By
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# Introduction

This primer presents, as we like to say in physics, the 0th order or most basic concepts about synchrotron X-ray beamline optics, equipment and layout. As shown in the illustration below, the process involves harvesting X-rays from a synchrotron source, modifying the X-rays with beamline optics and then directing them into an experimental station where they impinge on a sample, are detected and the resulting information is recorded and analyzed. All of this is done behind radiation shielding that protects the user from the harmful and sometimes lethal doses of radiation present in the beams.

Through this process, it is crucial to remember that, at the most fundamental level, the most important optical element in an X-ray beam-path is the *sample itself*. It is the job of the beamline designer to take the radiation from whatever source is available, operate on the beams to make them the right energy (wavelength), band-pass (ΔE), ray convergence, polarization, spot size, position and intensity to meet the needs of a particular experiment. There is no one-size-fits-all solution to the problem, which is why each beamline is unique. The requirements for each class of experiment determines the optical layout needed.

At the end of this primer, you can continue to sample the breadth and depth of synchrotron science and technology by using references listed in the resources section. These include a fantastic interactive CD called, ***Lumière Synchrotron Light*** [i] and the well-written text by Margaritondo, ***Introduction to Synchrotron Radiation***[ii]. Beyond that is the epic six-volume set ***Synchrotron Radiation***[iii] that presents all aspects of synchrotron X-ray production and scientific uses in minute scientific detail. For your bookshelf, we recommend a recent introductory book for X-ray physics by Jens Als-Nielsen[iv] and the standard introductory text by Cullity[v]. Finally, any serious X-ray user will want to find and carry a copy of the small 3" x 5" pocket reference, the ***X-ray Data Booklet*** [vi].

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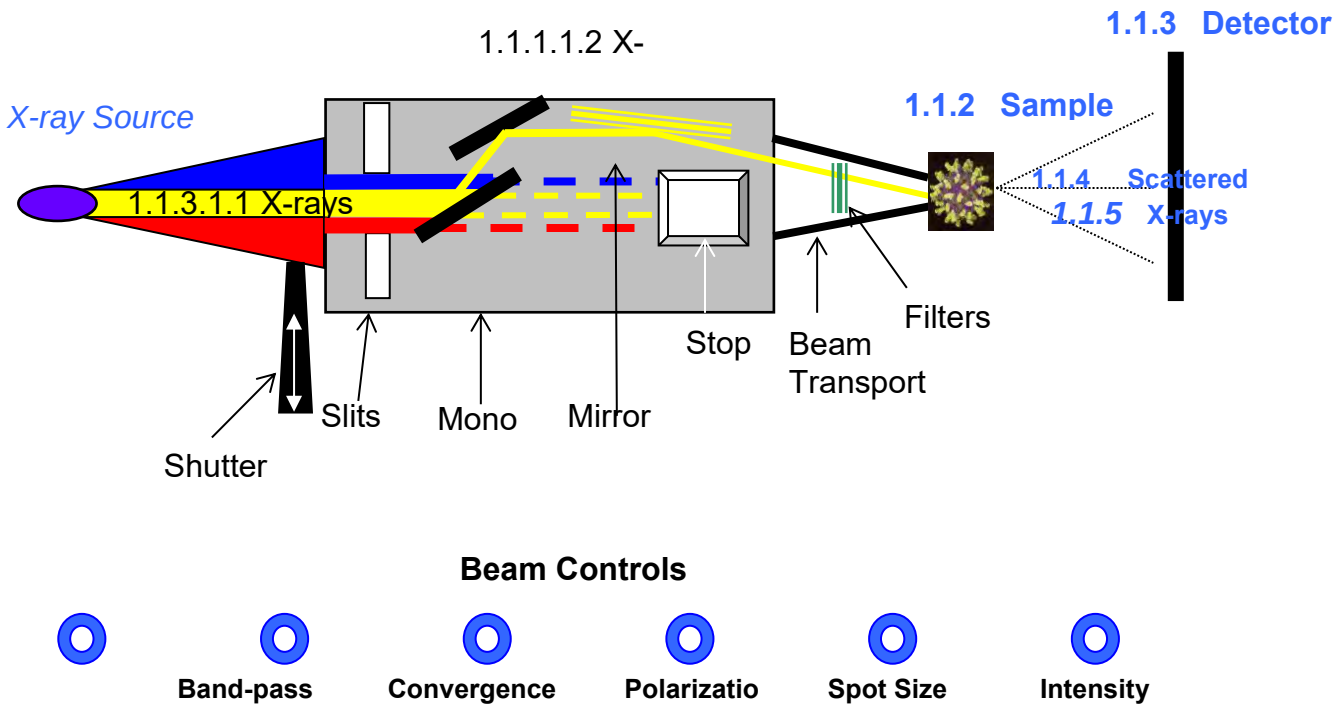


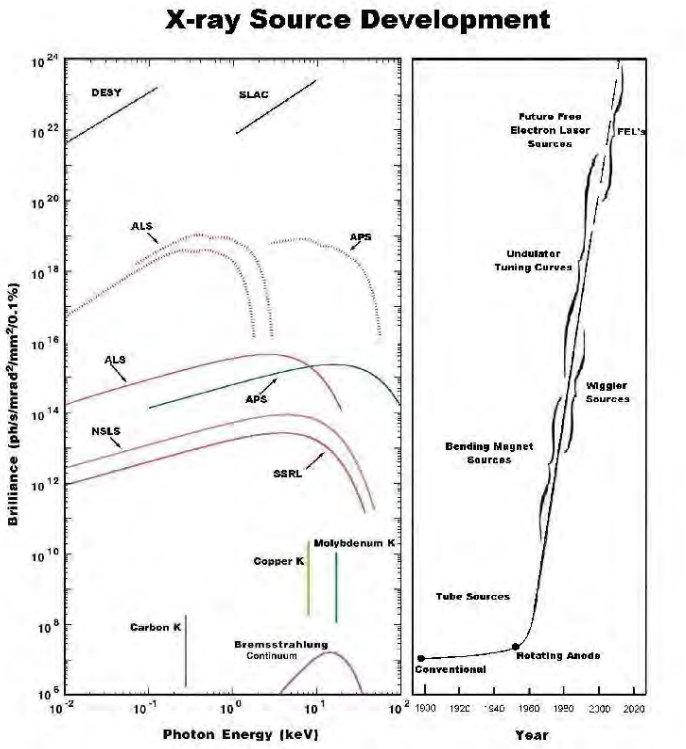
# Radiation Sources: Creating X-rays

X-rays are just short wavelength electromagnetic radiation, of the same general character as visible light. Throughout this primer, we will illustrate the basic concepts of X-ray interactions with beamline components by making analogies with visible light.

*The basic idea:* anytime that you accelerate (or de-accelerate) an electron, it produces X-radiation. In conventional tube sources, like those used for medical and dental diagnostics, electrons are smashed (rapidly decelerated) into metal anodes, giving off X-rays by two processes: the deceleration of the incident electron and the stimulation of characteristic radiation from the metal anode target. State-of-the-art micro-sources such as Z-pinch and flash tube sources squeeze hot electrons out of a strong electromagnetic field. In Synchrotrons[vii], Energy Recovery Linacs and future Free Electron Lasers (FELs), collections of relativistically moving electrons are accelerated by strong magnetic fields. The electrons lose energy by shedding X-rays as they pass through these fields. As the magnetic fields are made stronger and stronger, the intensity of these X-rays increases as seen in the brilliance and historical plots below. Each new generation of devices, starting with the X-ray tube, through the FEL sources of the near future, has and will produce more intense and well-collimated X-ray beams than its predecessor.

Since bending magnet sources are most prevalent at synchrotrons, it is important to understand that they provide a wide and uniform horizontal swath of radiation with a horizontal opening angle many milliradians wide. In the vertical direction, the radiation opening-angle varies inversely with the energy of the storage ring. More importantly, different energies exit the source at different vertical opening angles. The radiation is linearly polarized on the orbit plane of the synchrotron and has a greater component of circular polarization the further above or below the orbit you go.

It is important to understand that X-rays from tube and synchrotron sources are divergent. That is, they are spreading out in space as they travel away from the source. One of the important tasks for the beamline optics is to turn this beam into a parallel or a convergent beam as the experiment requires.



