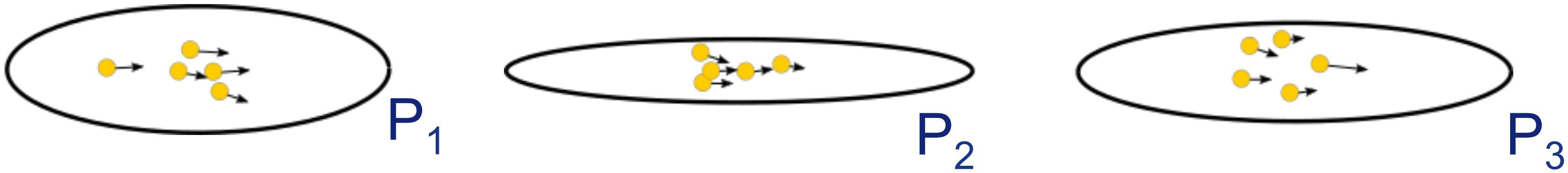
Synchrotron Sources

In storage rings, the electrons are statistically distributed inside bunches

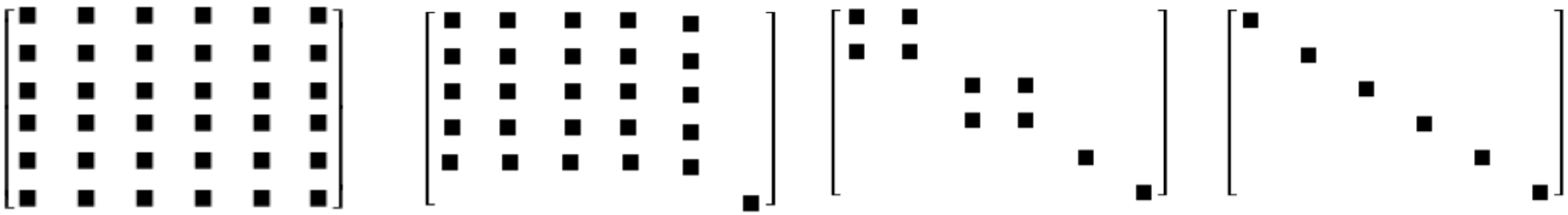


Order of 10^9 electrons per bunch

$$\boxed{f(\boldsymbol{r},\boldsymbol{\theta},\gamma,z) = C \cdot \exp\left(-\mathbf{u}^{\mathrm{T}}\Sigma^{-1}\boldsymbol{u}\right)}$$

Phase space vector $\boldsymbol{u} = (x, \theta_x, y, \theta_y, \gamma, z)$

6x6 covariance matrix Σ:

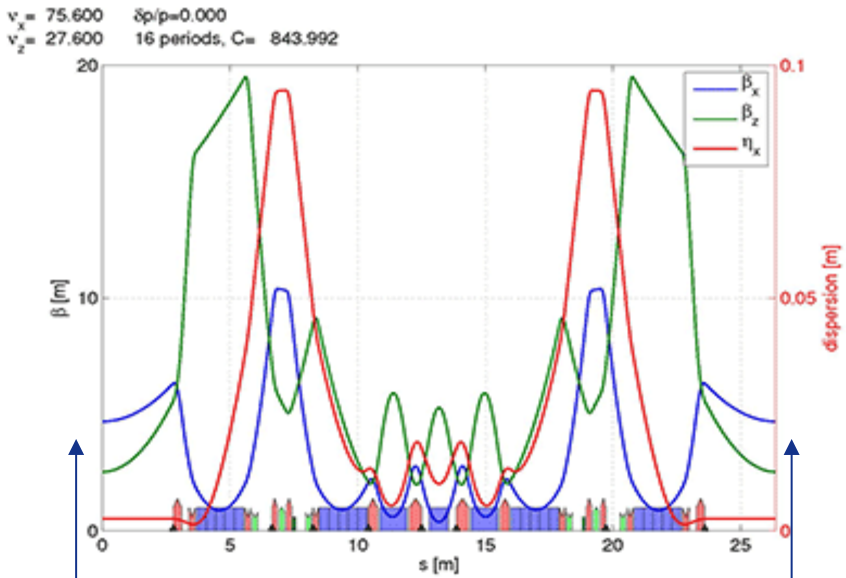


General No z-coupling Finite alpha Symmetry point

Stotage ring: electron beam sizes

Horizontal emittance = 147 pm

$$\Sigma = \begin{pmatrix} \langle x^2 \rangle & \langle xx' \rangle \\ \langle xx' \rangle & \langle x'^2 \rangle \end{pmatrix} = \begin{pmatrix} \beta_x \varepsilon_x & -\alpha_x \varepsilon_x \\ -\alpha_x \varepsilon_x & \gamma_x \varepsilon_x \end{pmatrix} + \eta^2 \sigma_\delta{}^2 I_{2x2}$$



With e the emittance (constant), and Twiss parameters:

$$\alpha = -\frac{1}{2}\frac{d\beta}{ds}; \quad \gamma = \frac{1+\alpha^2}{\beta}$$

At s (any point of the trajectory):

$$\sigma_x = \sqrt{\langle x^2 \rangle} = \sqrt{\beta_x \varepsilon_x}; \quad \sigma_{x'} = \sqrt{\langle x'^2 \rangle} = \sqrt{\gamma_x \varepsilon_x}; \quad \sigma_x \sigma_{x'} = \varepsilon_x \sqrt{1+\alpha_x^2}$$

At waist (zero correlation, r=a=0, b is minimum):

$$\sigma_x = \sqrt{\langle x^2 \rangle} = \sqrt{\beta_x \varepsilon_x}; \quad \sigma_{x'} = \sqrt{\langle x'^2 \rangle}\Big|_w = \sqrt{\frac{\varepsilon_x}{\beta_x}}; \quad \boxed{\sigma_x \sigma_{x'} = \varepsilon_x}$$

EBS (S28D):

b_x = 6.90 m

b_y = 2.64 m

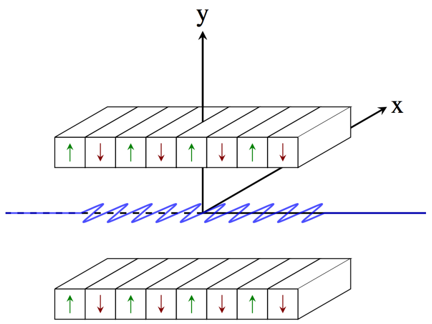
s_x = 30.2 mm

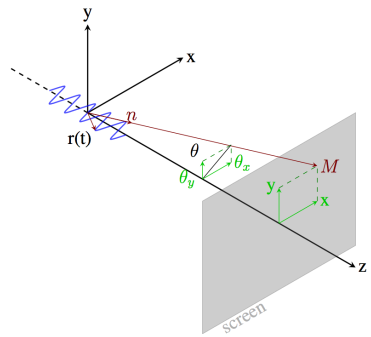
s_y = 3.64 mm

$s_{x'}$= 4.37 mrad

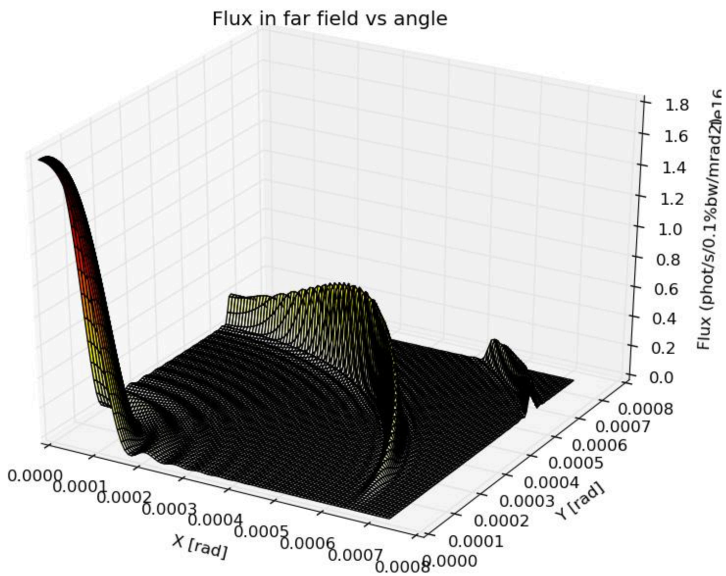
$s_{z'}$=1.37 mrad

Undulator emission, after classical electrodynamics (e.g., Jackson, etc)





$$\frac{d^2 I}{d\omega d\Omega} = \frac{eI}{8\pi^2 c\epsilon_0 h} 10^{-9} \left| \int_{-\infty}^{\infty} \left[\frac{n \times \left[(n-\beta) \times \dot{\beta} \right]}{(1-\beta \cdot n)^2} + \frac{c}{\gamma^2 R} \frac{(n-\beta)}{(1-\beta \cdot n)^2} \right] e^{i\omega(t' + R(t')/c)} dt' \right|^2$$



Undulator emission (single electron or filament beam or zero emmittance)

(after Onuki & Elleaume, Undulators, Wigglers and their applications, CRC press, 2002**)**

below resonance

on resonance

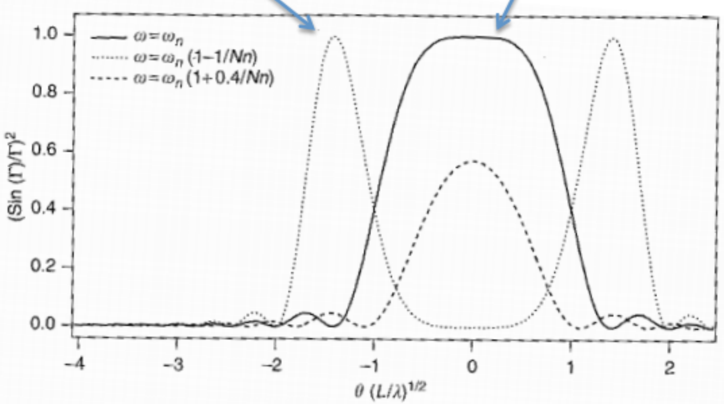


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2+\theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1(0,0)$.

