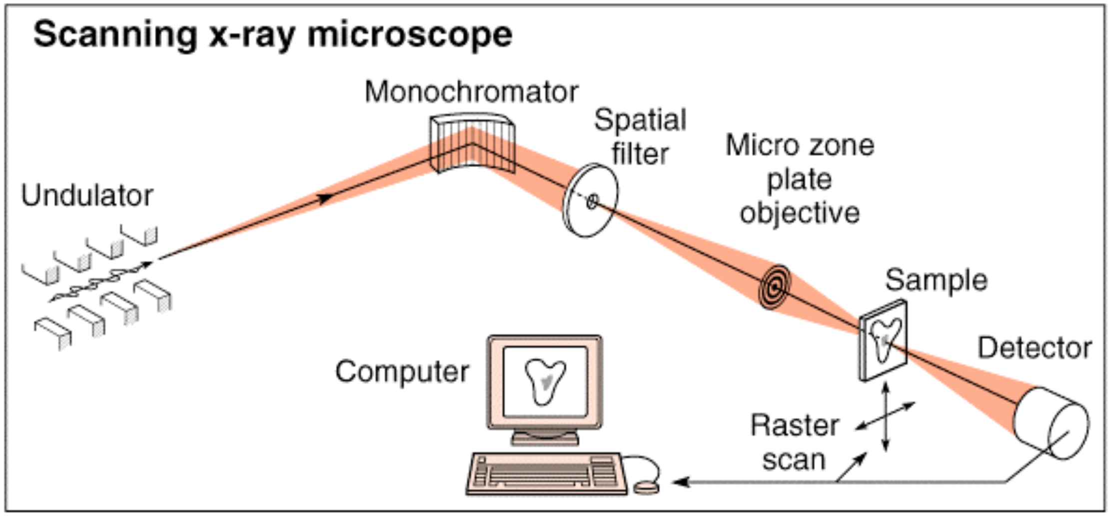


Figure from Center for X-ray Optics LBNL

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 100 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

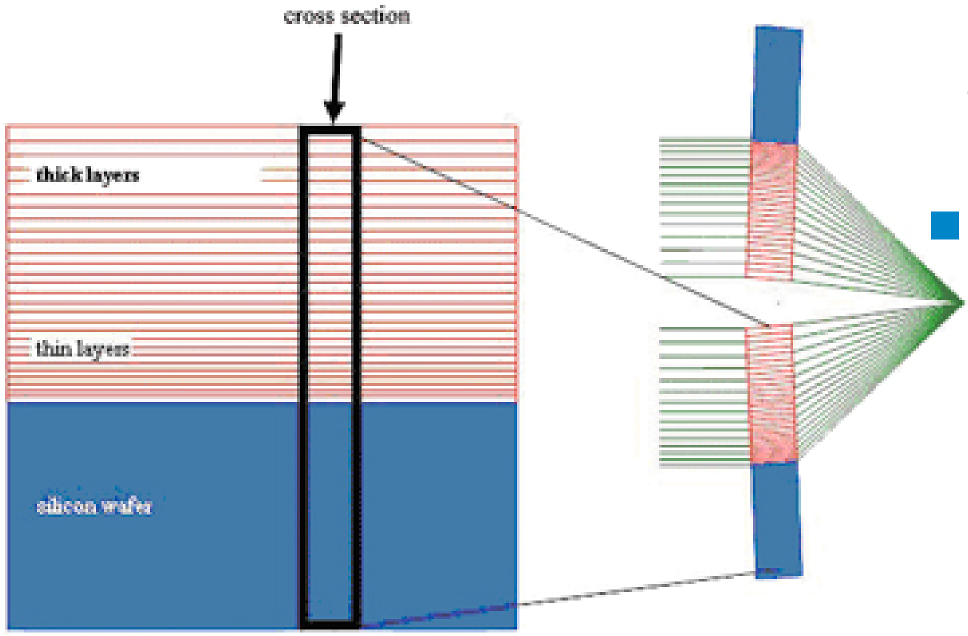
- An alternative to "blocking" out those rays that are out of phase (as in an amplitude zone plate), the thickness of the material can be adjusted so that the wave experiences a phase shift of π.

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

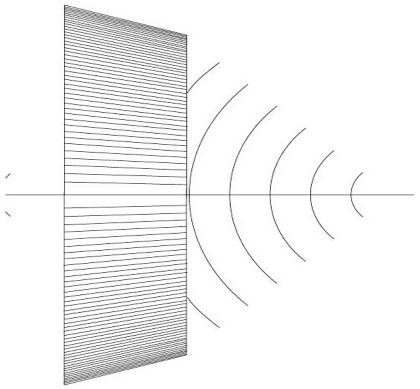
- The phase zone plates ease the thickness requirement (as compared to the amplitude zone plates) but the aspect ratio is still an issue.