## Shutter Systems: Stopping the Radiation that you just created

X-rays are absorbed by matter. To stop the intense X-ray beams that you have just created, you need to drop a chunk of material in its path. The chunk of material absorbs the X-ray photons and converts them into heat. If the absorber is too thin or light, some of the light passes through the material. The amount of light that passes through your material depends not only on the material thickness and density but also on its absorption properties for the wavelength or energy you are stopping. You can see from the important equation box below, that the higher the 'Z' or atomic number of the element (the heavier it is) the better X-ray absorber it is by $Z^4$ ! It is no wonder lead and tungsten are typically used for stopping X-rays. (In terms of stopping power, spent uranium would make the best shutter, beamstop or slit, but no one has ever gotten around to designing with it since lead and tungsten are so much cheaper.) You can also see that at shorter and shorter wavelengths (the higher the energy), X-ray absorption drops off rapidly. *Bottom line:* as the shutter gets lighter or as the X-ray energy goes higher, you will have to make the chunk of material thicker and thicker to stop the radiation. You can calculate this thickness by looking up the mass absorption coefficient, $\mu/\rho$ and density, $\rho$ from tables or by using a calculation engine, such as the one available at the Center for X-ray Optics (CXRO) web site.[viii]

The difficulty with any absorber is that, now that you have stopped the X-ray and turned its energy into heat, you must get rid of that heat or it will melt your shutter. It's not that a liquid metal will not stop X-rays but rather, that a puddle of liquid is more difficult to hold on to and move around in the beam. Therefore, shutters are typically engineered to match the power output of the source. If the radiation is from a tube or bending magnet source, the power density and total power can be readily stopped by a block of water-cooled copper. For the intense output from a wiggler, undulator or FEL source, one must get very tricky. Typically, we take the X-ray spot and spread it out over a highly inclined water-cooled dispersion strengthened copper surface. It is thus possible to keep the local temperature due to X-ray absorption well within safe temperature limits determined by the thermal conductibility of the copper.

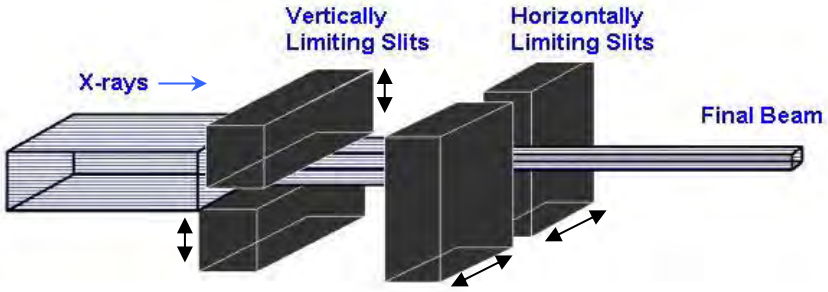
**Important Shutter, Slit and Absorber Equations:**

$I = I_o\, e^{-(\mu/\rho)*\rho*t}$ ⇐ Intensity of an X-ray pass through a body (I) is a function of the original intensity $I_o$ and an *exponential* reduction factor that depends on the material absorptivity, $\mu$, material density, $\rho$, and the material thickness, t. [$\mu$ is traditionally in units of 1/cm, density, $\rho$ in units of $gm/cm^3$ and thickness, t, is in units of cm.] You can interactively calculate absorption parameters using the resources found at the CSRO web-site[8] .

$\mu/\rho \propto Z^4\lambda^3$ ⇐ the ratio of absorptivity to density goes like Z, the atomic number of an element to the *fourth power* and like $\lambda$, the wavelength to the third power. $\mu/\rho$ is called the 'mass absorption coefficient' with units $cm^2/gm$. For historical reasons, you will find material absorption tabulated as $\mu/\rho$ vs. $\lambda$ in reference materials.

## Slit Systems: divergence delimiters, collimators, scatter guards

Slits are simply shutters that are put partway into the beam in order to clip, guard or shape the beam as needed. The majority of slits are made from combinations of copper, lead or tungsten although they can be made from any appropriate X-ray absorbing material. For example, biologists love X-rays roughly in the 5 to 20 keV range. Silver slits are excellent for this application since they are highly thermally conductive (they can be cooled easily), silver's fluorescence (secondary X-ray scatter) is outside of the 5 to 20 keV range, the slits are easy and safe to machine and a thick slice is relatively inexpensive.



Slit Operation

One needs to be careful with slit names, since there is no standard. What the figure shows as *vertically limiting slits*, some people call "horizontal slits" since the black absorber (slit) is lying horizontally, while others call them "vertical slits" because they cut the beam vertically.

*Important Concept:* Each time something physically intercepts an X-ray beam, it produces a new source of scattered (unwelcome) radiation and fluorescence (characteristic X-radiation from the material itself). Your beamline will have multiple sets of slits. The first slits in the beamline will define the beam coming from the source. Recall from Section 2 that different energies come off a bending magnet with different divergence angles. Here is a great application for slits. Adjust the slit width to match the opening angle for the radiation of the energy of interest and reject all of the rays and power that is of no use to your experiment. It is much more economical to have cheap slits manage your power load than to have expensive and sensitive monochromators or mirrors do it! Another critical use of slits is to 'guard' the beam. This refers to the practice of setting up a series of slits, the same size as the beam, all along the beam to absorb any parasitic scatter and pass just the 'clean' original beam on to the sample. Finally, slits can shape a beam to meet your needs. For example, if the full beam in your experimental station is 2 mm x 10 mm but your sample is 1 mm x 1 mm, all that beam missing your experiment creates a useless background signal for your sensitive and expensive detectors. Insert slits as far upstream of the sample as practical to reduce the beam size to a better match with your sample size.

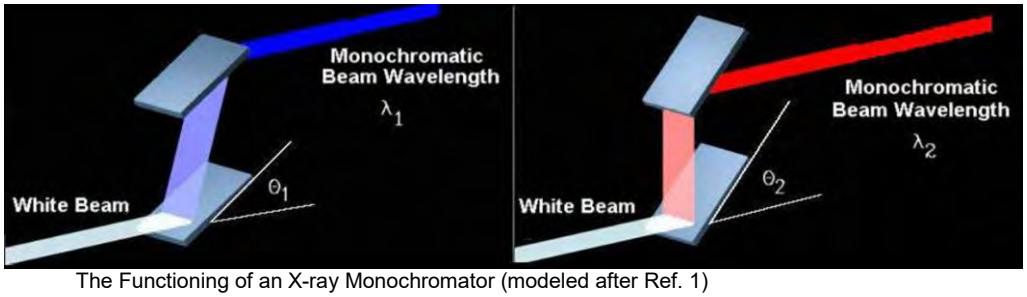
Slits are also critical for matching the beam divergence and the beam size after the sample as it travels to the detector. They help you to detect very weak signals by cleaning up the background scatter. Slits are also one of your simple beamline intensity controls. Too much intensity? Toss some of it away by closing slits.

# Monochromator Systems: choosing a wavelength

## *Wavelength Selection*

A monochromator selects one wavelength or 'color' from the broad 'white spectrum' of radiation that comes from a synchrotron source. Although a prism is a decent analogy for the concept of splitting the white radiation into components, the monochromator crystal acts more like a selector; it diffracts only the radiation with wavelength that satisfies Bragg's Law shown in the first important monochromator equation below. For a crystal (typically silicon, germanium or diamond at synchrotrons) with a given interplanar spacing, *d*, the incident or Bragg angle determines the diffracted wavelength. Using the visible light analogy again, the first monochromator in the illustration below at angle $\theta_1$ passes wavelength $\lambda_1$ (blue) and the second illustration with crystals at angle $\theta_2 > \theta_1$ passes longer wavelength (lower energy, red) radiation $\lambda_2 > \lambda_1$. Crystallographers tend to think in terms of X-ray wavelength and beamline scientists tend to think in terms of X-ray energy. The units are interchangeable. Conversion from wavelength to energy is done with the second important monochromator equation below. You will need to memorize the conversion.

