Synchrotron Beam Lines

Stanford-Berkeley Summer School

on Synchrotron Radiation

June 13-17th 2005

Tony Warwick

Advanced Light Source

Lawrence Berkeley National Laboratory

ALS delivers (soft) x-rays

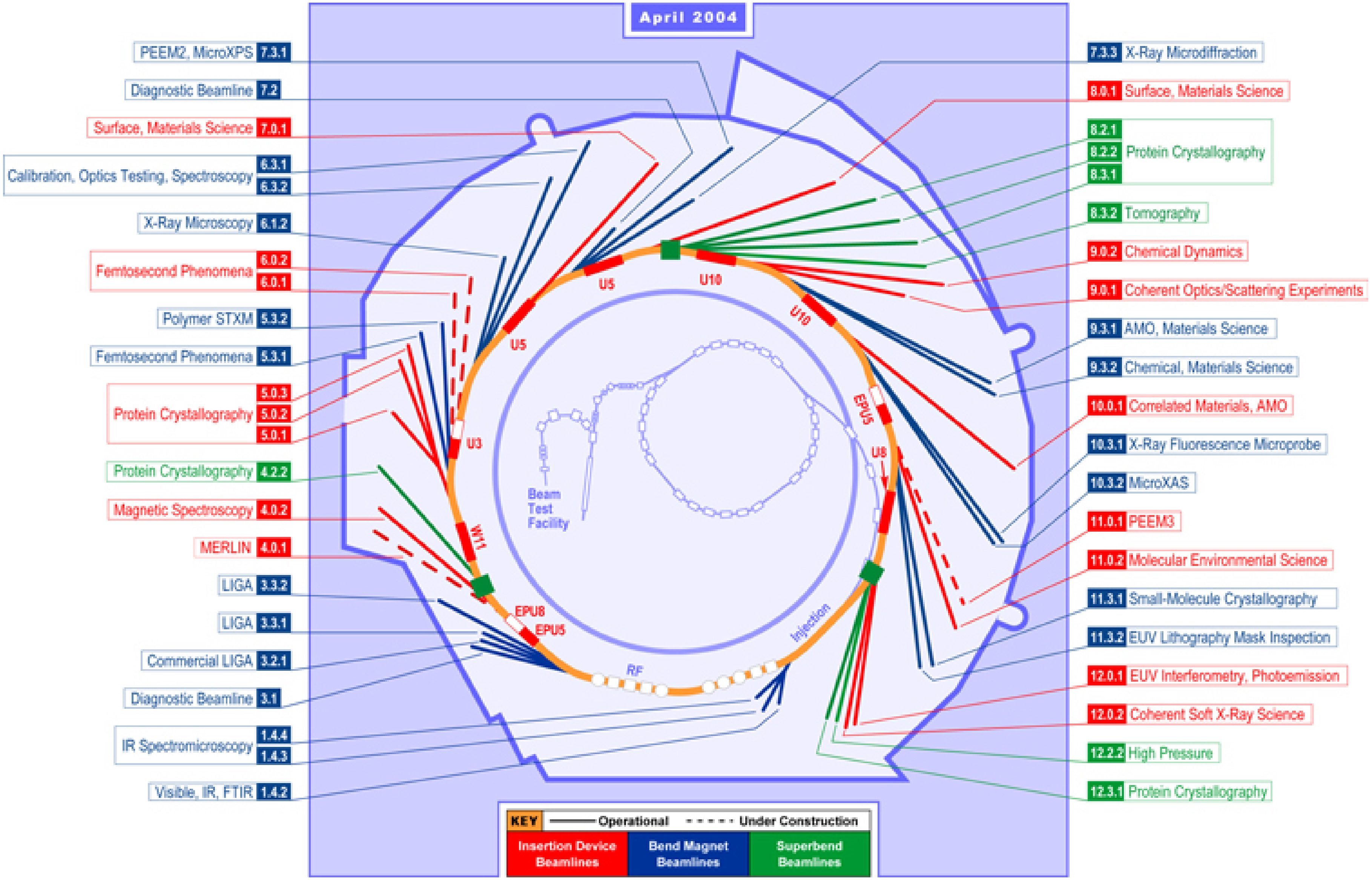
1.9 Gev storage ring, bend magnet critical energy = 2.5 keV

Undulator radiation from 10 to 2000 eV for spectroscopy and microscopy

Hard x-rays from wigglers and superbends for structure studies up to about 40keV

jc/ALSaerial/11-96

ALS Beam Lines



April 2004

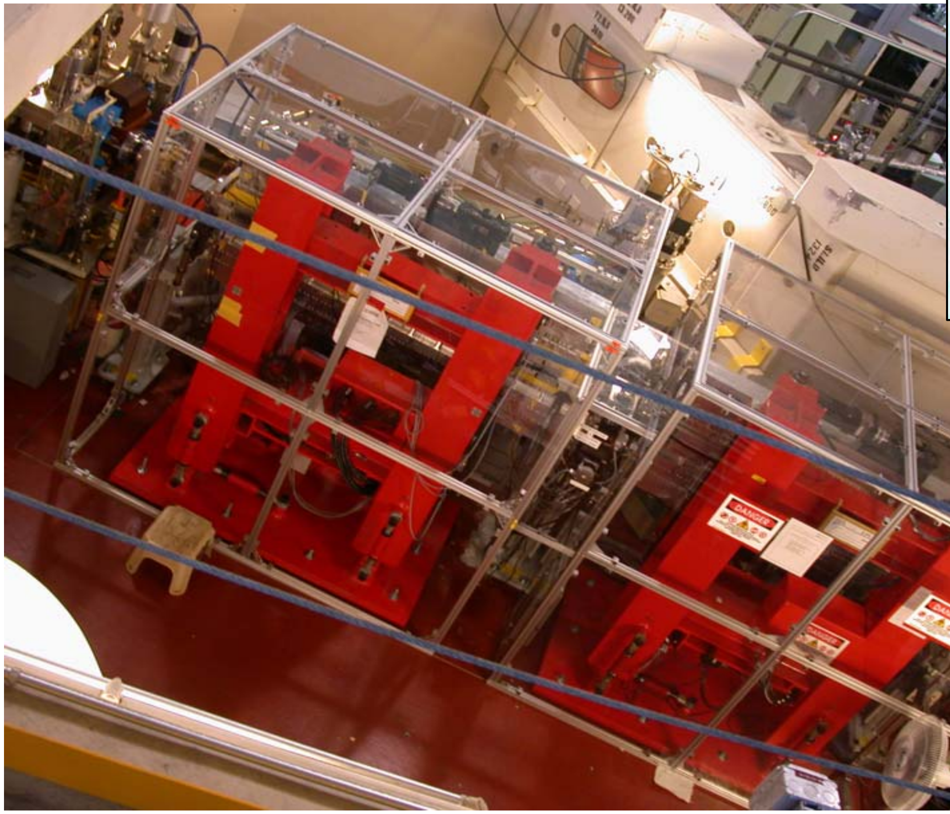
PEEM2, MicroXPS 7.3.1
Diagnostic Beamline 7.2
Surface, Materials Science 7.0.1
Calibration, Optics Testing, Spectroscopy 6.3.1
6.3.2
X-Ray Microscopy 6.1.2
Femtosecond Phenomena 6.0.2
6.0.1
Polymer STXM 5.3.2
Femtosecond Phenomena 5.3.1
Protein Crystallography 5.0.3
5.0.2
5.0.1
Protein Crystallography 4.2.2
Magnetic Spectroscopy 4.0.2
MERLIN 4.0.1
LIGA 3.3.2
LIGA 3.3.1
Commercial LIGA 3.2.1
Diagnostic Beamline 3.1
IR Spectromicroscopy 1.4.4
1.4.3
Visible, IR, FTIR 1.4.2

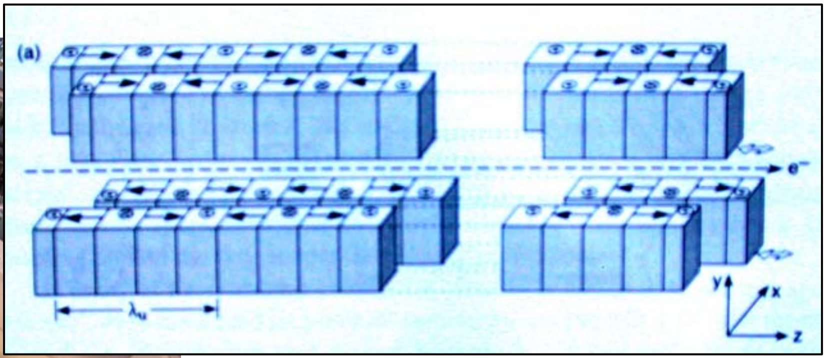
7.3.3 X-Ray Microdiffraction
8.0.1 Surface, Materials Science
8.2.1
8.2.2
8.3.1 Protein Crystallography
8.3.2 Tomography
9.0.2 Chemical Dynamics
9.0.1 Coherent Optics/Scattering Experiments
9.3.1 AMO, Materials Science
9.3.2 Chemical, Materials Science
10.0.1 Correlated Materials, AMO
10.3.1 X-Ray Fluorescence Microprobe
10.3.2 MicroXAS
11.0.1 PEEM3
11.0.2 Molecular Environmental Science
11.3.1 Small-Molecule Crystallography
11.3.2 EUV Lithography Mask Inspection
12.0.1 EUV Interferometry, Photoemission
12.0.2 Coherent Soft X-Ray Science
12.2.2 High Pressure
12.3.1 Protein Crystallography

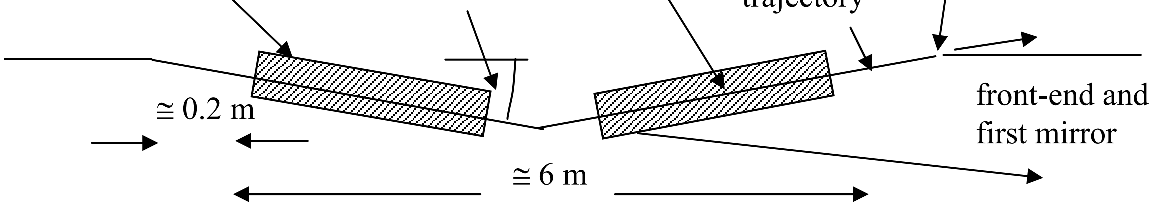
Synchrotron (soft x-ray) beam lines

- **undulator sources** *Maxwell's equations tell all*
- **diffractive structures for wavelength selection** *you need this, sorry*
- **diffraction gratings** *ancient practice*
- **aberration analysis** *a simple thing made complicated*
- **ray tracing** *a complicated thing made simple*
- **tuning and commissioning** *you really know what you are doing*
- **some beam lines** *optics of modern designs*
- **beam line technology** *engineering of modern designs*
- **micro-focusing** *you want this*
- **optimized user facilities** *you want this too*

Two Elliptically Polarizing Undulators







undulator in the upstream position

undulator in the downstream position

1.08 mrad

electron trajectory

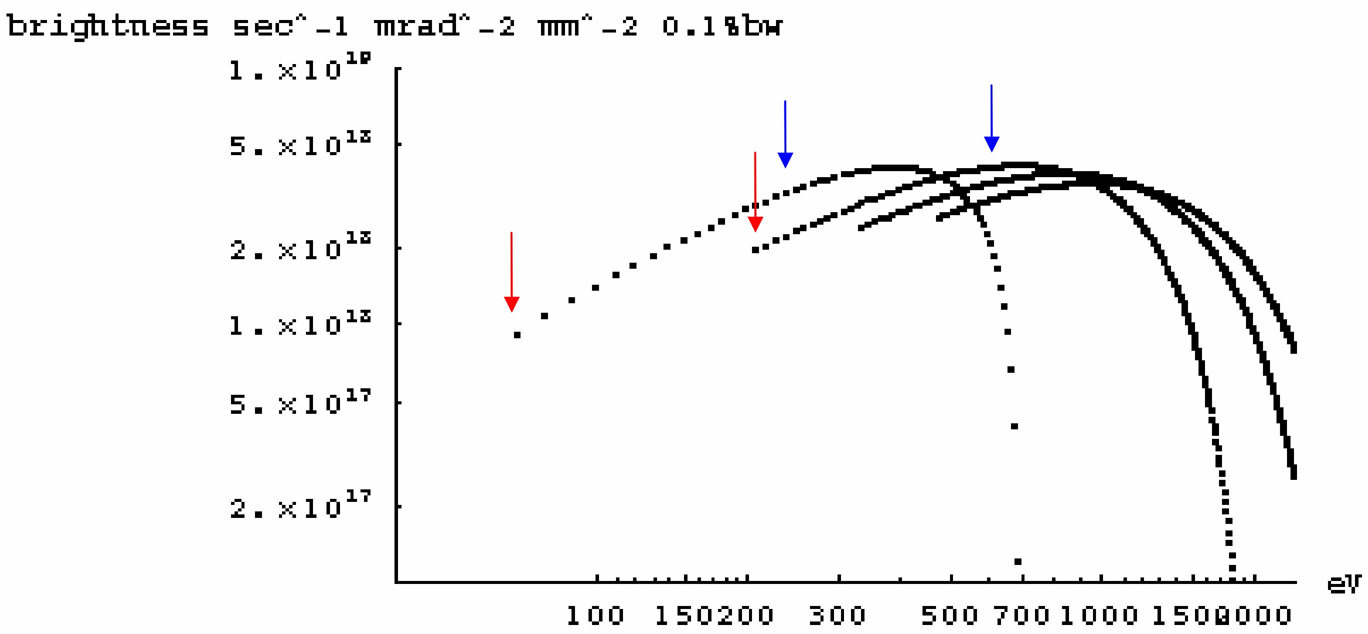
corrector magnet

≅ 0.2 m

≅ 6 m

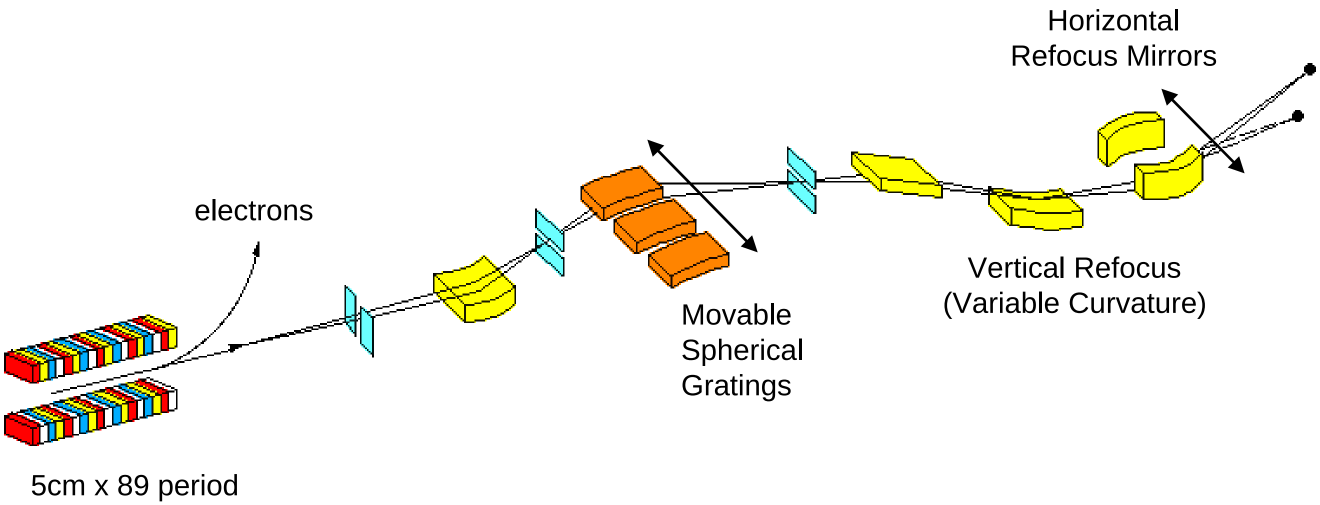
front-end and first mirror

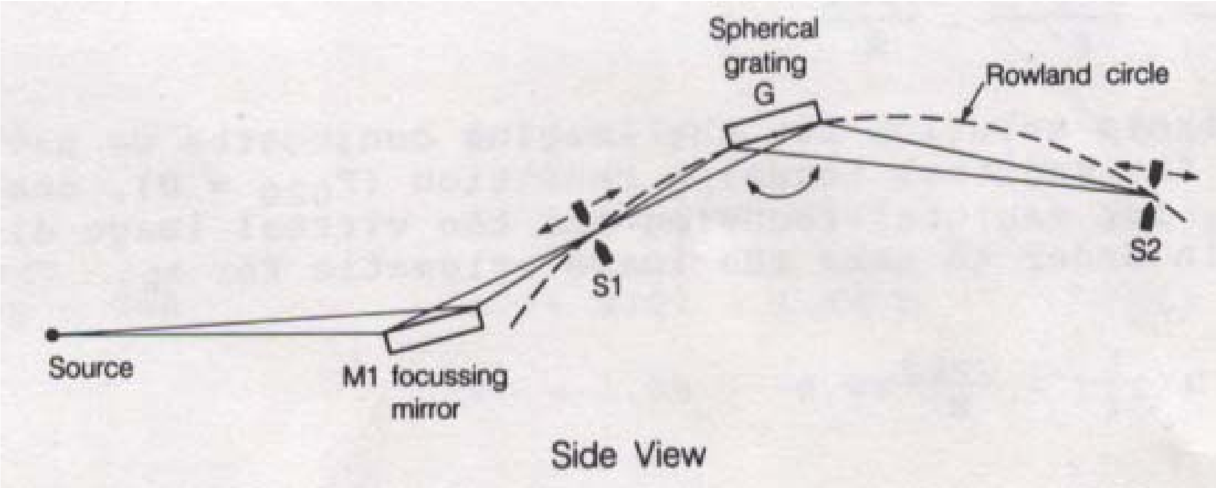
Elliptically Polarizing Undulator



Undulator brightness, harmonics 1 through 7, linear polarization.
5.0cm period, 37 periods, 400mA, 1.9GeV, 1x10^-4 dE/E
horizontal polarization:
13.0mm gap ky=4.307, lowest energy=66.753eV
vertical polarization:
13mm gap kx≈2.0, lowest energy=228.633eV
Note, the higher harmonics lose brightness if the energy spread increases.