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

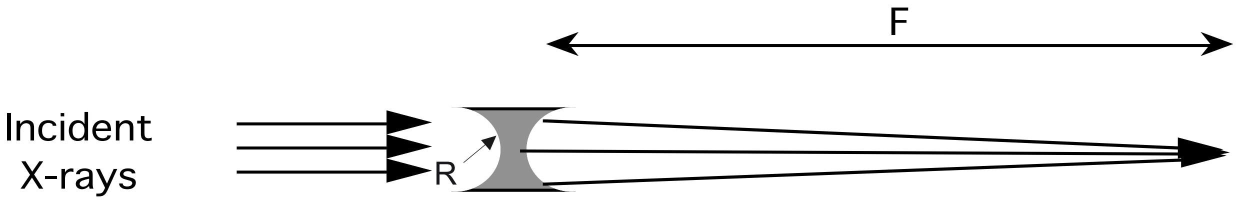
- **Each MLL comprises 1,588 layers (lines)**
- **The thinnest layer (line) is 5 nanometers thick**
- **The MLL has a current focus of 16 nanometers @ 19 keV!**

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).

Refractive Focusing Optics: X-ray Lenses

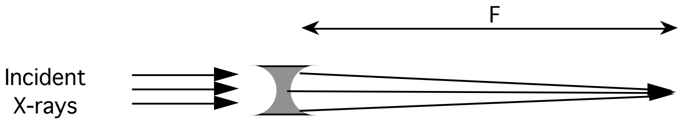
- Roentgen's first experiments convinced him that x-rays could not be concentrated by lenses; thirty years later his successors understood why.

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

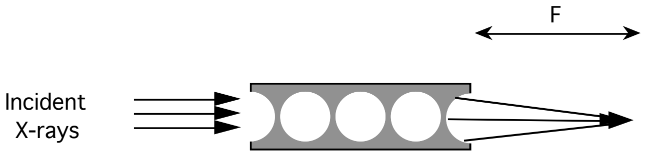


- What has happened over the last several years that now makes the compound lens not on feasible but now routinely used? The answer is high brightness synchrotron radiation beams.

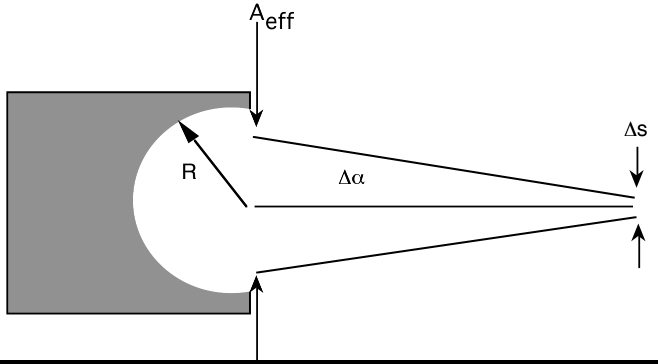
Compound Lenses



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:

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

Why Are They Applicable to SR?

- 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.

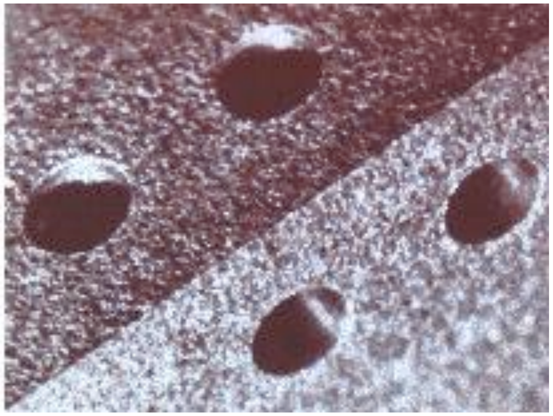
- Plugging in some numbers, suppose that:
  - $R = 1$ mm
  - $\delta \approx 10^{-6}$
  - $N = 50$

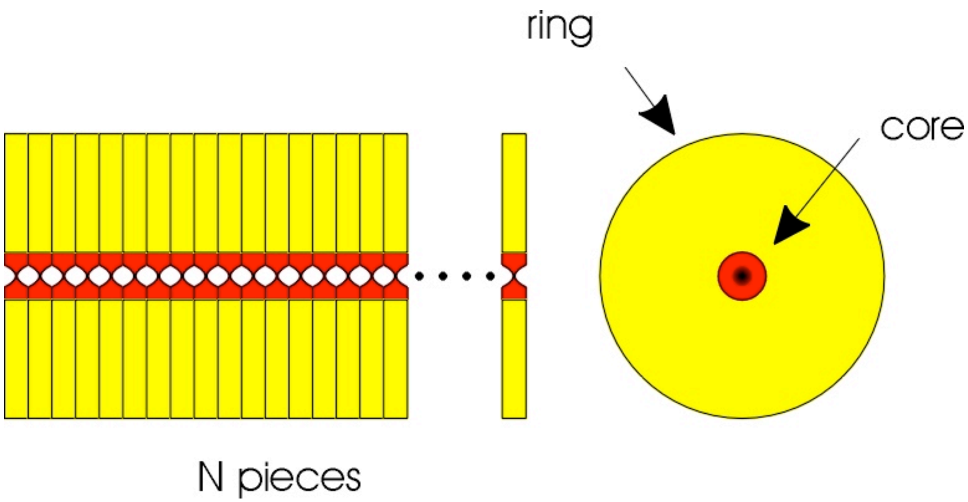
- Then the focal length, F, would be at 10 m.

- These lenses focus at rather larger distances and are be well adapted to the scale of synchrotron radiation beamlines.