It is important to note the integer, *n*, in Bragg's law, which tells you that, for any given monochromator angle setting, higher order harmonics are also passed. Your beam can consist not only of the *n* =1




The Functioning of an X-ray Monochromator (modeled after Ref. 1)

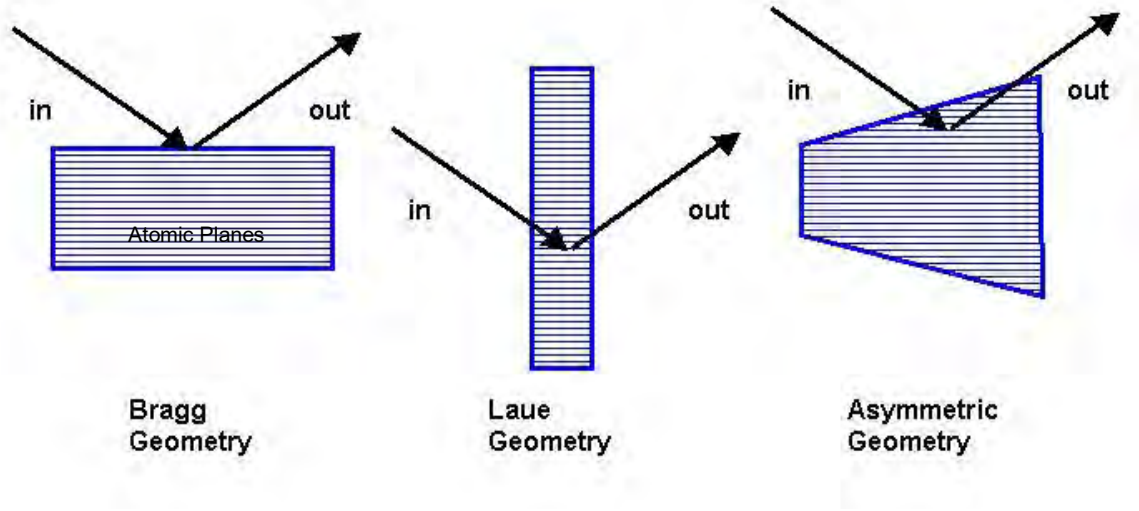
fundamental wavelength but also of discrete harmonics. It is not necessarily a perfectly pure single energy (wavelength) passed down the beamline by a monochromator.

You can think of X-rays as diffracting off the atomic planes in the monochromator crystal and you know that X-rays penetrate matter but, believe it or not, it is important to keep track of where the X-rays enter and leave the crystal's surface. I'll leave the nuances of why this is important for textbooks. Suffice it to say, the distinctions are so important that there are special names for the different cases as shown in the next illustration.

**Important Monochromator Equations:**

| | |
|---|---|
| $n\lambda[Å] = 2d_{hkl}[Å]\sin\theta_B$ | ⇐ Bragg's Law: tells you what wavelength is passed at $\theta_B$ |
| $E[keV] = 12.39854/\lambda[Å]$ | ⇐ Conversion between X-ray energy and wavelength |
| $\Delta E/E = [2r_e d_{hkl}^2/\pi V_e](\lvert P\rvert F_H e^{-M})$ | ⇐ Tells you the energy bandpass of a monochromator crystal |
| $d_{hkl}[Å] = a_o[Å]/\sqrt{h^2+k^2+l^2}$ | ⇐For Cubic systems only, d-spacing for any (h,k,l) lattice plane |
| Allowed mono reflections | ⇐ (hkl) all odd or (hkl) all even and h+k+l=4n |

*(variables are fully defined in Section 17, p80, Useful Equations and Constants)*




In the soft X-ray and VUV (vacuum ultraviolet) regions, grating monochromators are used. Since the wavelengths in these regimes are longer than for hard X-rays, the equivalent of Bragg's law must be satisfied, not by crystals of a given *d* spacing, but by gratings with a manufactured line-spacing..

Bragg's law leads you to believe that there is one wavelength for each angle of incidence, but actually there is a narrow range of wavelengths that pass. This range of wavelengths (or energies) can be calculated with the ΔE/E equation in the important monochromator equation box above. Typical numbers for ΔE/E in the hard X-ray region with a silicon (111) crystal are approximately $10^{-4}$, which means that for a 10 keV X-ray coming from a monochromator, a 1 eV range of energies is coming from the monochromator. The d-spacing is the most easily accessible variable for playing with the bandpass. X-ray optics people typically increase this d-spacing to increase ΔE/E by creating artificial crystals called Layered Synthetic Multilayers. These LSMs are vacuum-deposited alternating layers of high-Z and low-Z materials (W/C, Mo/C, W/Si are typical examples), that create an artificially stratified material, i.e., an artificial d-spacing. Wide bandpasses (ΔE/E up to 0.1) and >80% reflectivities are created this way. In essence, if you are not picky about a narrow energy span, you can pass a lot more photons to the experiment in this way.

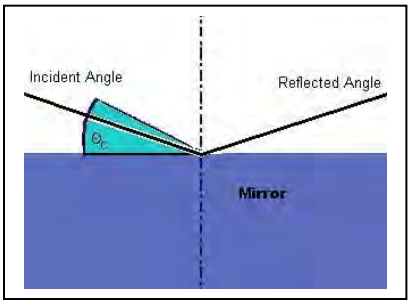
## *Focusing*

By bending monochromator crystals, so-called sagittal focusing, it is possible to re-direct a diverging or parallel beam of X-rays back into a converging spot. Asymmetrically cut crystals, bent Laue geometry crystals and bent Bragg geometry crystals all can be employed to focus X-rays. The principles are roughly the same, as will be demonstrated in the next section on mirror systems.

# Mirror Systems: X-ray bouncers

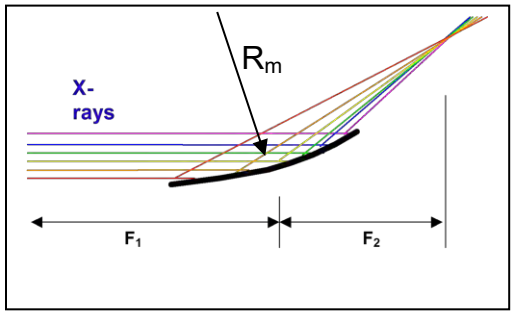
## *Reflectivity*

X-rays penetrate matter — a useful property isn't it? If you shine X-rays perpendicular to a mirror, they just go right through it without reflecting. The proper physics explanation for this is that the index of refraction for X-rays in solid materials is less than 1 by a small amount δ. The practical reality is that you can only reflect X-rays by skipping them off of a well polished surface at low angles, if that angle between the incident X-ray and the surface is less than a critical angle, $\theta_c$ as calculated by the first important mirror equation below. X-rays of a given wavelength impinging the surface at an angle greater than $\theta_c$ pass into the mirror surface and are transmitted or absorbed.




When we mentioned that the mirrors had to be well polished, we weren't kidding. Mirrors have two major classes of defects that impair their reflectivity: figure, measured by slope errors, and finish, measured as roughness. Today's state-of-the-art can produce mirrors up to 1 meter in length with slope errors of 2-5 microradians rms and roughness of 1Å! Most modern mirrors are made of single crystal Si, LTE Glass (Zerodur), Glidcop, SiC, or precipitation hardened stainless steel (PH-SS) although any finely polishable material is acceptable.

## *Focusing*[ix]




*Flat mirrors* can reflect X-rays at a shallow angle, a few milliradians depending on the mirror material. The first equation also tells you that, if you skip an X-ray beam with a wide range of wavelengths off of a mirror at some angle, only those with wavelengths $\theta_c > \theta$ will pass. The mirror acts like an energy low-pass (wavelength high-pass) filter. You can bend a flat mirror as shown to the right to focus a diverging or parallel beam. The second important mirror equation tells you the bending radius needed to focus incoming rays from distance $F_1$ to a location $F_2$ away. It is customary to use the term *bent flat mirror* to refer to meridional focusing in the vertical direction. The term *cylindrical mirror* is traditionally used to refer to a mirror not usually bent, but rather concave-figured in the other direction to horizontally focus the beam. Bending a cylindrical mirror along the long axis produces a *toroidal mirror* that focuses in both directions. Finally, the special case where you have two flat mirrors, one reflecting vertically, the next reflecting horizontally and both independently bendable is called a *Kirkpatrick–Baez (K-B) pair*.