Spherical Grating Monochromator Line at ALS

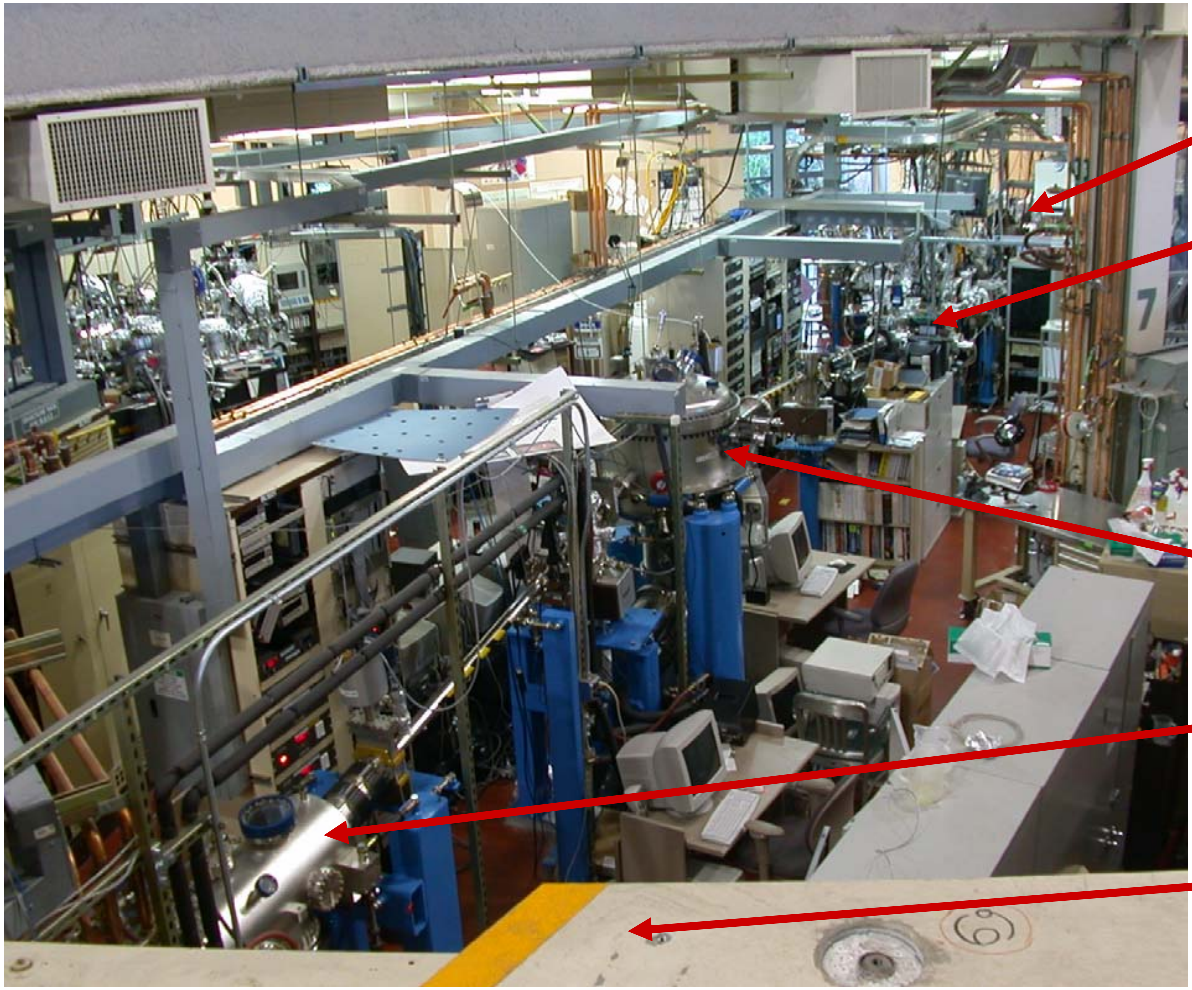




10^{12} photons
per second

$\Delta E/E = 2\ 10^{-4}$

Grating Monochromator Undulator Line



User area

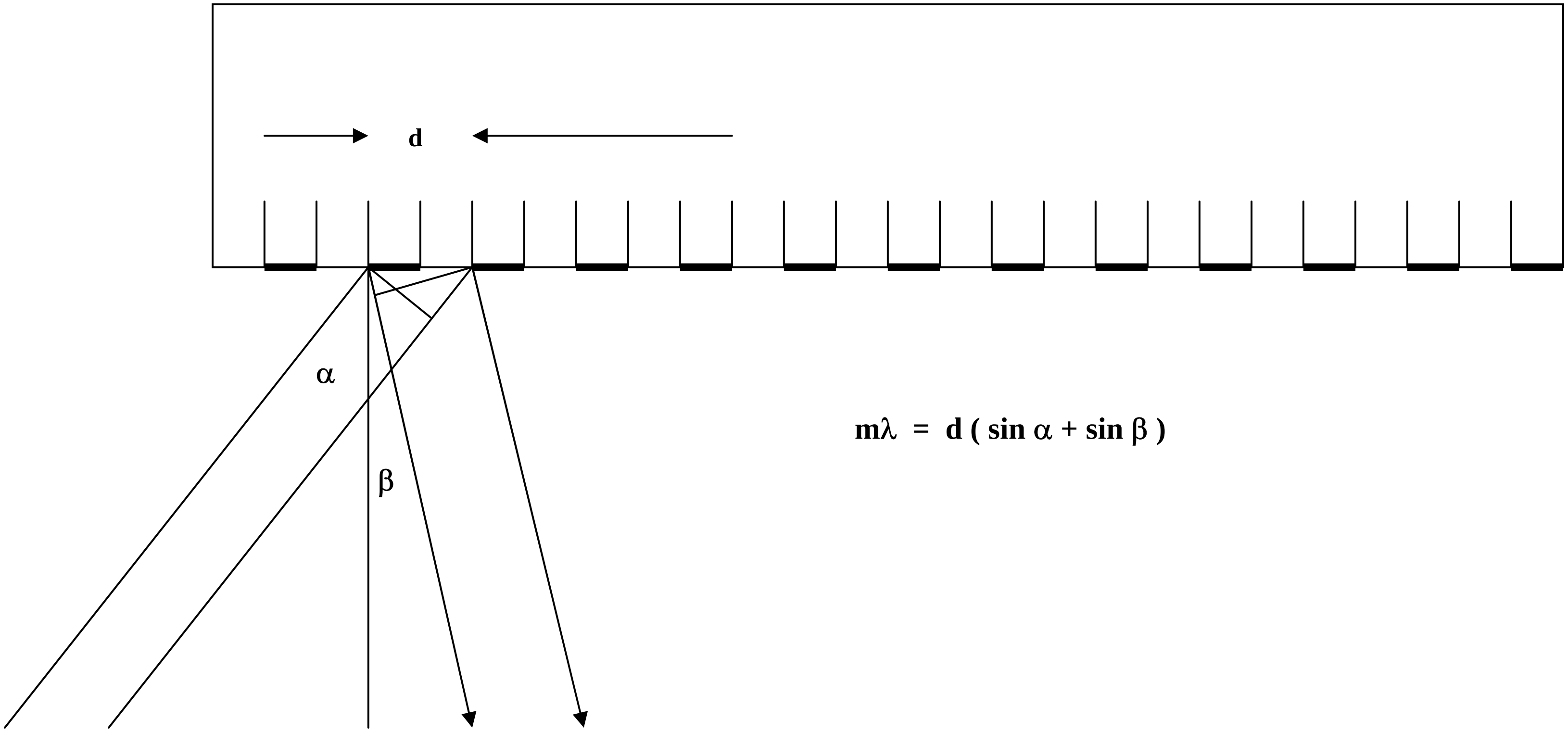
Exit Slits

Grating Chamber

First mirror

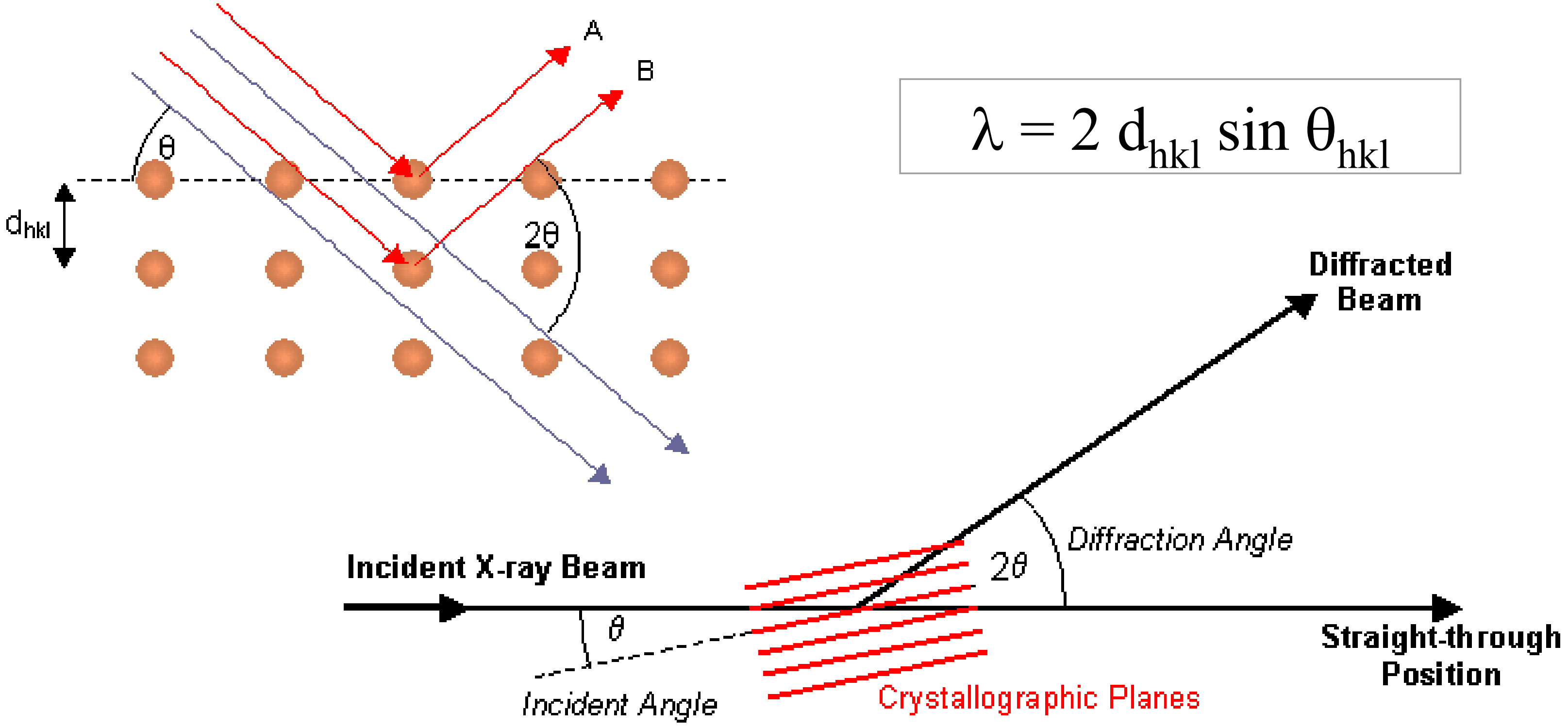
Storage ring shield wall

Diffraction Grating



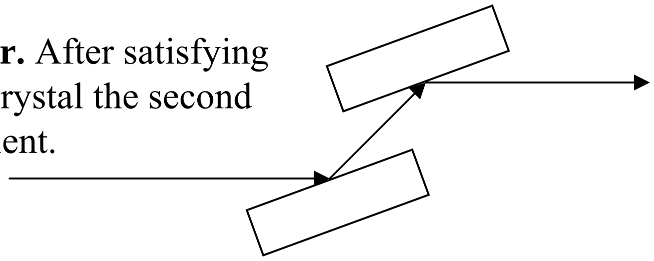
$$m\lambda = d(\sin\alpha + \sin\beta)$$

Crystal Diffraction



$$\lambda = 2\, d_{hkl} \sin \theta_{hkl}$$

Double crystal monochromator. After satisfying the Bragg condition at the first crystal the second diffraction is almost 100% efficient.



Data for selected crystals

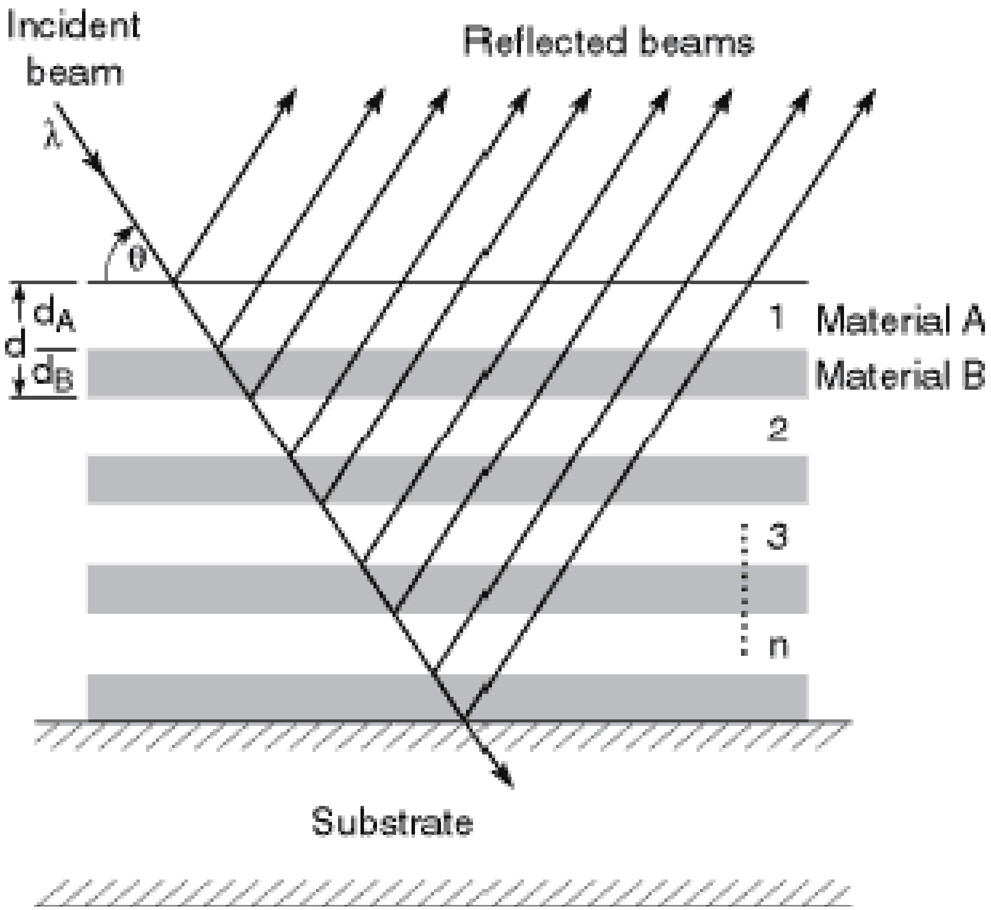
Data for selected crystals used as dispersive elements in x-ray spectrometers and monochromators.

Silicon	(111)*	6.2712	Si	Very rugged and stable general-purpose crystal. High degree of perfection obtainable. Cryogenic silicon has zero expansion.
Germanium	(111)*	6.532	Ge	Eliminates second order. Useful for intermediate- and low-*Z* elements where Ge $K\alpha$ emission is eliminated by pulse-height selection.
Indium antimonide	(111)	7.4806	InSb	Important for *K*-edge of Si at 1.8keV.
Diamond	(400)	1.742	C	General purpose substitute for silicon when heat load is very high, better thermal properties.

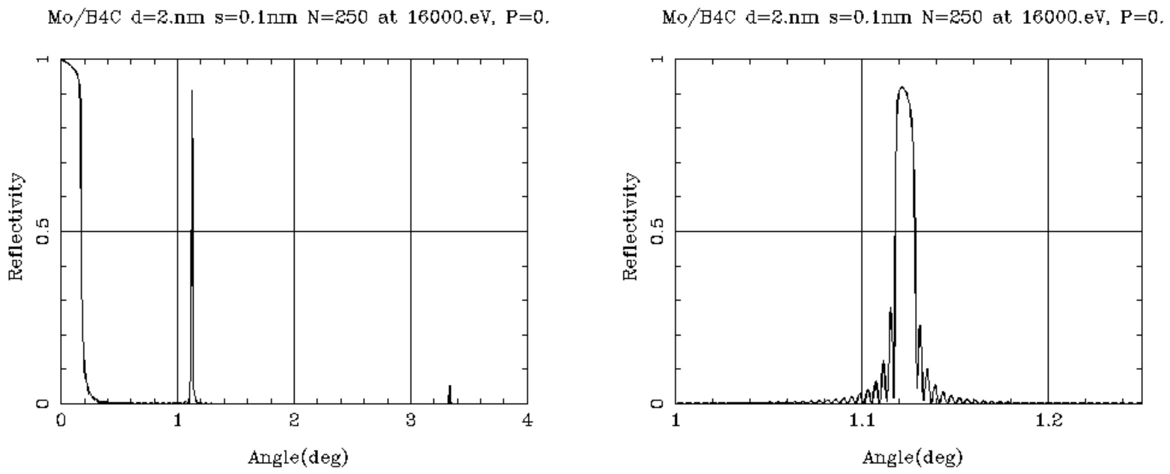
Side view of the Double Crystal Monochromator

Side view of the Double Crystal Monochromator for I.D. 31 at E.S.R.F. on 50° position. The resolution for the roll of both the groups is 1 µrad as the resolution of the coarse pitch of the secondary group. On this movement an additional piezo actuator allows a much fine movement (0.5 µrad). The translations perpendicular to the crystal surface have a resolution of 0.1 µm for both the crystal groups. The translation of the secondary group has also a resolution of 0.5 µm.

Diffraction from synthetic multilayers

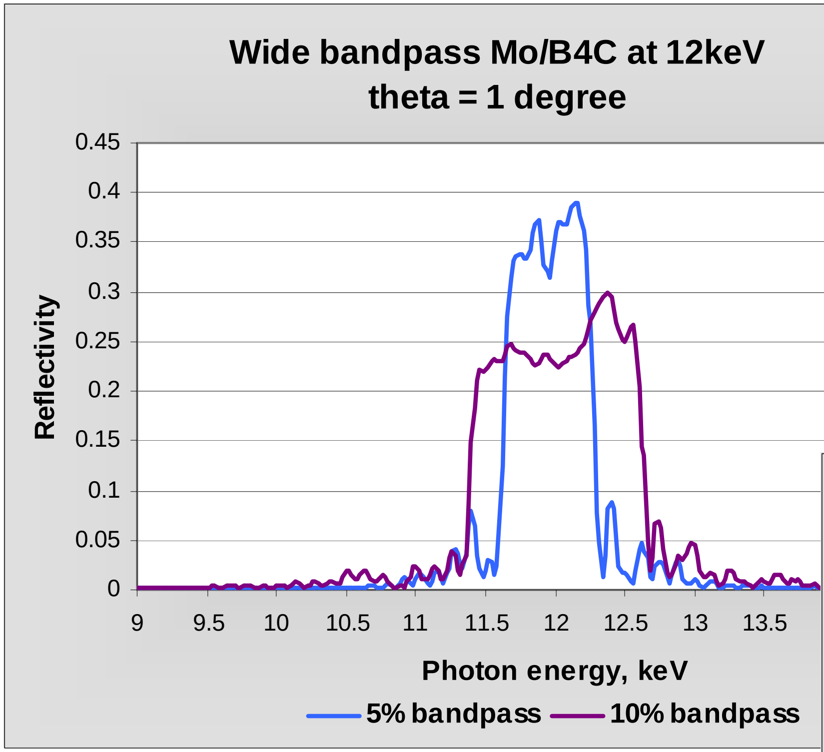


Diffraction from synthetic multilayers

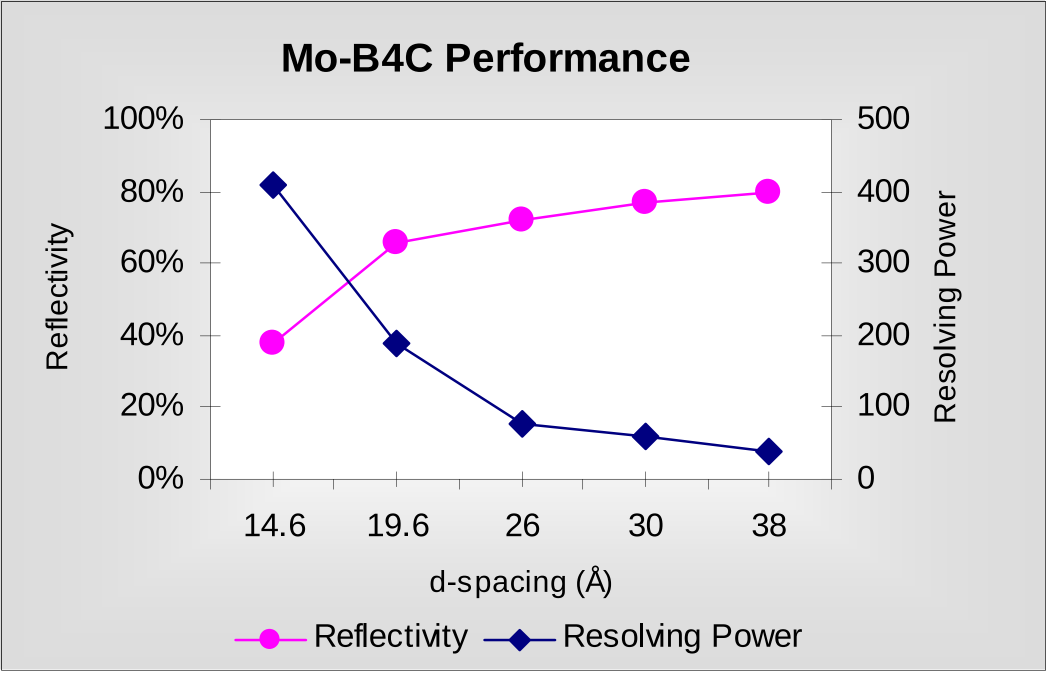


The Bragg angle is 1.122 degrees to maximize the reflectivity at 16 keV (92%). The 3rd order contamination is about 4%.