Focusing in Two Dimensions

- Two dimensional focusing can be achieved by using two arrays of cylinders at 90° to one another, but crossed cylinder geometries have the disadvantage that the x-rays need to traverse twice the thickness and this reduces the gain considerably (since we have the thickness in the exponent).



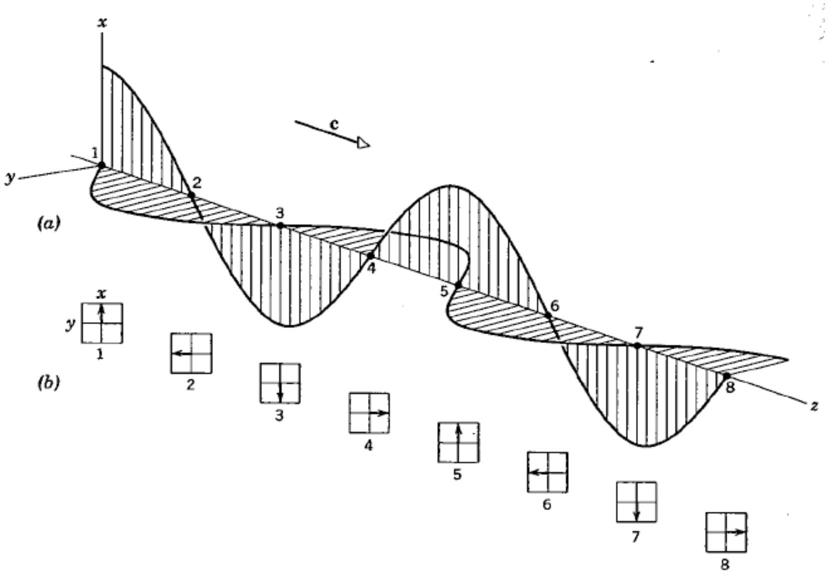


- Using spheres instead of crossed cylinders mitigates some of the absorption problems but increases the difficulty of fabrication. Paraboloids are the shapes we really want to eliminate spherical aberrations.

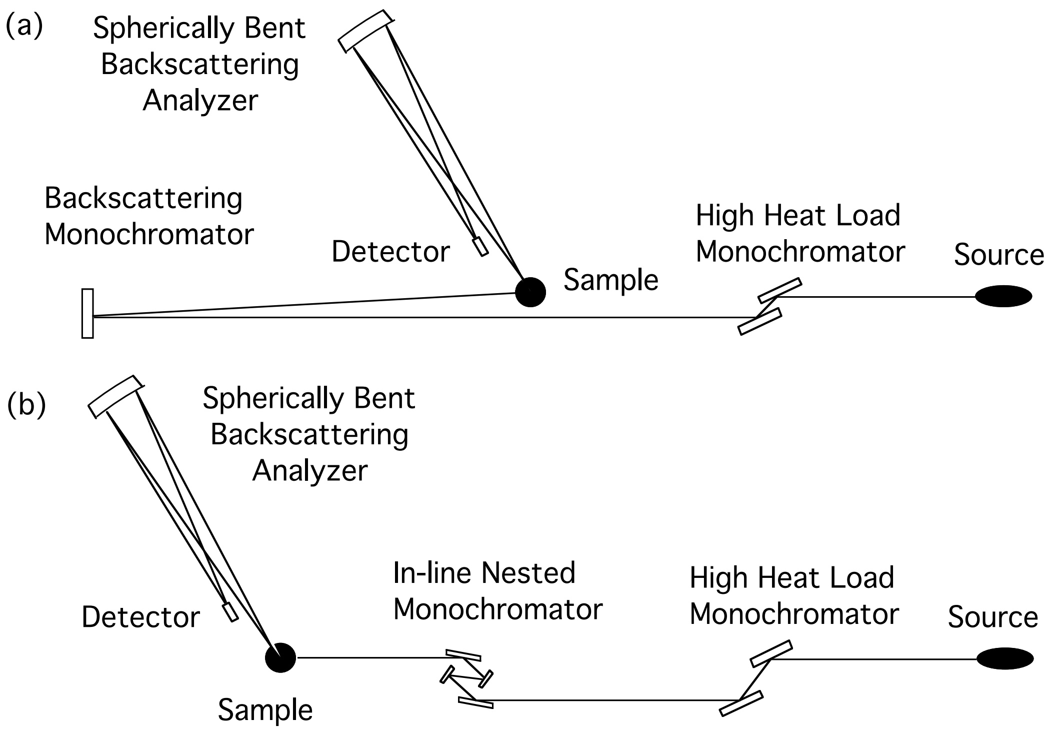
Figures from:
http://2b.physik.rwth-aachen.de/xray/imaging/main.php?language=en&frames=&content=crl#Focusingmethods

Other X-ray Optics

- Phase retarders (see Appendix 3):
  - Polarization analyzers and phase retarders for the determination and manipulation of the polarization, respectively, important for magnetic x-ray scattering.



