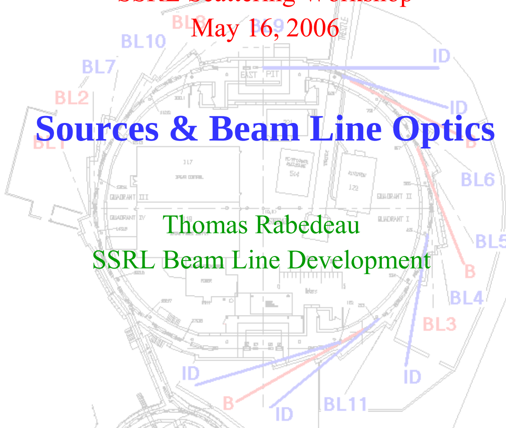
SSRL Scattering Workshop
May 16, 2006

Sources & Beam Line Optics



Thomas Rabedeau
SSRL Beam Line Development

Objective/Scope

Objective -

- *develop a better understanding of the capabilities and limitations of x-ray sources and optics to facilitate quality data collection at SSRL*

Scope –

- *relationship between the source characteristics and sample requirements*
- *x-ray mirrors*
- *crystal monochromators*
- *practical application on SSRL beam lines*

Source Characteristics & Sample Requirements
Two Sides of the Same Coin?

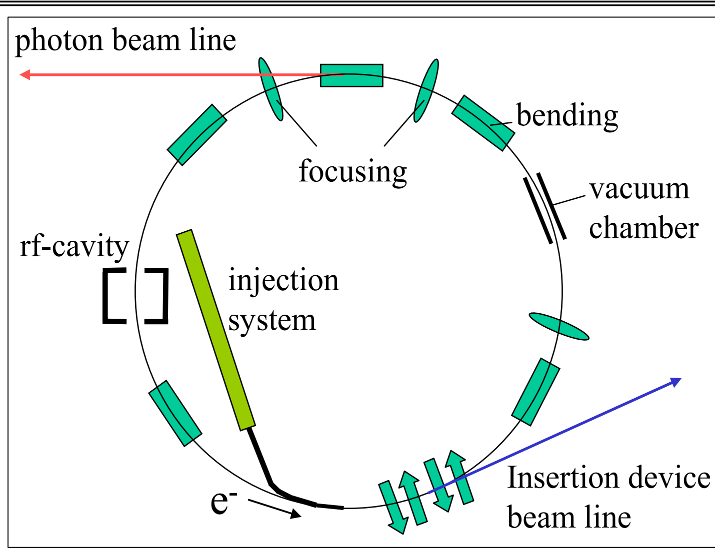
source (beam) characteristics:
- *size (x, y)*
- *angular divergence (x', y')*
- *energy content*
- *stability*
- *polarization*
- *time domain*
- *coherence*

sample (beam) requirements:
- *focus size (x, y)*
- *angular convergence (x', y')*
- *energy content*
- *stability*
- *polarization*
- *time domain*
- *coherence*

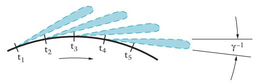
The job of x-ray optics is to transform the source beam characteristics to provide the best possible match to the sample requirements.

For most scattering experiments conducted at SSRL the first four characteristics listed are the central concern, so this talk with concentrate on how optics can manipulate these characteristics to best advantage.

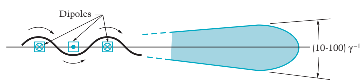
Generic Accelerator Components



Types of Sources



bending magnet - a “sweeping searchlight”



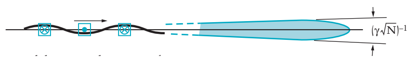
wiggler - incoherent superposition of radiation from an array of magnet poles

bend magnets & wigglers:

- continuous spectrum with so called “critical energy” …

ε_c(keV) = 0.665*B(T)E^2(GeV)

- intensity ~ N_{poles}
- broad horizontal fan



undulator - coherent interference of radiation from an array of magnet poles

undulator:

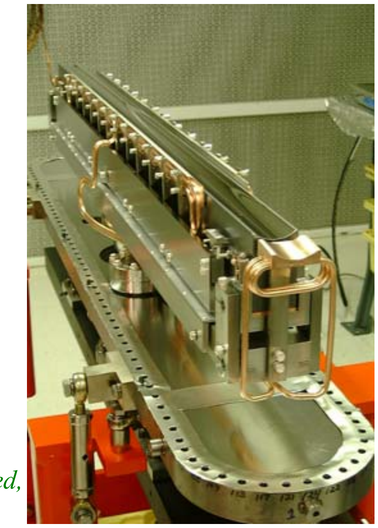
- quasi-monochromatic spectrum consisting of fundamental and higher harmonics
- intensity ~ $(N_{poles})^2$
- narrow horizontal emission cone