Engineered Bandpass Multilayer X-ray Optics



Figures from Osmic Inc.



Ruling Engines

Leonardo daVinci

c1475

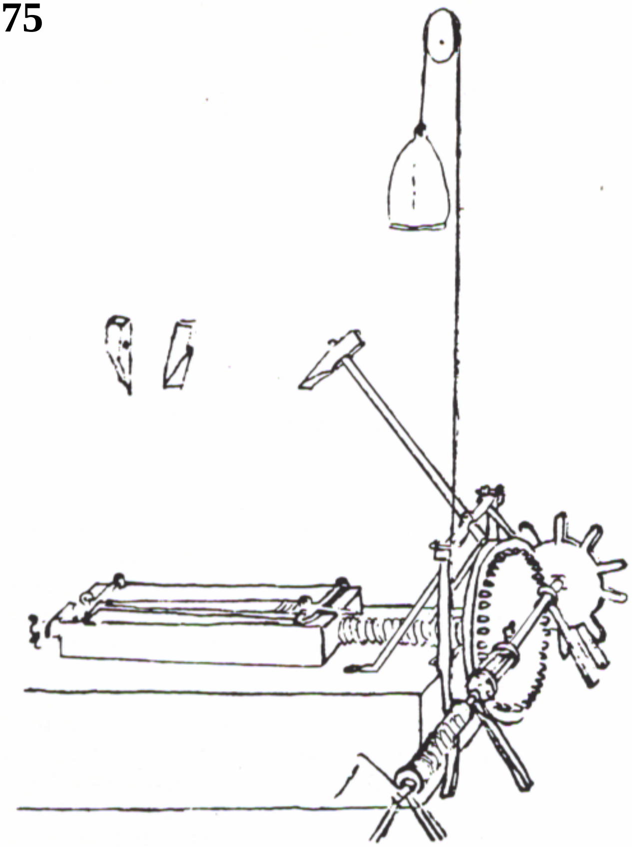


FIG 5.1 Leonardo's file making machine

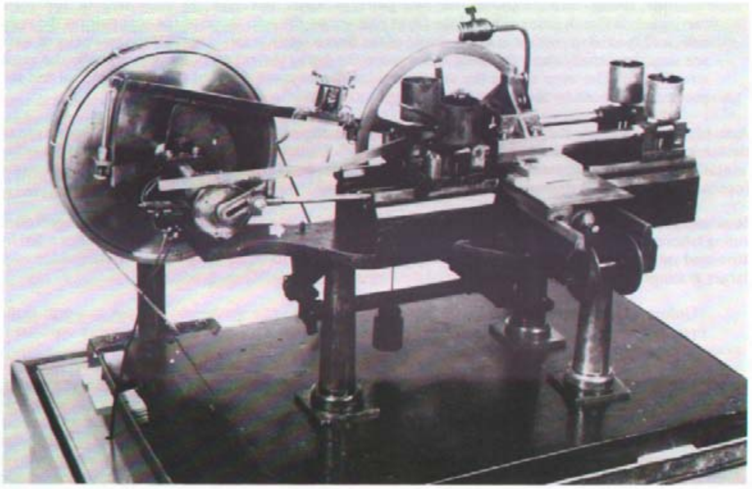
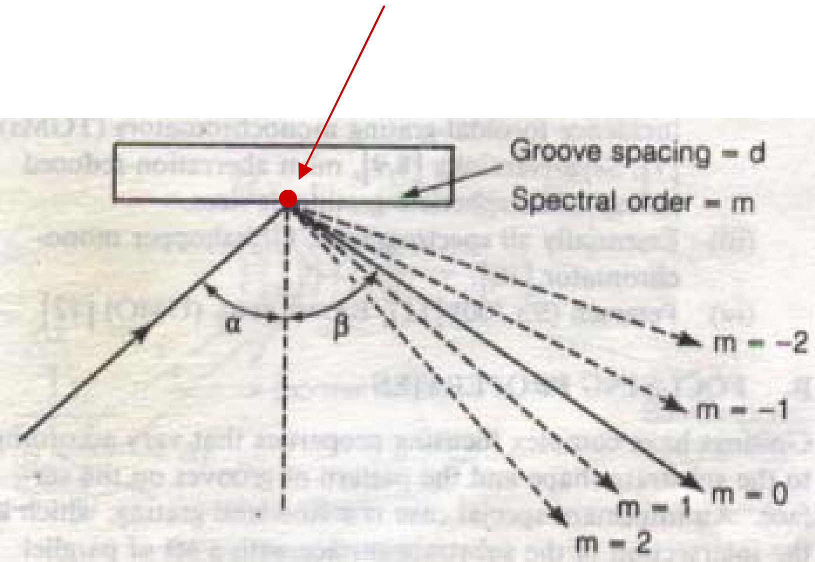


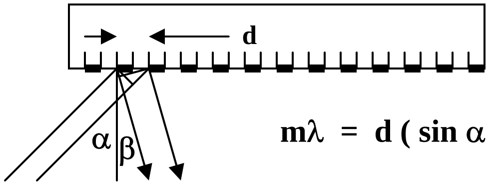
FIG 5.9 Rowland's ruling engine (Smithsonian Institution neg #72-7868)

Henry Rowland c1875

Water Cooled Copper Diffraction Gratings

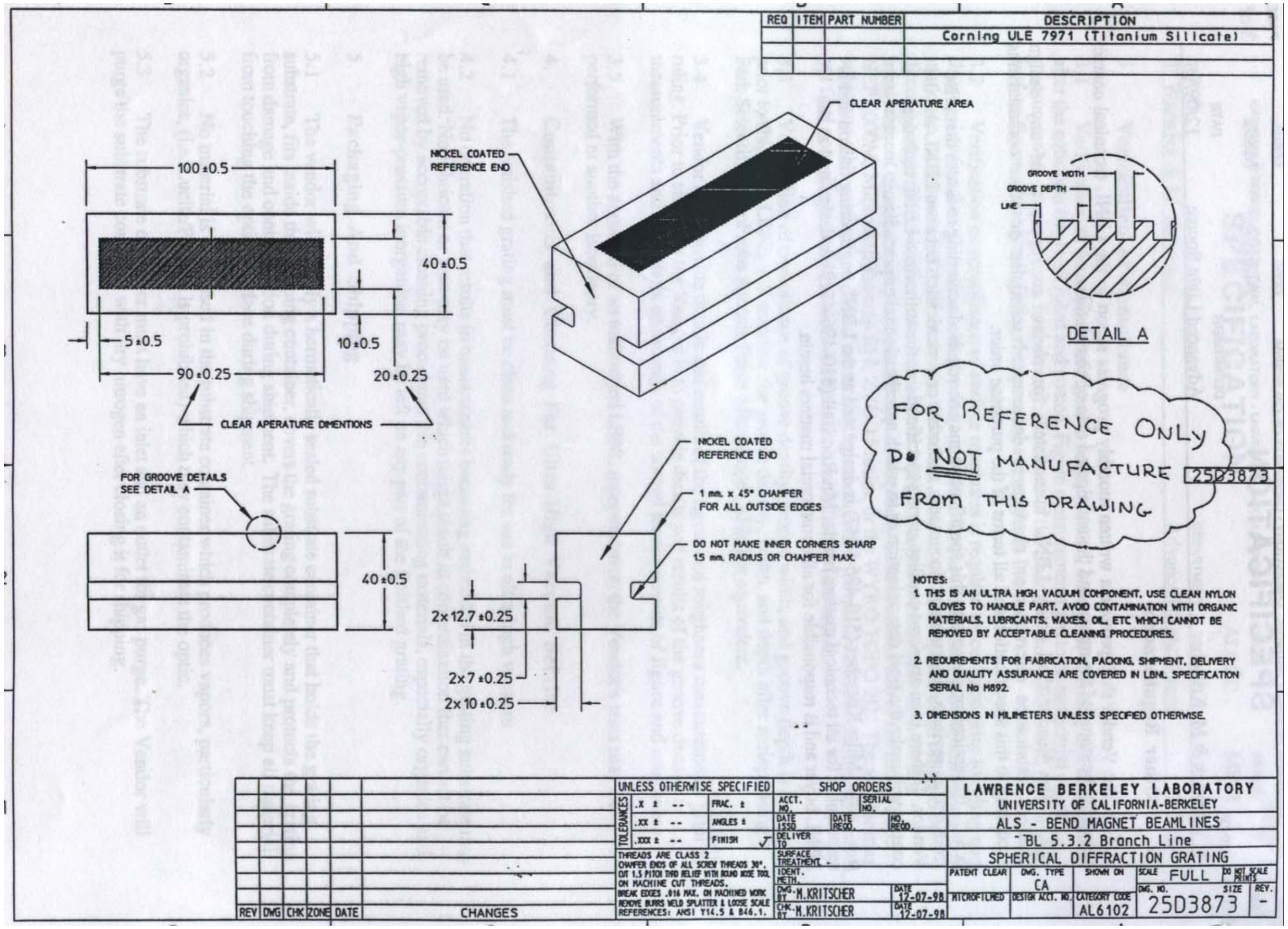
rotation axis





$$m\lambda = d\,(\sin\alpha + \sin\beta)$$

Grating Specification for Holographic Ruling



REQ	ITEM	PART NUMBER	DESCRIPTION
			Corning ULE 7971 (Titanium Silicate)

FOR REFERENCE ONLY
DO NOT MANUFACTURE
FROM THIS DRAWING

NOTES:

1. THIS IS AN ULTRA HIGH VACUUM COMPONENT. USE CLEAN NYLON GLOVES TO HANDLE PART. AVOID CONTAMINATION WITH ORGANIC MATERIALS, LUBRICANTS, WAXES, OIL, ETC WHICH CANNOT BE REMOVED BY ACCEPTABLE CLEANING PROCEDURES.
2. REQUIREMENTS FOR FABRICATION, PACKING, SHIPMENT, DELIVERY AND QUALITY ASSURANCE ARE COVERED IN LBNL SPECIFICATION SERIAL No M892.
3. DIMENSIONS IN MILIMETERS UNLESS SPECIFIED OTHERWISE.

REV	DWG	CHK	ZONE	DATE	CHANGES

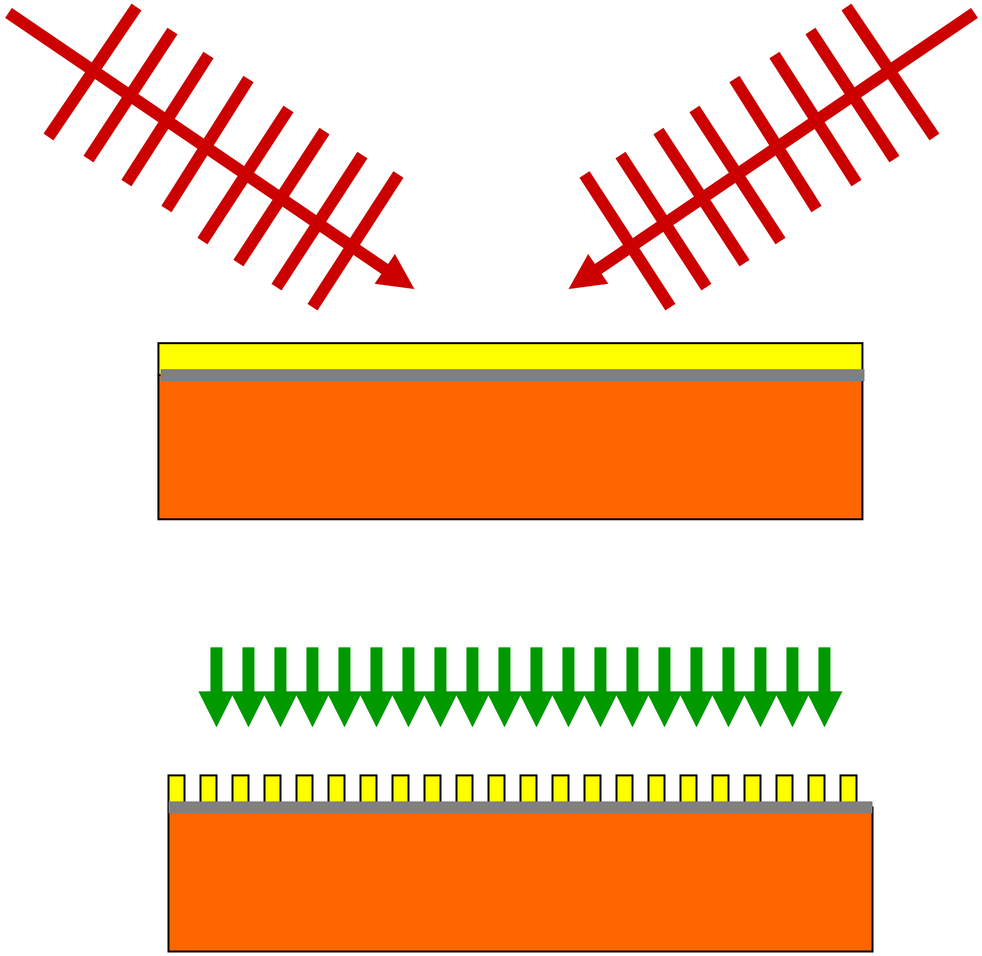
UNLESS OTHERWISE SPECIFIED
TOLERANCES
.X ± --
.XX ± --
.XXX ± --
FRAC. ±
ANGLES ±
FINISH √
THREADS ARE CLASS 2
CHAMFER ENDS OF ALL SCREW THREADS 30°.
CUT 1.5 PITCH THD RELIEF WITH ROUND NOSE TOOL ON MACHINE CUT THREADS.
BREAK EDGES .016 MAX. ON MACHINED WORK
REMOVE BURRS WELD SPLATTER & LOOSE SCALE
REFERENCES: ANSI Y14.5 & B46.1.

SHOP ORDERS
ACCT. NO.
SERIAL NO.
DATE ISSD
DATE REQD.
NO. REQD.
DELIVER TO
SURFACE TREATMENT -
IDENT. METH.
DWG. BY M.KRITSCHER DATE 12-07-98
CHK. BY M.KRITSCHER DATE 12-07-98

LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA-BERKELEY
ALS - BEND MAGNET BEAMLINES
BL 5.3.2 Branch Line
SPHERICAL DIFFRACTION GRATING
PATENT CLEAR
DWG. TYPE CA
SHOWN ON
SCALE FULL
DO NOT SCALE PRINTS
MICROFILMED
DESIGN ACCT. NO.
CATEGORY CODE AL6102
DWG. NO. 25D3873
SIZE
REV. -

Tony Warwick, Advanced Light Source

Holographic Ruling



interfering laser beams

photo resist

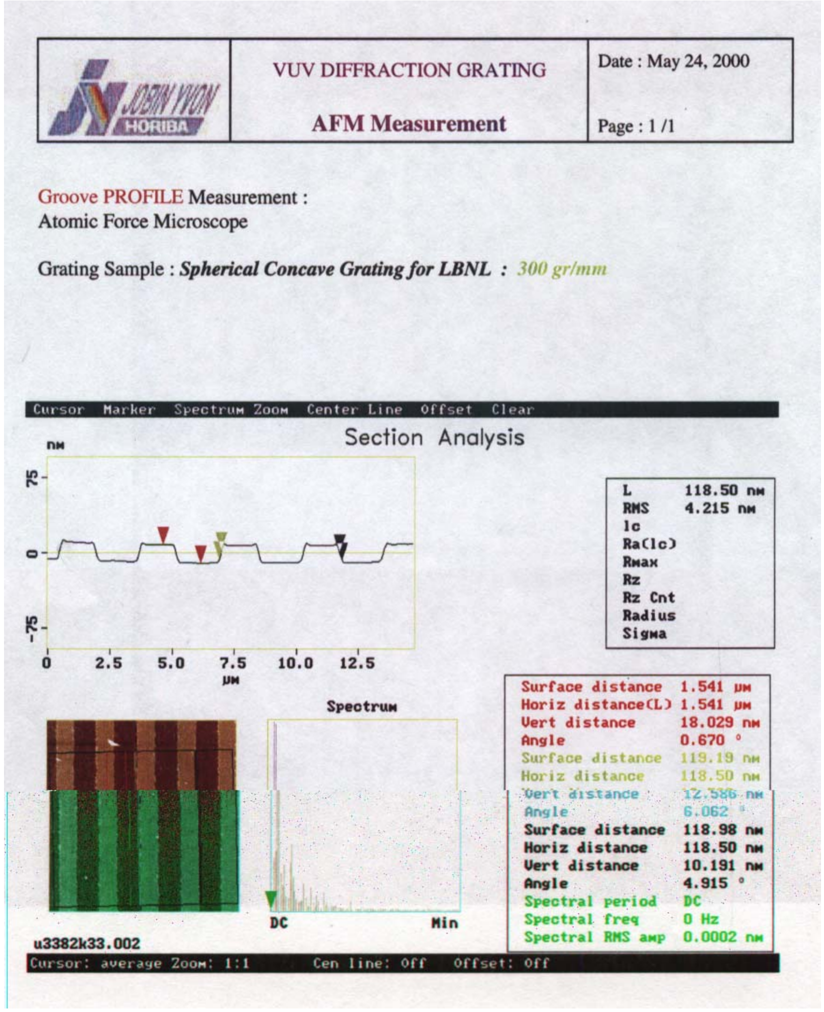
nickel

copper

ion etch

shallow grooves in nickel

High Quality Product, AFM Verification



VUV DIFFRACTION GRATING

AFM Measurement

Date : May 24, 2000

Page : 1 /1

Groove PROFILE Measurement :
Atomic Force Microscope

Grating Sample : ***Spherical Concave Grating for LBNL*** **:** *300 gr/mm*

Section Analysis

```
L          118.50 nm
RMS        4.215 nm
lc
Ra(lc)
Rmax
Rz
Rz Cnt
Radius
Sigma
```

```
Surface distance     1.541 μm
Horiz distance(L)    1.541 μm
Vert distance        18.029 nm
Angle                0.670 °
Surface distance     119.19 nm
Horiz distance       118.50 nm
Vert distance        12.586 nm
Angle                6.062 °
Surface distance     118.98 nm
Horiz distance       118.50 nm
Vert distance        10.191 nm
Angle                4.915 °
Spectral period      DC
Spectral freq        0 Hz
Spectral RMS amp     0.0002 nm
```

u3382k33.002

grooves about
1μm wide
20nm deep

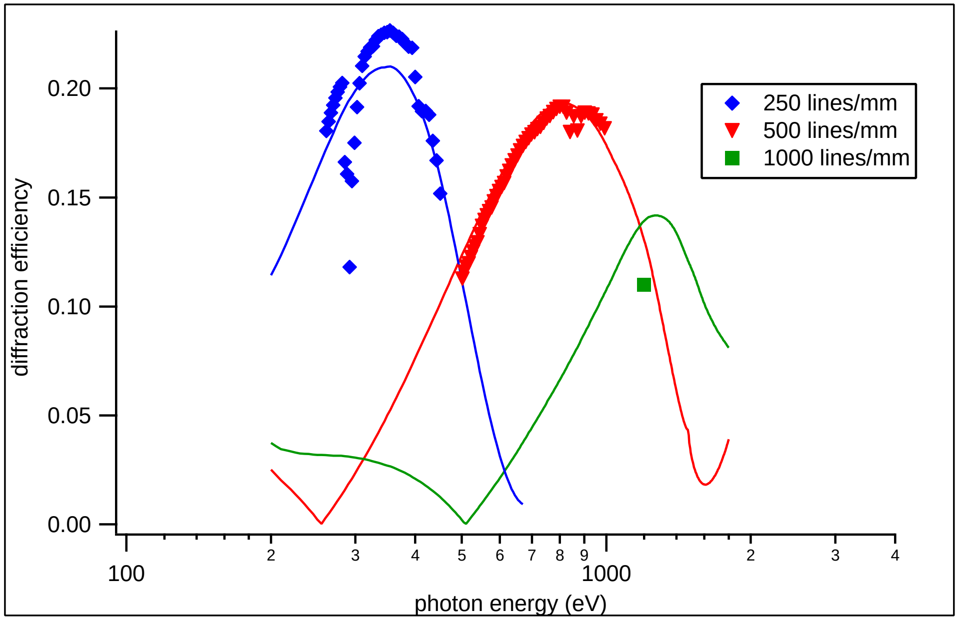
Triple VLS grating (Carl Zeiss)

Efficiency can be calculated:

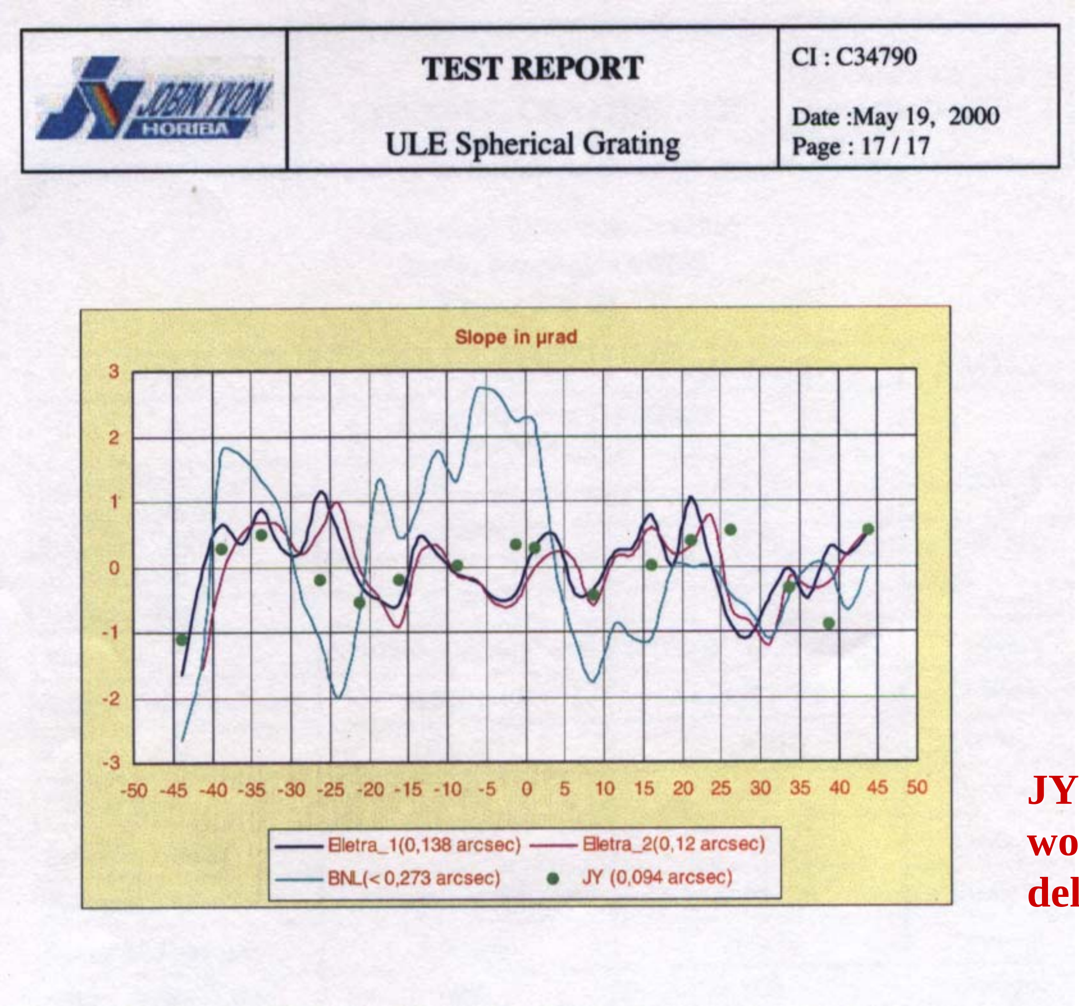
Just solve Maxwell’s equations with a conducting periodic boundary condition

(Neviere)

Zeiss triple VLS grating.
Neviere computations versus
measured diffraction efficiency
2 theta = 176 degrees



Surface Figure Error for Diffraction Gratings



TEST REPORT

ULE Spherical Grating

CI : C34790

Date :May 19, 2000
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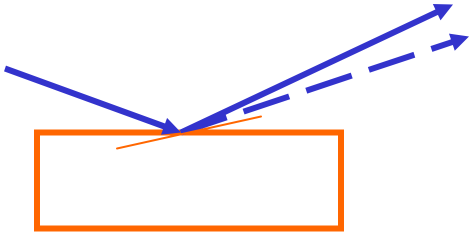


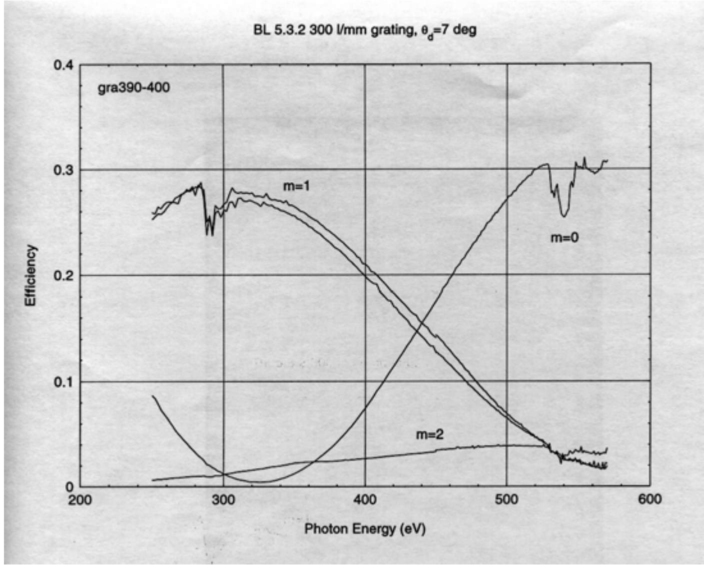
e.g. 1µrad @ 5m = 10µm

JY sent their product around the world to be measured before delivery to ALS

Cleanliness for Spectroscopy at C 1s edge 300eV

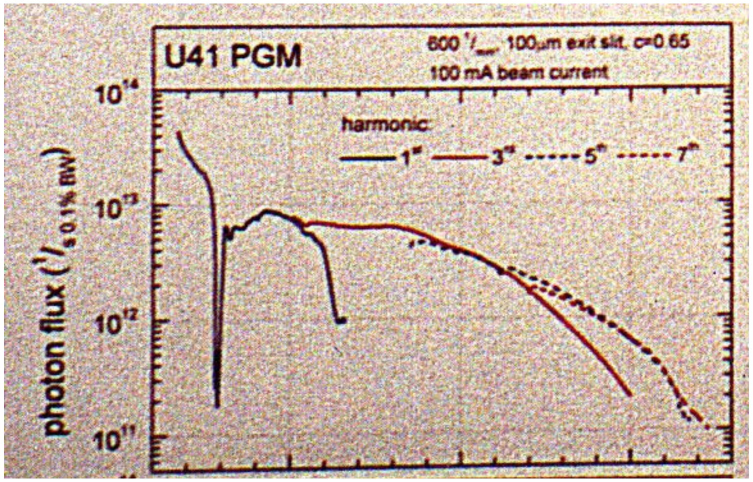
clean…..

New grating for ALS 5.3.2 (from Jobin-Yvon)

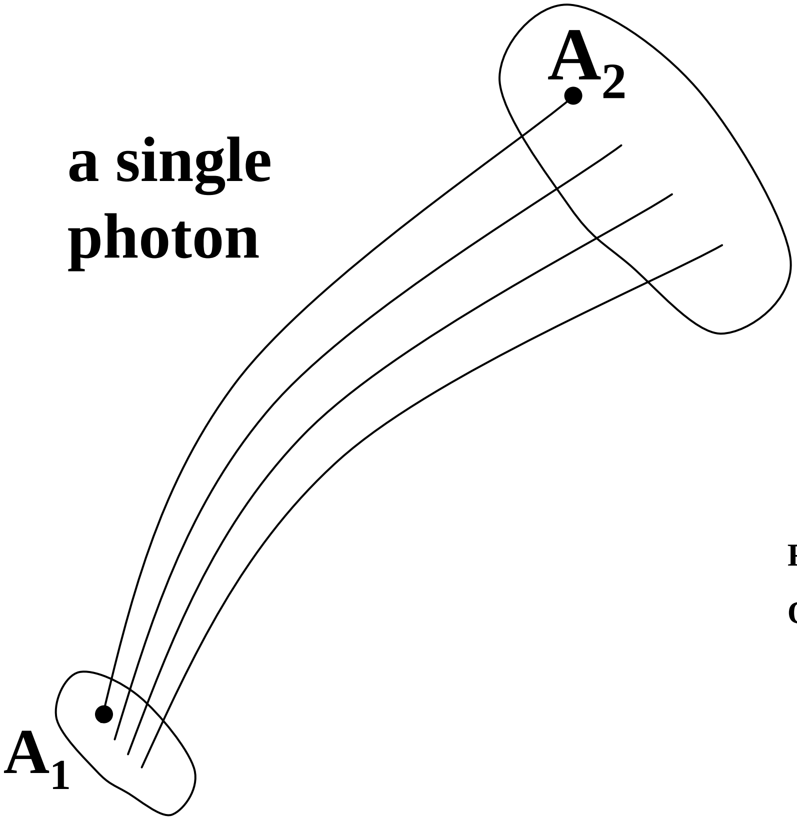


dirty…..

Jen-Optik mono at BESSY, ready for plasma cleaning



Aberration Analysis



Wavefront is a surface of specific phase.

It represents the uncertainty of the photon's transverse position.

Rays (Poynting vector) follow the 'optical path'.

They are all the same length, since the travel time at the speed of light must be the same, to maintain the phase condition as the wavefront advances.

Fermat's principle.

Optical path length is stationary.

$$\int_{A_1}^{A_2} n\,ds = c\int_{A_1}^{A_2} dt = const$$

Analysis: Express the optical path as a function of field and aperture variables, differentiate, and set the derivative to zero.

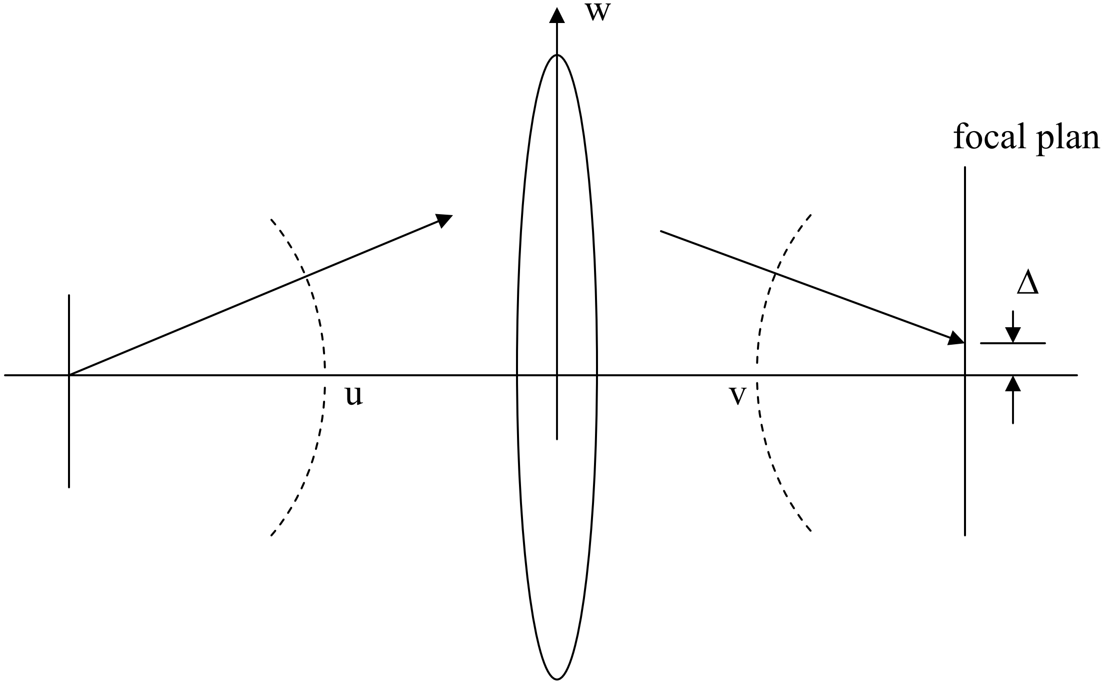
Aberration Analysis

For example: A single photon, emerging from a point source is focused by a lens.

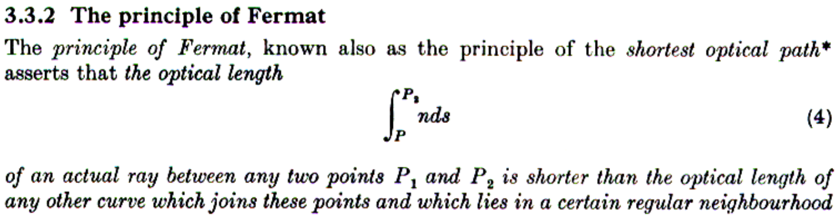
The lens (modifies the speed of light) has a thickness t(w) that is a function of the aperture variable 'w'.

Write down the length of the optical path passing through the lens at a distance 'w' from the axis in terms of t(w) and Δ.

Differentiate this with respect to w, set to zero, solve for Δ as a function of w, to describe the quality of the focus.



Aberration Analysis

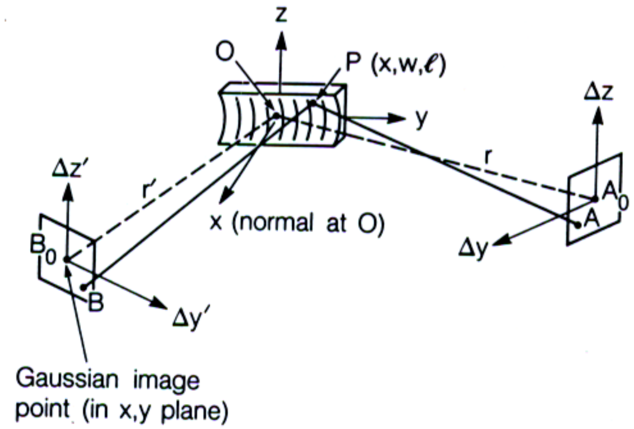


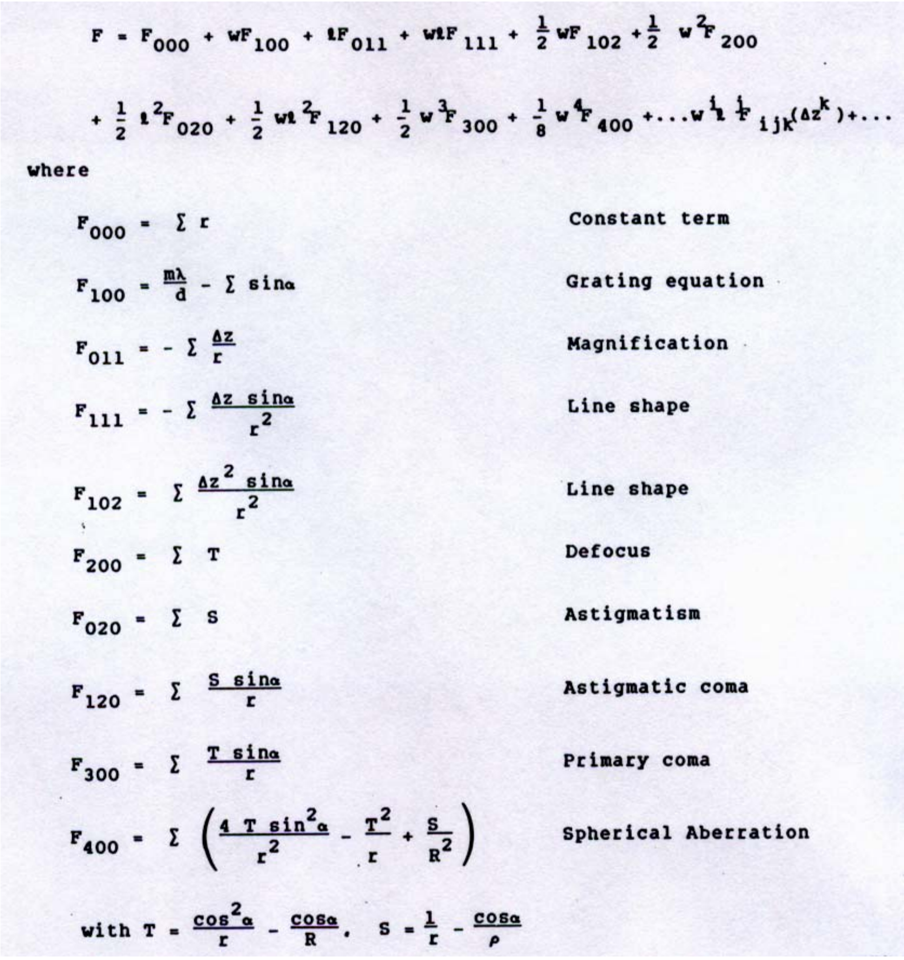
3.3.2 The principle of Fermat

The *principle of Fermat*, known also as the principle of the *shortest optical path** asserts that *the optical length*

$$\int_{P}^{P_2} n\,ds \qquad (4)$$

of an actual ray between any two points P_1 and P_2 is shorter than the optical length of any other curve which joins these points and which lies in a certain regular neighbourhood





$$F = F_{000} + wF_{100} + lF_{011} + wlF_{111} + \frac{1}{2}wF_{102} + \frac{1}{2}w^2F_{200}$$

$$+ \frac{1}{2}l^2F_{020} + \frac{1}{2}wl^2F_{120} + \frac{1}{2}w^3F_{300} + \frac{1}{8}w^4F_{400} + \ldots w^i l^j F_{ijk}(\Delta z^k) + \ldots$$

where

$F_{000} = \sum r$	Constant term
$F_{100} = \frac{m\lambda}{d} - \sum \sin\alpha$	Grating equation
$F_{011} = -\sum \frac{\Delta z}{r}$	Magnification
$F_{111} = -\sum \frac{\Delta z \sin\alpha}{r^2}$	Line shape
$F_{102} = \sum \frac{\Delta z^2 \sin\alpha}{r^2}$	Line shape
$F_{200} = \sum T$	Defocus
$F_{020} = \sum S$	Astigmatism
$F_{120} = \sum \frac{S \sin\alpha}{r}$	Astigmatic coma
$F_{300} = \sum \frac{T \sin\alpha}{r}$	Primary coma
$F_{400} = \sum \left(\frac{4T\sin^2\alpha}{r^2} - \frac{T^2}{r} + \frac{S}{R^2}\right)$	Spherical Aberration

with $T = \frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}$, $S = \frac{1}{r} - \frac{\cos\alpha}{\rho}$

If $F(w,l.....)$ is minimum

$\frac{\partial F}{\partial w}, \frac{\partial F}{\partial l}....$ must be zero

Conditions to be In-Focus and Coma-Free

Spherical grating focus condition:

$$T + T' = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \alpha}{R} \right) = 0$$

Spherical grating condition for vanishing of coma:

$$\frac{\sin \alpha}{r} \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) + \frac{\sin \beta}{r'} \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \alpha}{R} \right) = 0$$

(This condition is satisfied on the Rowland circle)

Rowland circle condition: $r = R \cos \alpha$ and $r' = R \cos \beta$

Plane grating case: $R = \infty$

$$r' = -r \frac{\cos^2 \beta}{\cos^2 \alpha} = -r\, c_{\mathrm{ff}}^2$$

Applications:

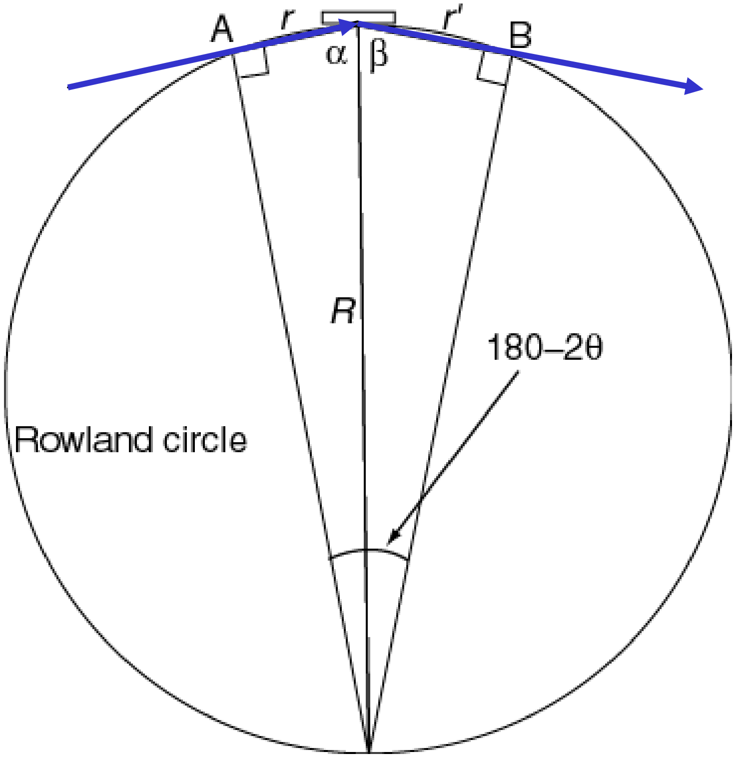
SGM’s, TGM’s

SGM’s

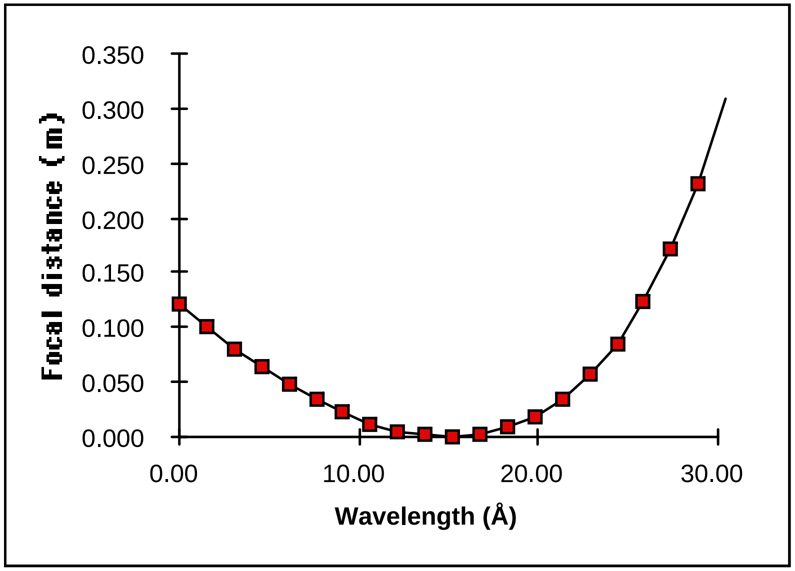
PGM’s, SX700 etc

Rowland Circle

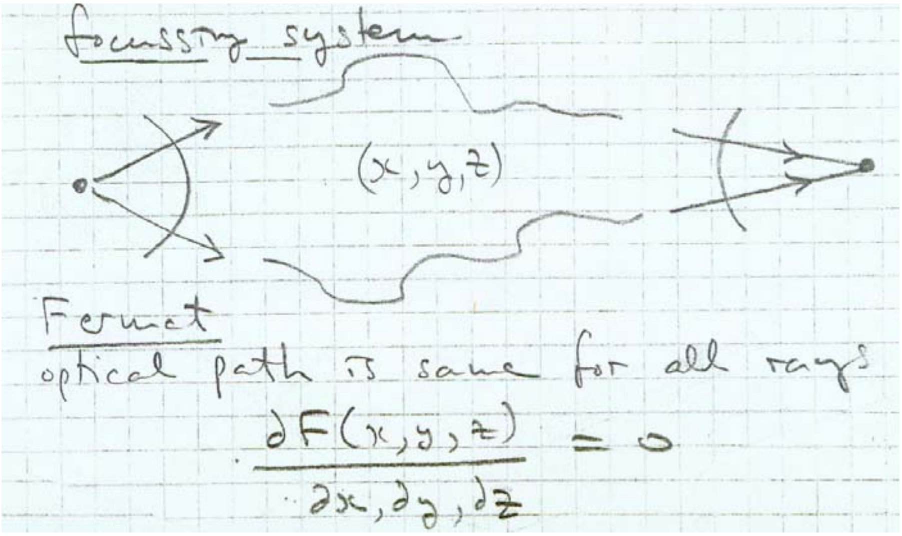
$$r = R\cos\alpha, \quad r' = R\cos\beta$$



- **Rowland Circle diameter equal to the grating radius**
- **Grating rotates, A and B need to move**
- **If A held fixed B moves to stay in focus and the Rowland condition is met at two points of the grating rotation**



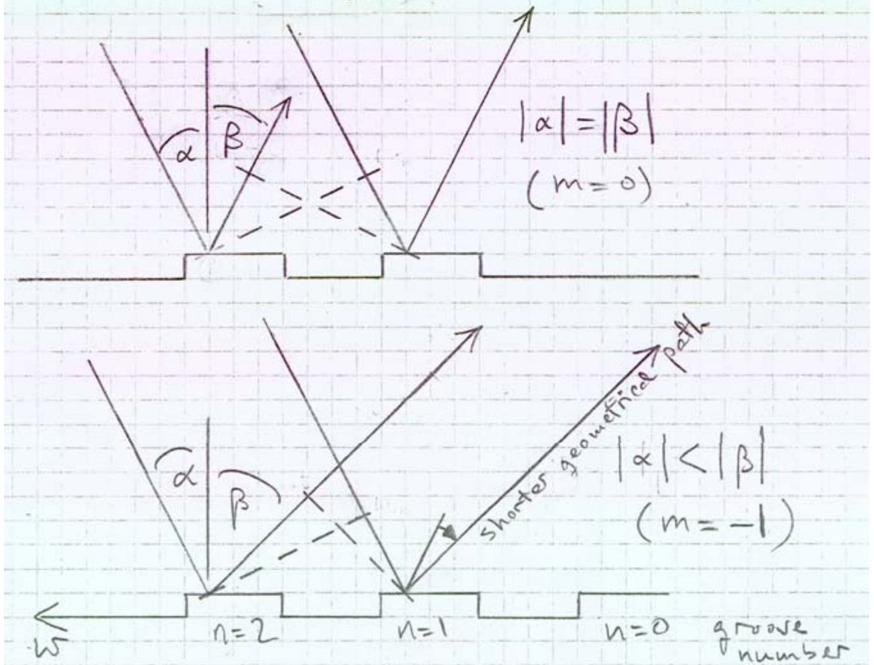
VLS features

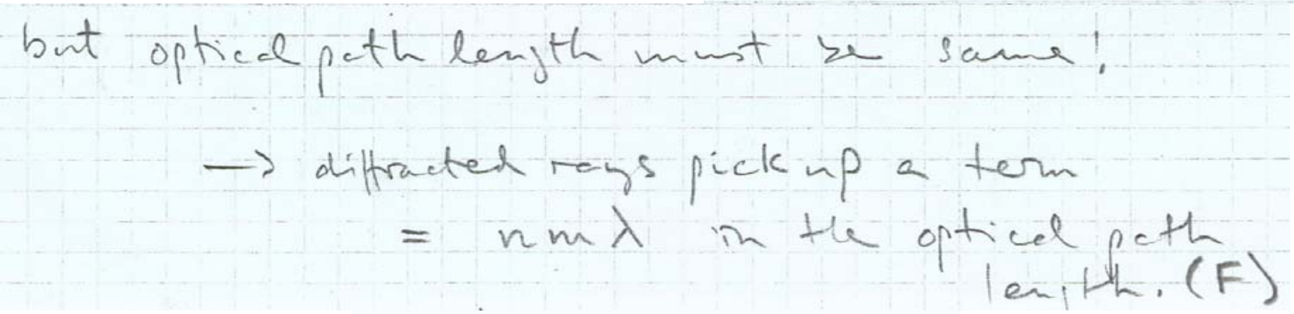


Fermat

optical path is same for all rays

$$\frac{\partial F(x,y,z)}{\partial x, \partial y, \partial z} = 0$$




but optical path length must be same!

→ diffracted rays pick up a term = $n m \lambda$ in the optical path length. (F)

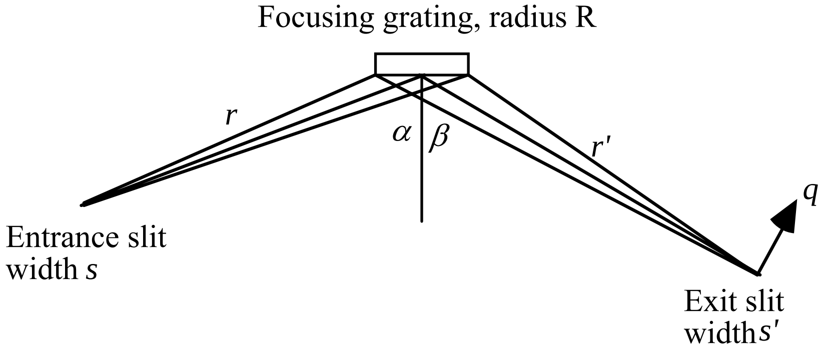

$\frac{\partial n}{\partial w}$ is groove density

Spectral Resolution of the Grating

$$m\lambda = d(\sin\alpha + \sin\beta)$$

$$\left(\frac{\partial\lambda}{\partial\beta}\right)_{\alpha} = \frac{d\cos\beta}{m}$$

$$\frac{d\lambda}{dq} = \frac{d\lambda}{d\beta}\frac{d\beta}{dq} = \frac{d\cos\beta}{mr'} \equiv \frac{10^{-3}d(\text{Å})\cos\beta}{mr'(\text{m})}\ \text{Å / mm}$$



From this we get the exit- and entrance-slit-width-limited resolutions

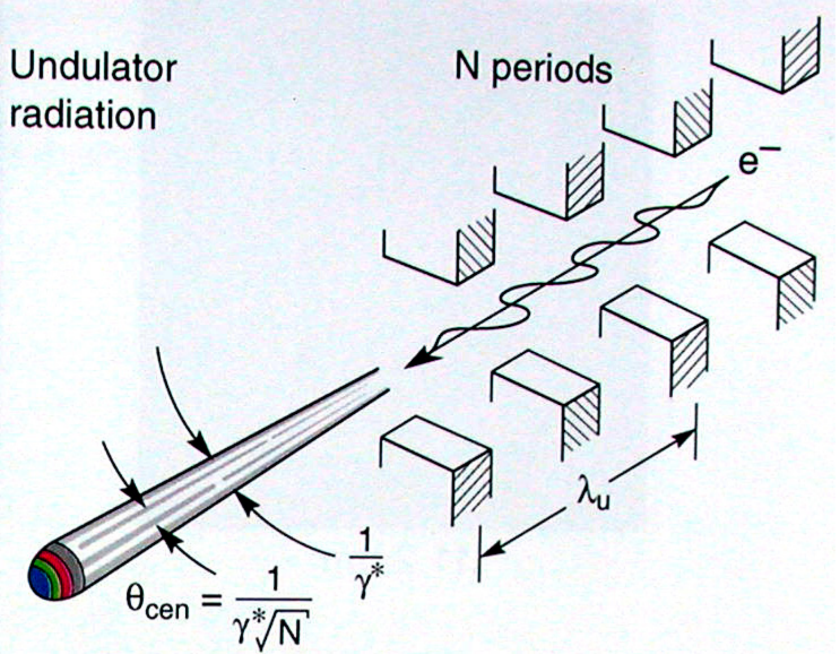
$$\Delta\lambda_s = \frac{d\cos\alpha\, s}{mr} \qquad \Delta\lambda_{s'} = \frac{d\cos\beta\, s'}{mr'}$$

Diffraction-limited resolution = 1/*N*

BUT

Provided the grating is big enough, the number of illuminated grooves is always sufficient to achieve the slit-width-limited resolution because of diffraction at the entrance slit

Undulator Radiation Patterns



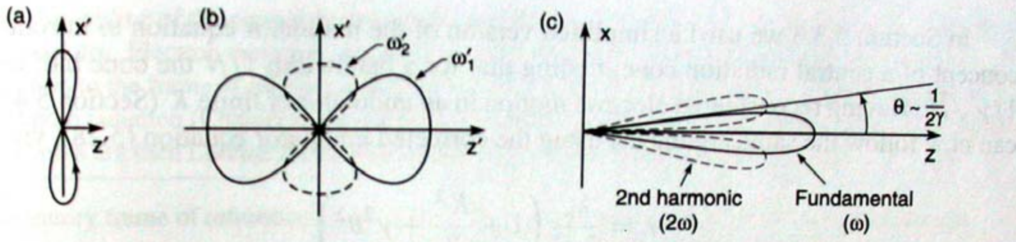
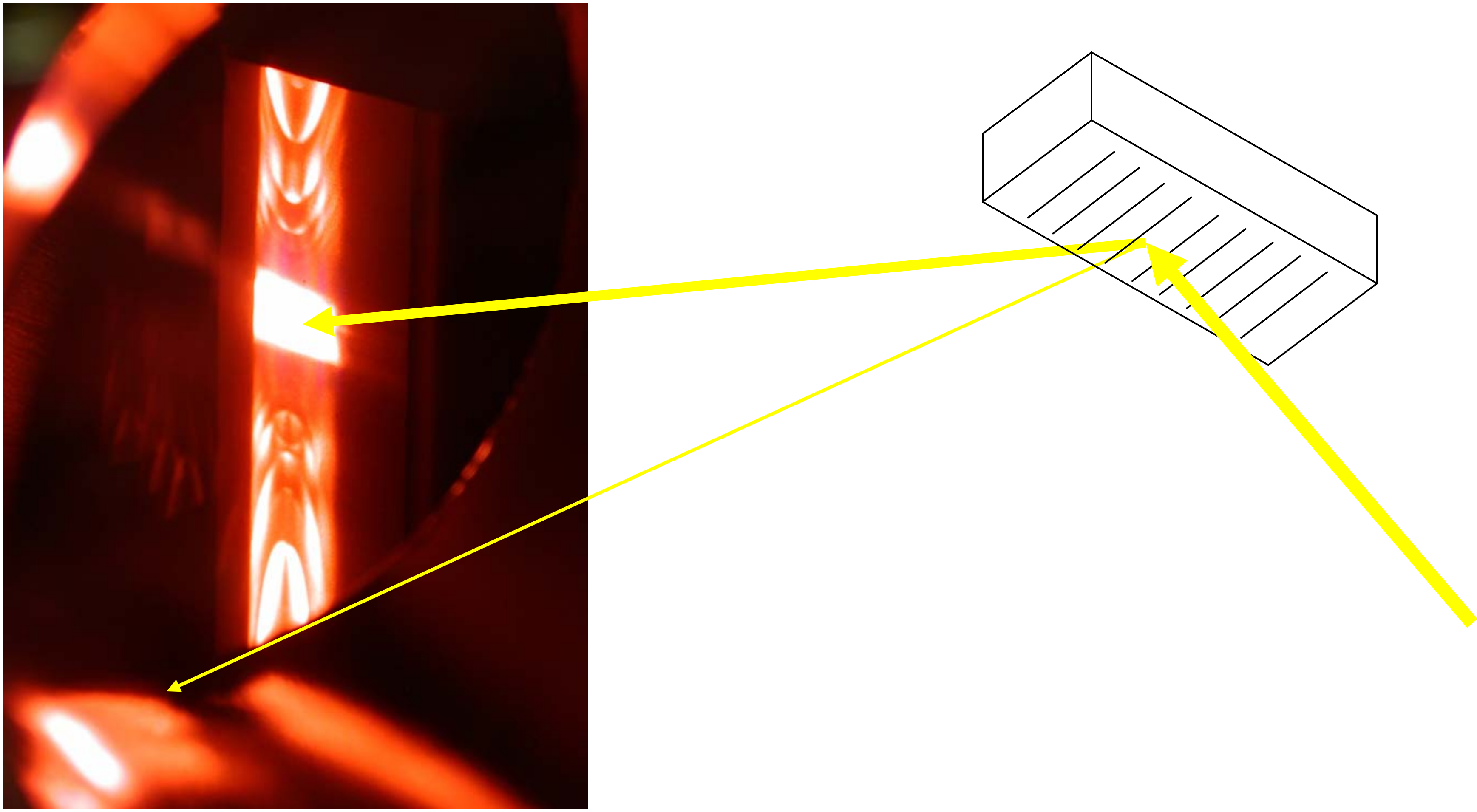
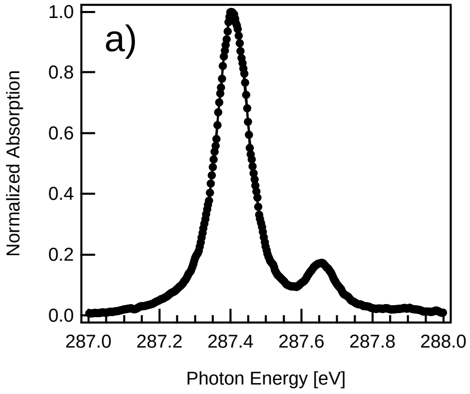


FIGURE 5.18. (a) Illustration of the figure eight electron motion in the frame of reference moving with the average electron velocity, and the resultant radiation patterns at the fundamental and second harmonic frequencies in both (b) the frame of reference moving with the electron and (c) the laboratory frame of reference.

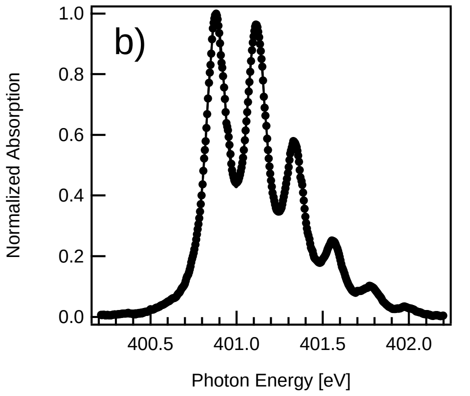
Undulator Harmonics Dispersed



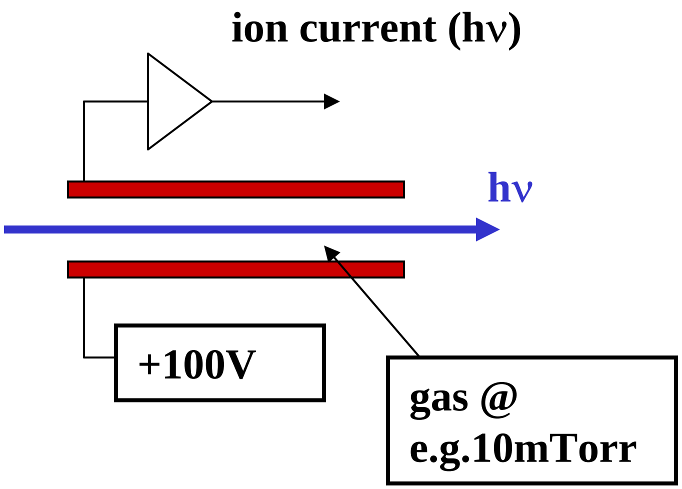
Spectral Resolution by Gas Phase Absorption



