Optics for Synchrotron Radiation

Introduction to the basic optical elements in synchrotron radiation beamlines

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Summer Student Program
Hamburg, 26. Jul 2013

HELMHOLTZ
ASSOCIATION

DESY

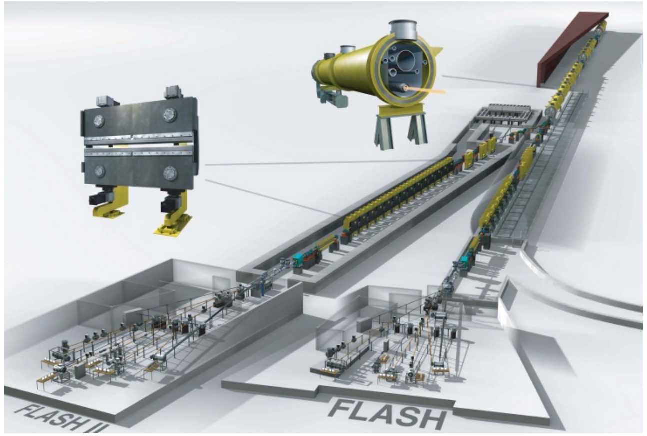
Synchrotron Radiation Sources at DESY

FLASH

FLASH II (civil construction in progress)

PETRA III

PETRA III extension project (start of civil construction 19 Dec. 2013)



FLASH / FLASH II experimental hall

(Courtesy: Ed. Züblin AG)

PETRA III experimental hall

PETRA III extension project Hall North and Hall East

Requirements of X-Ray Optics at a Third Generation Facility

Task: Preservation of the optical parameters of the source

Key parameters for the experiment

brightness
coherence
beam size and divergence at the sample

Challenges

mechanical stability of all components
heatload issues, thermal management
quality of optical surfaces

Realization

mechanical and optical design
manufacturing and infrastructure capabilities
optical and "at wavelength" metrology

PETRA III Photon Beam Parameters

	β_x [m]	β_y [m]	σ_x [μm]	σ_y [μm]	$\sigma_{x'}$ [μrad]	$\sigma_{y'}$ [μrad]	ID-length [m]
low-β 5 m	1.3	3	35.9	5.7	28	5.0	5
high-β 5 m	20	2.38	141	5.2	8.6	5.2	5

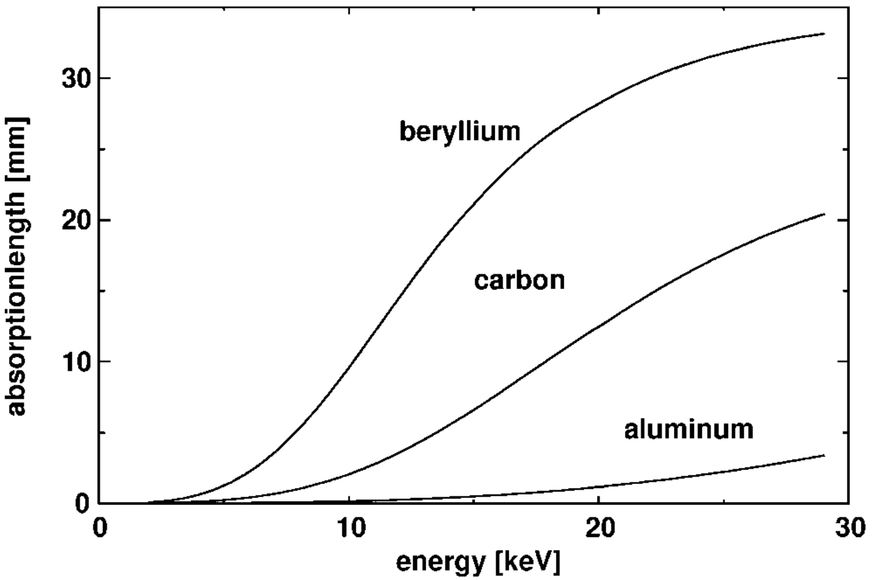
$\beta_x = \sigma_x / \sigma_{x'}$

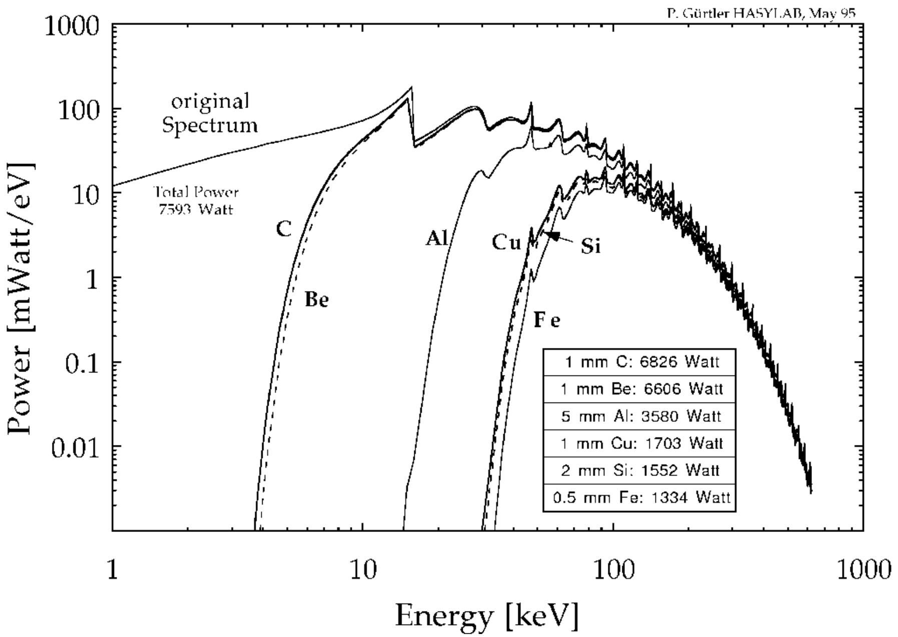
- **horizontal beam size (FWHM@12keV) in 100m distance: low-β: 6.7mm high-β: 2mm**
- **vertical beam size : 1.2mm**

- **total power (2m or 5m ID, 100mA) : 3kW - 7.5kW**
- **power density at monochromator : 60 - 150 W/mm²**
- **typical power at monochromator : 100 - 800 Watt**

Most beamlines will make use of the very small source size and will typically focus the beam down to values in the µm region and for special application into the 10nm-100nm range.

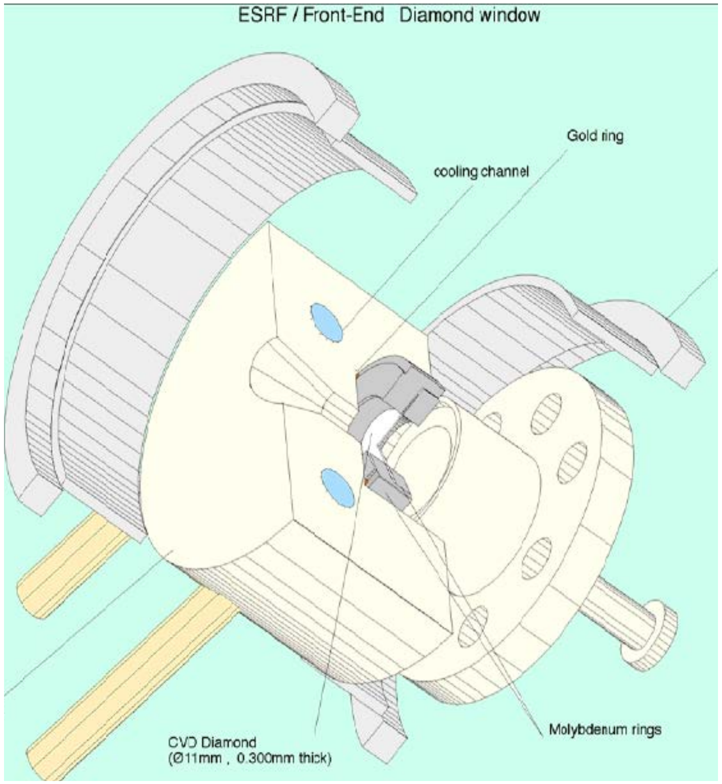
Thermal mangement: Filter





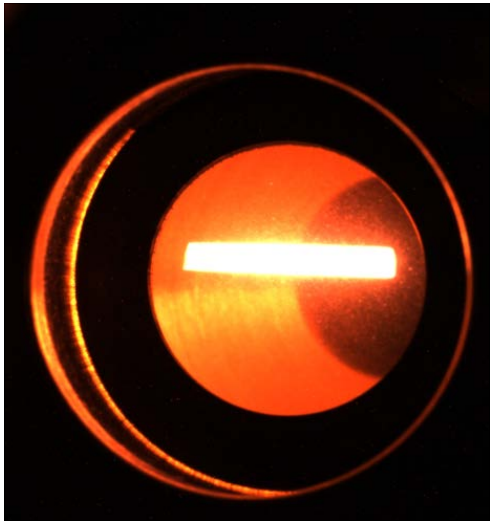
Absorption length (thickness for an attenuation to 1/e of the incoming flux) of common window materials Be, C, Al and the exemplary evolution of the total power along an undulator beamline due to sequential filtering of the undulator spectrum