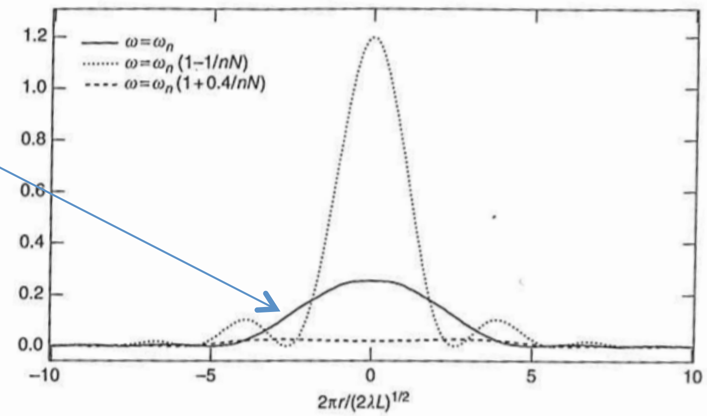
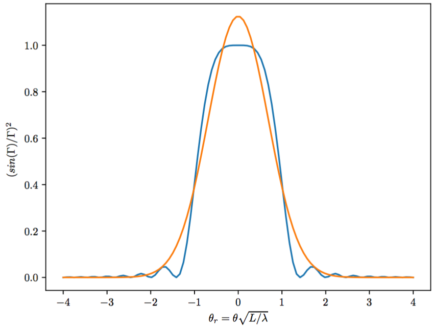


Figure 3.4 Spectral flux per unit surface in the middle of the undulator for three frequencies close to the on-axis resonant frequency $\omega_n = n\omega_1(0,0)$.

$$\sigma_r = \frac{2.704}{4\pi}\sqrt{\lambda L} \approx \sqrt{\frac{\lambda L}{2\pi^2}}$$

Even on resonance, beam is not fully Gaussian

But for resonance, can be reasonably approximated as Gaussian



$$\sigma_{r'} = 0.69\sqrt{\frac{\lambda}{L}} \approx \sqrt{\frac{\lambda}{2L}}$$

$$\sigma_r\sigma_{r'} = \frac{1.89\lambda}{4\pi} \approx \frac{\lambda}{2\pi}$$

- Undulator beams have not Gaussian profiles (even at resonances)
- These formulas are APPROXIMATED!

$$\boxed{K \equiv \frac{eB_0\lambda_u}{2\pi mc} = 0.9337\, B_0(\mathrm{T})\lambda_u(\mathrm{cm})}$$

$$\boxed{\lambda = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2} + \gamma^2\theta^2\right)}$$

$$E = \gamma m_\mathrm{e} c^2$$

$m_e c^2 = 0.51$ MeV

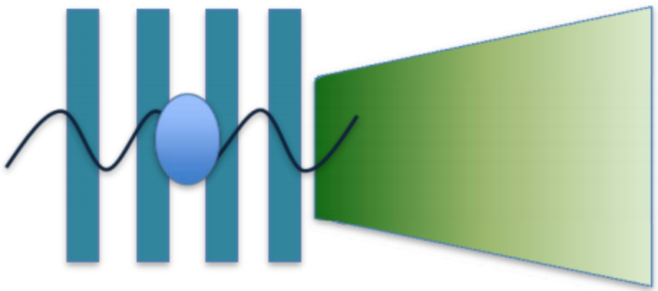
Photon beam size and divergence is determined by a combination of electron beam and single electron emission

$$\Sigma_x^2 = \sigma^2_{x,elec} + \sigma^2_{x,photon}$$

$$\Sigma_{x'}^2 = \sigma^2_{x',elec} + \sigma^2_{x',photon}$$

$$\Sigma_z^2 = \sigma^2_{z,elec} + \sigma^2_{z,photon}$$

$$\Sigma_{z'}^2 = \sigma^2_{z',elec} + \sigma^2_{z',photon}$$



Courtesy: Boaz Nash

These are at source. A distance D away, beam size become: $\Sigma_{x,0}^2 + \Sigma_{x',0}^2 D^2$

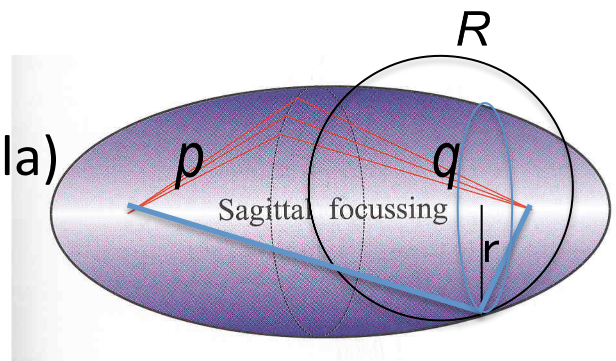
(FOR UNDULATORS, THESE FORMULAS ARE VALID AT THE WAIST, AT THE UNDULATOR RESONANCE, AND SUPOSSING GAUSSIAN EMISSION OF PHOTONS)

ShadowOui performs "numeric convolution" by Monte Carlo sampling of the electron beam [Gaussian] and photon emission [non Gaussian]

Mirrors

Mirror shape

- Ellipsoid: Point to point focusing
- Paraboloid: Collimating
- Focalization in two planes
  - Tangential or Meridional (ellipse or parabola)
  - Sagittal (circle)
- Demagnification: M=p/q
- Easier manufacturing:
  - 2D: Ellipsoid => Toroid
  - Only one plane: cylinder Ellipsoid (ellipse)=> cylinder (circle)
  - Sagittal radius: non-linear (ellipsoid) => constant (cylinder) or linear (cone),
- All mirrors produce aberrations



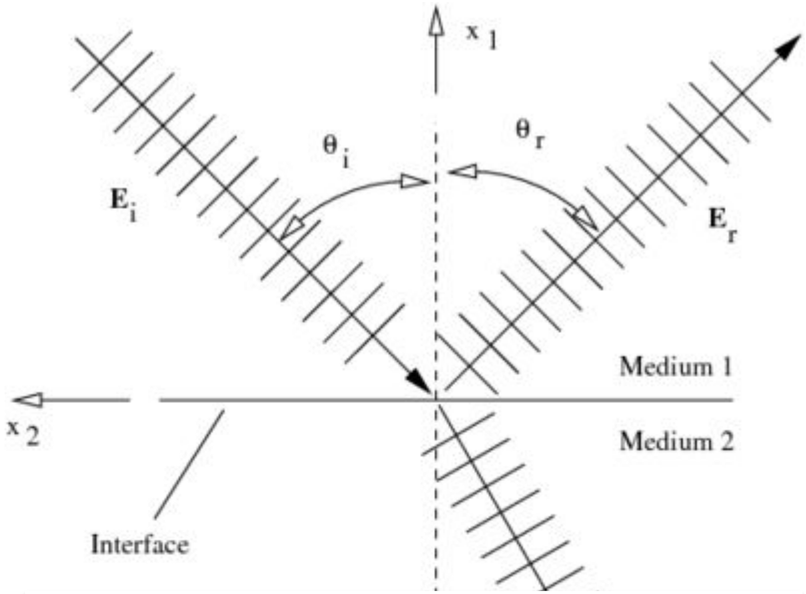
$$\frac{1}{p}+\frac{1}{q}=\frac{2}{R\sin\theta}$$

$$\frac{1}{p}+\frac{1}{q}=\frac{2\sin\theta}{\rho}$$

Mirrors

Geometrical model

Specular reflection



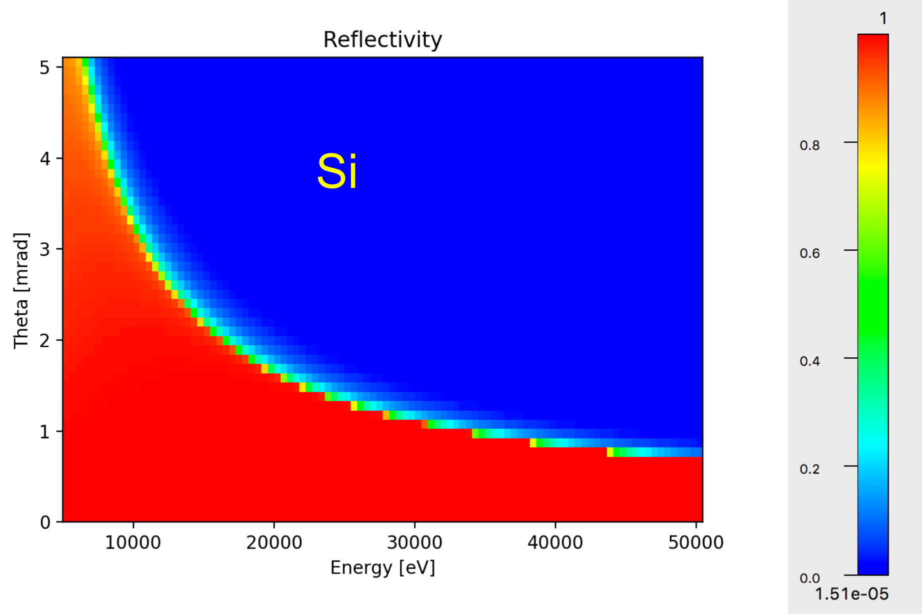
$$\hat{\mathbf{d}}_{\mathrm{s}} = 2\left(\hat{\mathbf{d}}_{\mathrm{n}} \cdot \hat{\mathbf{d}}_{\mathrm{i}}\right)\hat{\mathbf{d}}_{\mathrm{n}} - \hat{\mathbf{d}}_{\mathrm{i}},$$