Carbon in CO2



Nitrogen in N2



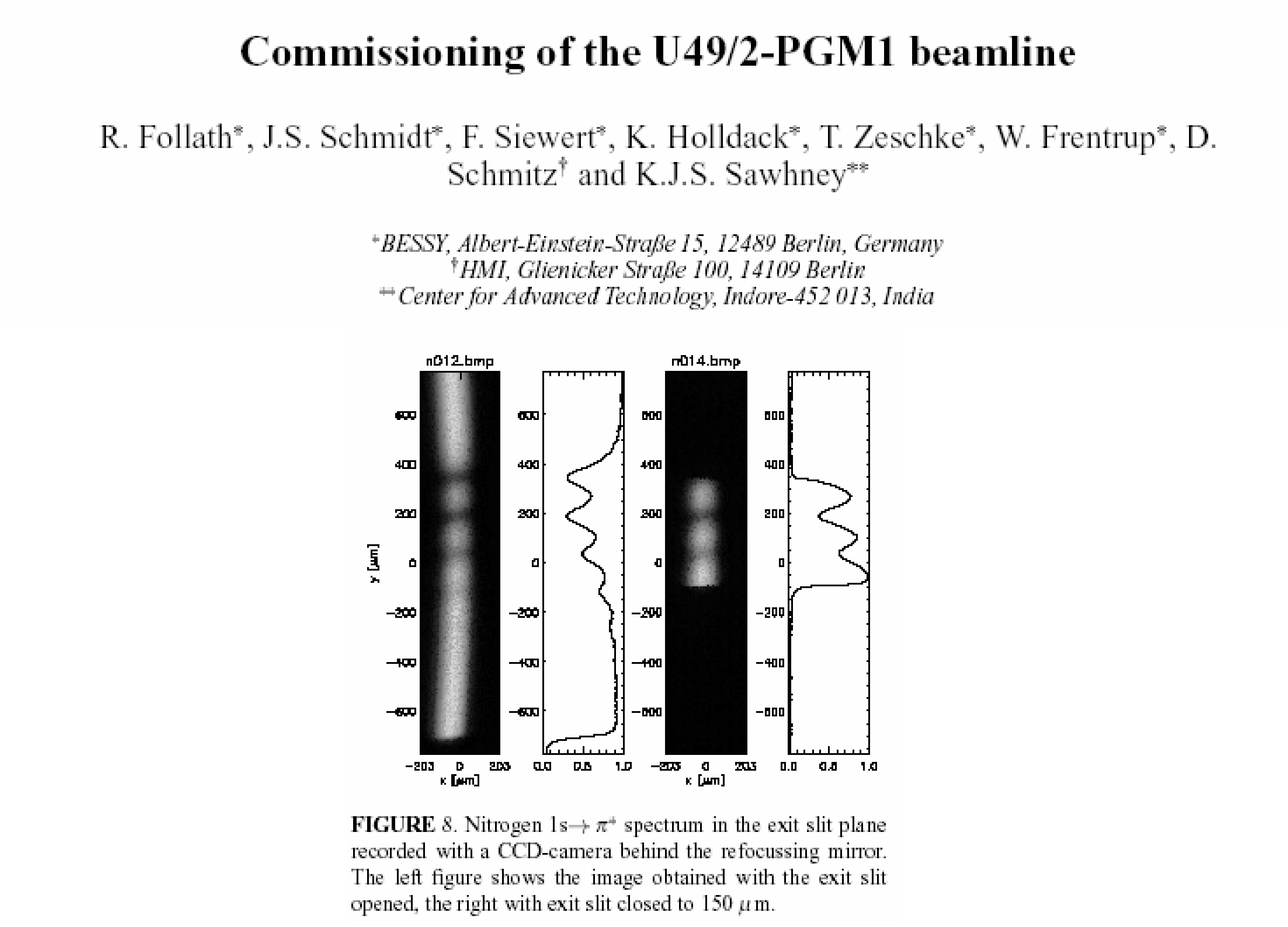
ion current (hν)

hν

+100V

gas @
e.g.10mTorr

Open the exit slits



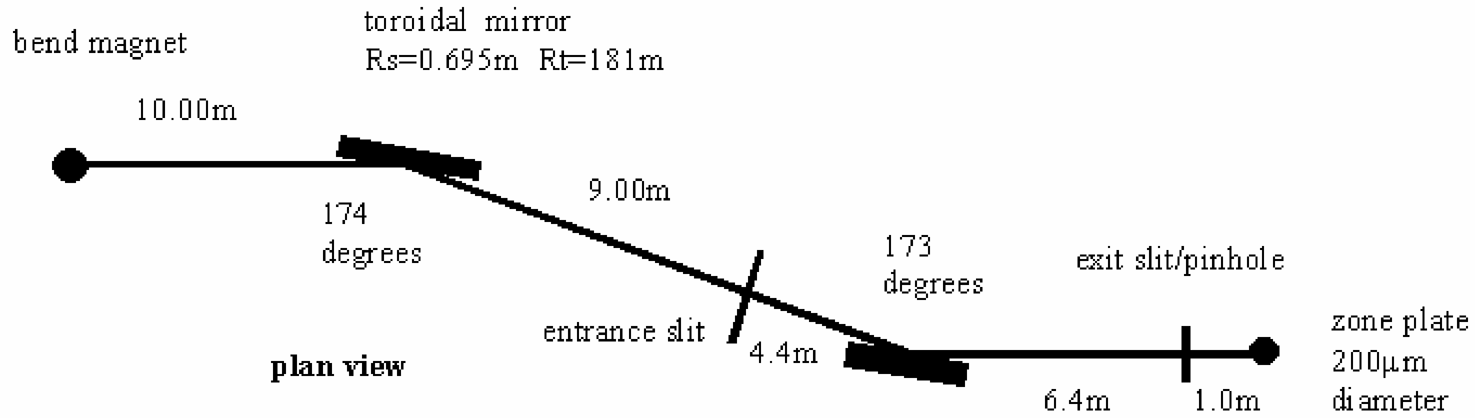
Commissioning of the U49/2-PGM1 beamline

R. Follath*, J.S. Schmidt*, F. Siewert*, K. Holldack*, T. Zeschke*, W. Frentrup*, D. Schmitz† and K.J.S. Sawhney**

*BESSY, Albert-Einstein-Straße 15, 12489 Berlin, Germany
†HMI, Glienicker Straße 100, 14109 Berlin
**Center for Advanced Technology, Indore-452 013, India

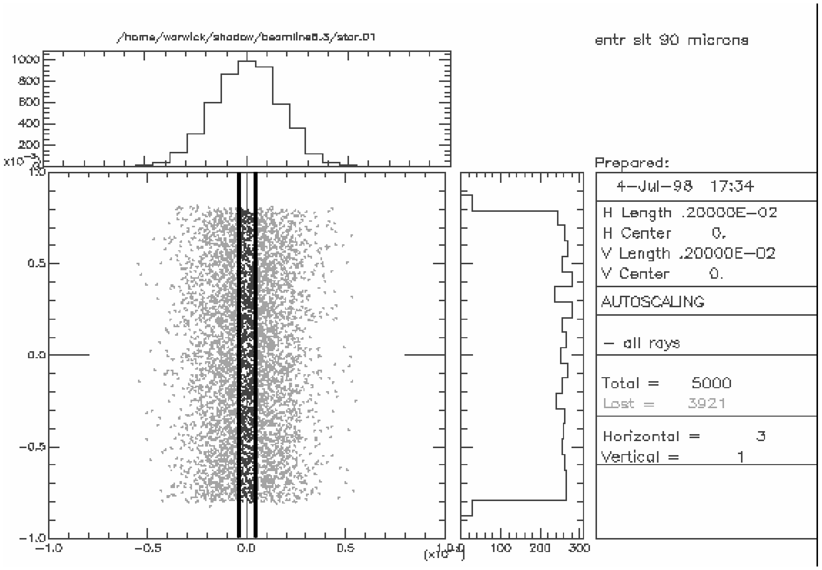
FIGURE 8. Nitrogen 1s→ π^* spectrum in the exit slit plane recorded with a CCD-camera behind the refocussing mirror. The left figure shows the image obtained with the exit slit opened, the right with exit slit closed to 150 μm.

A Simple Beam Line



built for bend magnet illumination of Scanning Transmission Xray Microscope

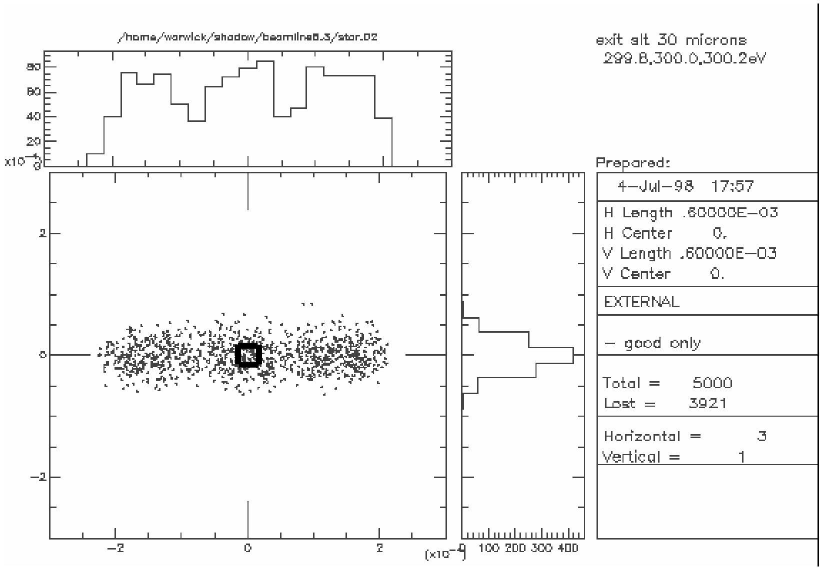
Ray Trace



entr slit 90 microns

Prepared:
4−Jul−98 17:34
H Length .20000E−02
H Center 0.
V Length .20000E−02
V Center 0.
AUTOSCALING
− all rays
Total = 5000
Lost = 3921
Horizontal = 3
Vertical = 1

entrance slit



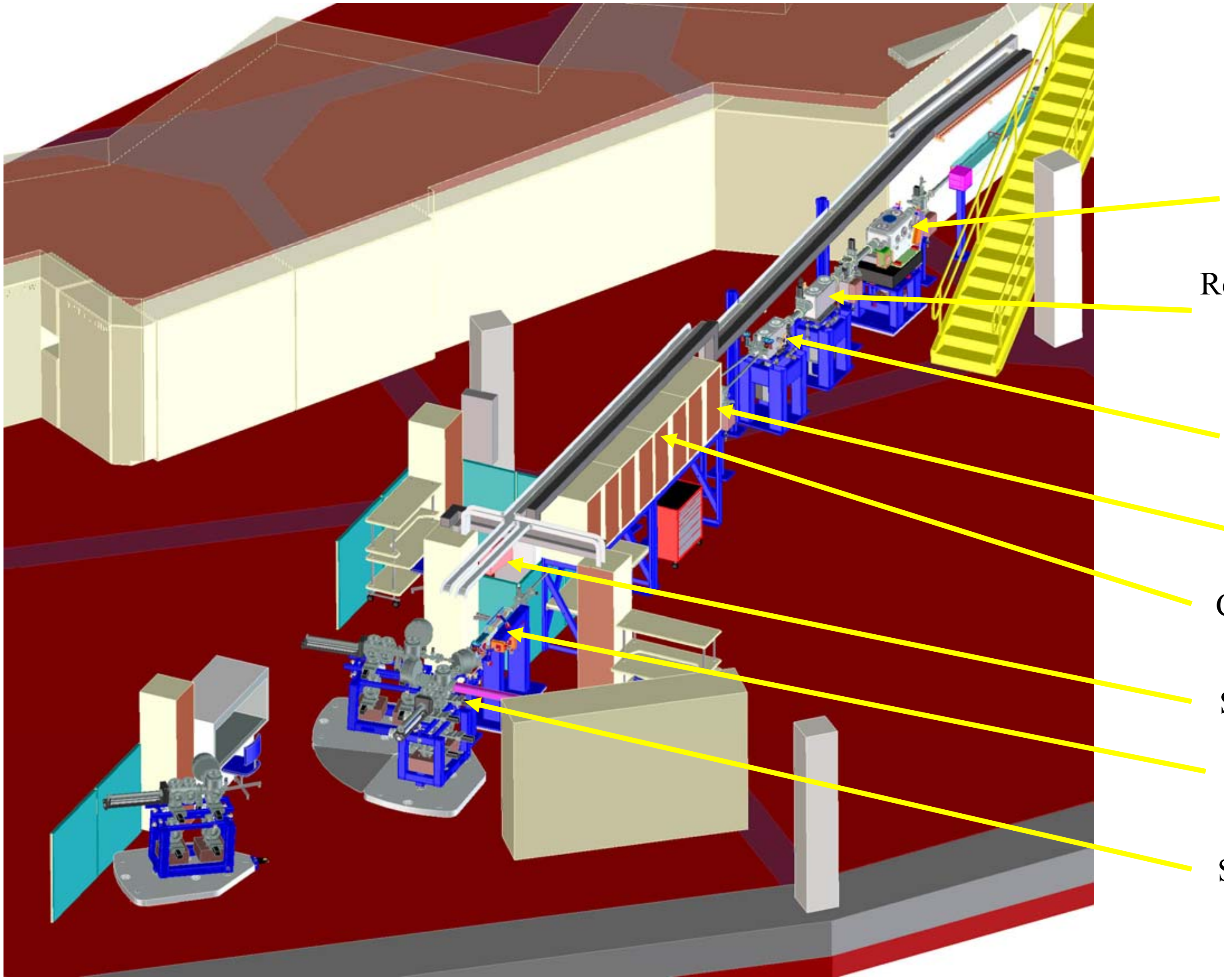
exit slit 30 microns
299.8,300.0,300.2eV

Prepared:
4−Jul−98 17:57
H Length .60000E−03
H Center 0.
V Length .60000E−03
V Center 0.
EXTERNAL
− good only
Total = 5000
Lost = 3921
Horizontal = 3
Vertical = 1

exit slit

299.8 eV 300.0 eV 300.2 eV

Modern Designs (variable included angle)



Monochromator

Retractable focus mirror (deflecting right)

Fixed focus mirror (deflecting left)

Exit slits (x2)

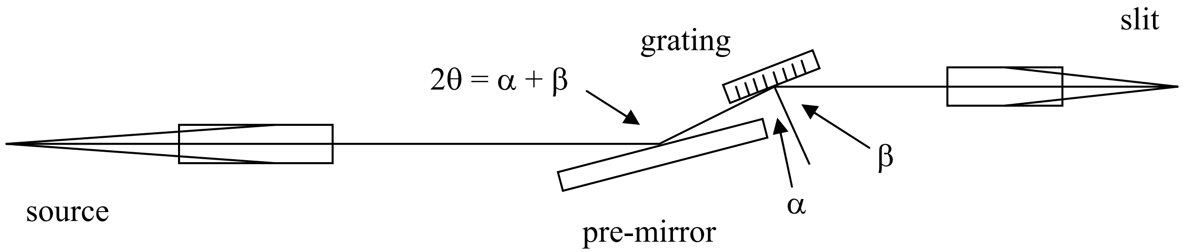
Control racks (above the beam line)

Scanning microscope

KB refocus mirrors

Spectroscopy stations

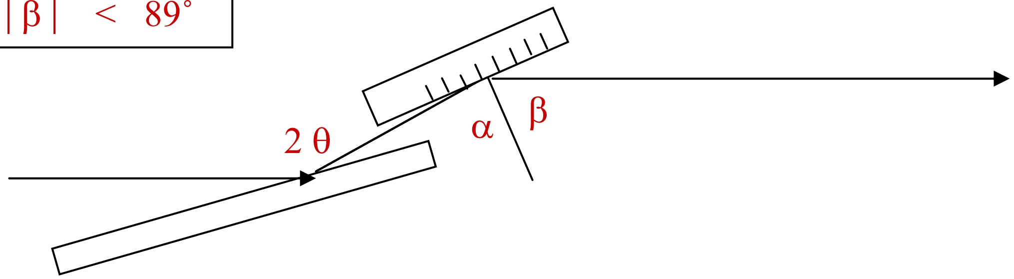
Collimated Variable-Included-Angle PGM



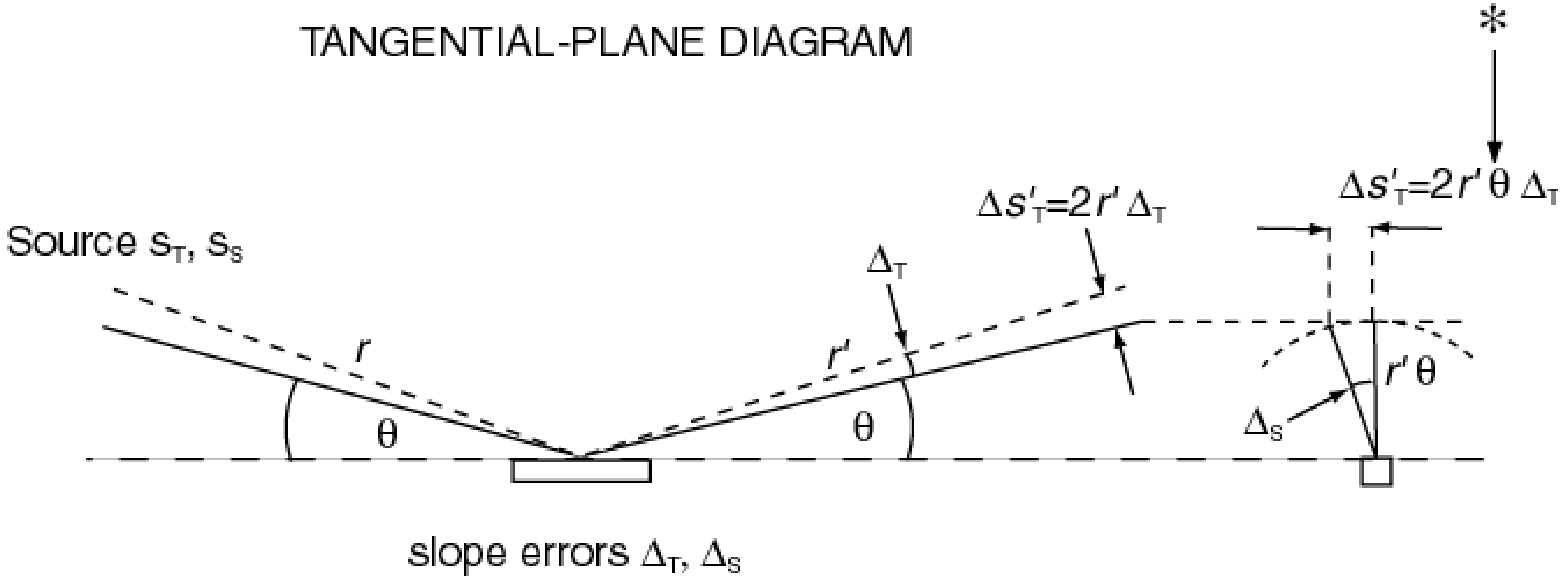
$$Cff = \cos\beta \;/\; \cos\alpha \qquad\qquad m\lambda = \sin\alpha - \sin\beta$$