Diamond Windows



ESRF front end window,
Jean-Claude Biasci, MEDSI-2004

PETRA III CVD diamond window
(Diamond Materials, Freiburg)

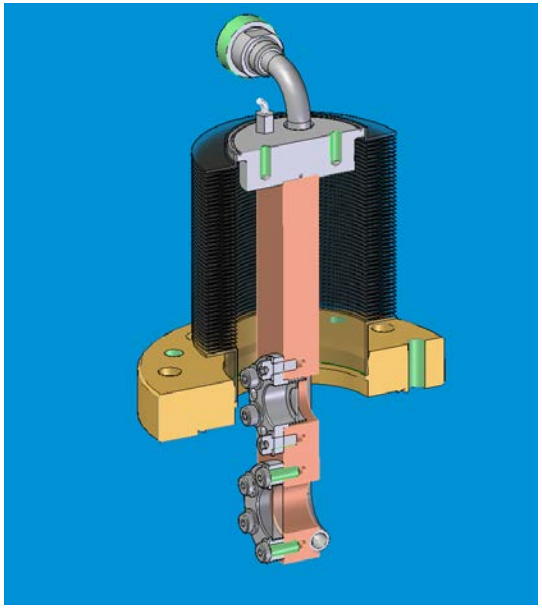


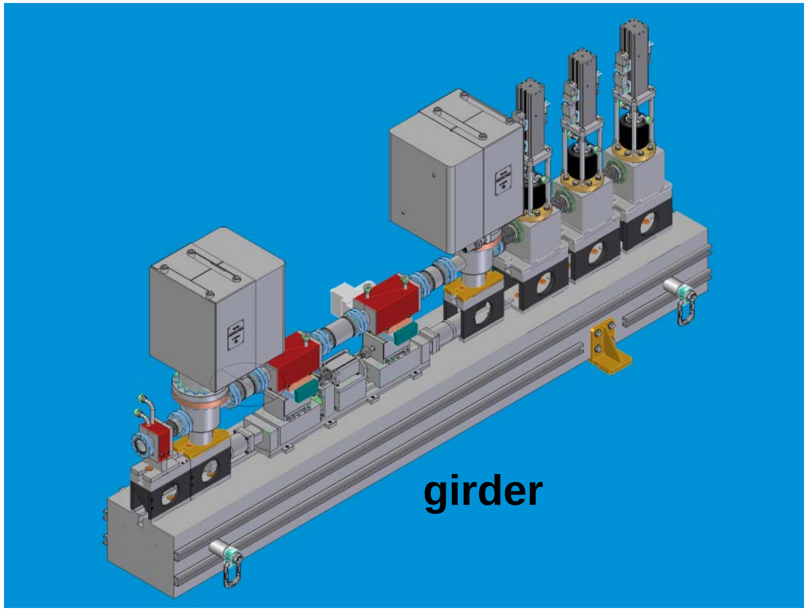
White beam at P13
(M.Degenhardt and EMBL/P13)

Free window apertures from Ø2 mm, thickness from 20 µm to 300 µm, in CVD and single crystal diamond technology.

CVD Diamond White Beam Filter Units

Water cooled, up to 3 units with two filters each in all 14 PETRA III front-ends





CVD diamond, 300µm thickness (Diamond Materials, Freiburg)

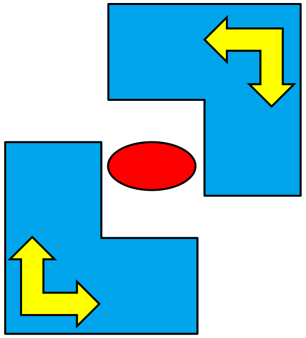
CVD diamond 300µm with 25µm Copper on both sides

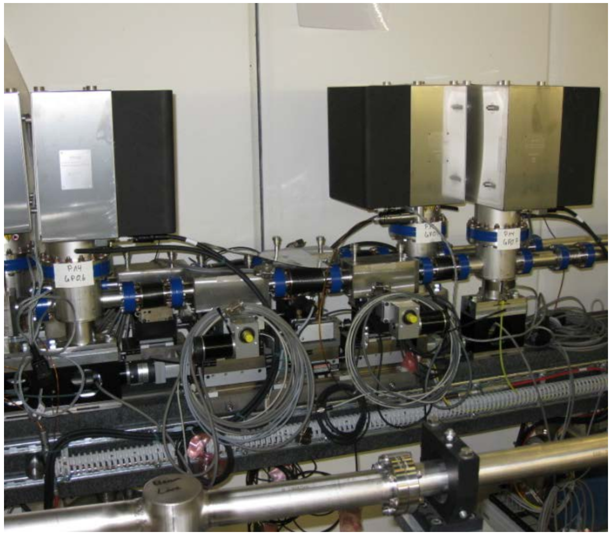
0.5mm, 0.6mm, 0.9mm, 1.0mm, 4mm polished Glassy Carbon

High Power Slit Systems for PETRA III

High Power Slit Systems for PETRA III undulator beamlines

- **High precision roll angle**
- **Safety Shutter function**
- **Compact design for canted undulator beamlines**



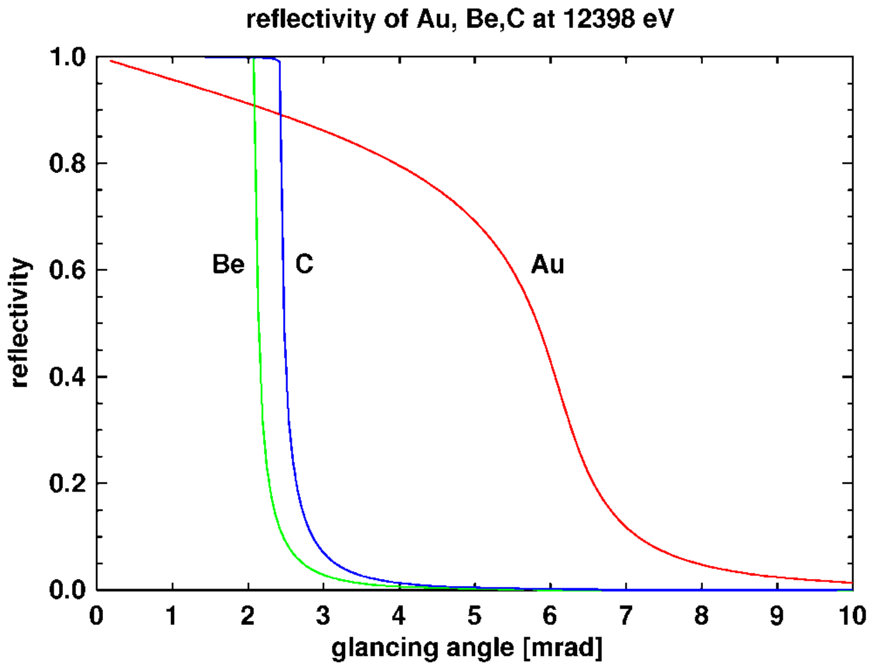


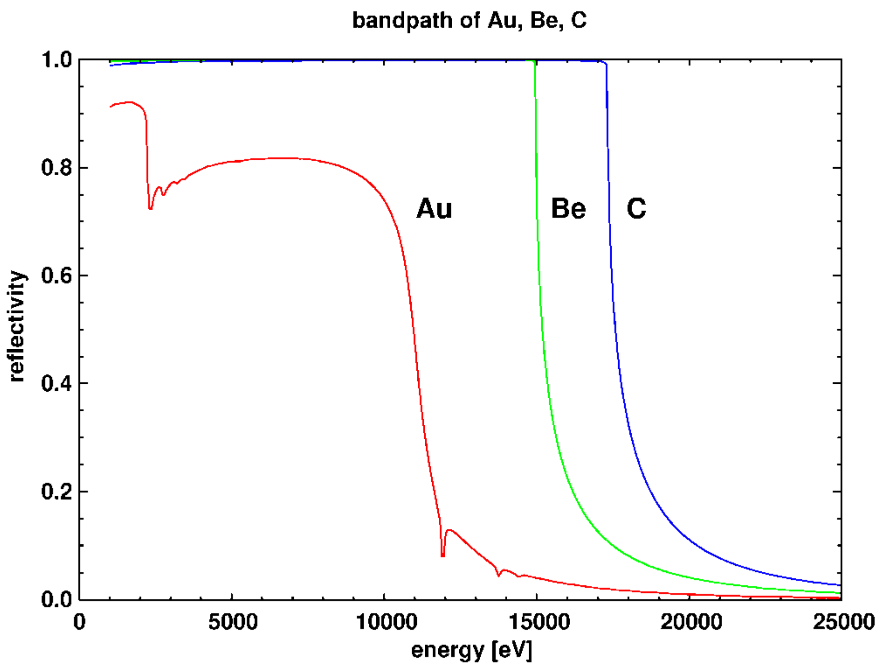
Glidcop® slits

Basic Optical Elements: Mirrors

mirrors	multilayers	single crystals
total external reflection	Bragg diffraction $2dsin(\theta_B + \delta) = n\lambda$	
reflection	reflection	reflection, transmission
$\theta_C \approx 0.4^\circ$, Au at 10keV	$\theta_B \approx 1^\circ$	$4^\circ \leq \theta_B \leq 90^\circ$
	functions	
focusing	$\Delta E/E : 10^{-3}...10^{-1}$	$\Delta E/E : 10^{-2}...10^{-8}$
high energy cut-off	focusing	focusing

Mirrors: Optical Properties





Reflectivity at 1Å and energy bandpath at the critical angle for Au, Be, and C coatings acting as a high energy cut-off.