**Important Mirror Equations:**

$\theta_c[°] = 1.6\ \lambda[Å]\ \sqrt{\rho}\ [g/cm^3]$ ⇐ Critical angle for mirror reflection of X-rays

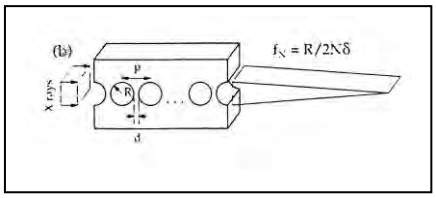
$R_m[m] = (2/\sin\theta)[F_1F_2 / (F_1 + F_2)]$ ⇐ Bending radius for meridional focus

$R_s[m] = R_m \sin^2\theta$ ⇐ Bending radius for sagittal focusing

$M = F_2/F_1$ ⇐ Magnification (demagnification) factor definition

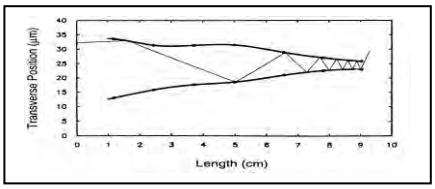
# Other Focusing Optics: special methods for making small spots

## *Compound Refractive Lenses*



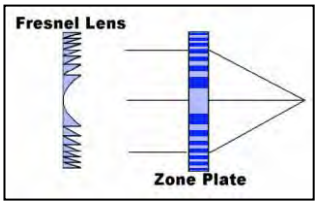

Compound Refractive Lenses (CRL's or Snigirev[x] Lenses) can focus X-rays. We discussed in the last section that X-rays have an index of refraction <1 by a small amount δ. You can make the analogy with light, if you do it backwards from your intuitive feel. For example, light traveling through vacuum or air that comes upon a standard double-convex glass lens, (), is refracted and focused. Flipping this around for X-rays, if an X-ray traveling through glass comes upon a lens-shaped pocket of vacuum or air, it is bent and focused in the same manner. Vacuum or gasses can be thought of as 'more optically dense' than solid matter for X-rays! The focusing effect for X-rays is small, because the index of refraction is almost unity but, for small parallel beams traveling many tens of meters in a typical modern beamline, the focusing effect is useful.

## *Capillaries*



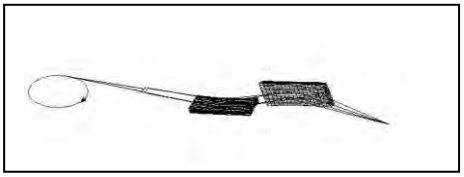

Just as X-rays can be 'skipped' off the surface of a mirror, they can also be transmitted down a hollow glass tube[xi]. The trick is to bring the X-rays in at a shallow enough angle to allow for complete reflection and to taper the tube from a wide entrance end to a narrow exit end. In this way, X-rays can be 'concentrated', that is, made to have a smaller spot size at the tube exit (at the expense of having a larger divergence at the exit.). You can make a large and precise 'lens' of hundreds of these capillary tubes collecting a large solid angle from a laboratory X-ray source and concentrating them to a small focal spot size. Devices of this type are usually called Kumokhov Lenses after the originator.

## *Fresnel Zone Plates*




Just as for visible light optics, focusing can be done with a Fresnel lens, which is just a folded parabolic optic. For X-rays, we make the binary equivalent of this lens and call it a *zone plate*. Using either absorption or phase retardation techniques, the zone plate focuses X-rays at very high demagnification ratios.

## *Kirkpatrick-Baez Mirrors*

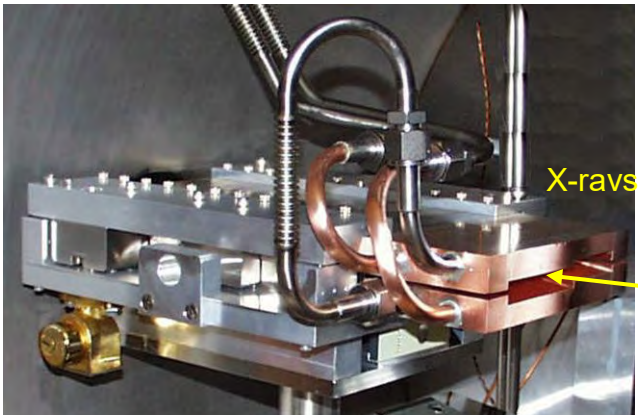


Recall that at the end of Section 6, we mentioned K-B mirrors? These devices are so elegantly simple, separating the vertical and horizontal focusing functions onto two separate flat mirrors, that they can be used in the experimental end-station to greatly de-magnify X-ray beams, producing micro spot sizes.

# Beam Stops: 'last resort' stop for runaway radiation

Modern synchrotrons produce X-rays up to the energy of the synchrotron ring itself through a process called *bremsstrahlung* radiation. For the newest generation of hard X-ray synchrotrons this means that there are 6 to 8 *GeV* ($10^9$ eV) X-rays in the direct beam to stop. As you can imagine, the absorbers designed for this duty are high Z and thick. At the Advanced Photon Source (APS), 300 mm of lead or 180 mm of tungsten are required to stop this 7 GeV radiation.

Again, the exact name that you call these 'last resort' beam blockers depends on where you work. At some facilities, they are called 'stops', at others 'safety bricks' and at yet others 'Bremsstrahlung shielding blocks.' The purpose is the same, however, to stop every last X-ray photon before it penetrates through the line, the shielded station and into personnel. The photo to the right shows a beamstop used at the APS Sector 14 undulator line. The stop is made-up of a tapered four-inch thick water-cooled copper absorber, to stop synchrotron radiation, followed by twelve inches of tungsten, to stop bremsstrahlung radiation. Any radiation passing through optical components upstream of this device is stopped here.



Beamstop

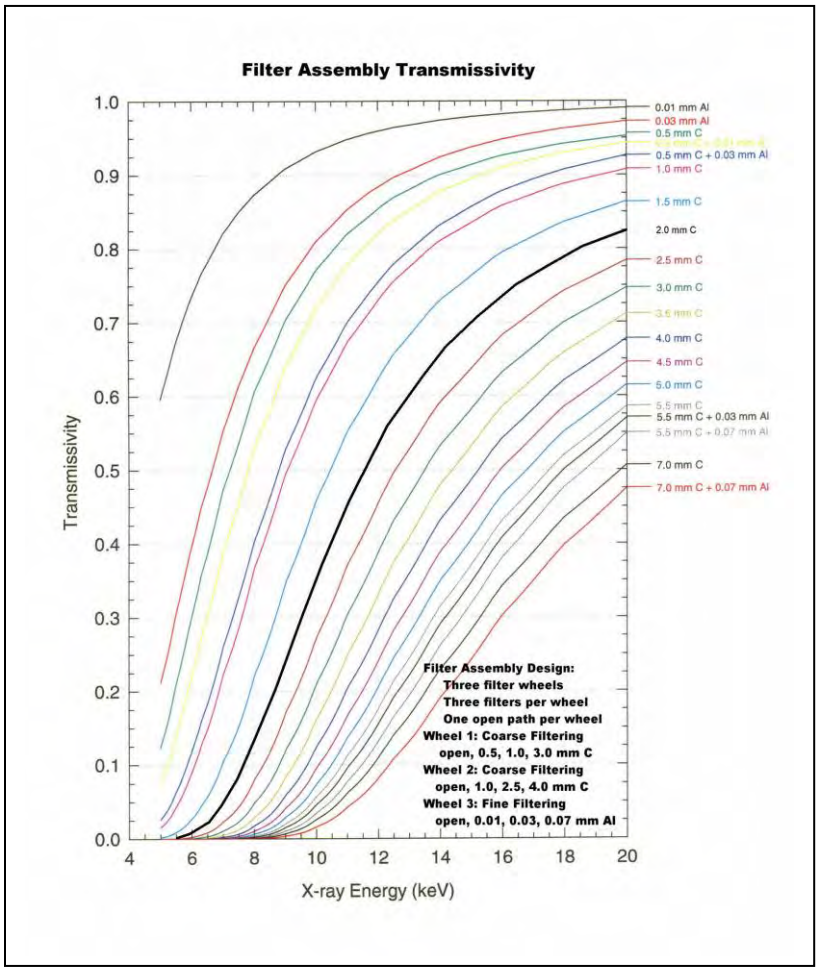
This device is designed to stop all of the direct on-orbit white radiation. You may be thinking "this is good, except that my experiment is now also 'safe' from any of that same radiation needed to do an experiment!" Fortunately, it is a simple task to select out only the radiation of interest using mirrors and monochromators, and to physically offset the useful beams from the direct on-orbit beam. Thus Bremsstrahlung radiation and undesired synchrotron radiation can hit the beam stop, while the useful radiation jogs around the stop on its way to the experimental station.

In the experimental station, you may also find devices on the downstream wall called 'stops' or 'safety bricks'. These serve a similar purpose. Any radiation that the station is capable of receiving can be fully stopped before penetrating the walls of the station, in the unlikely event of a run-away beam.