SSRL Source Characteristics
Current Generation of SSRL Scattering Facilities

- *source size*
  - *typical ID 430um x 30um rms (1010um x 70um fwhm)*
  - *bend 160um x 50um rms (380um x 120um fwhm)*
- *angular divergence (bends/wigglers not undulators)*
  - *horizontal divergence limited by slits to 1-3mrad typical*
  - *vertical divergence is energy dependent - typical x-ray divergence ~110urad rms (250urad fwhm)*
- *broad (white) energy content (bends/wigglers not undulators)*
- *stability - ~20um horz x ~5um vert (rms)*
- *polarization – dominantly horizontal*
- *time domain – fast pulsed (~250MHz)*
- *coherence – very slight*

X-ray Mirrors

above: BL11-1 1.0m Si flat, side-cooled M0 mirror



right: BL10-2 1.2m Si cylindrical, side-cooled, M0 mirror

X-ray Mirrors
Reflectivity at Grazing Angles

refractive index

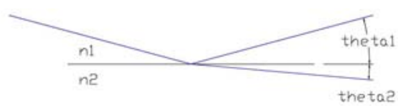
$n = 1 - r_0 \rho \lambda^2 / 2\pi - i\, \mu\lambda / 4\pi$

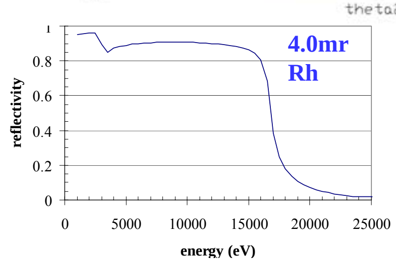
where

r_0 *is classical* e^- *radius (2.82e-13cm)*

ρ *is electron density*

μ *is linear absorption coefficient*



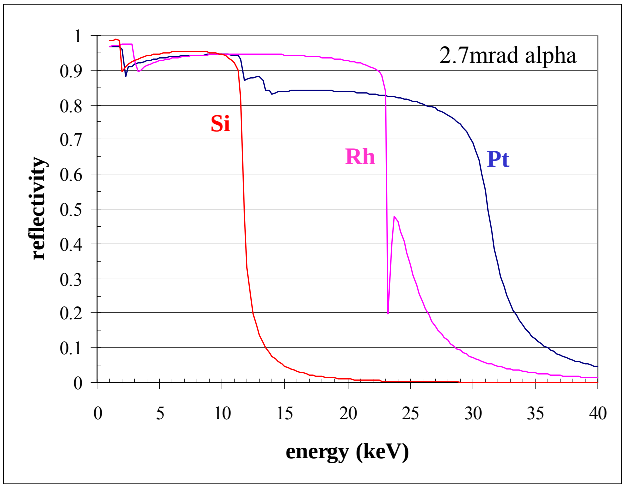


By Snell's law [$n_1 \cos(\theta_1) = n_2 \cos(\theta_2)$ with θ the grazing angle] in the absence of absorption, we find total external reflection for angles less than

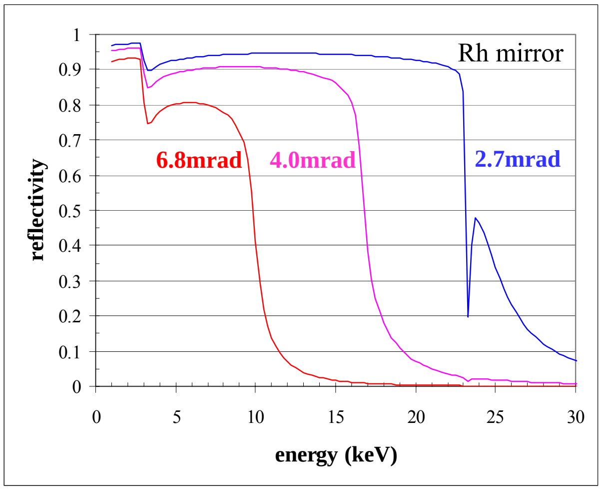
$\theta_c \approx \lambda(r_0 \rho / \pi)^{1/2}$

θ_c is typically a few mrad for x-ray mirrors. As a consequence x-ray mirrors tend to be quite long. For example, a 250urad fwhm beam intercepted at 15m by a mirror at 3mrad results in 1250mm beam footprint.