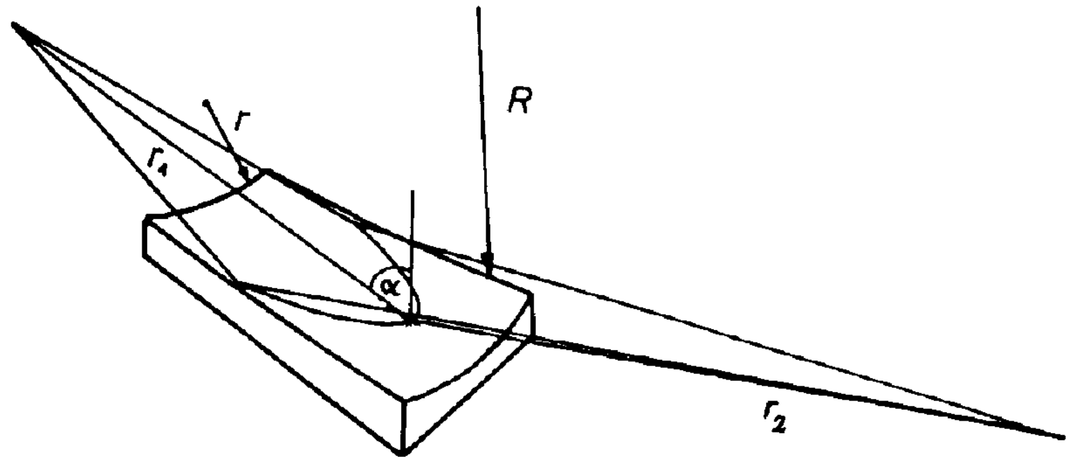
Mirrors: Geometrical Properties

plane mirrors used for deflection/offset and filtering

point to point focusing mirror example: toroidal mirror

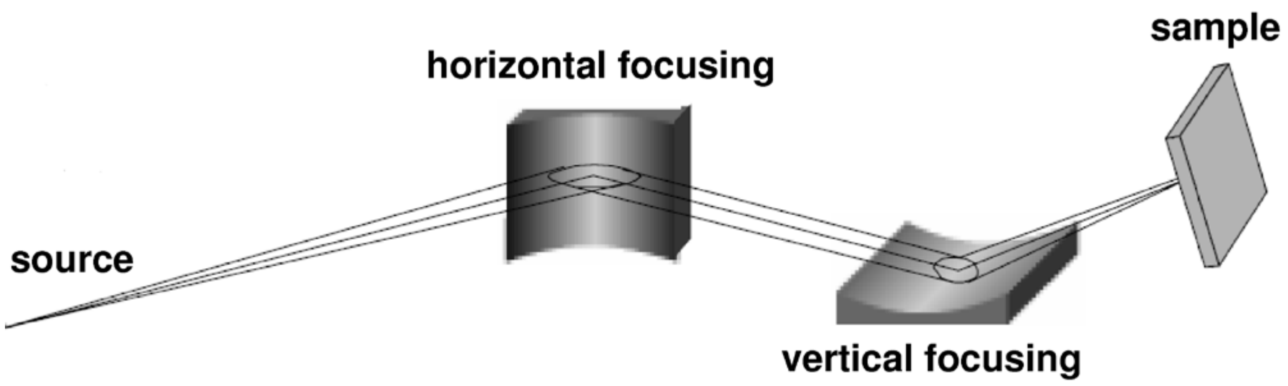
$$\text{sagittal: } \frac{1}{r_1} + \frac{1}{r_2} = \frac{2\cos\alpha}{r} = \frac{1}{f_{sag}}\text{, tangential: } \frac{1}{r_1} + \frac{1}{r_2} = \frac{2}{R\cos\alpha} = \frac{1}{f_{tan}}$$

$$\Longrightarrow \text{ one angle } \alpha \text{ at which } f_{sag} = f_{tan} \Longrightarrow \cos\alpha = \sqrt{\frac{r}{R}}$$

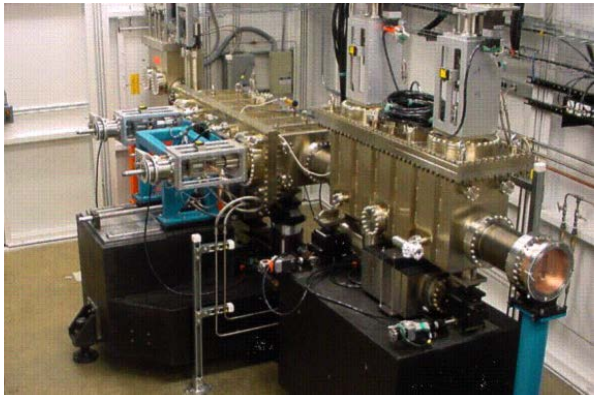


typical values: r_1=20m, r_2=10m, $\alpha = 89.6^\circ$, r=93mm, R=1.9km

Mirrors: Kirkpatrick-Baez system

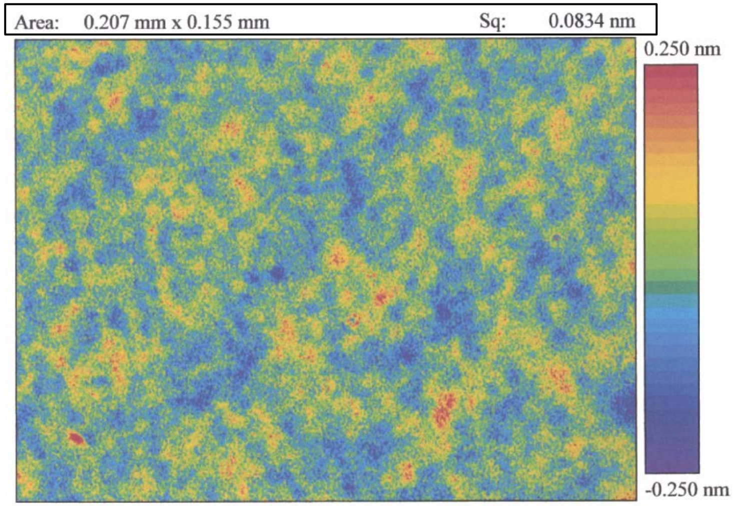


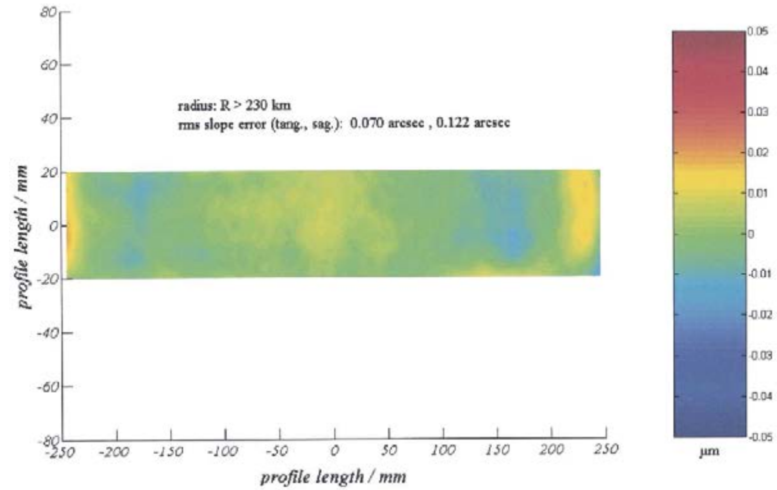
from 100mm mirrors (left: XRADIA) to 1m long mirrors (right: IDT)



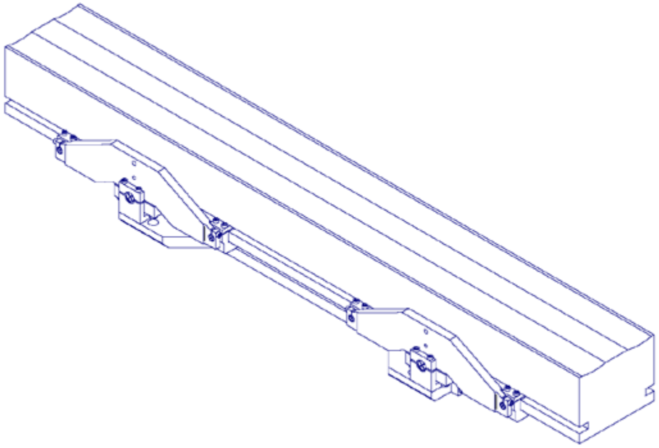
Error free focusing can only be achieved with an ellipsoidal mirror surface. The Kirkpatrick-Baez (KB) mirror system circumvents the fabrication of this complicated shape by separating the vertical and horizontal focusing into two steps using elliptically bent plane mirrors.