# Filter Systems: adjusting beam intensity and harmonics

When synchrotron users ask to modify the beam intensity for their experiment, this author's favorite saying is, "Less beam intensity is easy, down to zero… but if you want *more* beam, now that's difficult." One of the tricks for modifying beam intensity without using slits or complex optical elements is to use filters. As we discussed in the important equations of section 3, any given radiation wavelength can be reduced to intensity $I$, of the incident intensity $I_o$, by choosing a filter of the right thickness and density. Sheets of aluminum, aluminum foil, carbon, copper, etc. are commonly found at beamlines to perform this task.

Filters can also be used to: 1) absorb low energy photons and thus pull out power from the white beam to reduce the heat load on downstream optical components such as Be windows, monochromators and mirrors, 2) selectively filter higher harmonic radiation by taking advantage of the fact that there are 'step increases' in the absorption properties of all materials at their absorption edges, 3) preferentially absorb the softer, lower energy radiation and effectively 'harden the beam' enhancing the throughput of higher harmonics.




At left, you will find the results of an exercise of building a three-wheel filter system that would give fine control of beam attenuation over a large energy range. The results show how beam intensity can be reduced to practically any desired value if you have enough combinations of materials and material thickness. (This example only used carbon and aluminum as filter materials to avoid 'step' increases in attenuation in the 5 to 20 keV energy range.)

# Diagnostic Tools: how to see and measure the beam

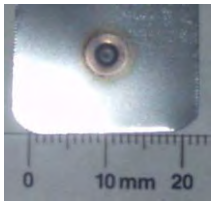
## *Imaging*

*Fluorescent Screens:* There are numerous compounds that will fluoresce in visible wavelengths when struck with hard X-rays. The oldest is zinc sulfide, a yellow powdery substance that when affixed to a backing material, can be inserted into the beam to visualize it. In the same family, cadmium sulfide (Zn,Cd)S:Ag also works well. The new workhorse for fluorescent screens is terbium-doped gadolinium oxysulfate ($GdO_2S:Tb^{3+}$), which has much higher efficiency and light output than ZnS. Single crystals of cadmium tungstate ($CdWO_4$) have also been used for years to image X-rays.

*Instant Reading Papers and Films:* There are many times when you want to have a quick permanent beam image to measure, insert into your log book or to examine under magnification. 'Burn papers' and instant developing films fill this role. Kodak makes pink and Sessions-of-York (England) makes green, self-developing or direct print papers. When exposed to X-rays, the paper color changes in proportion to the X-ray intensity passing through it without need for any development chemicals. Photographic film makes a high spatial resolution and dynamic range X-ray detector. Beamlines have used POLAROID® Type 57 and 53 instant developing sheet film packs for years. This method requires that you expose the film to radiation either with or without a fluorescent image enhancement screen, process the film like in the POLAROID® film cameras of the 1970's and, thirty seconds later, open the film pack with the image of your beam.

A "Green Paper" Burn

Beam Burn in Glass




Beam Burn on Stainless

For very intense beams such as broad spectrum (pink beam) or full spectrum (white beam), use standard glass microscope slides or pieces of stainless steel shim stock to image the beam. Strong beams cause color centers in the glass slides, making the glass brown. The power from strong beams causes local heating and temper coloring (right) of the poor thermally conducting stainless steel to produce an image.

## *Power Measurement*

The easiest way to measure beam power is with a Cu block bolometer (also called a calorimeter). Essentially, you absorb all photons in a well-insulated block of metal, usually copper, of known mass, turning them into heat and measure the rate of temperature rise. If the $\Delta T$ is small, a few tens of degrees C, the heat capacity of the copper can be considered a constant so the power, P (Watts) is equal to a constant x $\Delta T$ (°) / $\Delta t$(sec). The constant is exactly known from the heat capacity and mass of the bolometer block.

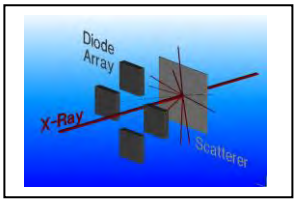
## *Photon Flux Measurement*

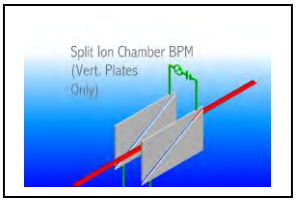
Ion Chambers (right) and PIN diodes are the most economical and simplest way to qualitatively and quantitatively measure photon flux without energy discrimination. For energy resolved measurements, invest in more expensive Ge, Si(Li) or diode (Amptek™) detectors.

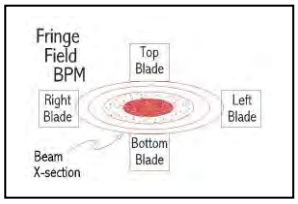
An Ion Chamber

## *Beam Position Measurement*

To measure a beam's position without blocking it (as a fluorescent screen does) requires a beam position monitor (BPM) sensitive to beam motion in two dimensions. Diode arrays, split ion chambers or fringe-beam blades are commonly used to provide beam positions. Each works in a different way, taking a small bit of the beam to determine its location in space. Diode arrays typically look at the small amount of radiation scattered from a thin filter. Four diodes, positioned in a plane 90° from each other and perpendicular to the beam, measure and then compare the intensity of that scattered radiation at each diode location. Split ion chambers work similarly. Four split ion chamber plates, again oriented 90° from each other, measure the difference in ion current as the X-ray beam passes through a gas in the BPM chamber. The more current a given plate sees, the closer the beam is to that plate. A measurement of the individual plate currents allows you to triangulate the beam position to a few micrometers. Fringe-beam detectors actually touch the very edges, the fringe field (i.e., the left, top, right and bottom) of the beam. As the beam hits the metal blade, photoelectrons are ejected and a current is created. The more beam that an individual blade intercepts, the higher the current in that blade. Usually, the extremes of the beam will chopped out of the final beam with slits, so impact on final intensity is minimal.

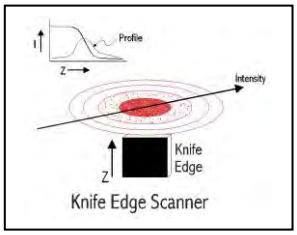


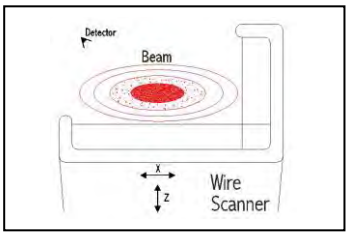



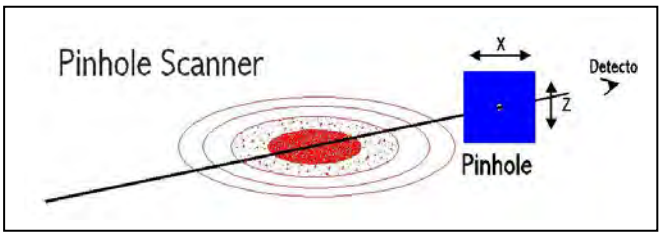




## Beam Size Measurements

For an accurate measurement of the beam's size, shape and intensity, you must pass something through the beam itself. Knife-edge scanners, wire scanners and pinhole scanners are the traditional workhorses. Knife-edge scanners are the simplest. Since your beamline already has slit systems in it, the trick is to just pass one blade of the slit, either horizontally or vertically, through the beam and measure the transmitted intensity as a function of slit position. The measurement is just an integrated intensity through the beam. A first derivative fit to that intensity profile is the beam profile. Wire scanners are more straightforward. In this method, a fine metal wire is mechanically scanned through the beam. By watching the wire fluorescence or photocurrent, you have a direct measurement of the beam intensity at any cut through the beam. Pinhole scanners provide the most intuitively simple method of beam profiling. Here, you mechanically raster scan in 2D a pinhole through the beam and measure the transmitted intensity. Just as in a television, you create a pixel-by-pixel map of the beam shape and intensity convoluted with the pinhole size.



# Transport & Shielding: containing the radiation

Modern synchrotron X-ray sources are situated remotely from the samples under study, as much as one kilometer away in the case of three Spring-8 beamlines! As powerful as these sources are, it would be a shame to waste all those expensive photons by having them absorbed in the air and turned into heat and ionized gases; air is an absorber just like any of the filters discussed in Section 9.