X-ray Mirrors
Reflectivity vs. Composition



X-ray Mirrors
Reflectivity vs. Angle



X-ray Mirrors
Figure

X-ray mirrors are either polished or bent to obtain desired figure.

- *elliptical figure provides point to point focusing*
- *parabolic figure collimates beam from source point or focuses parallel beam to a point*
- *focusing equations*

  $R_{tangential} = 2\ F_{in}\ F_{out}\ /\ (F_{in} + F_{out})\ \alpha$

  $R_{sagittal} = 2\ F_{in}\ F_{out}\ \alpha\ /\ (F_{in} + F_{out})$

Most x-ray BL mirrors at SSRL fall into two classes:

- *polished flats bent to approximate an ellipse or parabola to provide one dimensional beam shaping (eg., BL7-2 & BL11-3)*
- *polished cylinders bent into a toroidal figure to provide two dimensional beam shaping (eg., BL2-1)*

Typical radii of curvature:

- $R_{tangential} = 2\text{-}8\ km$
- $R_{sagittal} = 35\text{-}100\ mm$

X-ray Mirrors
Applications

- focusing
  - *condense beam to source dimensions on sample (1:1 focusing)*
  - *demagnify source image to better couple photons on small sample at the expense of greater angular convergence on sample (n:1 demagnification results in n-fold convergence)*
- collimation
  - *collimate divergent beam to improve energy resolution of crystal monochromator as discussed below*
- power filter
  - *absorb waste power at low power density on grazing incident optic rather than high power density on crystal monochromator*
- harmonic filter
  - *suppress higher energy contamination of beam (low pass filter)*

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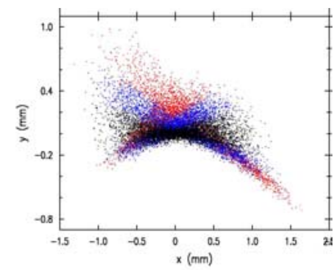
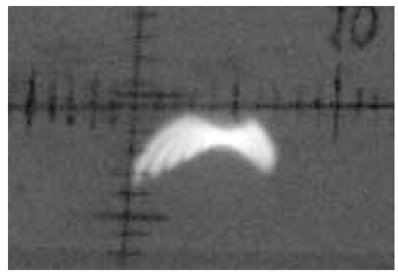
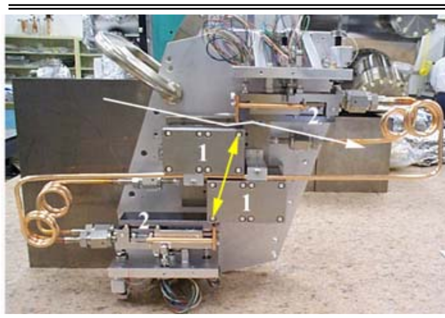
X-ray Mirrors Non-idealities

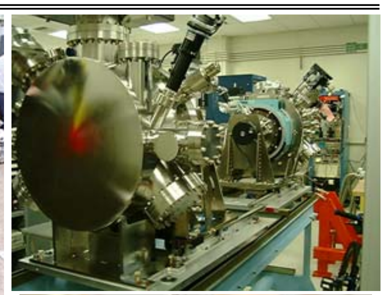
- grazing incidence optics introduce focus aberrations particularly when used to focus in horizontal and vertical planes simultaneously (function of accept.)
- toroidal mirrors located upstream of a crystal monochromator can significantly limit the energy resolution of the mono as discussed below
- mirror polish errors introduce focus blowup (eg., 2ur rms error on mirror 15m from focus broadens beam 60um rms)
- absorbed power can distort mirror surface resulting in focus degradation and time dependent focus changes
- beam stability crucially dependent upon mirror stability (eg., 1um differential motion at mirror ends can steer beam 20-30um at sample)