Physical model

Fresnel formulas

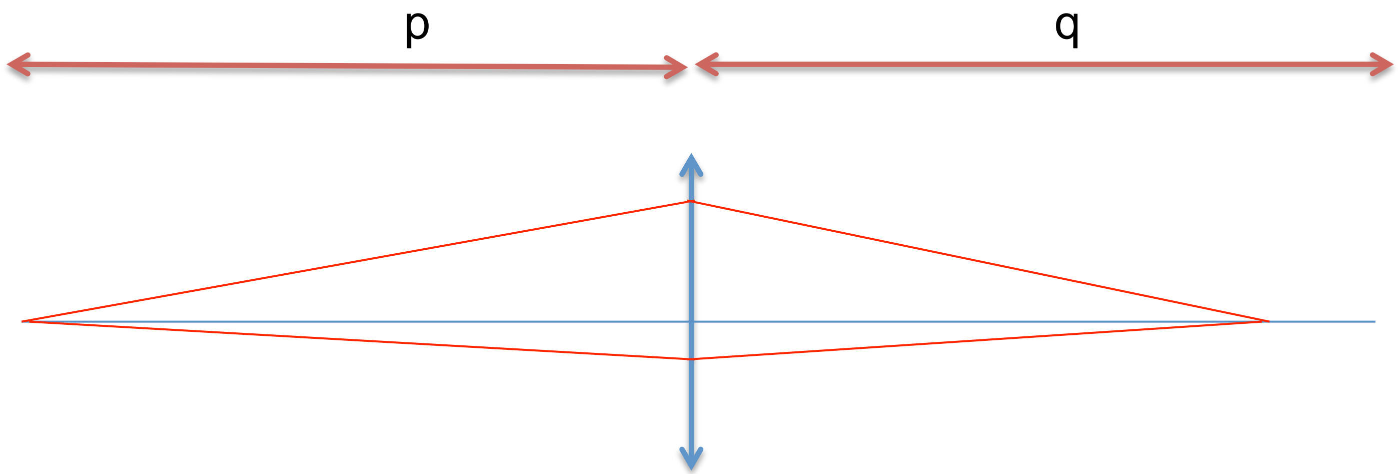
Fresnel equations give the reflectivity as a function of angle and photon energy. As a consequence, one gets the critical angle:

$$1 = \left(\frac{n_1}{n_2}\right)^2 \cos^2\theta_c \quad \Leftrightarrow \quad \sin\theta_c = \sqrt{2\delta - \delta^2} \approx \sqrt{2\delta}$$

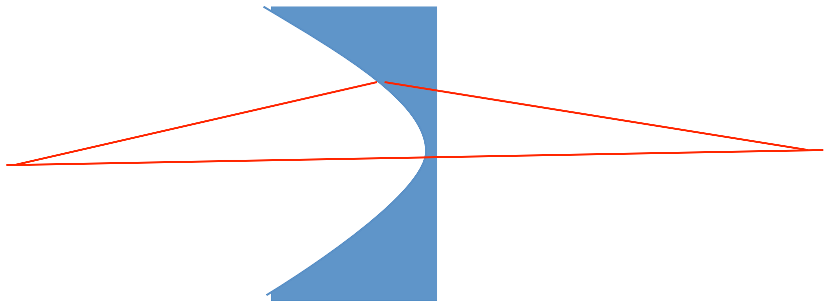


Lenses

LENS

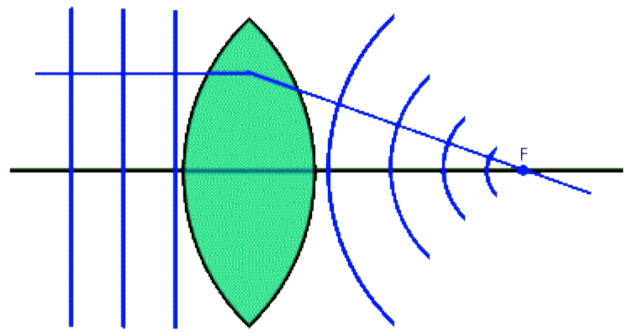


$$\frac{1}{F} = \frac{1}{p} + \frac{1}{q}$$



$$\sin\theta_1 = (1-\delta)\sin\theta_2$$

$$\frac{1}{F} = (n-1)\left(\frac{1}{R_1} - \frac{1}{R_2} + \frac{(n-1)d}{nR_1R_2}\right) \approx \frac{\delta}{R_1}$$



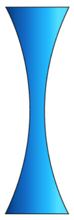
$$E = E_0 e^{i\frac{kr^2}{2f}}$$

CRL (COMPOUND REFRACTIVE LENSES) = replicate N lenses

Single interface

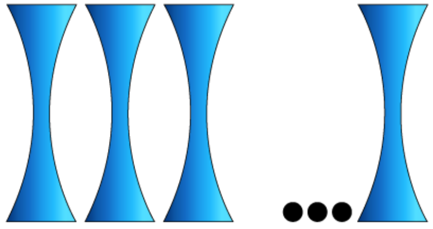
$$F = \frac{R}{\delta}$$

Lens



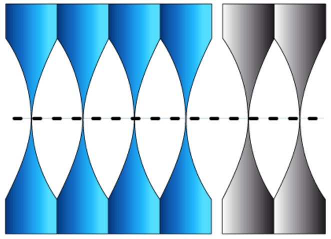
$$F = \frac{R}{2\delta}$$

Compound Refractive Lens (CRL)



$$F = \frac{R}{2N\delta}$$

Transfocator



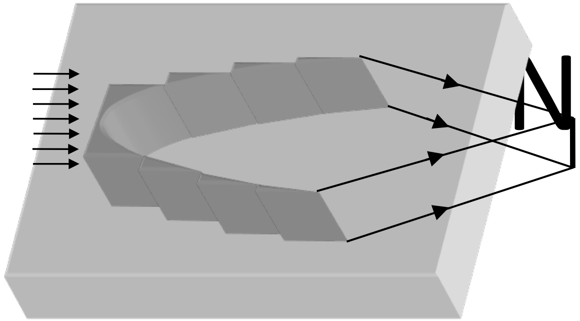
$$\frac{1}{F} = \frac{1}{F_1} + \frac{1}{F_2} + \ldots$$

1996 Experimental demonstration of CRL

- A. Snigirev *et al* Nature 384 (1996) 49

2011 Transfocator

HIGH DEMAGNIFICATION with NGL



	material->air	air->material
Collimated to convergent	Ellipse	Hyperbola
Divergent to convergent	Cartesian oval	Cartesian oval

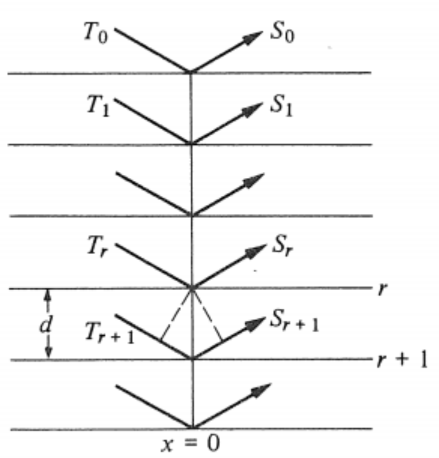
K. Evans-Lutterodt *et al*
Single Element elliptical hard X-ray micro-optics
Opt. Expr. **11**, 8, 919-926 (2003).