- High-energy resolution (from eV to milli-eV) optics for inelastic x-ray scattering (see Appendix 4):


(a)

Spherically Bent Backscattering Analyzer

Backscattering Monochromator

Detector

Sample

High Heat Load Monochromator

Source

(b)

Spherically Bent Backscattering Analyzer

Detector

In-line Nested Monochromator

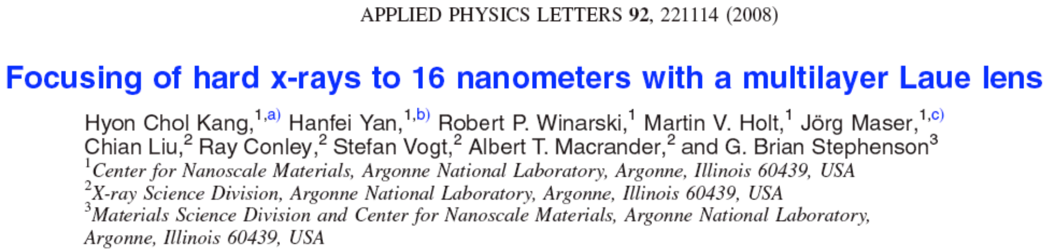
High Heat Load Monochromator

Source

Sample

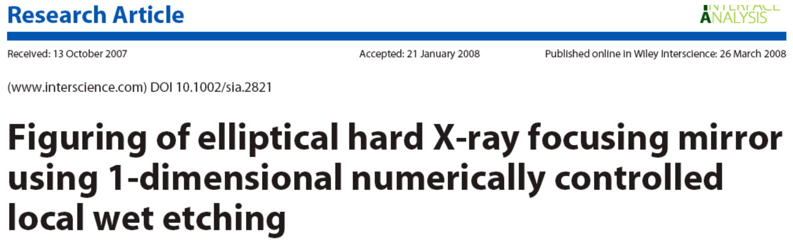
There is still stuff to do……

Although the basic equations the govern x-rays have been around for a while, not all x-ray optical components were invented 50 years ago and that there is still plenty of opportunities for the researchers in the field of x-ray optics.


APPLIED PHYSICS LETTERS **92**, 221114 (2008)

Focusing of hard x-rays to 16 nanometers with a multilayer Laue lens

Hyon Chol Kang,[1,a)] Hanfei Yan,[1,b)] Robert P. Winarski,[1] Martin V. Holt,[1] Jörg Maser,[1,c)]
Chian Liu,[2] Ray Conley,[2] Stefan Vogt,[2] Albert T. Macrander,[2] and G. Brian Stephenson[3]
[1]*Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[2]*X-ray Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[3]*Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA*


Research Article ANALYSIS

Received: 13 October 2007 Accepted: 21 January 2008 Published online in Wiley Interscience: 26 March 2008

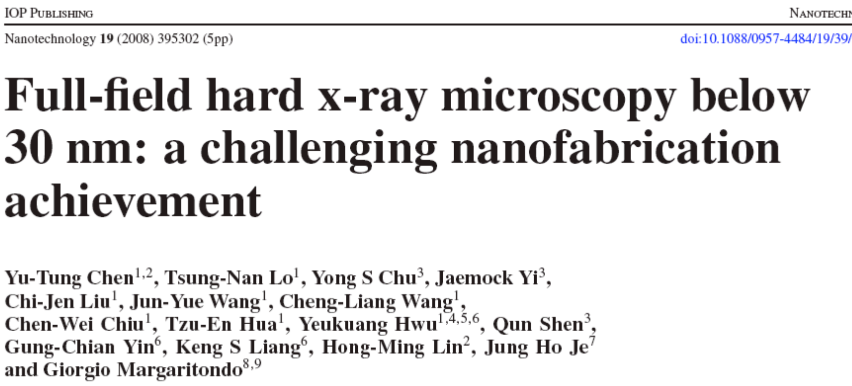
(www.interscience.com) DOI 10.1002/sia.2821

Figuring of elliptical hard X-ray focusing mirror using 1-dimensional numerically controlled local wet etching


Wave-optical simulation of hard-x-ray nanofocusing by precisely figured elliptical mirrors

Cameron M. Kewish, Lahsen Assoufid, Albert T. Macrander, and Jun Qian

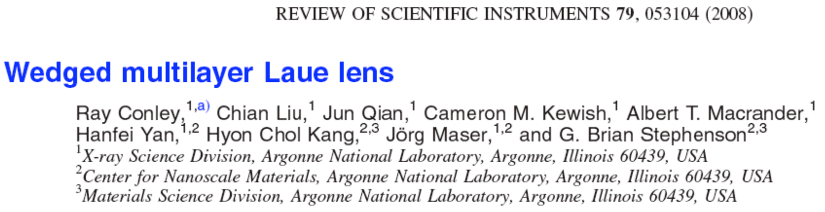
2010 APPLIED OPTICS / Vol. 46, No. 11 / 10 April 2007


IOP PUBLISHING NANOTECHNOLOGY

Nanotechnology **19** (2008) 395302 (5pp) doi:10.1088/0957-4484/19/39/395302

Full-field hard x-ray microscopy below 30 nm: a challenging nanofabrication achievement

Yu-Tung Chen[1,2], Tsung-Nan Lo[1], Yong S Chu[3], Jaemock Yi[3], Chi-Jen Liu[1], Jun-Yue Wang[1], Cheng-Liang Wang[1], Chen-Wei Chiu[1], Tzu-En Hua[1], Yeukuang Hwu[1,4,5,6], Qun Shen[3], Gung-Chian Yin[6], Keng S Liang[6], Hong-Ming Lin[2], Jung Ho Je[7] and Giorgio Margaritondo[8,9]