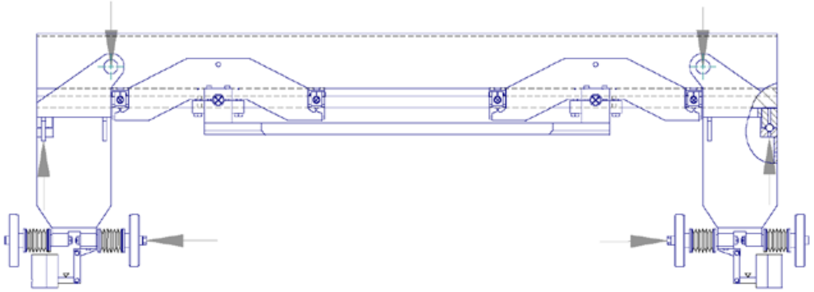
Mirrors: Figure, Roughness, Mechanical Design





Slope error and roughness of a 500mm long plane Si mirror





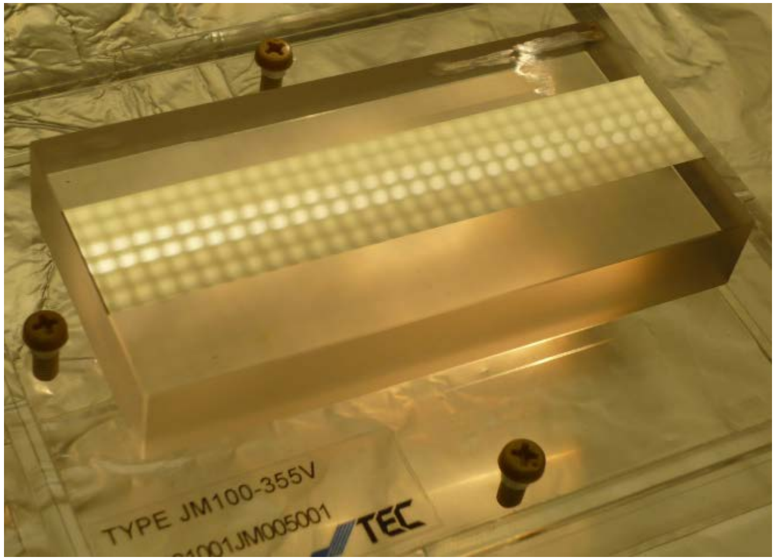
Mirror support and bender design for 1m long bendable plane mirrors

Mirrors: Metrology at a Kirkpatrick-Baez system

Parameter of a JTEC planar ellipse made for PETRA III, beamline P06

Specifications:
Source distance r: 93595 mm, Focus distance r`: 355 mm, Incidence angle θ: 2.7 mrad
Metrology result:
r: 93594.98 mm, r`: 355 mm, θ: 2.71 mrad

Residual slope error: 0.041 µrad rms
In meridional direction, (inspected aperture length: 87.4 mm)
Residual figure error: meridional: **0.39 nm rms / 1.1 nm pv**



Measurements by F.Siewert, HZB

Mirrors: Metrology Tools

The measured quantities are figure or shape, slope-error, and micro-roughness.

Standard optical metrology instruments used to inspect synchrotron radiation optical components are:

long trace profiler (LTP) or nanometer optical component measurement machine (NOM)

LTP (commercial,Ocean Optics) or NOM (HZB, F.Siewert) for measuring surface slope error and curvature in a line scanning mode over the full optics length (~m).

figure interferometer

Figure measuring over a larger area. Figure interferometers are manufactured by ZYGO, and Veeco. The aperture is about 150mm. Stitching methods are under development which may overcome this limitation towards larger optics sizes.

optical interference roughness microscope

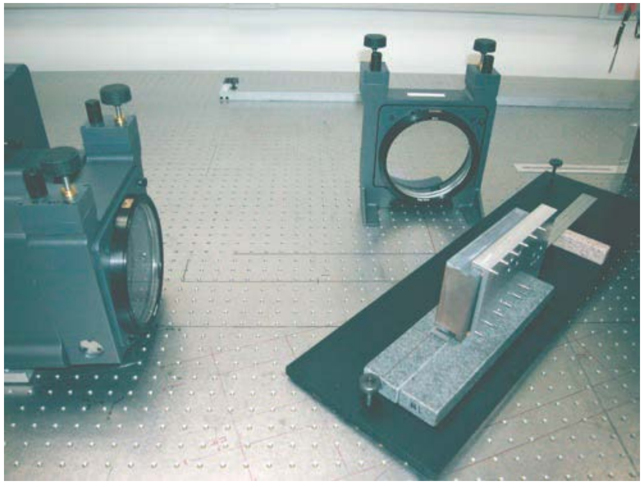
Local measurement (sub-mm) of the roughness on an sub-Å scale. Interference microscope (based of phase shifting technique) are manufactured by Veeco-Wyko, ZYGO, Phase Shift, Micromap.

Mirrors: Metrology Tools

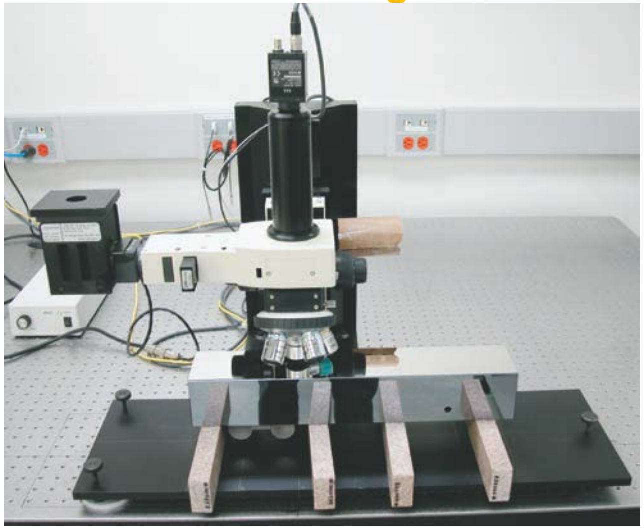
long trace profiler (LTP)

nanometer optical component measurement machine (NOM)