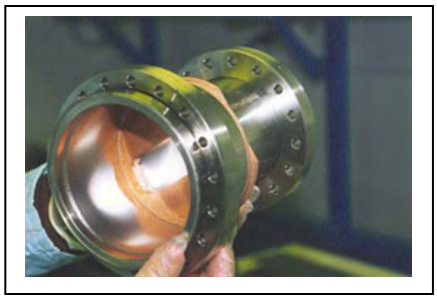
The least expensive way to save these photons is by creating tubes of helium or vacuum to minimize parasitic air scatter and absorption. For quick transport of monochromatic radiation inside of a shielded station, you will typically see PVC pipe with aluminum or kapton end-covers, filled with helium as a beam transport. Some scientists get pretty fancy with their 'sewer pipe' transport lines, adding segments with O-ring seals for length adjustability, beryllium end-windows and fancy flow gauges or fittings. Some scientists only care about function and wrap a tube with lead tape, stick a hose in the end, rubber band a plastic bag on and go. Heck, many times I've put He filled plastic trash bags around my experiments to lower background scatter and argon fluorescence! The X-rays just don't care. As long as they see low atomic number, they don't scatter.

For high intensity, polychromatic or white radiation or for transport outside of shielded stations, the transport itself will need to be shielded and most likely, vacuum. The most basic method for making this beam-pipe involves a long, usually stainless steel, vacuum pipe, covered with an appropriate thickness of lead. Some designers wrap it in one thick lead sheet, some wrap multiple thin layers of lead sheet, some build lead brick tunnels, some fabricate fancy and exotic lead housings —
I've even seen concentric pipes filled with lead shot used. The basics remain the same: an evacuated tube to protect the beam from scatter covered with thick enough lead to stop whatever beam *is* scattered by the remaining gasses in the vacuum or accidental venting of the pipe.


UHV Beam Transport

Because these pipes are lead-wrapped, they become very heavy and proper design of the supporting pillars as well as proper design of the joint shielding is critical. On top of all of that, in order to reach ultra-high vacuum ($10^{-9}$ torr or better) the pipes must be 'baked' at 100°C or higher temperature, complicating the shielding design. This is a commonly needed piece of beamline hardware, however, and numerous commercial vendors, including Advanced Design Consulting, Inc., have experience with construction of beam transports.

# X-ray Windows and Vacuum Systems: beamline support



A Beryllium Window

At some point, your beamline may end in a room containing the experiment. Perhaps your equipment is configured so that you must devise a way to separate sections of the beamline that are at different vacuum levels, or even vacuum from helium sections. Either way, an X-ray window is the right component for the job. For photons above 6 keV in energy, beryllium is a strong, stiff metal that is virtually transparent to X-rays. A thin, 250 micron foil brazed to a cooled copper holder is capable of holding back the one atmosphere pressure and will allow the beam to exit your vacuum or He beamline and impinge on your sample situated in another environmental chamber or at the center of a goniometer.

Beamlines are usually under vacuum for two main reasons. First, as we discussed in the last section, air absorbs X-rays and causes undesirable and unusable background scatter. By evacuating the air, you remove both of these problems. Realize, however, that vacuum is just very 'thin air'. The difference in photon transmission down a beamline with $10^{-3}$ torr vacuum (rough vacuum) and $10^{-9}$ torr (ultra high vacuum) are negligible. If 1 Einstein ($\equiv 6.02252 \times 10^{23}$ photons) of 12 keV ($\sim$ 1 Å wavelength) photons are sent down 50 meters of beamline at $10^{-3}$ torr, $6.0225189 \times 10^{23}$ photons still come out the other end. At $10^{-9}$ torr, you may get most of that two-parts-in-$10^{7}$ of the beam back, even though you have probably paid a factor of 10X or more for the better vacuum. (Just for comparison, if the beamline were filled with helium, losses would be more like 14% of the incoming photons.) The reason beamlines strive for the best attainable vacuum have to do with a second reason: when intense beams pass near optical elements, even in vacuum, the X-rays 'crack' or disassociate any hydrocarbon molecules remaining in the vacuum and deposit a thin carbon layer on all surfaces. Recall that in Section 6.1, the high quality needed for X-ray mirrors was discussed. Poor vacuum still contains many residual hydrocarbons that crack and turn into a carbon layer deposited on expensive mirror surfaces, increasing the absorption and effective roughness and degrading the ultimate focusing properties of the mirror. The longer the beam is on, the heavier the carbon deposit becomes.

*"Unlike the case for wines and cheeses,*
*nature does not improve the quality of*
*X-ray mirrors with time."*

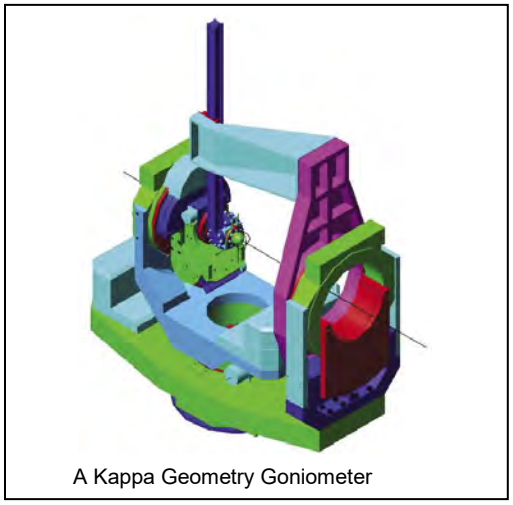
If your beamline does not require the ultimate in focal spot size nor the maximum obtainable flux, by all means don't suffer the expense and complexity of an ultra high vacuum beamline. Many excellent scientific experiments have been done with helium-filled beamlines and a little extra time.

If your experiment does require the best vacuum technology available (and some do) then an entire 'windowless' beamline can be constructed by connecting a UHV end chamber through a UHV beamline directly to synchrotron vacuum. Distributed differential pumping and on-line mass spectrometry is then used to monitor and maintain these ultra-clean conditions.

# End-station Equipment: manipulating your samples

## Goniometers

Very few experiments require that your sample sit statically, at atmospheric pressure and temperature in the beamline end-station for analysis. Most often, you will need to move your sample in 3D and/or subject it to various environments to get the information you need. Additionally, you will need to simultaneously and independently move your detector around. We use mechanical devices called goniostats, diffractometers, goniometers, and spectrometers to move the sample in 3D allowing it to come into various diffraction conditions. We tend to swing the sample around, only because moving the radiation source in a synchrotron is very difficult. These sample-manipulation devices come in all sizes and configurations. The two most basic goniometer orientations are Eulerian and Kappa geometry. Eulerian geometry goniometers have multiple circles, usually φ, ω and θ situated at right angles from each other. The detector independently rides on a 2θ arm with its own adjustment angles. The entire device sits on X, Y, Z motion platforms. The Kappa geometry goniometer, shown in the illustration above, has non-orthogonal φ, κ and Ω axes. Both types can situate your sample in any 3D orientation. The spectrometer, at lower right, is designed to manipulate a sample in θ, X, Y, Z angles while precisely moving a detector on the long 2θ arm.



A Kappa Geometry Goniometer

## Motion translation systems

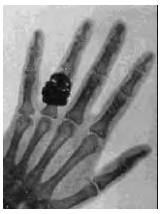
One doesn't need every type of rotation and translation for every experiment; just invest in the motions that are required. Many stations just rely on a single or a few rotation motions riding on numerous translation stages. Routine beamline hardware is readily available, and numerous commercial vendors, including Advanced Design Consulting, Inc., provide translation and rotation solutions for any combination of required motions.

A 3 m Diameter Spectrometer

## Sample environment chambers

There are many sample environments available at X-ray facilities. Ultra high vacuum, ultra high pressure, ultra hot, cryogenic, high magnetic field, liquid, corrosive, ultra fast laser pulsed, etc. The great advantage to using X-rays is that they can probe the structure of matter in all of these conditions with relative ease.