M. Sánchez del Rio & L. Alianelli,
J. Synchr. Rad. 19 (2012) 366

1) When illuminating with coherent light, reducing acceptance decreases N.A. therefore increases coherent diffraction ~0.61 l/ (h/q)
2) The rays become very grazing to there is total reflection. Not a limitation for kinoform lenses (K. Evans-Lutterodt *et al* Phys. Rev. Lett. 99 (2007)). For standard lenses one can reverse the lens.
3) There is a lot of absorption => remove material and convert it to a Fresnel lens (W. Jark *et al* J. Synchr. Rad. 13 (2006))
4) Use the lens shape adapted for your needs

Crystals

DARWIN TREATMENT OF DYNAMICAL THEORY (1914) – the darwin width

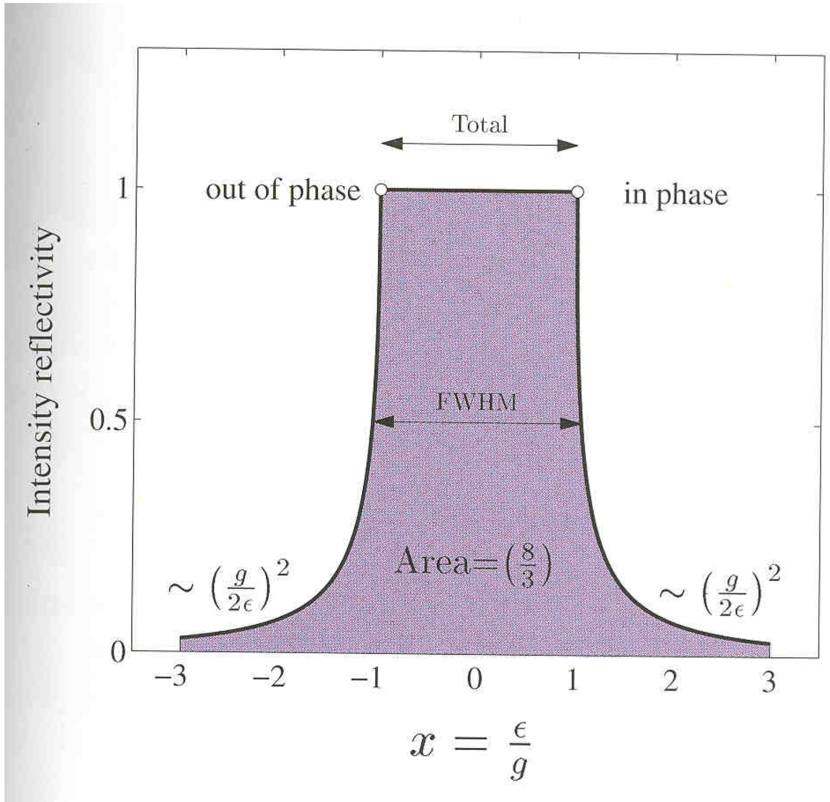


$$S_r = \frac{T_r - (1 - h + iq_0)T_{r-1}e^{-i\phi}}{iqe^{-i2\phi}}$$

$$R(x) = \begin{cases} \left(x - \sqrt{x^2 - 1}\right)^2 & \text{for } x \geq 1 \\ 1 & \text{for } |x| \leq 1 \\ \left(x + \sqrt{x^2 - 1}\right)^2 & \text{for } x \leq -1 \end{cases}$$

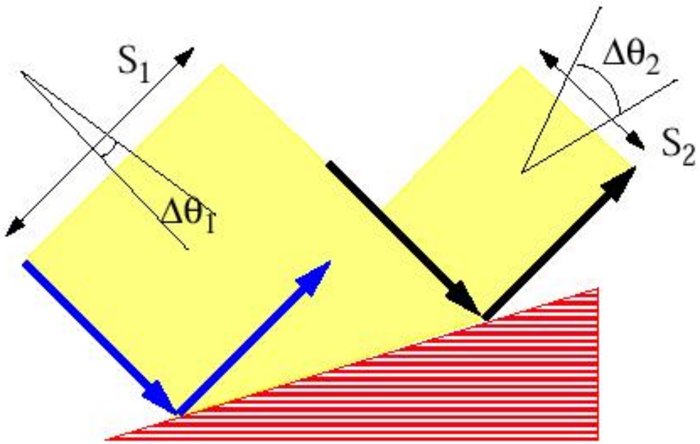
$$(\Delta\theta)_\mathrm{D} = 2\left|\frac{P|\Psi_H|}{(|b|)^{1/2}\sin(2\theta_\mathrm{B})}\right|$$

$$\Psi_H = \frac{-r_0\lambda^2}{\pi v_\mathrm{c}} F_H, \quad r_0 = \frac{e^2}{mc^2}$$



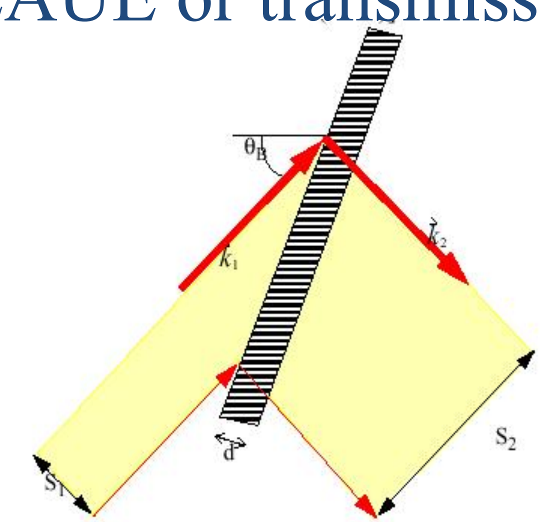
The Zachariasen treatment for plane Crystals

BRAGG or reflection

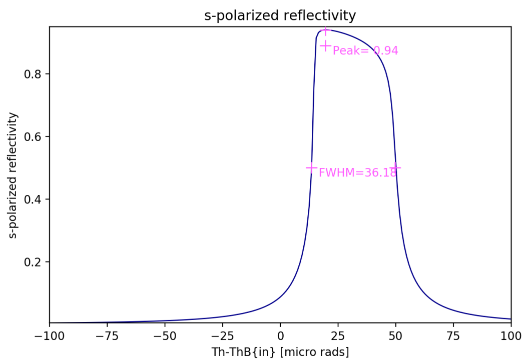


$$r^{\text{Bragg}}(\alpha_Z) \equiv \frac{1}{|b|}\frac{I^H}{I^0} = \frac{1}{|b|}\left|\frac{x_1 x_2 (c_1 - c_2)}{c_2 x_2 - c_1 x_1}\right|^2$$

LAUE or transmission



$$r^{\text{Laue}}(\alpha_Z) \equiv \frac{1}{|b|}\frac{I^H}{I^0} = \frac{1}{|b|}\left|\frac{x_1 x_2 (c_1 - c_2)}{x_2 - x_1}\right|^2$$



$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{-z \pm (qP^2 + z^2)^{1/2}}{P\Psi_{\overline{H}}}$$

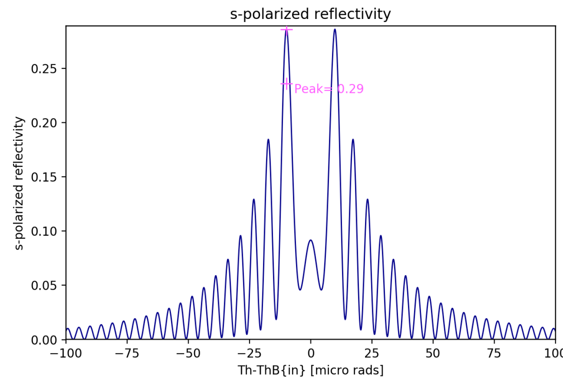
$$z = \frac{1-b}{2}\Psi_0 + \frac{b}{2}\alpha_Z.$$

$$c_1 = \exp(-i\varphi_1 T), \quad c_2 = \exp(-i\varphi_2 T),$$

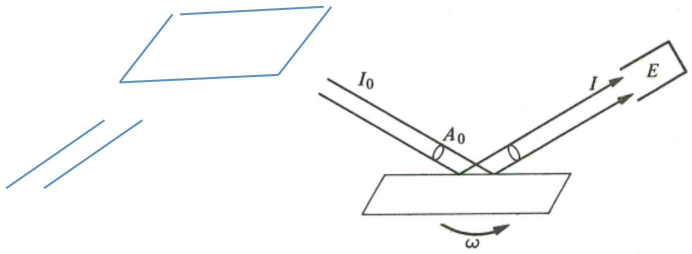
$$\varphi_1 = -\frac{2\pi k^0 \delta_0'}{\gamma_0}, \quad \varphi_2 = -\frac{2\pi k^0 \delta_0''}{\gamma_0},$$

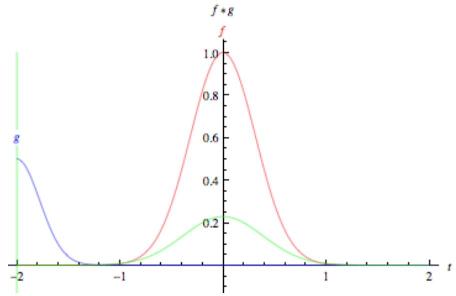
$$\begin{pmatrix} \delta_0' \\ \delta_0'' \end{pmatrix} = \frac{1}{2}\left[\Psi_0 - z \pm (qP^2 + z^2)^{1/2}\right]$$

$$\alpha_Z = \frac{1}{|\mathbf{k}^0|^2}\left(|\mathbf{H}|^2 + 2\mathbf{k}^0 \cdot \mathbf{H}\right)$$