figure interferometer



optical interference roughness microscope

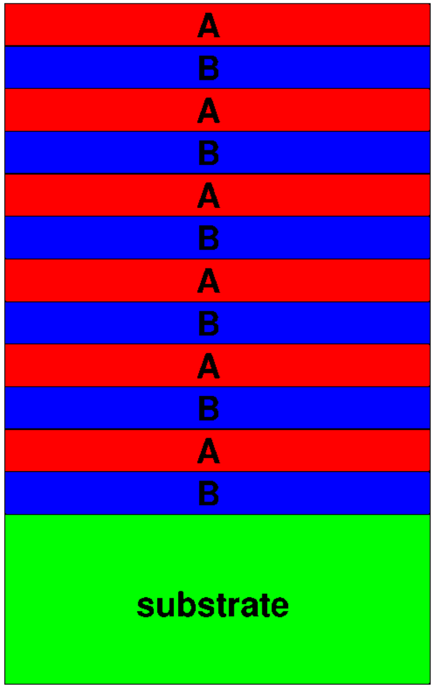


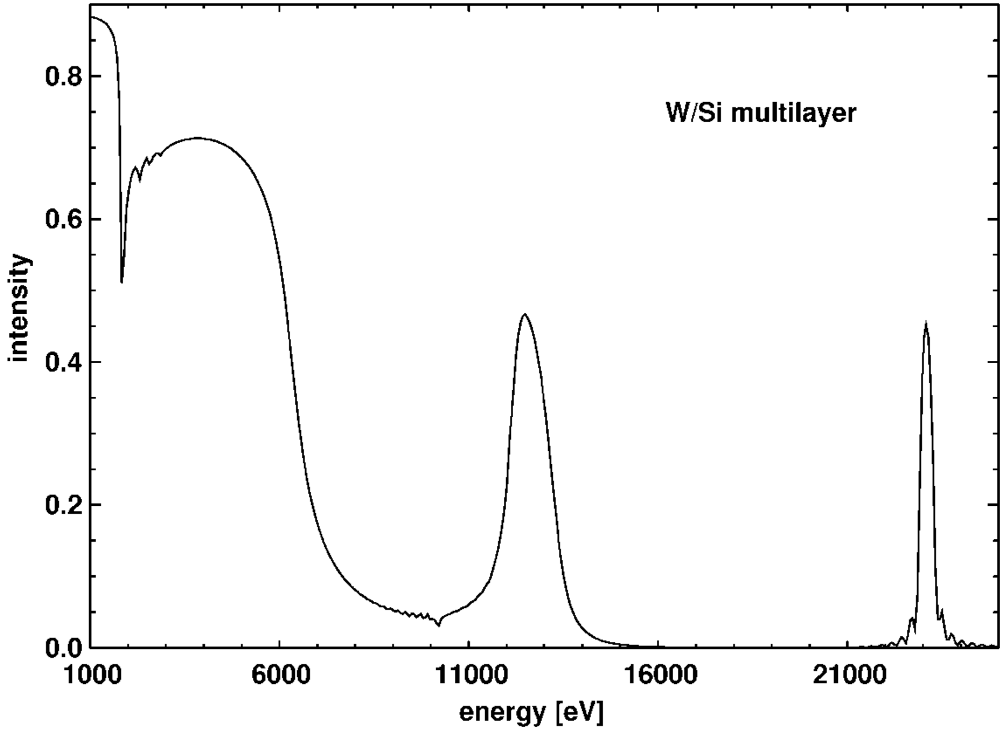
(pictures from CLS Optical Metrology Laboratory 2001-2004 activity report and F.Siewert, HZB)

Basic Optical Elements: Multilayers

mirrors	multilayers	single crystals
total external reflection	Bragg diffraction $2d\sin(\theta_B + \delta) = n\lambda$	
reflection	reflection	reflection, transmission
$\theta_C \approx 0.4^\circ$, Au at 10keV	$\theta_B \approx 1^\circ$	$4^\circ \leq \theta_B \leq 90^\circ$
	functions	
focusing	$\Delta E/E : 10^{-3} \ldots 10^{-1}$	$\Delta E/E : 10^{-2} \ldots 10^{-8}$
high energy cut-off	focusing	focusing

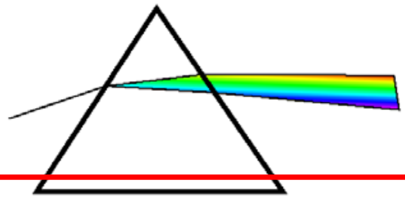
Multilayer



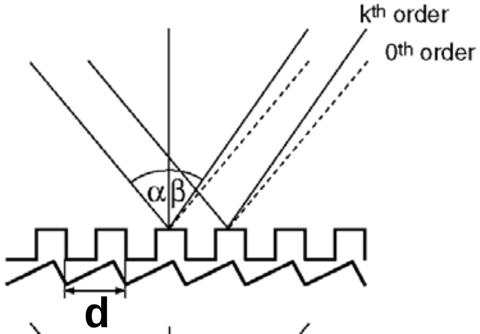


Multilayer principle and reflectivity curve of a typical W/Si multilayer. The present limit in the d-spacing of an AB-layer is in the 15 Å range.

Gratings

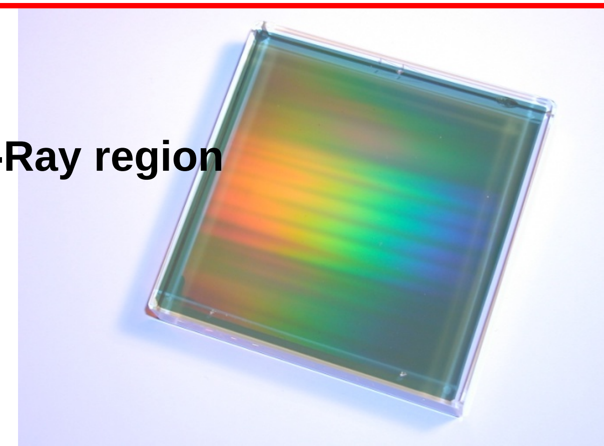


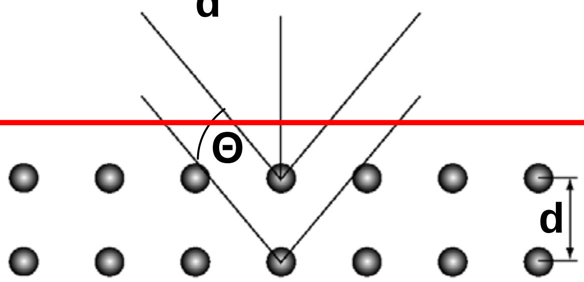
Prism: visible light and UV.
Heavily absorbing in the VUV/XUV and soft-X-Ray region.
Weak effect in the hard-Xray region: X-Ray Lenses



Grating: VUV/XUV and soft X-Ray region

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





Crystal: Hard X-Ray region

$$n\lambda = 2d\,(\sin \Theta)$$

Basic Optical Elements: Crystals

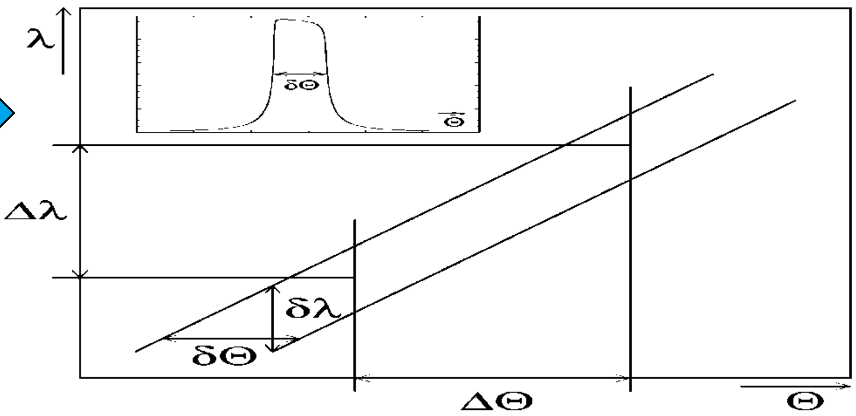
mirrors	multilayers	single crystals
total external reflection	Bragg diffraction $2d\,sin(\theta_B + \delta) = n\lambda$	
reflection	reflection	reflection, transmission
$\theta_C \approx 0.4^\circ$, Au at 10keV	$\theta_B \approx 1^\circ$	$4^\circ \leq \theta_B \leq 90^\circ$
	functions	
focusing	$\Delta E/E : 10^{-3}...10^{-1}$	$\Delta E/E : 10^{-2}...10^{-8}$
high energy cut-off	focusing	focusing

Crystals and Bragg´s Law

$$2d \sin\theta_B = \lambda \Longrightarrow \frac{\delta\lambda}{\lambda} = \frac{\delta E}{E} = \delta\theta \cot\theta_B$$

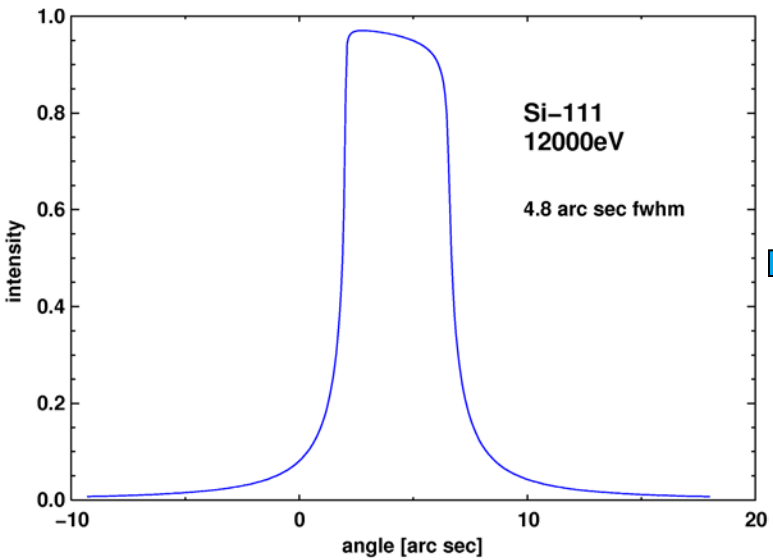
Basic treatment:

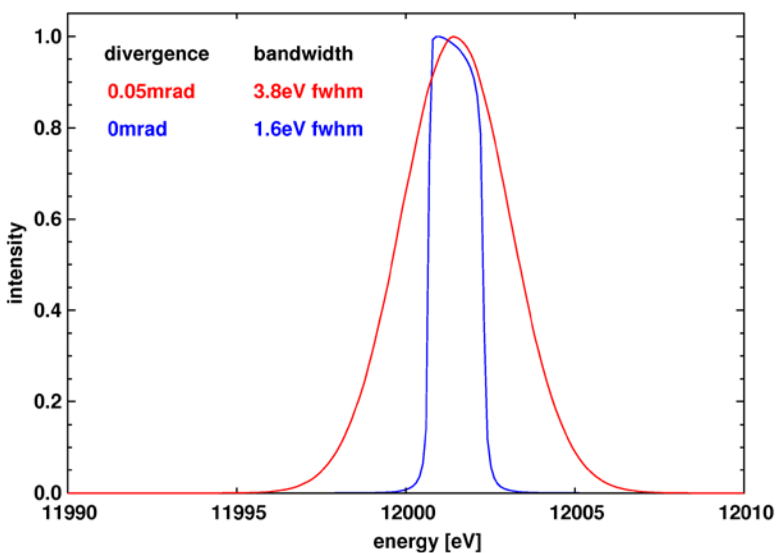
Du Mond diagram



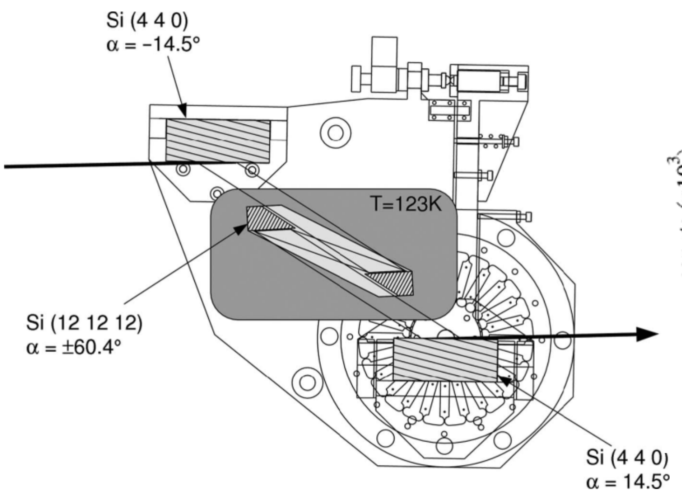
Extended treatment:

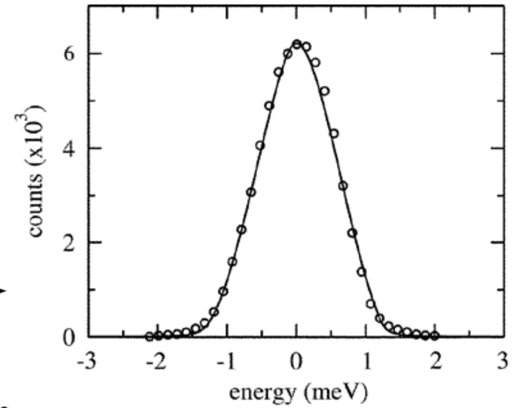
dynamical scattering theory





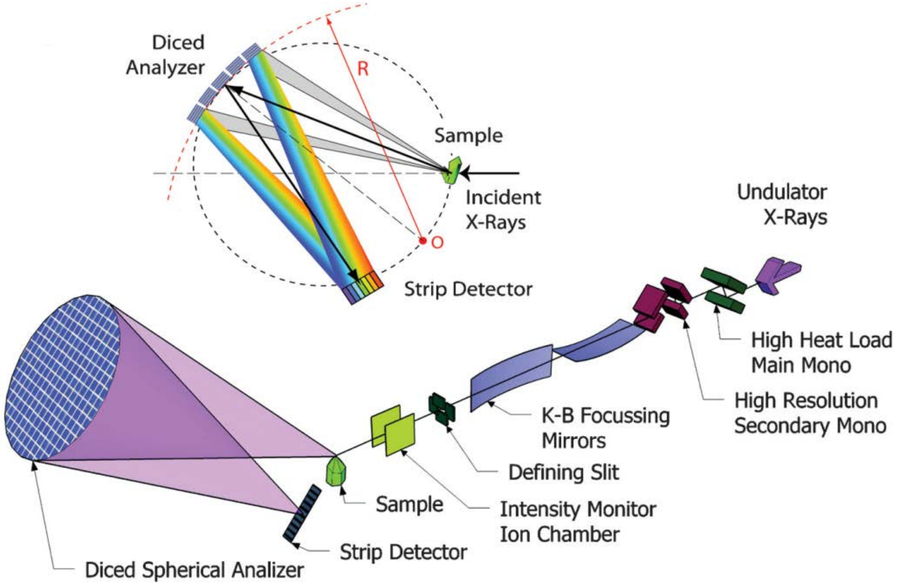
Ultrahigh Energy Resolution Monochromators and Analysators

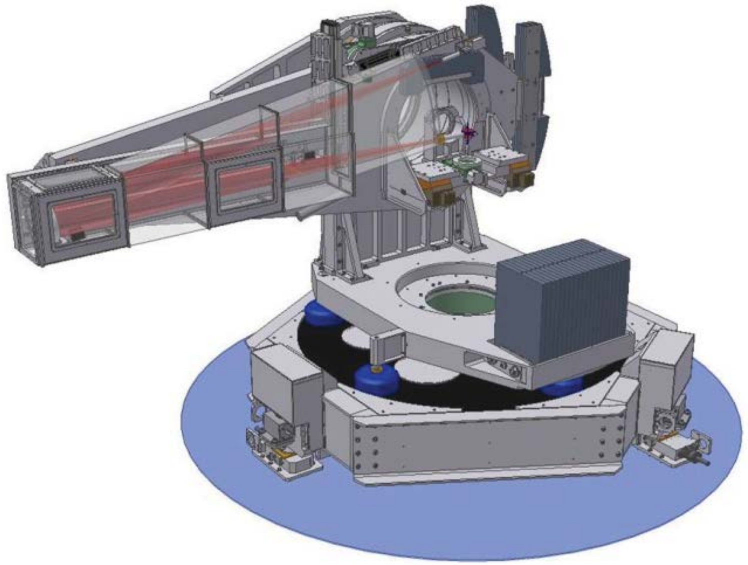




A cryogenically stabilized meV-monochromator for hard X-rays
T. S. Toellner,* A. Alatas, A. Said, D. Shu, W. Sturhahn and J. Zhao
J. Synchrotron Rad. (2006). 13, 211–215

Resonant inelastic x-ray scattering studies of elementary excitations
Luuk J. P. Ament et al.
Reviews of Modern Physics, Vol. 83, April–June 2011, 705-726





Monochromator System Design: Double Crystal Options

The non-dispersive (+/-) setting of two crystals is the most common realization of an X-ray monochromator in the hard X-ray energy range starting from ~2.4keV.

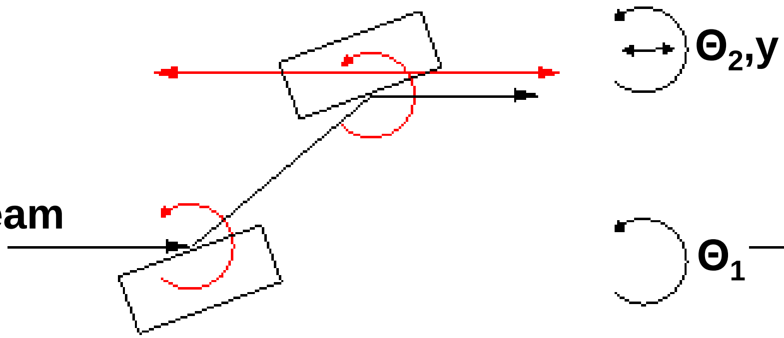
Basic fixed-exit monochromatic beam options:

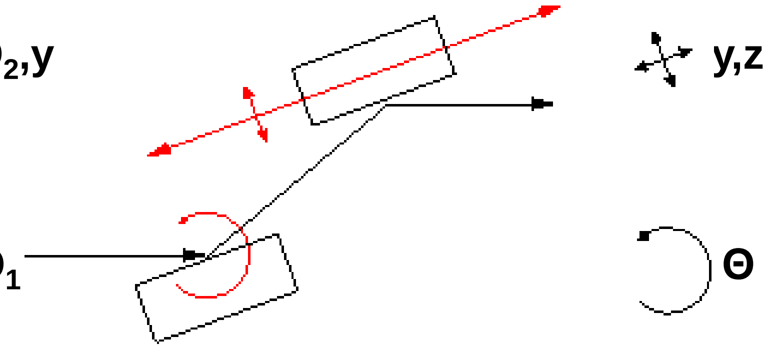
- **separated movement of both crystals**
- **central rotation and short or long 2nd crystal**

Channel-Cut type (monolithic or Pseudo) providing better intrinsic beam stability, but with limited energy range and moving, not fixed exit, monochromatic beam.