# Detectors: systems for gathering data



Mrs. Roentgen's Hand 1896

Section 10.3 discusses simple detectors for measuring intensity. The oldest method for detecting X-rays, the one that lead to the *discovery* of X-rays by Roentgen, was the use of photographic film. X-rays passing through the silver halide emulsion of the film ionized the silver. Developing the film fixed the silver into a photographic image of the beam's passing. The detection channel here is ionization and detection of that ionized element. As technology progressed, reliable photon counting methods with Geiger-Müller gas filled proportional counters ("Geiger counters" for short) and ion chambers were developed. There have been improvements in, and modifications to, these techniques over the years, but the general method for X-ray detection remained at this level through the 1970's. For example, the Geiger counter is simply a positively charged wire in a gas-filled tube. X-rays entering the tube ionize the gas, the electron is swept to the (+) charged wire and the ion is swept to the (-) charged cylinder wall, creating a measurable electrical current. Again, the detection method is based on the fact that X-rays ionize materials. If one takes many, many wires and arranges them in a grid pattern, you have a multi-wire detector that can produce 2D images of the X-ray distribution. If you make the (+) and (-) electrodes into two parallel plates, you have an ion chamber.

Storage Phosphor

2x2 CCD

Somewhere early in the development of the field, it was noticed that X-rays will visibly fluoresce certain minerals. A detection method in which X-rays are absorbed and visible light is emitted was created. X-rays still ionize the mineral; however, the cascade to re-fill the empty electron shell generates visible light. This detection channel is used in scintillation counters. Materials like sodium iodide crystals are connected to photomultiplier tubes. An X-ray photon hits the NaI, creates a photon which strikes a charged metal plate. That photon creates a cascade of electrons in the photomultiplier tube and is detected as a current proportional to the energy of the original photon. Later, photographic companies like Kodak and Fuji developed storage phosphors. When struck by X-rays, these materials 'store' energy and, at a later time, are read out by stimulating the release of that stored photon by a small laser. Today, a variation of this X-ray-to-light process is the most popular method for area detection of X-ray patterns. Photons strike a thin phosphor screen, the light is carried to a solid state CCD camera chip and turned, pixel by pixel, into an image of the beam.

A Ge Detector

Today with silicon solid state technology, direct X-ray photon detection is undergoing rapid development. Basically, an X-ray striking a Si-diode or a Ge or Si(Li) detector directly creates electron-hole pairs. These pairs are swept away under the influence of electric potentials and create a measurable current. Sound familiar? This is once again an ionization detection process. The next generation of detectors, so called pixel array detectors, relies on this technology with micron size diode to directly create 2D images.

## Computing: controlling the beamline, the experiment and your data

Since modern synchrotron beamlines carry lethal doses of X-rays to the experiment, all optics and specimen motions must be done under remote control inside of locked, shielded stations. This usually means use of computerized stepper motor-controlled motions for whatever needs manipulation, although some of us have been known to run ropes, tubes and an occasional extension cord through the station labyrinth in order to control some aspect of the experiment. A few beamlines have experimented with DC servo motor controls but the vast majority of facilities use stepper motors.

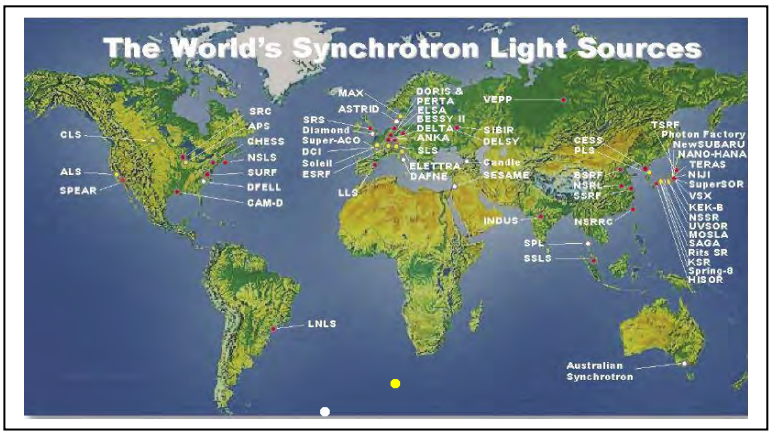
Remote manipulation is a problem encountered on every beamline, so there are software packages and hardware controllers available to help you to interface your motion automation with your computers. Before the 1980's, most experimental control software was written by individual laboratory personnel to solve a particular experimental problem. Since the explosion of computing resources in the 1990's, experimental control is becoming more user-friendly and standardized, but there are still many software/hardware/computer combinations from which to choose.

In the US, the newest and most common beamline control software packages are: *Spec* commercialized by Gerry Swislow, *MX* pioneered by Bill Lavender, *Blu-ICE* originated by Tim McPhillips, *EPICS* (Experimental Physics and Industrial Control System) an international collaboration and *MatLab* a commercial control system product. Search the web for these package keywords for more information. The combinations of motions, controls, computers, operating systems, software, hardware and warm-ware are ever-changing. We advise you to check the beamline documentation and personnel for help. You are going to need a computer specialist if you want to tackle this area of experimental control.

Data formats: there are no standards to date. There is a standard data format used by imaging sciences for complex collections of data called Hierarchical Data Format (HDF) created by the National Center for Supercomputing Applications, but it has not been adopted by the synchrotron community. Each control and data collection program's output is in its unique format and we typically run conversion programs to re-format the file for input into the unique form required for each analysis program.

# Uses of Synchrotron Radiation

X-rays have substantially contributed to every field of scientific and engineering endeavor over the past 105 years: from macroscopic examination of welds on the Space Shuttle, to medical diagnostics, to structures of proteins and bonding of chemical compounds, to studies of the nuclear states of atoms. Every industry, government and university laboratory has X-ray facilities available. Their astounding usefulness is evident in the hard X-ray, soft X-ray and vacuum ultraviolet synchrotrons that have been built all around the world as shown below. A lot has been discovered with X-rays and exciting new research is forthcoming every day. Now that you have a taste for the basics of synchrotron radiation, see whether you can apply it to your own area of interest.



# Useful Equations and Constants

## General X-Ray Formulas

Wavelength and photon energy relationship:

$$\hbar\omega \cdot \lambda = hc = 1239.842 eV \cdot nm$$

Number of photons required for 1 joule of energy:

$$1 \text{ joule} \Rightarrow 5.034 \times 10^{15} \lambda \text{ [nm] photons.}$$

## X-Ray Scattering and Absorption

Thomson cross section for a free electron:

$$\sigma_e = \frac{8\pi}{3} r_e^2 \qquad r_e = \frac{e^2}{4\pi\varepsilon_0 mc^2} = 2.82 \times 10^{-13} cm$$

and $r_e$ is the classical electron radius.

Scattering cross section for a bound electron:

$$\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma\omega)^4}$$

Rayleigh cross section $(\omega^2 \langle\langle \omega_s^2)$:

$$\sigma_R = \frac{8\pi}{3} r_e^2 \left(\frac{\omega}{\omega_s}\right)^4 = \frac{8\pi}{3} r_e^2 \left(\frac{\lambda_s}{\lambda}\right)^4$$

Scattering by a multi-electron atom:

$$\frac{d\sigma(\omega)}{d\Omega} = r_e^2 |f|^2 \sin^2\Theta \qquad \sigma(\omega) = \frac{8\pi}{3} |f|^2 r_e^2$$

where the complex atomic scattering factor represents the electric field scattered by an atom, normalized to that of a single electron:

$$f(\Delta\vec{k}, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\Delta\vec{k}\cdot\Delta\vec{r}_s}}{(\omega^2 - \omega_s^2 + i\gamma\omega)}$$

For forward scattering or long wavelength this reduces to:

$$f^0(w) = \sum_{s=1}^{Z} \frac{\omega^2}{(\omega^2 - \omega_s^2 + i\gamma\omega)} = f_1^0 - i f_2^0$$

Refractive index for x-ray radiation is commonly written as*:

$$n(\omega) = 1 - \delta + i\beta = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left(f_1^0 - i f_2^0\right)$$

where

$$\delta = \frac{n_a r_e \lambda^2}{2\pi} f_1^0(\omega) \qquad \beta = \frac{n_a r_e \lambda^2}{2\pi} f_2^0(\omega)$$

Absorption length in a material:

$$l_{abs} = \frac{\lambda}{4\pi\beta} = \frac{1}{2 n_a r_e \lambda f_2^0(\omega)}$$

Mass-dependent absorption coefficient:

$$\mu = \frac{2 r_e \lambda}{A m_u} f_2^0(\omega)$$

Atomic absorption cross section:

$$\sigma_{abs} = 2 r_e \lambda f_2^0(\omega) = A m_u \mu(\omega)$$

Relative phase shift through a medium compared to a vacuum:

$$\Delta\phi = \left(\frac{2\pi\delta}{\lambda}\right)\Delta r$$

where $\Delta r$ is the thickness or propagation distance.