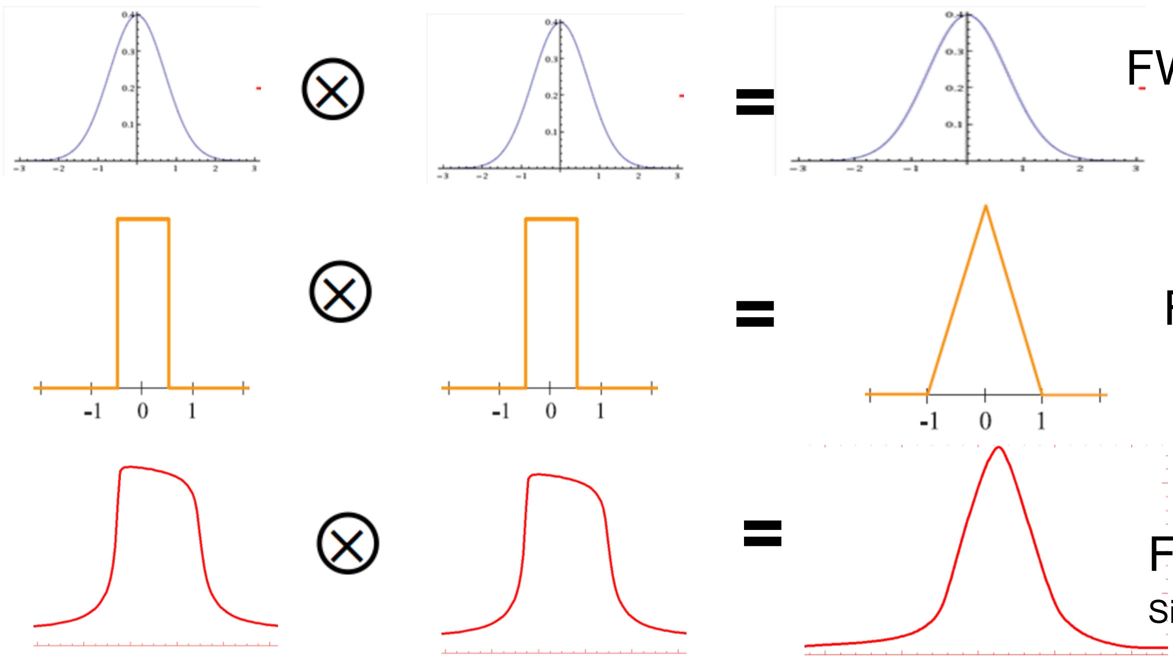


ROCKING CURVES





The rocking curve is the **CONVOLUTION** of the two diffraction profiles.



$FWHM_R = 1.4\ FWHM_1$

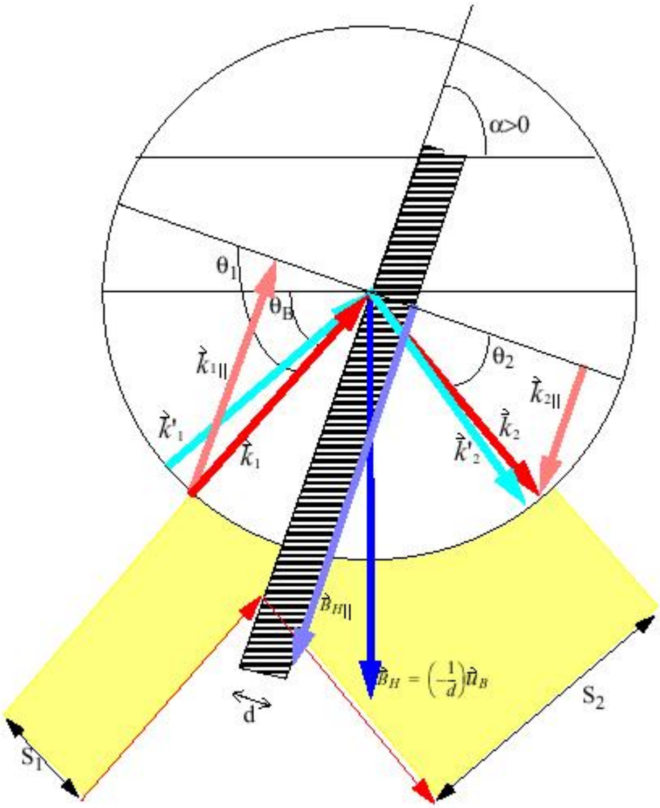
$FWHM_R = 1\ FWHM_1$

$FWHM_R \sim 1.5\ FWHM_1$

Si111 8 keV

For a full discussion about rocking curves see: Masiello *et al.* J. Appl. Crystall. 47, 1304-1314 (2014)

ON THE DIRECTION OF THE OUTCOMING WAVE



The change in the direction of any monochromatic beam (not necessarily satisfying the diffraction condition or Laue equation) diffracted by a crystal (Laue or Bragg) can be calculated using (i) elastic scattering in the diffraction process:

$$|\mathbf{k}^0| = |\mathbf{k}^H| = {}^{1} \qquad (2)$$

with $\mathbf{k}^{0,H} = (1/\lambda)\mathbf{V}^{0,H}$ and $\mathbf{V}$ a unitary vector; and (ii) the boundary conditions at the crystal surface:

$$\mathbf{k}_{\parallel}^{H} = \mathbf{k}_{\parallel}^{0} + \mathbf{H}_{\parallel}. \qquad (3)$$

$$-|\sin\theta_2| = |\sin\theta_1| - \frac{\lambda}{d}\sin\alpha$$

A crystal behaves like a grating or prism, except the Bragg Symmetric crystal that behaves like a mirror.

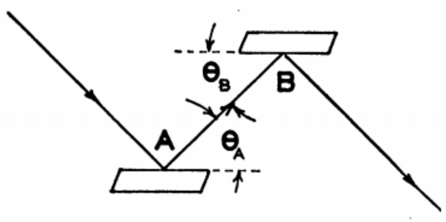
$$\frac{d}{\sin\alpha} = \frac{d_{Grating}}{m}$$

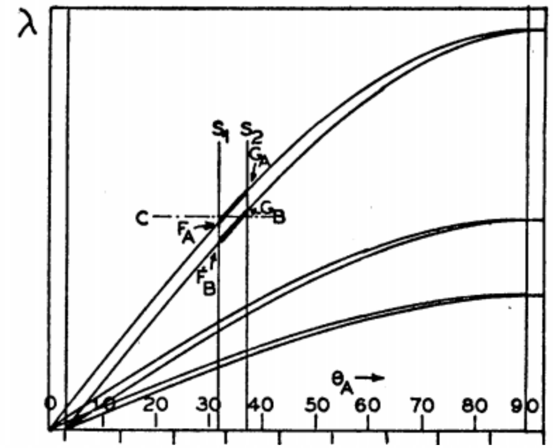
When combined with reflectivities from dynamical theory we can do ray tracing (beam decomposed in plane waves) ex17_crystalmono.ows

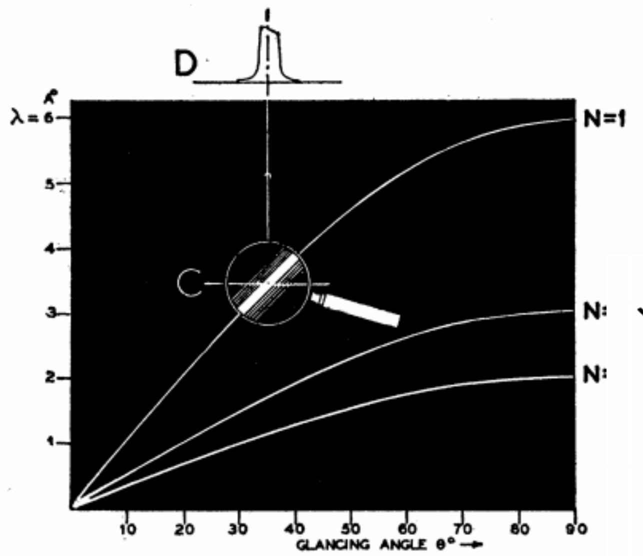
Theory of the Use of More Than Two Successive X-Ray Crystal Reflections to Obtain Increased Resolving Power

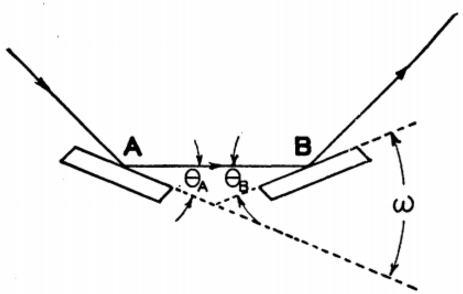
J W. M. DuMond Phys. Rev. **52**, 872 – (1937)

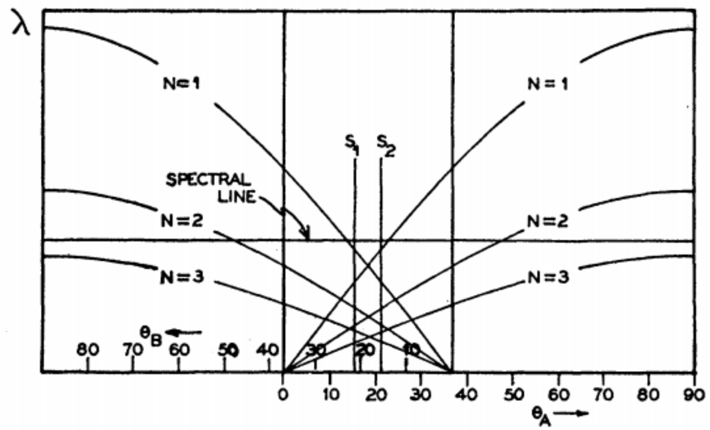
http://dx.doi.org/10.1103/PhysRev.52.872











Energy Resolution

$$\frac{\Delta\lambda}{\lambda_0} = \frac{\Delta E}{E_0} = (\Delta_{src} + \omega_D)\cot\theta_0$$