Monochromator System Design: Double Crystal Options

white beam

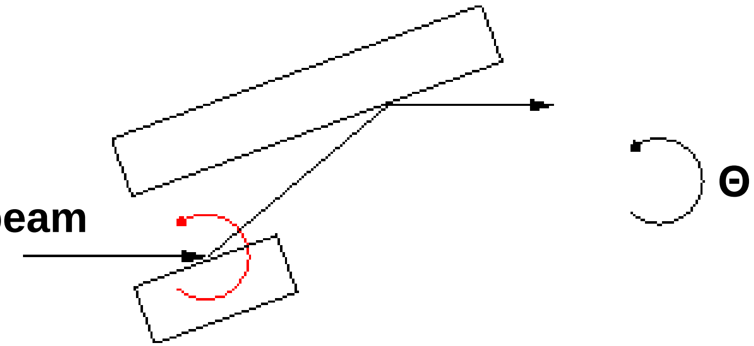




basic fixed exit setup with separated crystals

fixed exit setup with central rotation Θ, both crystals on rotating backplate

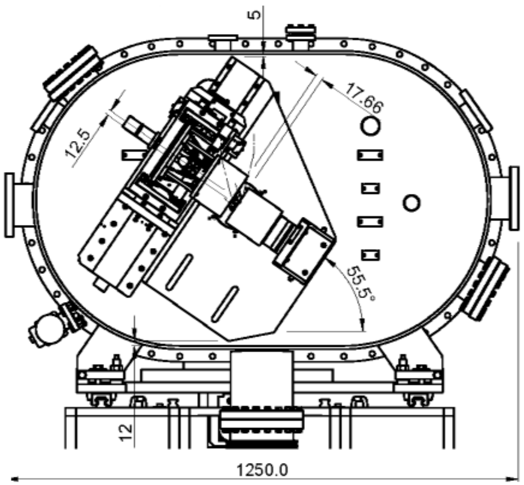
white beam

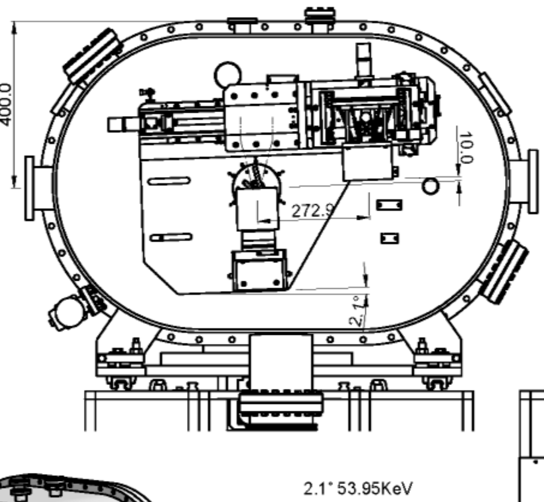


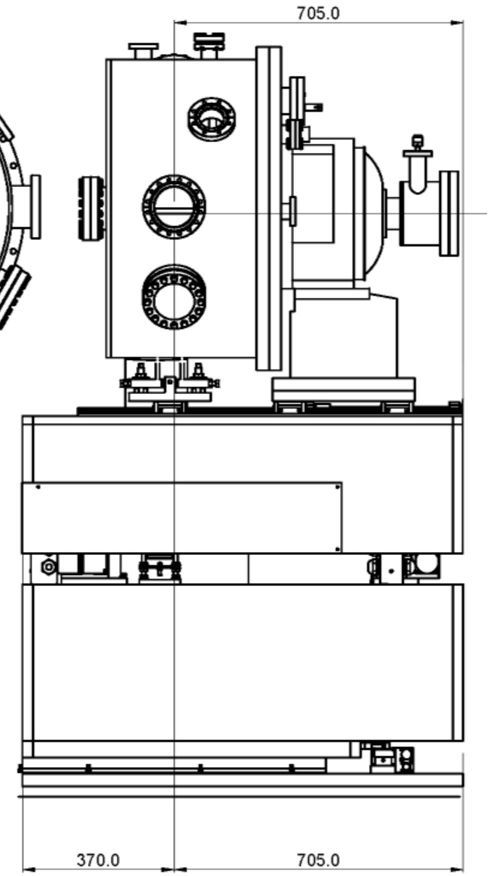
Channel-Cut (monolithic or pseudo) setup with one rotation axis only.
Energy range limited by crystal size and monochromatic beam not fixed exit