Snell's law:

$$\sin\phi' = \frac{\sin\phi}{n}$$

Critical angle for total external reflection of x-rays:

$$\theta_c = \sqrt{2\delta} = \sqrt{\frac{n_a r_e \lambda^2 f_1^0(\lambda)}{\pi}}$$

Brewster's angle (or polarizing angle):

$$\phi_B \cong \frac{\pi}{4} - \frac{\delta}{2}$$

## Multilayer Mirrors

Bragg's law:

$$m\lambda = 2d \sin\theta_b$$

Correction for refraction:

$$m\lambda = 2d\sin\theta\sqrt{1 - \frac{2\bar{\delta}}{\sin^2\theta}} = 2d\sin\theta\left(1 - \frac{4\bar{\delta}d^2}{m^2\lambda^2}\right) \text{ where}$$

$\bar{\delta}$ is the period-averaged real part of the refractive index.

$$\Gamma = \frac{\Delta t_H}{\Delta t_H + \Delta t_L} = \frac{\Delta t_H}{d}$$

| Unit Cell Length for Diamond-like monochromator materials: | |
|---|---|
| Material | $a_0$[Å] |
| Si | 5.4307 Å |
| Ge | 5.6580 Å |
| C (diamond) | 3.5597 Å |

| Allowed Reflections from Diamond Lattice Crystals: | | |
|---|---|---|
| If hkl mixed | $F_{hkl} = 0$ | |
| If hkl all odd | $F_{hkl} = \sqrt{32}$ | |
| If hkl all even: | h+k+l = 4n | $F_{hkl}$=8f |
| | h+k+l = 4n±2 | $F_{hkl}$=0 |

* The choice of $+i\beta$ is consistent with a wave description $E = E_0 exp[-i(\omega t - kr)]$. A choice of $-i\beta$ is consistent with $E = E_0 exp[i(\omega t - kr)]$.

**Note:** Values contained in square brackets [ ] denote appropriate unit for the connected variable

**Important Shutter, Slit and Absorber Equations: (Section3)**

Attenuation of X-ray intensity: $I = I_o e^{-(\mu/\rho)[cm^2/g]\rho[g/cm^3]t[cm]}$

General form - mass absorption coefficient: $\mu/\rho[cm^2/g] \propto Z^4\lambda^3$

Web source for tabulated μ/ρ and ρ data:
http://www-cxro.lbl.gov/optical_constants/pert_form.html

**Important Monochromator Equations: (Section 5)**

Bragg's Law: $n\lambda[\text{Å}] = 2d_{hkl}[\text{Å}]\sin\Theta_B$

Energy to Wavelength conversion: $E[keV] = \frac{12.39854}{\lambda[\text{Å}]}$

Interplanar Spacing for cubic materials: $d_{hkl}[\text{Å}] = \frac{a_o[\text{Å}]}{\sqrt{h^2+k^2=l^2}}$

General form for Monochromator Intrinsic Bandpass: $\frac{\Delta E}{E} = \left(\frac{2r_e d_{hkl}^2}{\pi V_c}\right)\cdot|P|F_H e^{-M}$

Simplified form for Intrinsic Bandpass - Si only: $\frac{\Delta E}{E} = 2.24\times10^{-7}F_H d_{hkl}^2$

General form for the Darwin Width: $\omega_D = \left(\frac{r_e\lambda^2}{\pi V_c}\right)\cdot\frac{F_H}{\sin(2\Theta_B)}$

Simplified form for the Darwin Width -Si only: $\omega_D = \frac{0.023F_H d_{hkl}^2}{\sqrt{\left(\frac{E[keV]d_{hkl}}{6.2}\right)^2 - 1}}$

| Approximate structure factors, $F_H$ for Si in the hard x-ray region: | |
|---|---|
| Reflection h,k,l | FH |
| 111 | 60 |
| 220 | 71 |
| 311 | 48 |
| 400 | 62 |

**Terms not previously defined:**
P = Lorentz Polarization Factor
$e^{-M}$ = Debye-Waller temperature factor
$F_H$ = crystal structure factor
$F_1$ = distance [m] from source to optic
$F_2$ = distance [m] from optic to focus
$V_C$ = volume of crystalline unit cell

**Important Mirror Equations: (Section 6)**

Critical angle for mirror reflection: $\Theta_C[^\circ] = 1.6\lambda[\text{Å}]\sqrt{\rho[g/cm^3]}$

Bend radius for meridional focusing: $R_m[m] = \left(\frac{2}{\sin\Theta}\right)\cdot\frac{F_1[m]F_2[m]}{(F_1[m]+F_2[m])}$

Bend radius for Sagittal focusing: $R_s[m] = R_m[m]\sin^2\Theta$

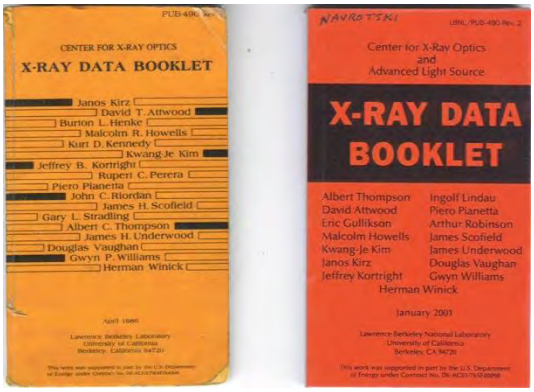
# Summary

There are as many variations to the basic concepts presented in this primer, as there are beamline scientists and engineers. Each area has specialists interested in detailed optimization of physical beamline components.

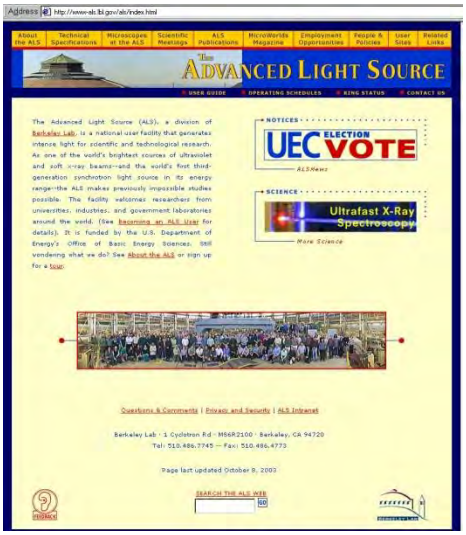
The next step in your education is to obtain a copy of *Lumière Synchrotron Light*i and interactively browse areas of interest to you. Look at the breadth of physical, chemical, biological, geological, engineering, materials, atomic, agricultural and archeological science being done with synchrotron radiation. Next, familiarize yourself with the expanse of technical information presented in the X-ray data bookletvi. This is a great starting point from which to leap into the detailed synchrotron literature record. Finally, talk to a specialist in your field. We've all been through the academic system at one time or another and there is a little bit of teacher in most of us that is happy to start you up the long learning curve.

# Resources: Where to get more information


• This interactive CD, *Lumière Synchrotron Light*[i] (in English and French), covers the spectrum of synchrotron radiation science and technology with wonderfully presented animations, illustrations and narration. The user can jump between historical, technical and scientific aspects of the field with ease. It is a great introductory resource for both the specialist and the non-scientific curious. http://synchrotron.imediasoft.fr/indexEN.htm




• These are the X-ray data booklets[vi] that any serious synchrotron user must have. The older 1986 Rev 1, sometimes called the 'Yellow Book' is to the left, and the newer 2001 Rev 2 is to the right. The book is also available in an on-line version at http://xdb.lbl.gov . Get one from your synchrotron User Office or from the Lawrence Berkeley Laboratory, Publication 490, through their on-line ordering system.




• Go to the web site for any synchrotron. A quick search there will provide you with links pointing to all other major synchrotron and X-ray information compilations. (The Advanced Light Source page, http://www-als.lbl.gov/als/index.html is the easiest for novices to navigate. Then go to the 'related links' tab at http://www-als.lbl.gov/als/worldwide.html for extensive reference information.)

# References:

[i] *Lumière Synchrotron Light*, http://www.springer.de/synchro, with a flash preview at http://synchrotron.imediasoft.fr/indexEN.htm
[ii] G. Margaritondo, Introduction to Synchrotron Radiation, Oxford (1988).
[iii] Handbook on Synchrotron Radiation, (Kotch, Sadaki and Winick, series eds.), North-Holland (1991).
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