REVIEW OF SCIENTIFIC INSTRUMENTS **79**, 053104 (2008)

Wedged multilayer Laue lens

Ray Conley,[1,a)] Chian Liu,[1] Jun Qian,[1] Cameron M. Kewish,[1] Albert T. Macrander,[1]
Hanfei Yan,[1,2] Hyon Chol Kang,[2,3] Jörg Maser,[1,2] and G. Brian Stephenson[2,3]
[1]*X-ray Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
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[3]*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*

Appendix 1: Dielectric Constant

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:

$$p = -ex \text{ and } P = -exn_e$$

where n_e is the number of electrons/unit volume. In a simple harmonic approx:

$F = ma = mx'' = -eE - kx$ **where k is the "spring constant" associated with ω_o ($= \sqrt{k/m}$).**

If x has the form $x = Ae^{i\omega t}$, x will be:

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

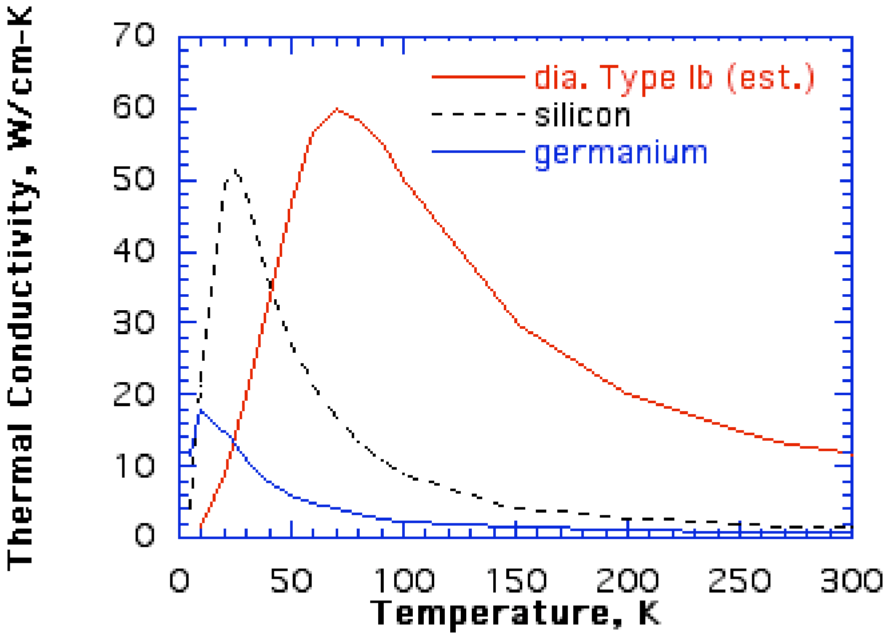
$$P = -(e^2/m)n_eE/(\omega_o^2 - \omega^2)$$

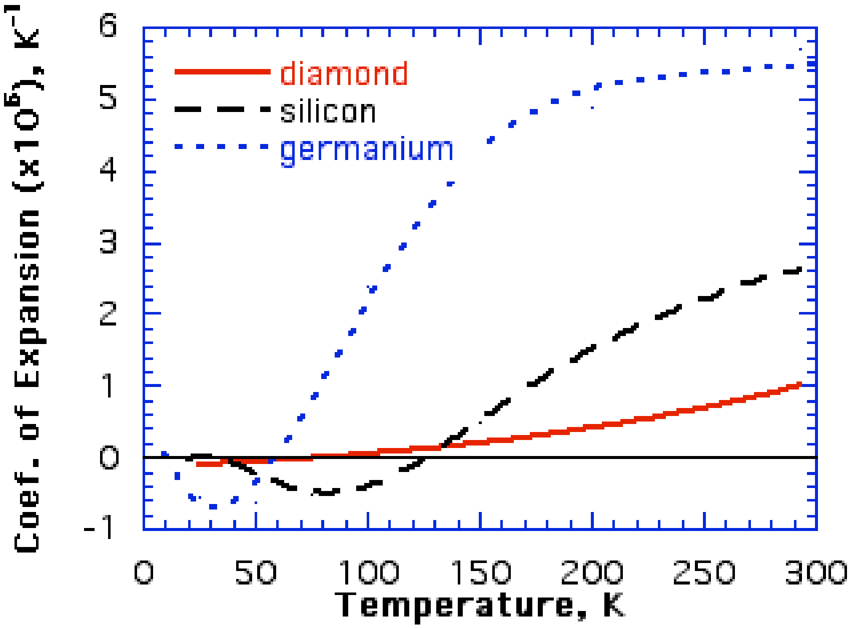
Appendix 2: Physical Properties of Si, Ge, and C(diamond)

- 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.