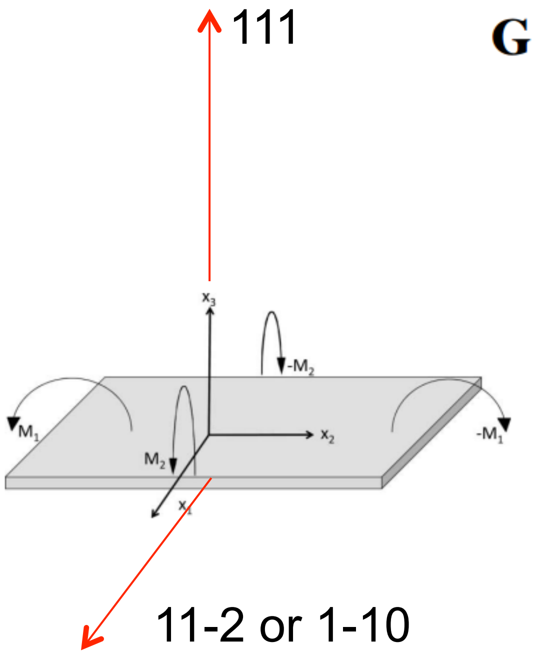
$$\frac{\Delta\lambda}{\lambda_0} = \frac{\Delta E}{E_0} \approx \sqrt{\omega_D^2 + (\Delta_{geom} + \Delta_{ss})^2}\cot\theta_0 = \sqrt{\omega_D^2 + \left[\left(\frac{p}{R\sin\theta_1} - 1\right)\Delta_{src} + \frac{s_1}{p}\right]^2}\cot\theta_0$$

EFFECT OF CRYSTAL ANISOTROPY in bent crystals

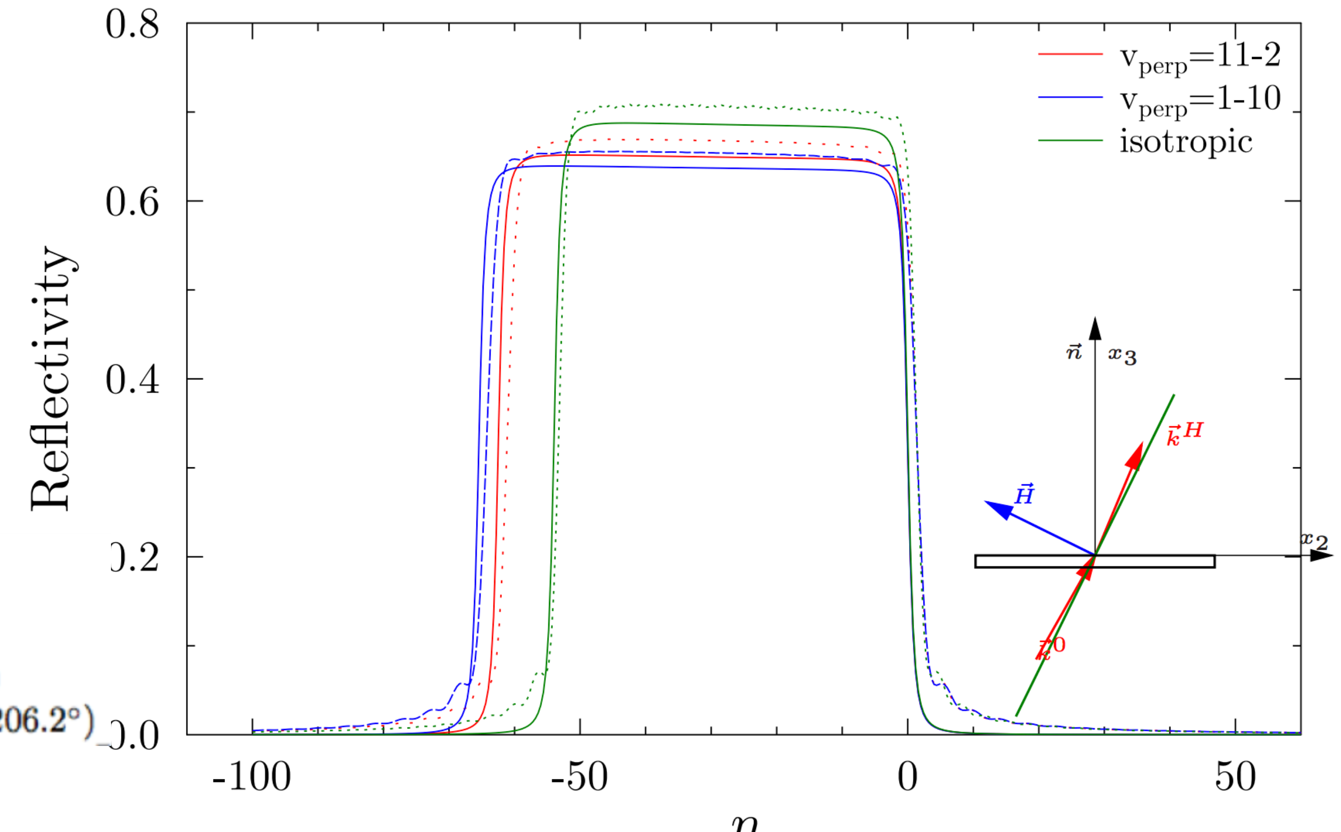
$$\mathbf{G} \equiv \frac{\partial^2(\mathbf{H}\cdot\mathbf{u})}{\partial V_0 \partial V_H}$$

$$\begin{aligned}
u_1 &= \frac{1}{I}[(s_{11}M_1 + s_{12}M_2)x_1x_3 + (s_{51}M_1 + s_{52}M_2)x_3^2/2 \\
&\quad + (s_{61}M_1 + s_{62}M_2)x_2x_3/2], \\
u_2 &= \frac{1}{I}[(s_{21}M_1 + s_{22}M_2)x_2x_3 + (s_{41}M_1 + s_{42}M_2)x_3^2/2 \\
&\quad + (s_{61}M_1 + s_{62}M_2)x_1x_3/2], \\
u_3 &= \frac{1}{2I}[-(s_{11}M_1 + s_{12}M_2)x_1^2 - (s_{21}M_1 + s_{22}M_2)x_2^2 \\
&\quad - (s_{61}M_1 + s_{62}M_2)x_1x_2 + (s_{31}M_1 + s_{32}M_2)x_3^2].
\end{aligned}$$

$$\frac{M_1}{I} = \frac{1}{s_{12}s_{21} - s_{11}s_{22}}\left(\frac{s_{12}}{R_2} - \frac{s_{22}}{R_1}\right),$$
$$\frac{M_2}{I} = \frac{1}{s_{12}s_{21} - s_{11}s_{22}}\left(\frac{s_{21}}{R_1} - \frac{s_{11}}{R_2}\right).$$



Si 111
33170 eV
0.07 cm
325 cm (convex to the beam)
$\alpha_X = 296.2°$ ($\alpha = -116.2°$, $\chi = -206.2°$)

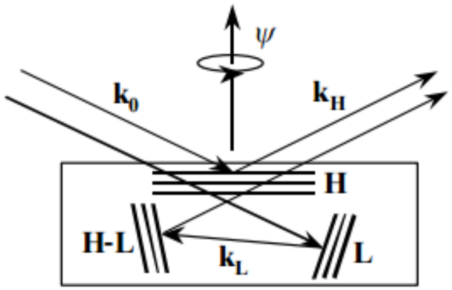


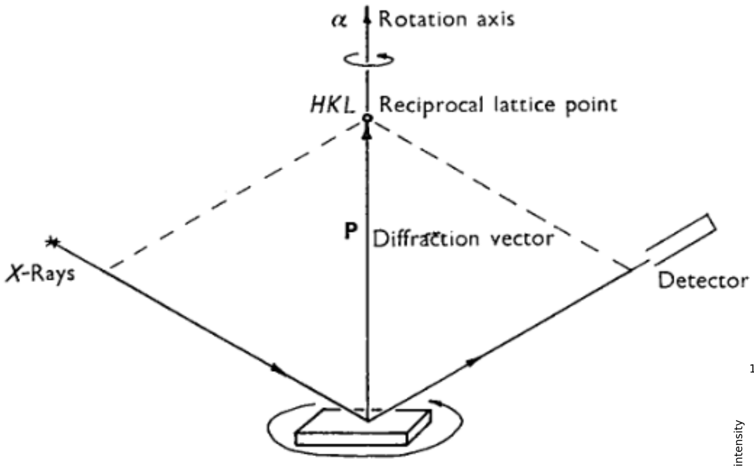
M. Sanchez del Rio, N. Perez-Bocanegra, X. Shi & V. Honkimaki, J. Appl. Cryst. (2015). 48, 477-491

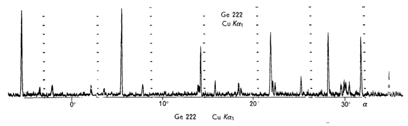
Multiple BRAGG Diffraction

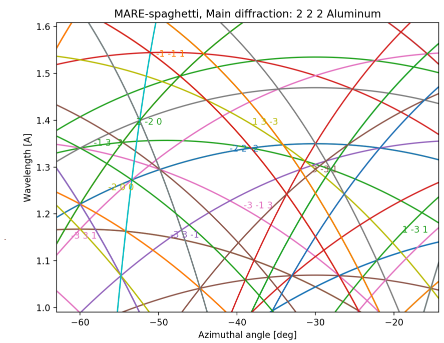
Simultaneous multiple diffraction occurs when the incident wave finds several sets of planes satisfying the Bragg law.