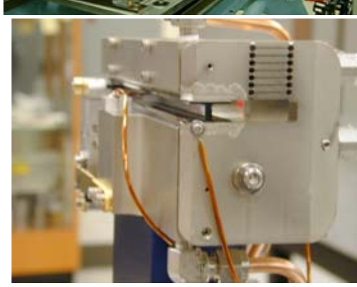


X-ray Crystal Monochromators





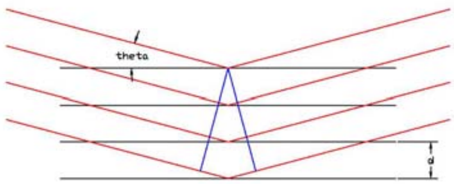
above left - LN mono crystal mount plate
above right - two LN monos awaiting installation



right: BL11-1 focusing mono crystal (BL11-3 similar)

X-ray Crystal Monochromators
Bragg Equation

- *diffraction from a crystal is obtained when radiation scattered from successive atomic planes adds constructively (ie., nλ path difference)*
- *Bragg Equation (real space)*
  $2d \sin \theta = n\lambda$
- *Bragg Equation (k space)*
  $(4\pi / \lambda) \sin \theta = q$ *where*
  $q = (2\pi / a_0)(h^2 + k^2 + l^2)^{1/2}$
  a_0 *is unit cell dimension &*
  h, k, l are reciprocal lattice vectors



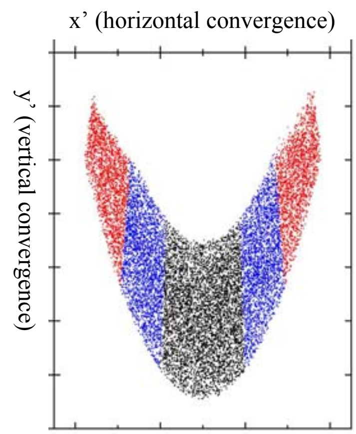
- *consequence of the Bragg equation … crystal monochromators pass not only the fundamental energy of interest but also allowed higher order harmonics, so harmonic rejection becomes important function of optics*

X-ray Crystal Monochromators
Energy Resolution

- *the function of the monochromator, oddly enough, is to monochromate the beam or select a narrow energy bandpass from a broad spectral source; typical energy resolution ~1e-4 (or better)*
- *energy resolution obtained by taking derivative of Bragg equation wrt θ, divide by Bragg eq., and rearrange terms …*
  $\delta\lambda / \lambda = \delta \theta / \tan \theta = \delta\varepsilon / \varepsilon$
- *better energy resolution obtained by using higher index reflections to obtain larger θ for a given energy*
  $\sin \theta = (\lambda / 2a_0)(h^2 + k^2 + l^2)^{1/2}$
- *so what contributes to δ θ?*
  - *beam divergence or convergence on monochromator*
  - *crystal intrinsic rocking width (Darwin width)*

X-ray Crystal Monochromators
Focusing Mirror Effects on Resolution

- toroidal focusing mirror upstream of monochromator will degrade monochromator energy resolution with increasing horizontal acceptance by increasing beam vertical convergence
  - *even in the limit of zero vertical beam divergence, a horizontally focusing toroidal mirror will generate vertical beam convergence of order* $\sim \varphi^2 F_{in} (F_{in}+F_{out}) / (2\alpha F_{out}^2)$ *where* φ *is the horizontal half acceptance angle*
- typically this effect is reasonably modest when the beam horizontal acceptance is restricted to ~1 mrad



X-ray Crystal Monochromators
Improving Energy Resolution

- *employ higher index monochromator crystal (eg., 1/tan θ scaling)*
- *use a collimating mirror upstream of monochromator to reduce vertical angular spread (eg., BL7-2 M0 mirror can be used to collimate the beam at the expense of vertical spot size)*
- *reduce horizontal angular acceptance if monochromator is preceded by toroidal focusing mirror (eg., BL2-1)*
- *reduce horizontal angular acceptance on side deflecting monochromators (eg., BL11-3) and optimize crystal bend*
- *reduce vertical angular acceptance*
  - *BL w/o mirror optics upstream on mono*
  - *BL w/ focusing mirrors upstream of mono (BL2-1, BL7-2)*
  - *BL w/ collimating mirrors to reduce mirror aberration effects*

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X-ray Crystal Monochromators
Harmonic Content