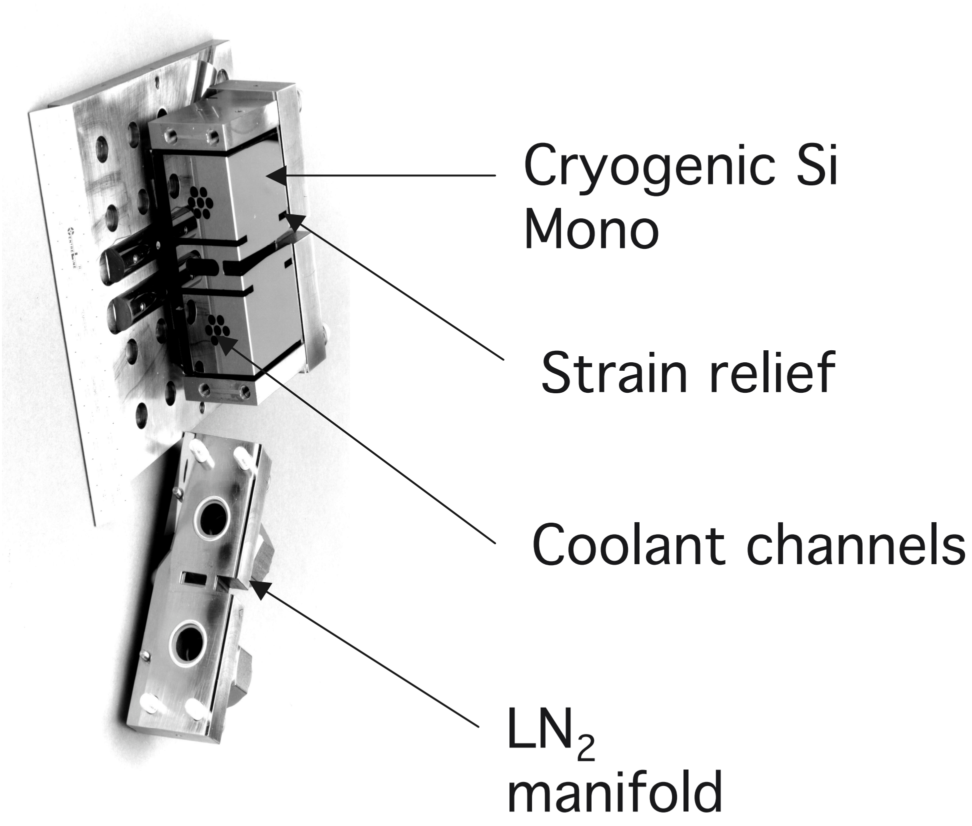
Appendix 2: Figure of Merit (FOM) for Various Materials and Temperatures

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

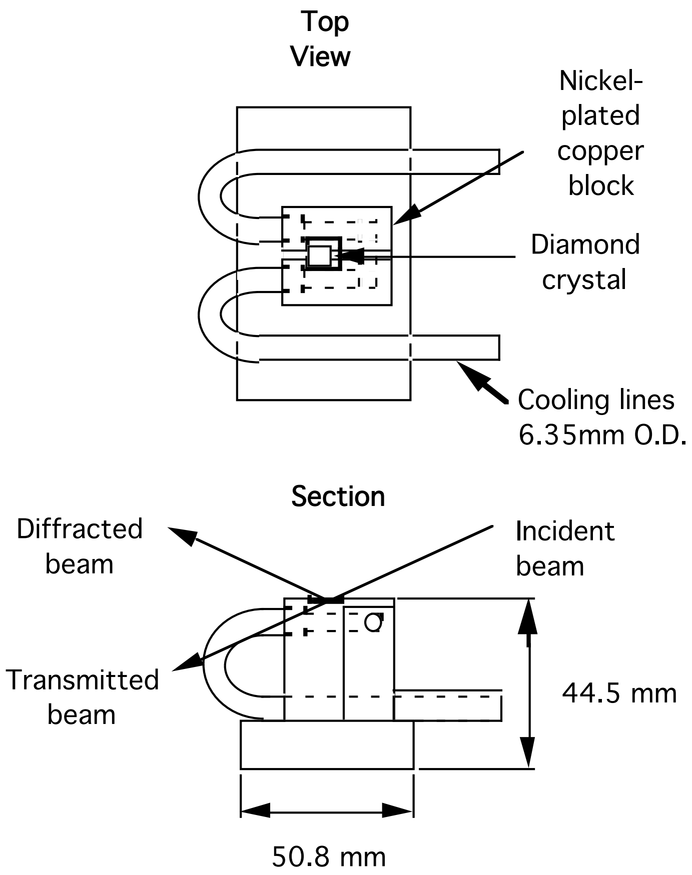
FOM of various materials

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 2: Cooled Monochromators



Cryogenically Cooled Si Mono



Water Cooled Diamond Mono

Appendix 3: Index of Refraction Variation near the Bragg Angle

- At x-ray wavelengths, the index of refraction of all materials is isotropic and so you cannot use the same approach as with visible light (i.e. birefringence) to change the phase of the electric field with one polarization direction relative to the electric field of the other polarization.

- However, near the Bragg condition, the σ and π polarizations "feel" or interact with the atoms in the crystal to different degrees and hence the the indices of refraction are slightly different for σ and π polarized waves. This small effect can be used to make phase retarders at x-ray wavelengths.