$170^\circ < 2\theta < 178^\circ$

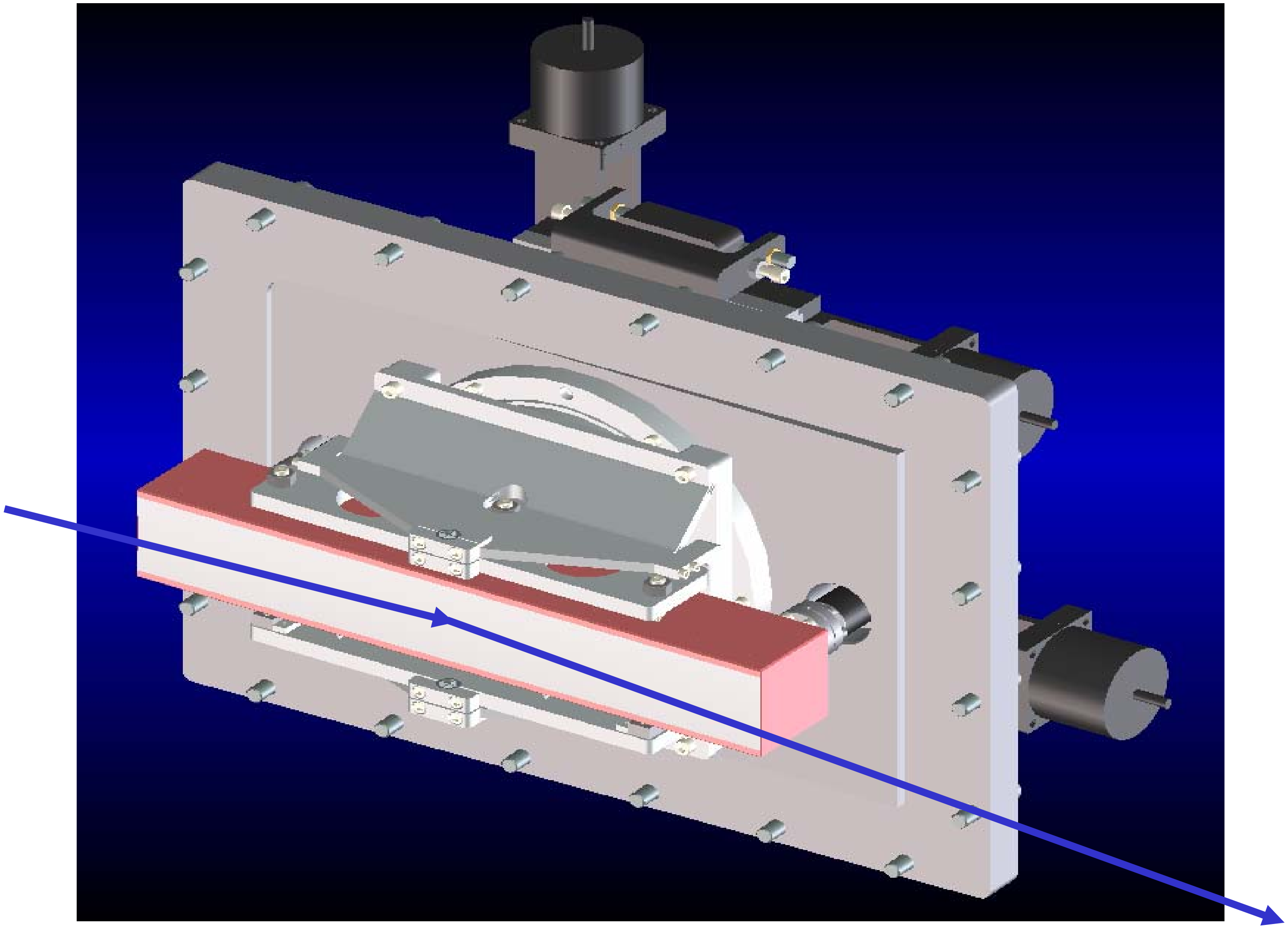
$80^\circ < |\beta| < 89^\circ$



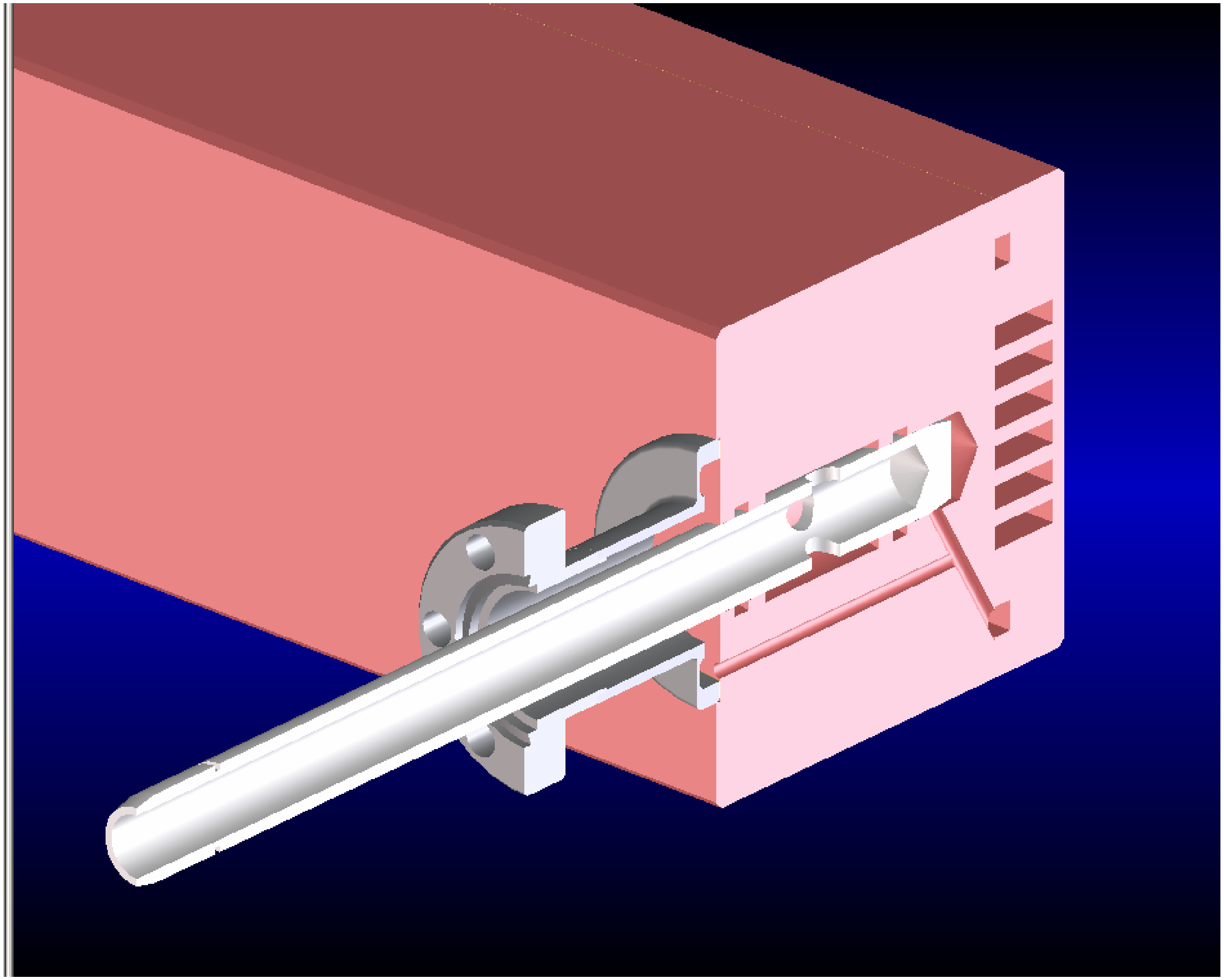
Forgiveness Factor in Sagittal Focusing



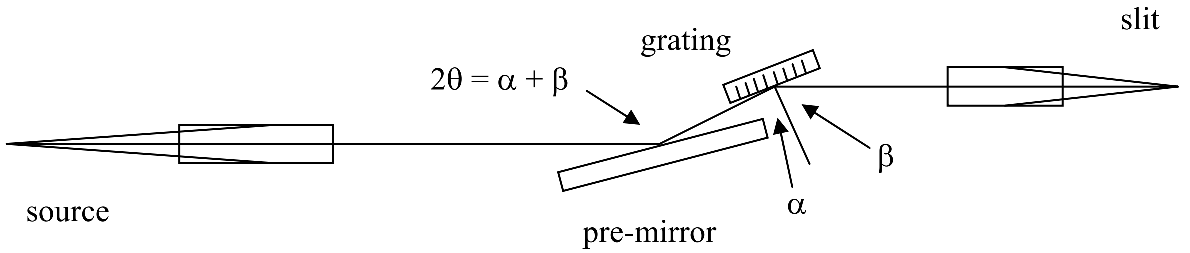
Sagittal Focusing Water Cooled Mirror



Mirror Cooling for High Heat Load



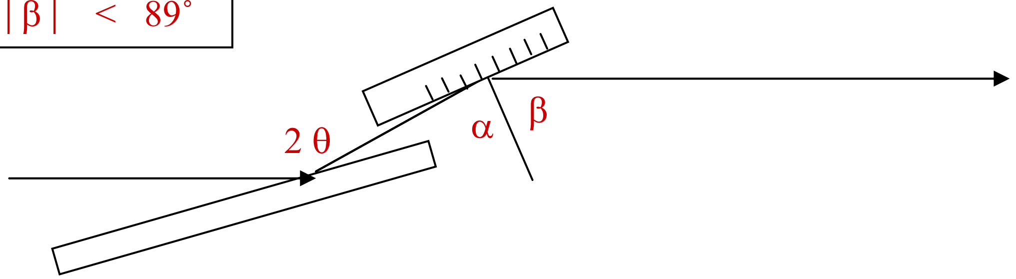
Collimated Variable-Included-Angle PGM



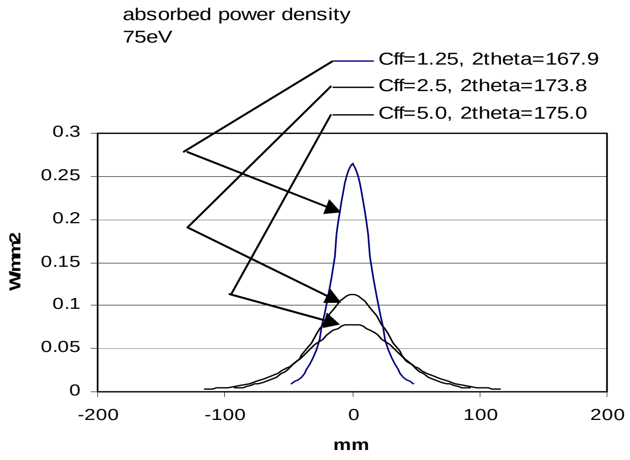
$$Cff = \cos\beta \;/\; \cos\alpha \qquad\qquad m\lambda = \sin\alpha \;-\; \sin\beta$$

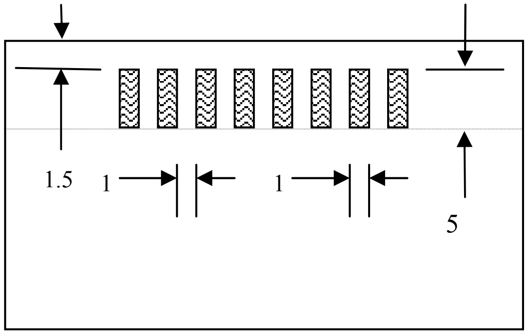
$170^\circ < 2\theta < 178^\circ$

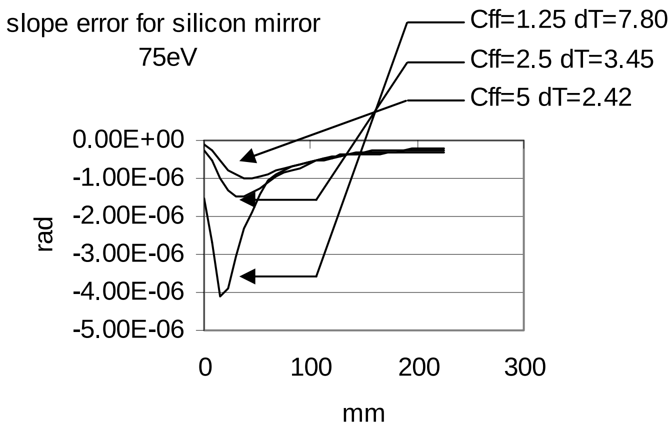
$80^\circ < |\beta| < 89^\circ$



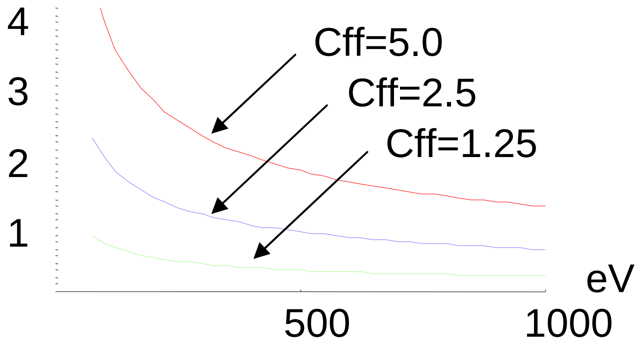
Optic Cooling for High Heat Load



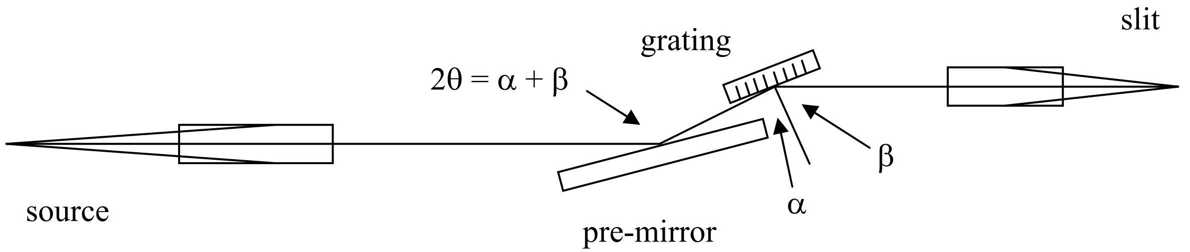




The rms slope error (μrad) of the pre-mirror corresponding to a resolving power R=7500 (FWHM) from the 150l/mm grating.



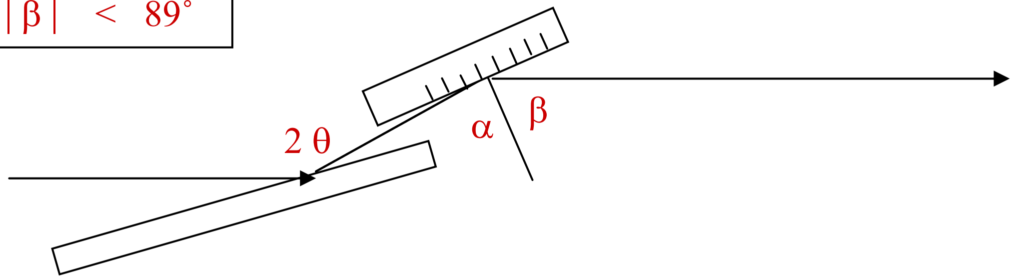
Collimated Variable-Included-Angle PGM



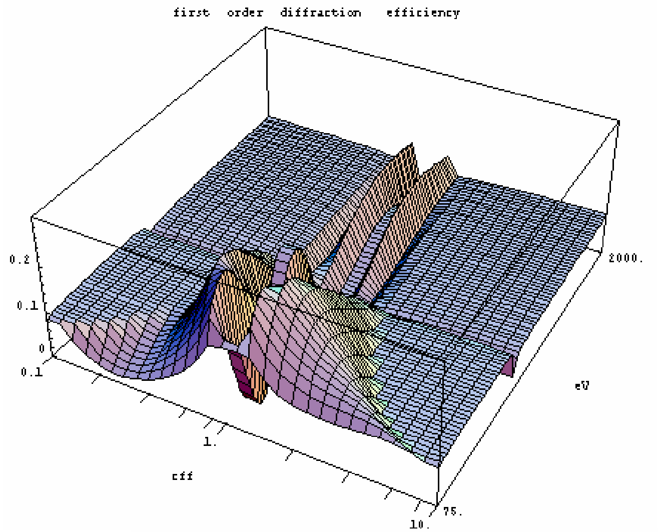
$$\mathrm{Cff} = \cos\beta \;/\; \cos\alpha \qquad\qquad m\lambda = \sin\alpha \;-\; \sin\beta$$

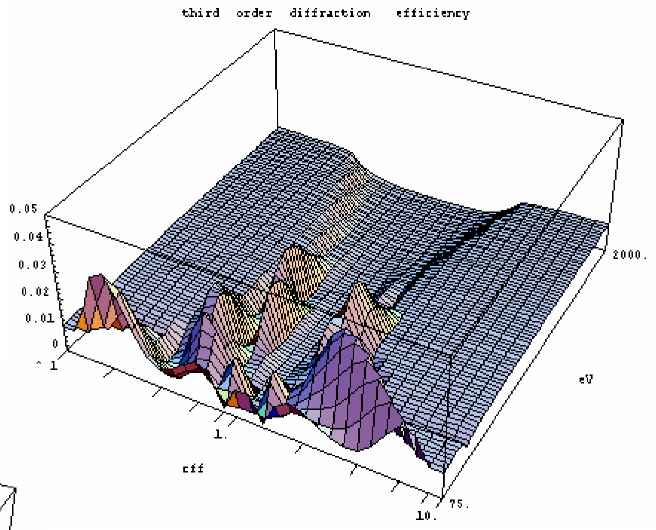
$170^\circ < 2\theta < 178^\circ$

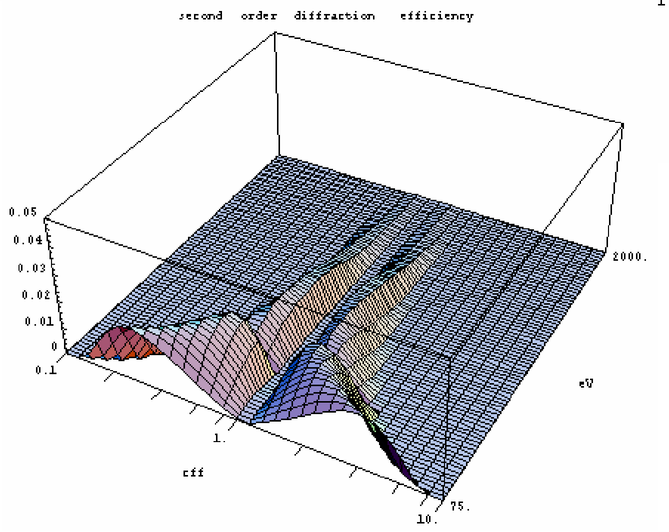
$80^\circ < |\beta| < 89^\circ$



Computed Diffraction Efficiency



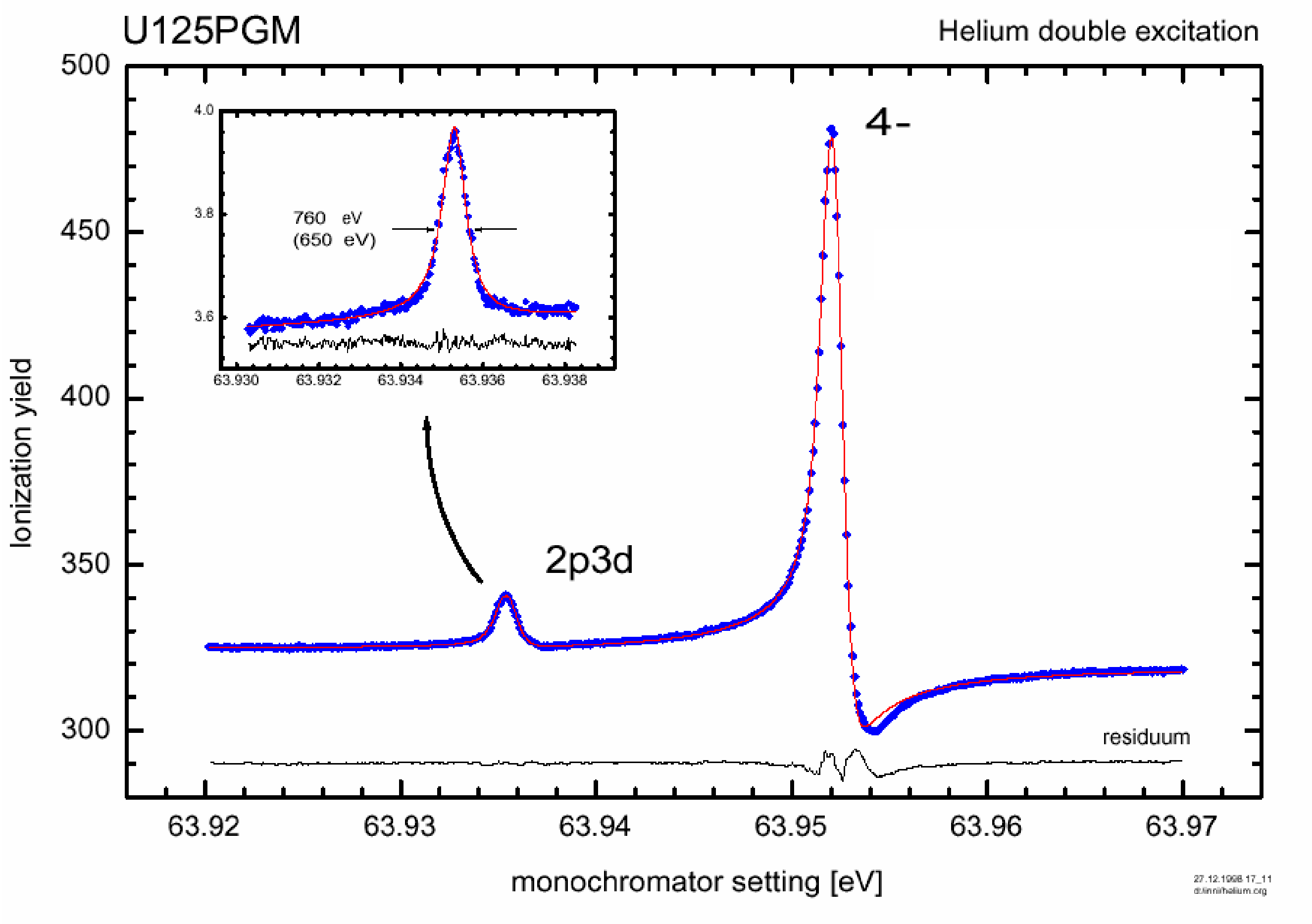




First, second and third order efficiency calculations for a laminar grating 150 lines/mm