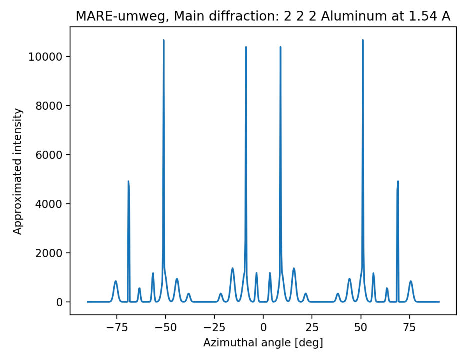
- They were first discovered by Renninger (1937) so they are called Renninger reflections of detour reflections (umweganregung).
- Kinematical theory (Cole, Acta Cryst.15 138 (1962); Rossmanith PSILAM; XOP/ MARE)
- Beyond kinematical theory (Colella, Acta Cryst. A30, 413 (1974); Shen; Stepanov http://x-server.gmca.aps.anl.gov)











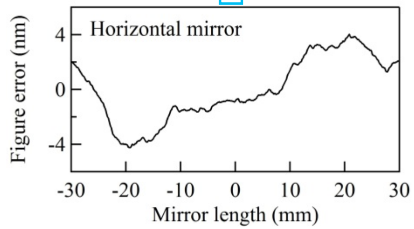
Coherence

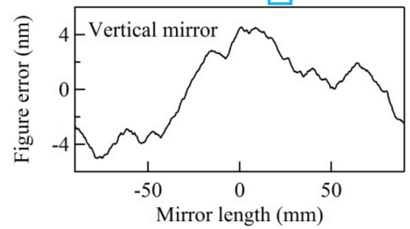
HYBRID METHOD IN SHADOW (X. Shi *et al.*)

Combining ray tracing and wavefront propagation

$$\text{Plane wave} \times \exp\left[-ik\left(\frac{x^2}{2f_x}+\frac{z^2}{2f_z}\right)\right] \times \exp[-i2k\sin\theta_x \cdot \text{Height}(x)] \times \exp[-i2k\sin\theta_z \cdot \text{Height}(z)]$$

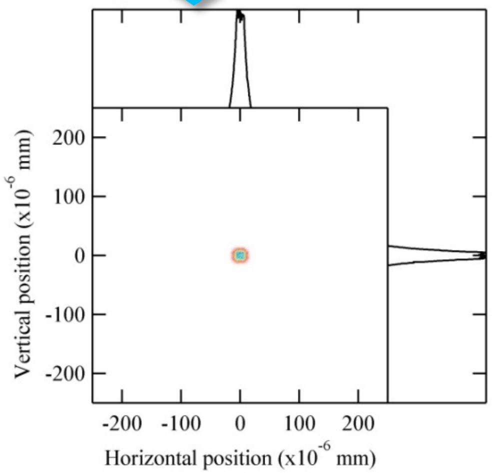
Ideal lens with focal lengths of f_x and f_z



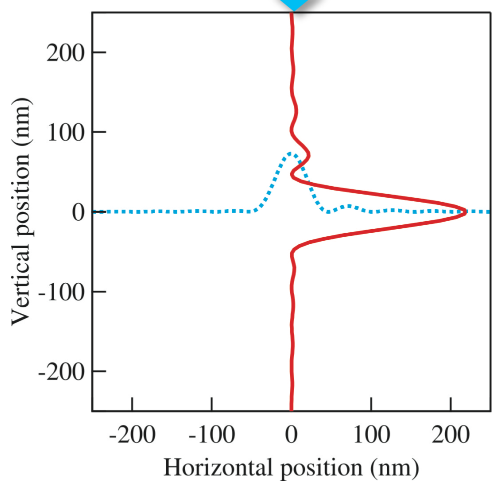


$$E(x,z) \rightarrow \boxed{\text{FFT}} \xrightarrow{\mathcal{F}(u,v)} \boxed{\times \exp\left[-\frac{i2\pi^2}{k}(u^2+v^2)y\right]} \xrightarrow{\mathcal{F}'(u,v)} \boxed{\text{Inverse FFT}} \rightarrow E(x',z')$$

Ray tracing of the beamline



$\otimes$



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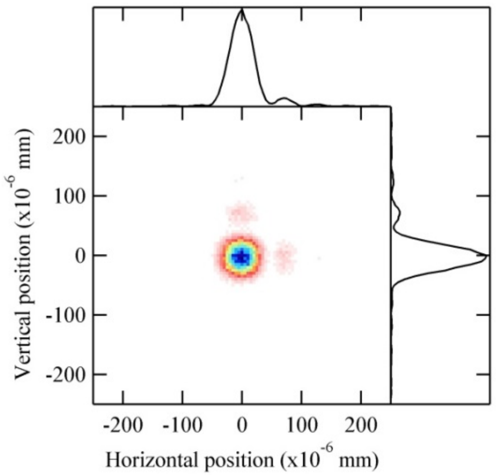

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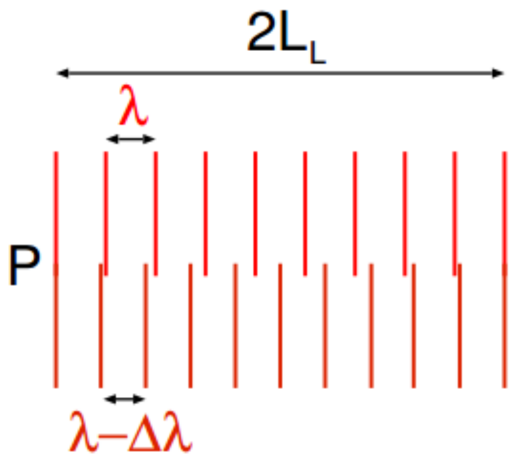
COHERENT LENGTHS - TWO WAVES http://www.csrri.iit.edu/~segre/phys570/10F/lecture_04.pdf

Starting with TWO well defined (thus coherent) waves with THE SAME intensity:

LONGITUDINAL (TEMPORAL) COHERENCE LENGTH L_L

Distance over which two waves from the same source point with slightly different wavelengths will completely dephase.



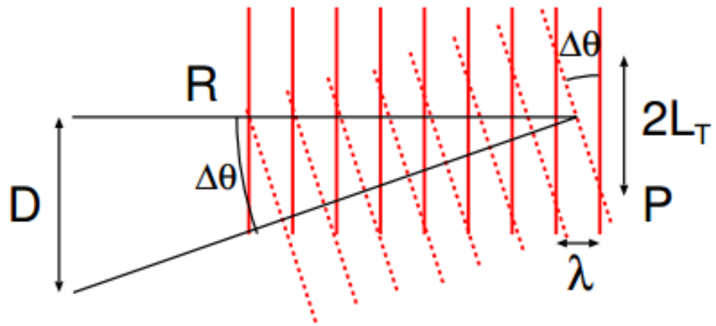
$$2L_L = N\lambda$$

$$2L_L = (N+1)(\lambda - \Delta\lambda)$$

$$0 = \lambda - N\Delta\lambda - \Delta\lambda \longrightarrow \lambda = (N+1)\Delta\lambda \longrightarrow N \approx \frac{\lambda}{\Delta\lambda} \longrightarrow \boxed{L_L = \frac{\lambda^2}{2\Delta\lambda}}$$

TRANSVERSE COHERENCE LENGTH L_T

The lateral distance along a wavefront over which there is a complete dephasing between two waves of the same wavelength, which originate from two separate points in space



$$\frac{\lambda}{2L_T} = \tan\Delta\theta \approx \Delta\theta \qquad \frac{D}{R} = \tan\Delta\theta \approx \Delta\theta$$

$$\boxed{L_T = \frac{\lambda R}{2D}}$$

correlation lengths for a typical synchrotron

- the synchrotron beam ***is not*** formed by two single monochromatic plane waves
- But we give some ***approximated*** values…

LONGITUDINAL COHERENCE

Imagine that a typical monochromator:

•Produces a typical of $\Delta\lambda/\lambda = 10^{-4}$ (Si 111) peak distribution (Gaussian)

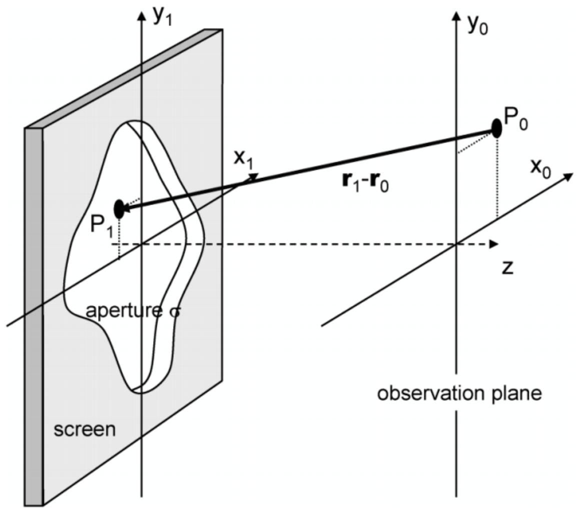
•For main wavelength of λ = 1Å we select two lines thus separated its width $\Delta\lambda = 10^{-4}$ Å