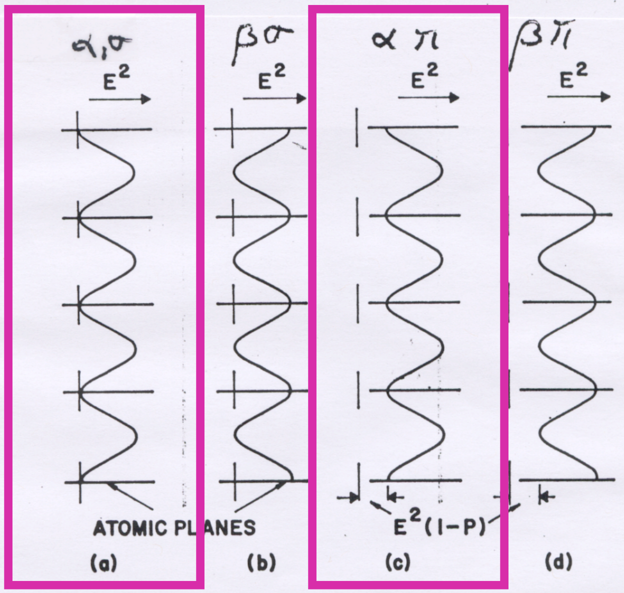
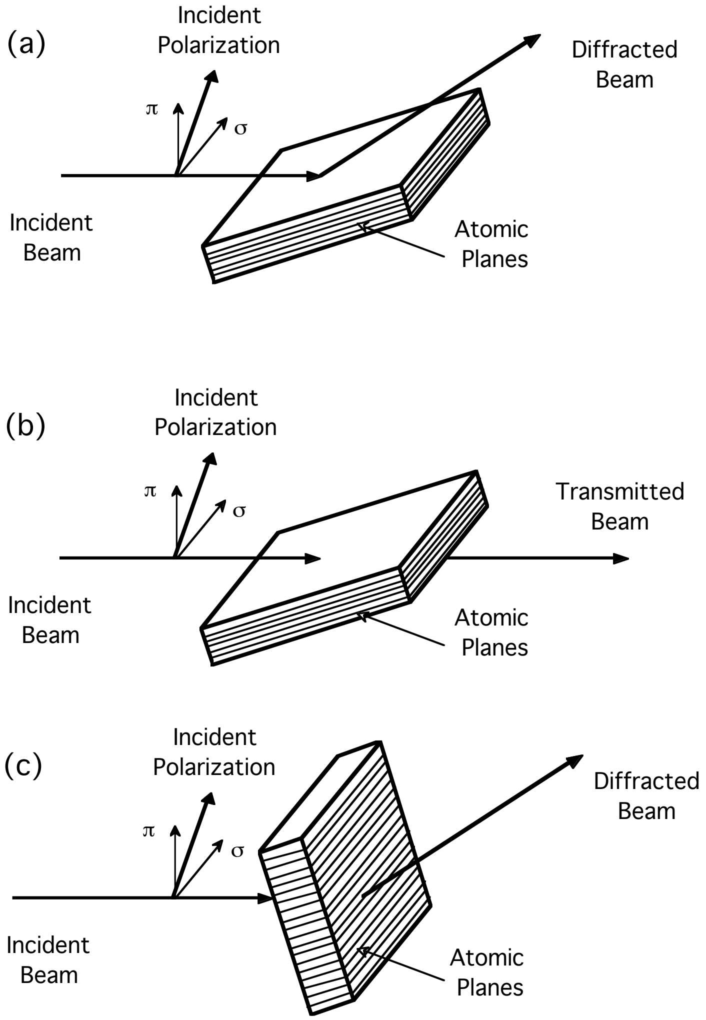
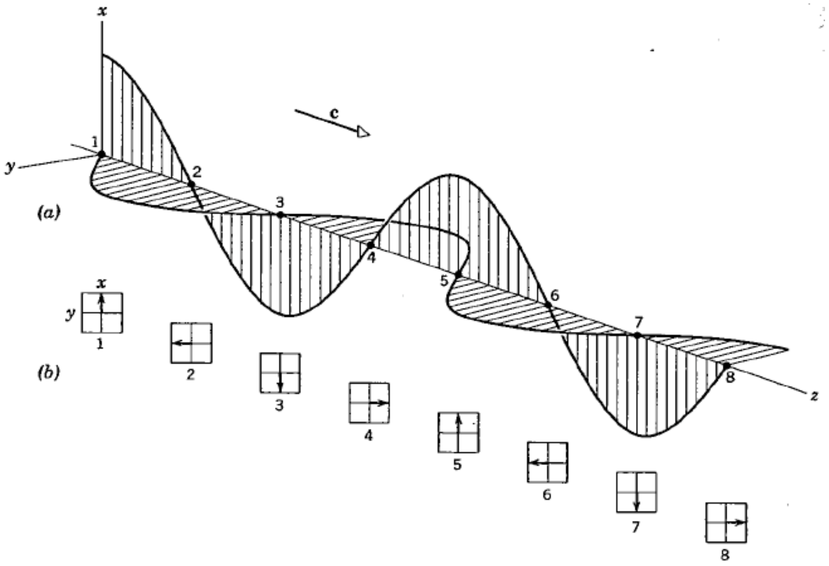


FIG. 19. Possible configurations of the standing wave patterns, assuming that the nodes of the α branch pattern, σ polarization, coincide with the atomic planes. (a) α branch, σ polarization (b) β branch, σ (c) α branch, π state (d) β branch, π state.