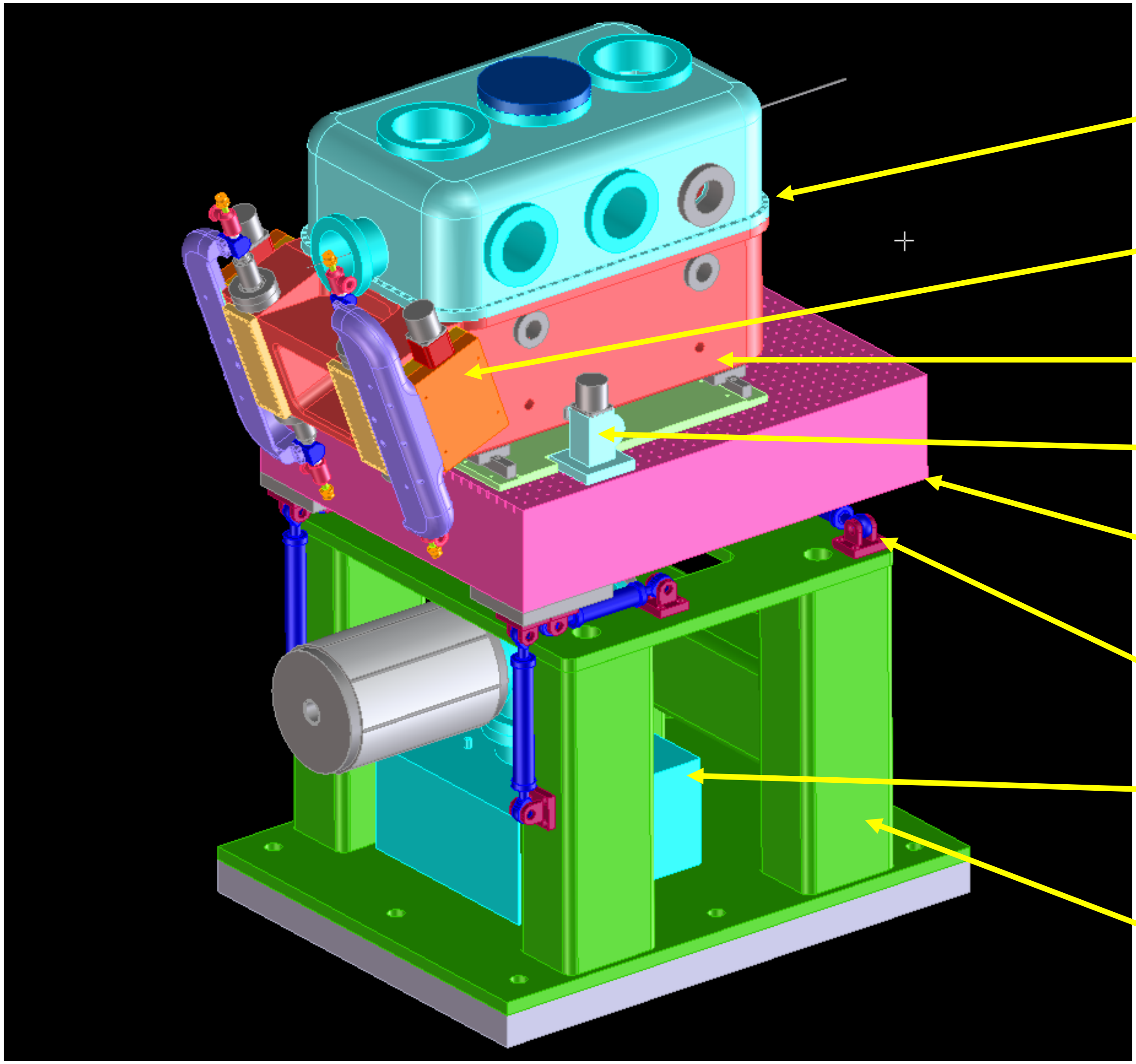
Collimated SX700 Capable of Very High Resolution

Picture from R. Follath, BESSY



- Doppler width 0.4 meV
- Monochromator contribution 0.65 meV
- Resolving power=$1.0\text{x}10^5$
- Rotation increments
  - grating: 17 nrad
  - mirror: 9 nrad
- Measured with 1200/mm grating at c_{ff} =10 to 12

New Implementation of SX700 Monochromator



Seal joint below beam height for alignment access

External sine-bar drives and linear encoders

Aluminum structural vessel

External grating changer

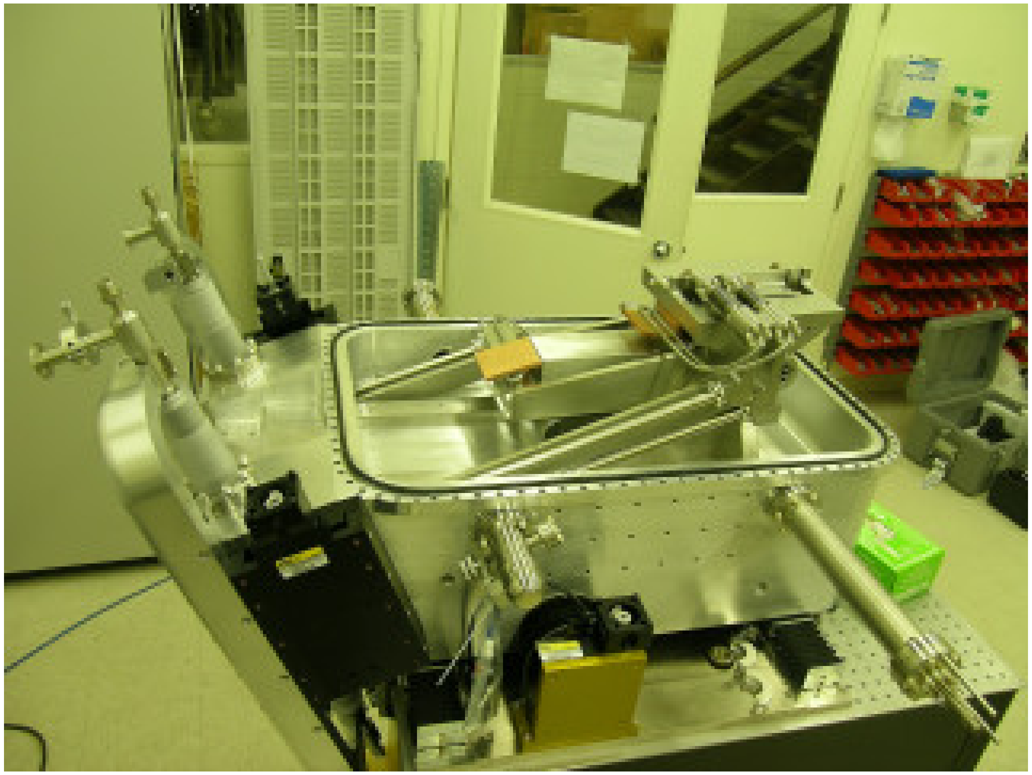
Lightweight rigid honeycomb table

6-strut alignment

Heavy pump below bellows on separate support

Legs filled with epoxy granite

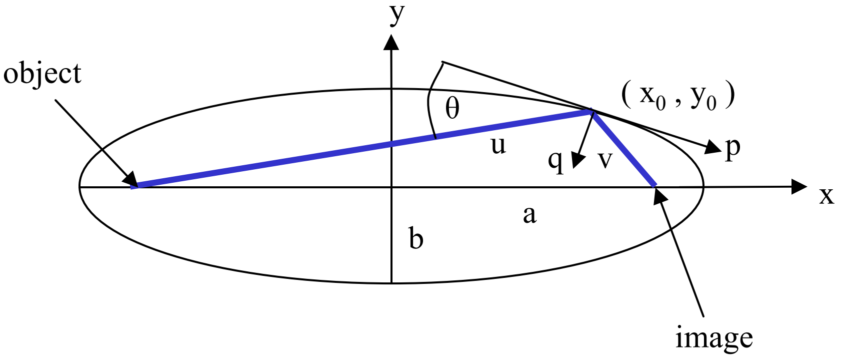
Monochromator fabrication by Johnsen Ultravac



successful factory motion tests and preparation for final vacuum qualification September 10th 2004

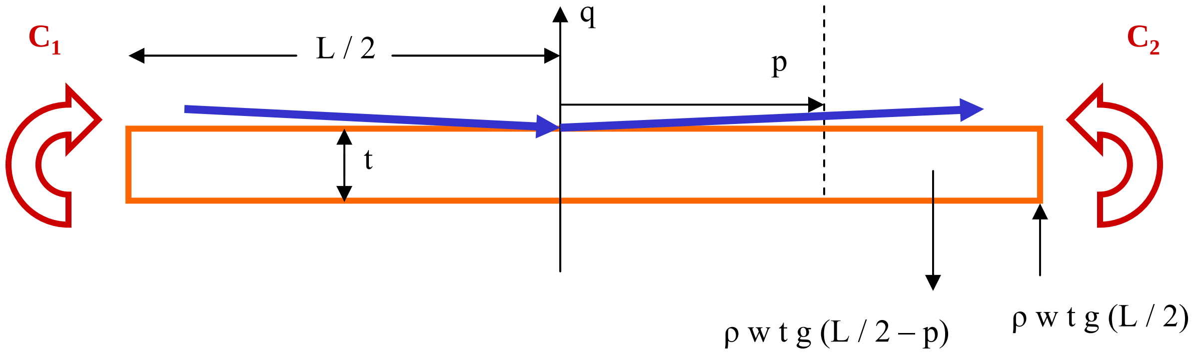
accepted, ready for shipment October 12th 2004

Bending Mirrors to Approximate an Ellipse



$$x(p) \approx p \left\{ 1 + \left(x_0^2\, b^2 / a^2 \right) / \left(a^2 - x_0^2 \right) \right\}^{-1/2} + x_0$$

$$1/\rho_{\mathrm{ellipse}} = \pm\, a\, b \left\{ a^2 - x(p)^2 + x(p)^2\, b^2 / a^2 \right\}^{-3/2}$$

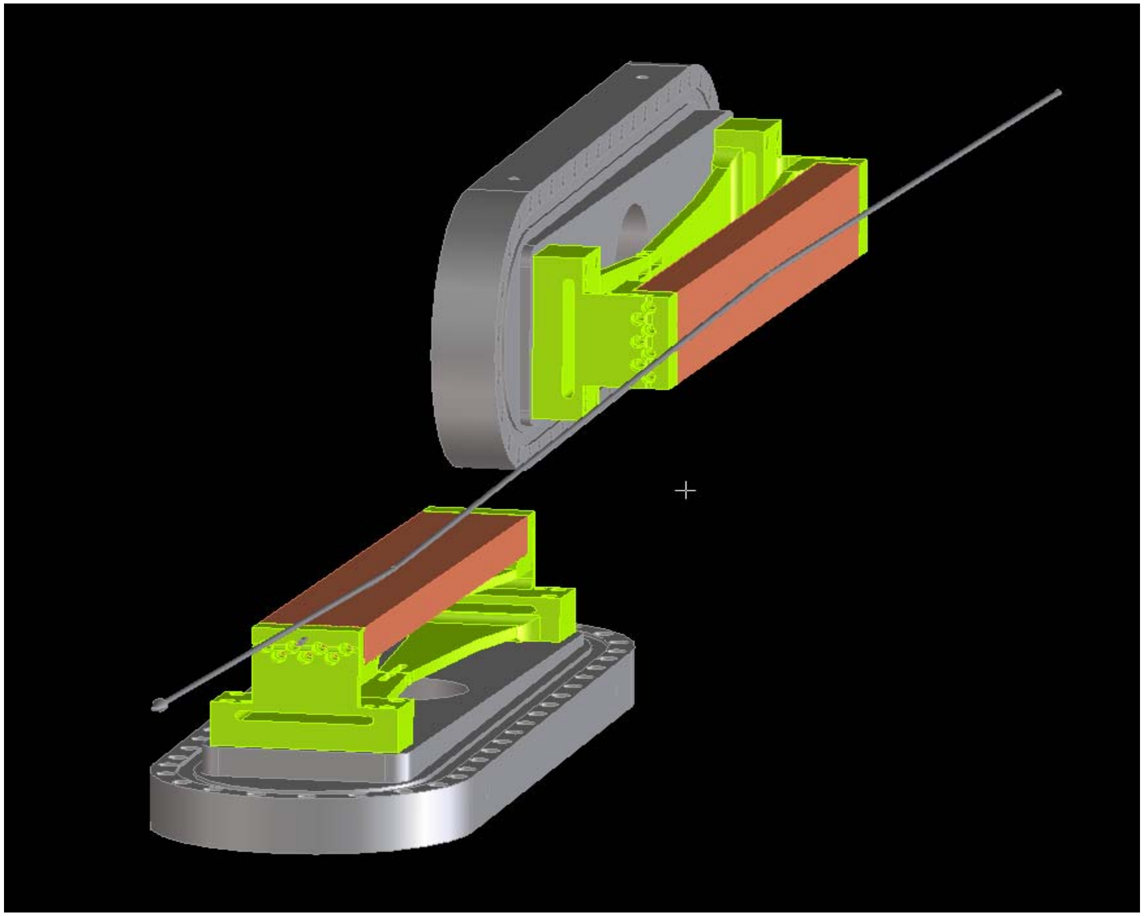


$$M(p) = \left\{ C_1 (L/2 - p) + C_2 (L/2 + p) \right\} / L + (\rho\, w\, t\, g / 2)\, (L/2 - p)\, (L/2 + p)$$

$$1/\rho_{\mathrm{bender}} \approx d^2q/dp^2 = 12\, M(p) / E\; w(p)\; t^3$$

Bending Mirrors to Approximate an Ellipse

Kirkpatrick-Baez Mirror Pairs for Micro-Focus



for focussed spot size down to about 0.5 μm

Final focus spot size

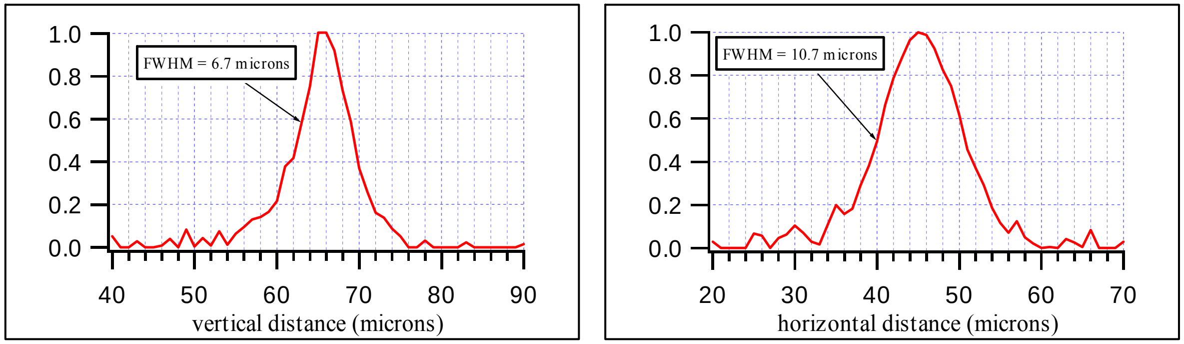


Figure 3. Measured x-ray spot profiles at the focus.

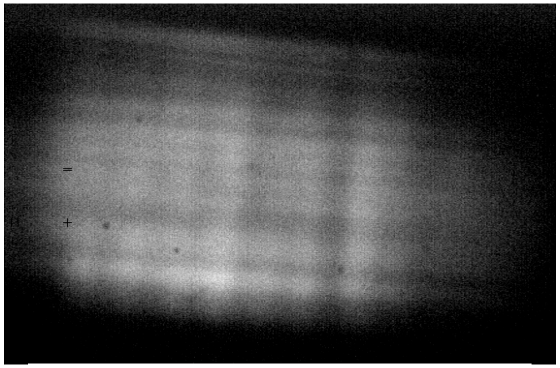
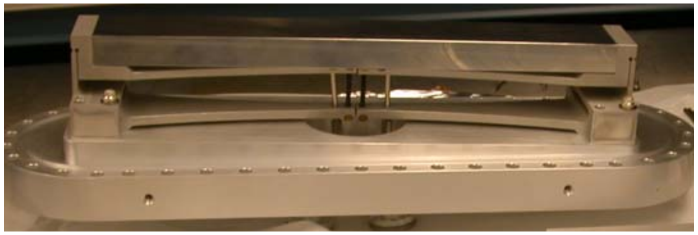
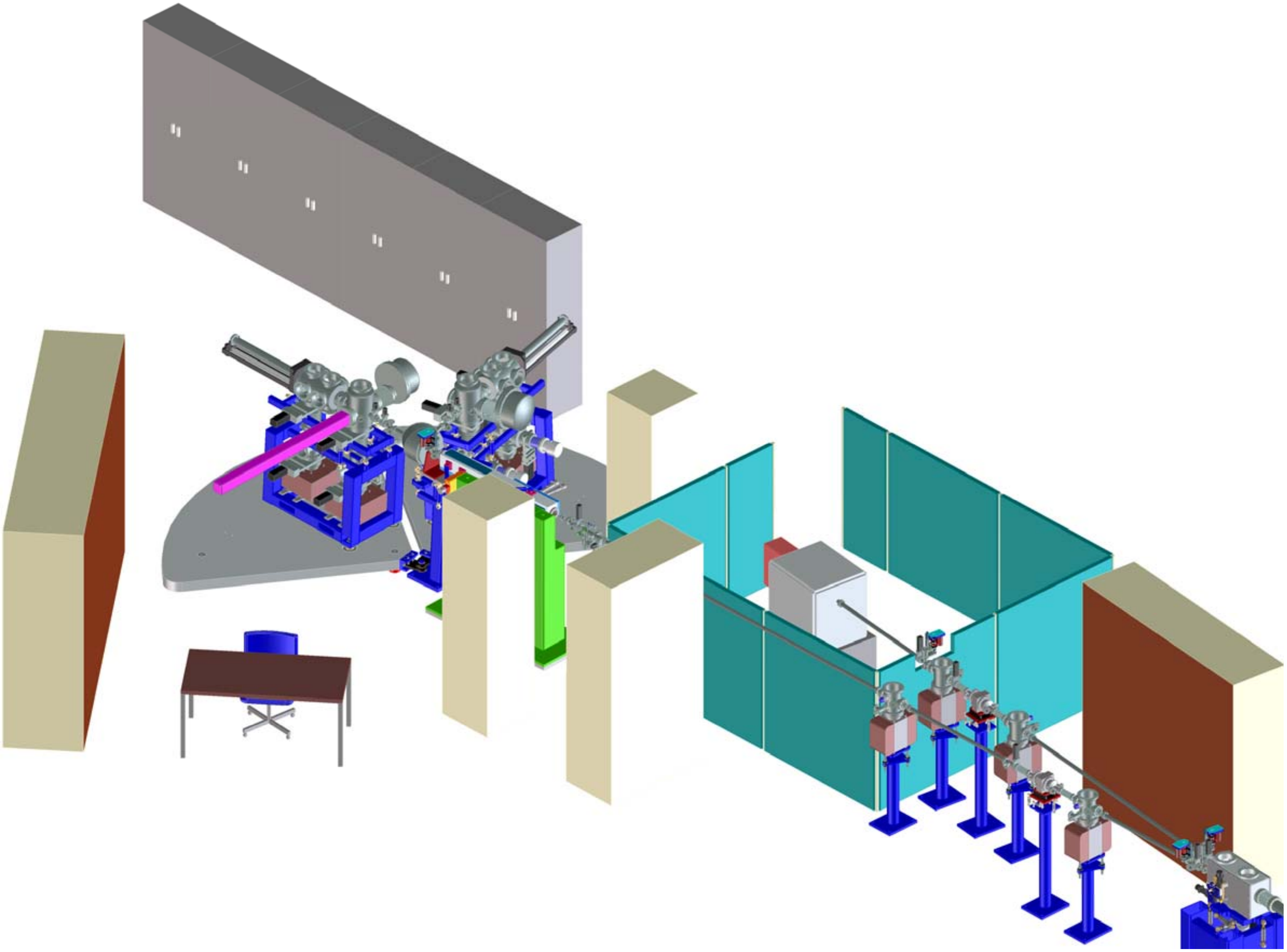


Figure 4. Defocused spot 500μm diameter.



Optimized Experiment Stations Keep Users Busy



Synchrotron Beam Lines

Stanford-Berkeley Summer School

on Synchrotron Radiation

June 13-17th 2005

Tony Warwick

Advanced Light Source

Lawrence Berkeley National Laboratory