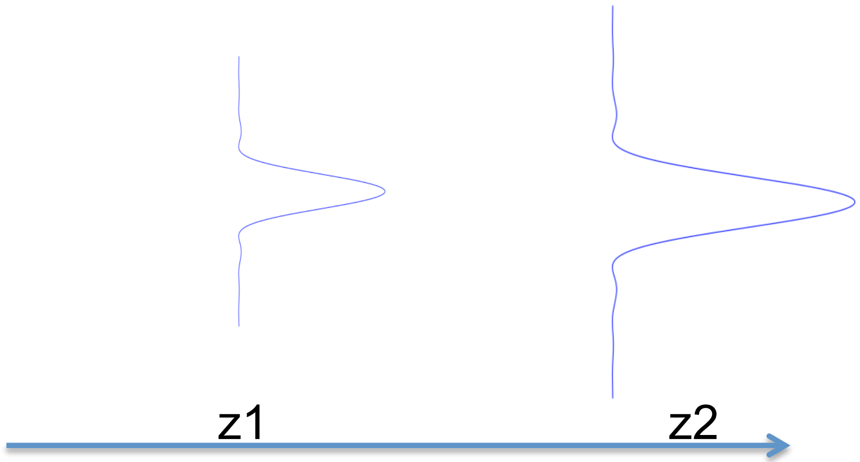
•The wavefronts of these two monochromatic waves are plane and identical

$$L_L = \frac{\lambda^2}{2\Delta\lambda} = 0.5\mu\mathrm{m} \qquad \tau = \frac{L_L}{c} = \frac{1}{6}10^{-14} \sim \mathrm{fs}$$

STATIONARY: This correlation time is much smaller than "bunch time" ~ 15 10^{-3} / c ~10^{-12} s~ ps

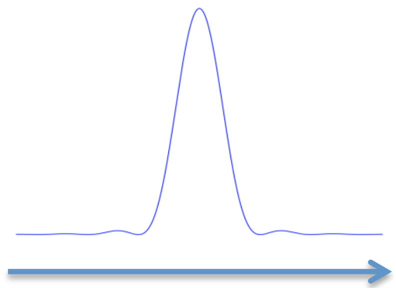
FRAUNHOFER DIFFRACTION





$$U(x_0, y_0) = \frac{-e^{-jkz}}{j\lambda z} e^{-\frac{jk}{2z}[x_0^2+y_0^2]} \int \int_{-\infty}^{+\infty} U(x_1, y_1) e^{j\frac{2\pi}{\lambda z}[x_0 x_1 + y_0 y_1]} dx_1 dy_1$$

Fourier transform with conjugated variables:
x ; f_x=x/(l z) ~ sinq/l (same for y)

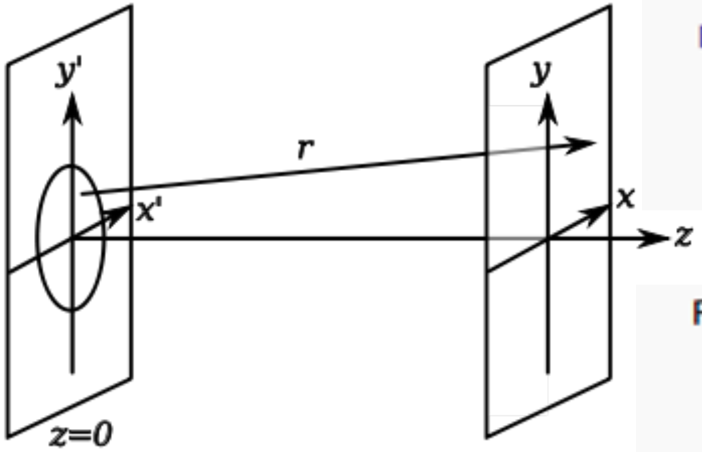


The same shape for different distances

f_x=x/(l z) ~ sinq/l ~ q/l

```
F1 = np.fft.fft2(image)  # Take the fourier transform of the image
```

FRESNEL DIFFRACTION

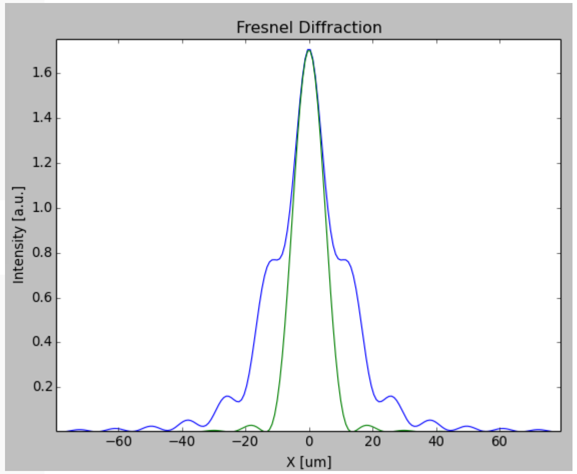


Fraunhofer diffraction occurs when:

$$F = \frac{a^2}{L\lambda} \ll 1$$

Fresnel diffraction occurs when:

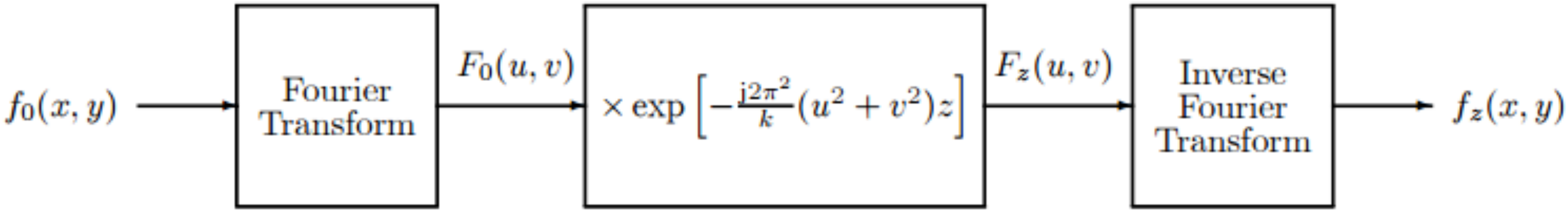
$$F = \frac{a^2}{L\lambda} \geq 1$$



$$f_z(x,y) = \frac{1}{\mathrm{j}\lambda z}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_0(x_0,y_0)\boxed{\exp\left[\frac{\mathrm{j}k}{2z}\left((x-x_0)^2+(y-y_0)^2\right)\right]}\,\mathrm{d}x_0\,\mathrm{d}y_0.$$

Numeric calculation: convolution with a Gaussian kernel

CONVOLUTION



Quantifying efficiency of the source to emit coherent radiation:

coherent fraction for SR lattices (Undulator emission)

$$\boxed{CF = CF_h CF_v = \frac{(\lambda/2\pi)^2}{\Sigma_x \Sigma_{x'} \Sigma_y \Sigma_{y'}}}$$

$$CF_{H,V} = \frac{\sigma_\gamma \sigma_\gamma{}'}{\sqrt{\sigma_\gamma{}^2 + \sigma_{H,V}{}^2}\sqrt{\sigma_\gamma{}'^2 + \sigma'_{H,V}{}^2}} = \frac{\lambda/(2\pi)}{\sqrt{\frac{\lambda L}{2\pi^2} + \sigma_{H,V}{}^2}\sqrt{\frac{\lambda}{2L} + \sigma'_{H,V}{}^2}}$$

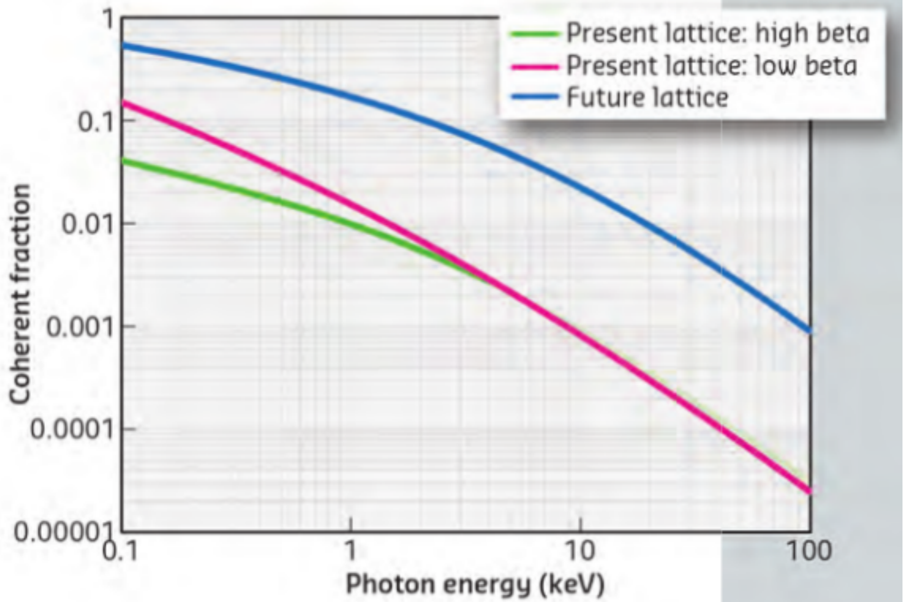


Figure 4.01: Comparison of the variation of the coherent fraction of X-ray emission with energy for the current insertion devices (low-β and high-β source points) and the proposed source.