Appendix 3: X-ray Phase Retarders



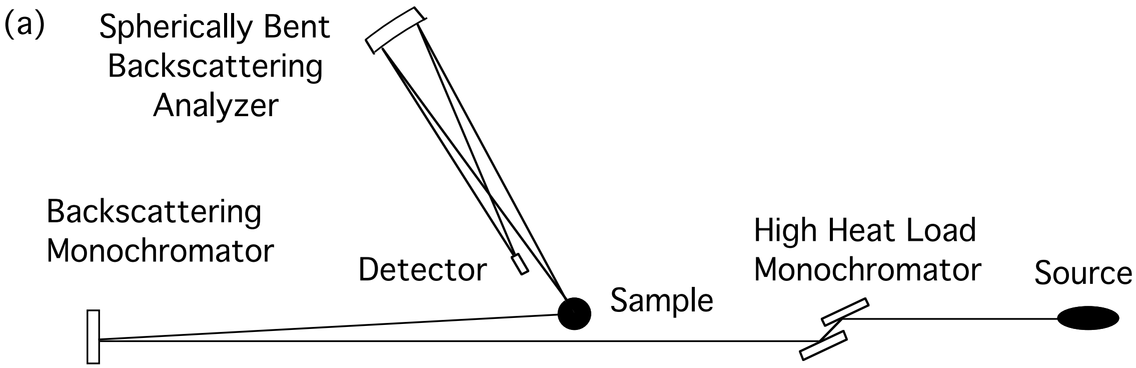
Polarization analyzers and phase retarders for the determination and manipulation of the polarization, respectively, important for magnetic x-ray scattering.



Appendix 4: High Energy-Resolution Optics

- Recall that a Si (111) crystal has a energy resolution ΔE/E ≈ 10^{-4}.

- However milli-electron volt resolution monochromators and analyzers are often required for inelastic scattering.



- If you look at the equation for energy resolution:

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

as θ approaches 90°, $\cot(\theta)$ goes to zero and the energy spread, ΔE, gets very small and so a backscattering geometry is employed.

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).

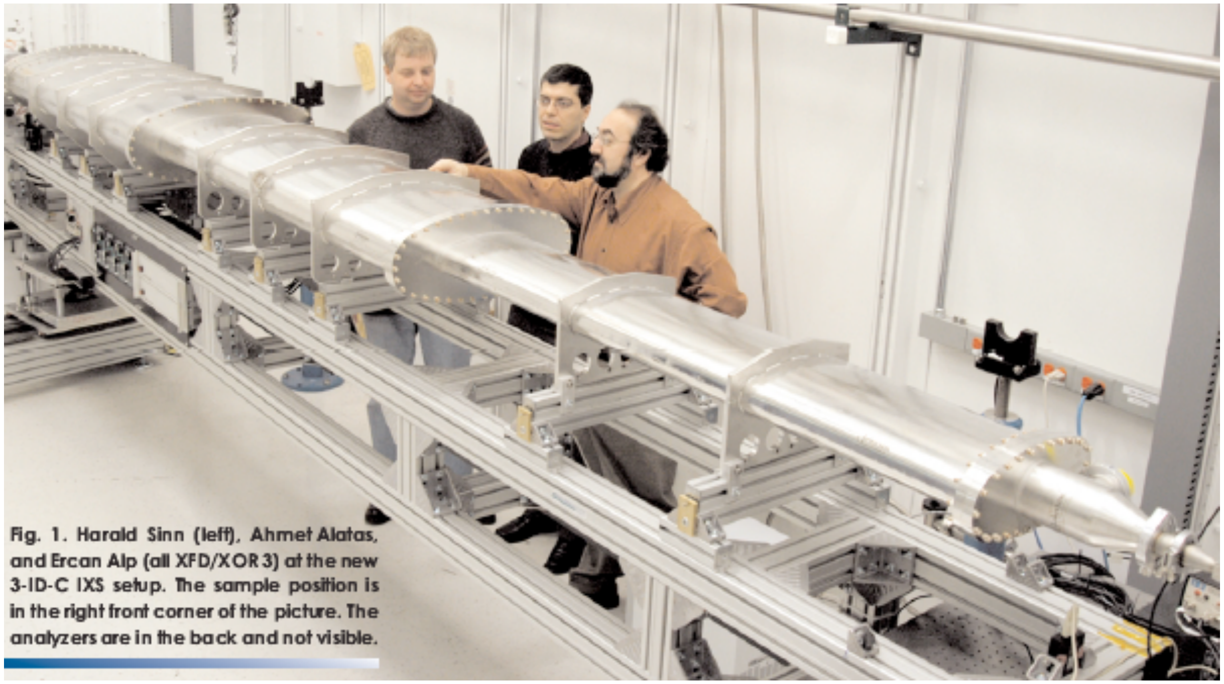


Fig. 1. Harald Sinn (left), Ahmet Alatas, and Ercan Alp (all XFD/XOR 3) at the new 3-ID-C IXS setup. The sample position is in the right front corner of the picture. The analyzers are in the back and not visible.

The inelastic scattering beamline at the APS.