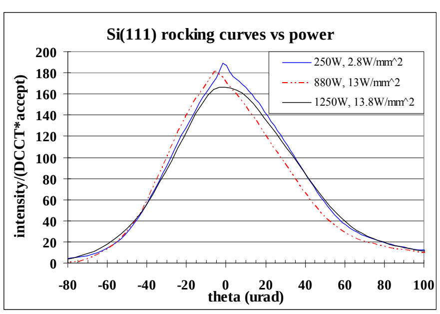
- *crystal monochromators pass not only the fundamental energy of interest but also allowed higher order harmonics since*
  $\sin\theta = (\lambda / 2a_0)(h^2 + k^2 + l^2)^{1/2}$
- *fortunately the narrower intrinsic (Darwin) rocking curve width of higher order harmonics decreases the diffracted intensity as a function of peak index*
- *Si(220) example with fundamental at 12keV (15.607 deg):*

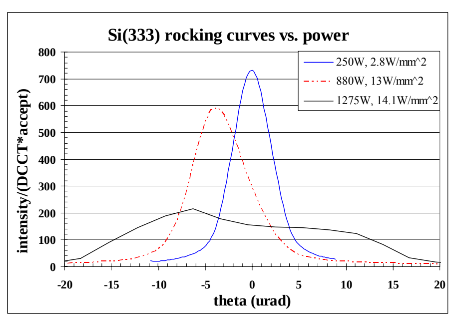
index	energy (keV)	Darwin (urad)	δε/ε
220	12.0	15.99	5.72E-05
440	24.0	2.55	9.15E-06
660	36.0	0.645	2.31E-06

- *narrower rocking curves also facilitate slightly detuning double crystal pair in monochromator to suppress diffraction from harmonics while retaining most of diffracted intensity of fundamental*
  - *detuning maximizes mono sensitivity to crystal angular misalignment!*
  - *it is always better to use mirrors to harmonic reject when feasible (eg., variable incidence M0 on BL7-2 and fixed incident M0 on BL2-1 & 11-3)*

X-ray Crystal Monochromators
Other Non-Idealities & Mitigation

- high power on monochromators tends to create thermal distortions of the crystals which reduce double crystal mono diffracted intensity and degrade harmonic rejection obtained by detuning
  - *LN monos, though expensive, have proved capable of handling significant power (>1000W tested) with acceptable distortions*





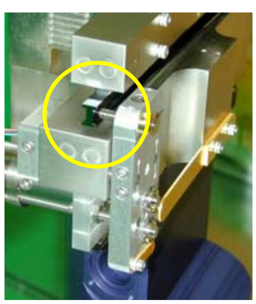
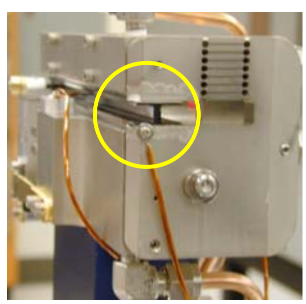
BL6-2 LN mono 500mA power test results from 8/1/05

X-ray Crystal Monochromators
Other Non-Idealities & Mitigation

- SSRL employs quasi channel cut double crystal monochromators as this approach tends to make for quieter monos; however…
  - *diffracted beam height varies as 2*channel height*cos θ so hutch table or downstream optics need to compensate for beam motion*
- roll misalignment between the first and second crystal in a double crystal monochromator results in beam horizontal motion with energy
  - *roll misalignment is particularly troublesome when the mono is followed by a toroidal focusing mirror as beam horizontal motion results in a focusing mirror yaw error such that the focus shape changes with energy*
  - *the LN monochromators include a remote roll adjustment capability*
  - *the crystals in the older double crystal monochromators have been polished to minimize miscuts and carefully aligned such that the first and second crystal surfaces are parallel*

X-ray Crystal Monochromators
Other Non-Idealities & Mitigation

- high power on side deflecting monochromator crystals tends to create thermal distortions which degrade the focus and energy resolution
  - *cubed-root, I beam cross section crystals employed in SPEAR3 side scattering monochromators (BL7-1, 9-1, 11-1, 11-3) have been designed to minimize thermal deformation by locating power footprint near crystal neutral axis*

A Few Closing Thoughts -
Some Keys to Optimal BL Performance

- *your BL request should reflect careful consideration of the experiment requirements vs. the source/optics capabilities (ie., the best BL for a given experiment isn't always the most familiar BL)*
- *plan/communicate needs in advance such that the BL is configured optimally for your experiment (mirror cutoffs, mono crystal cuts, etc.)*
- *avoid depositing waste power in optics, rather use slits and filters to best advantage!*
- *utilize the BL mirrors to optimize performance*
  - *power filtering*
  - *harmonic rejection*
  - *beam shaping*
- *avoid mono detuning whenever possible to minimize mono instability*

Questions?