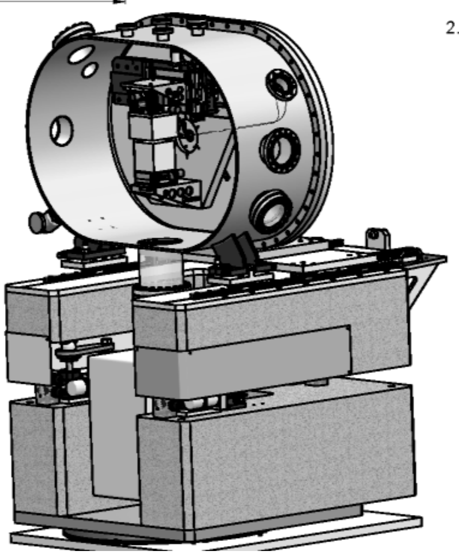
PETRA III High Heatload Monochromators

FMB-Oxford Systems for PETRA III





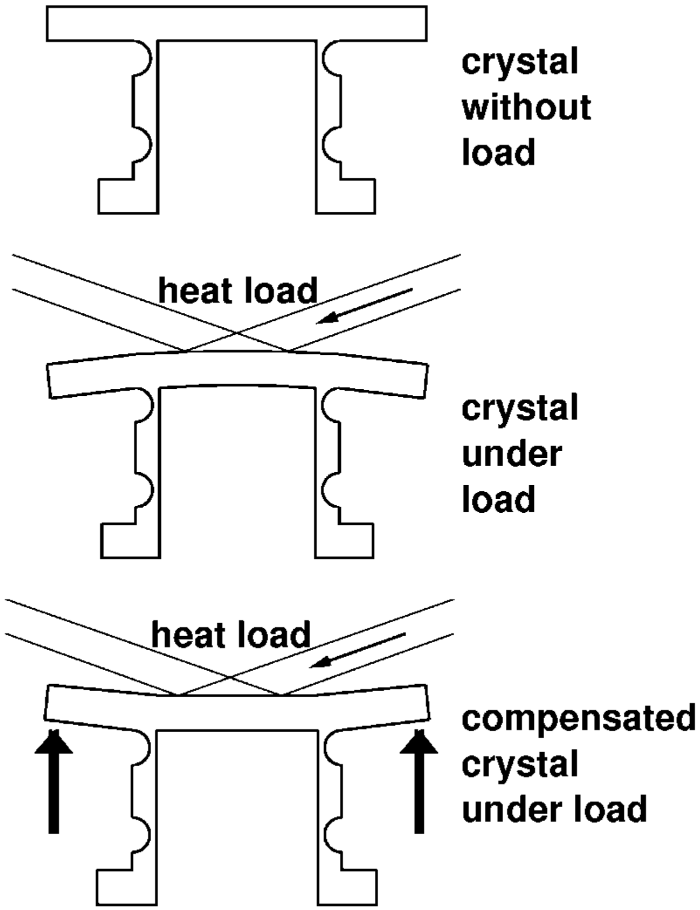




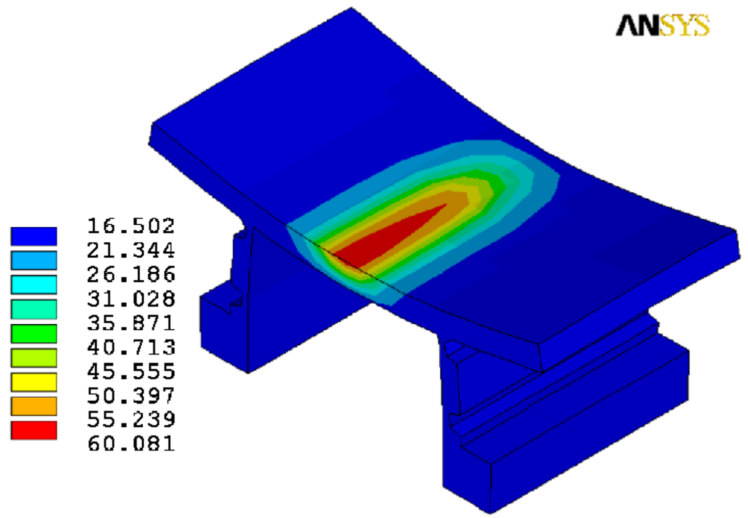
Si 111 **2.4keV – 54keV**

Si 311 **4.6keV -103keV**

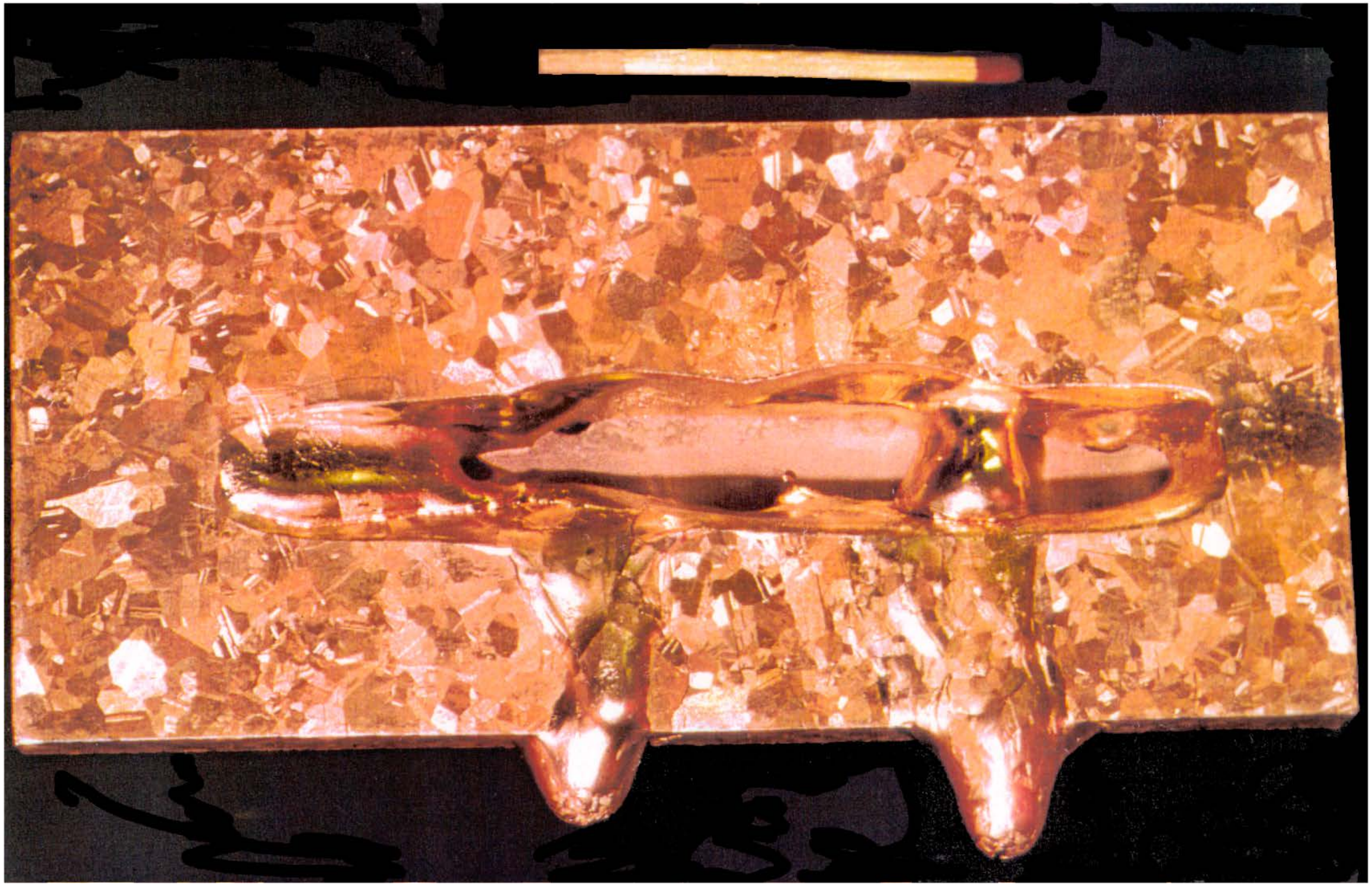
Heatload Issues: Water cooling



adaptive bending

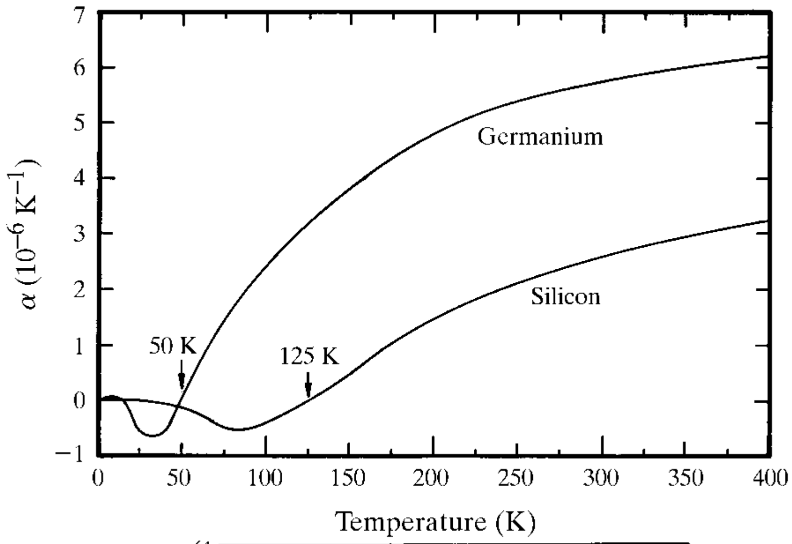


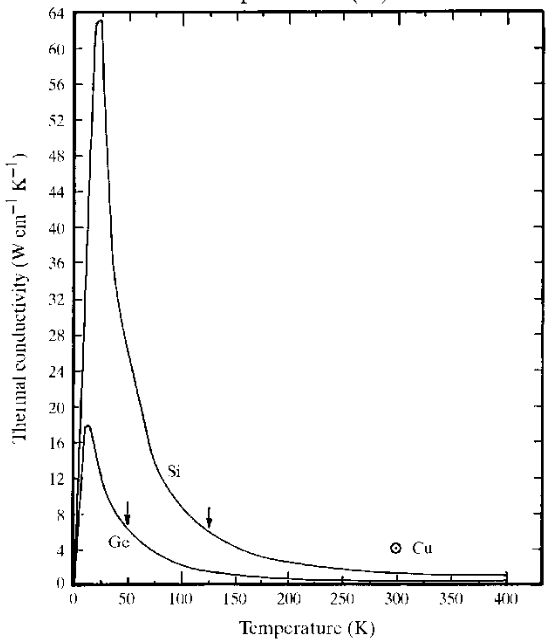
Heatload Issues: Damage



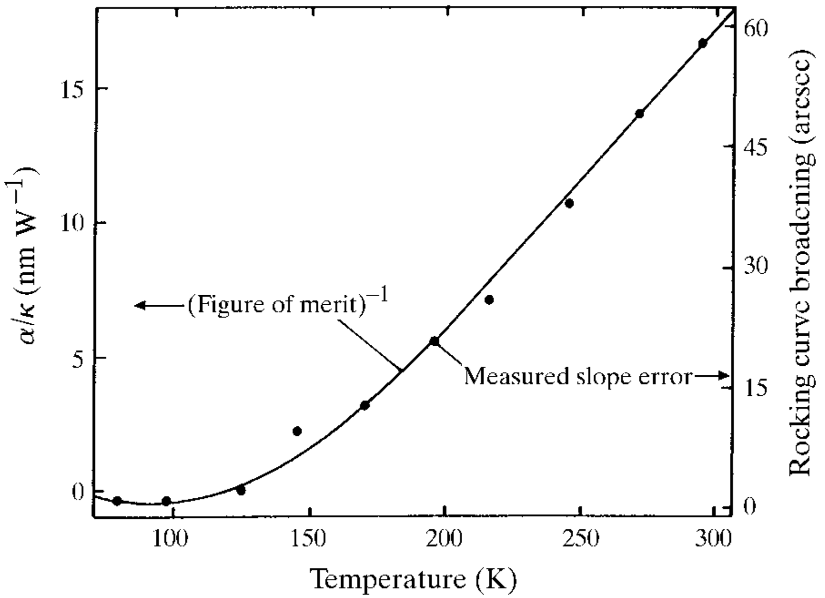
Re-crystallized copper absorber damaged by a white synchrotron light beam after a failure of the water cooling system

Heatload Issues: Liquid Nitrogen Cryo-Cooling

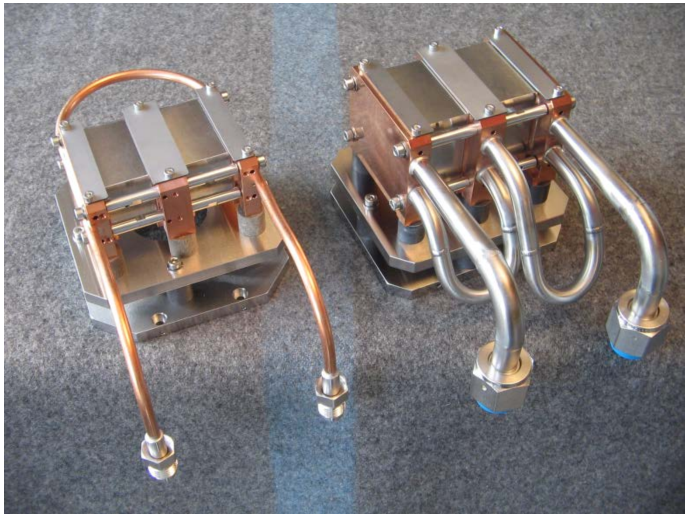




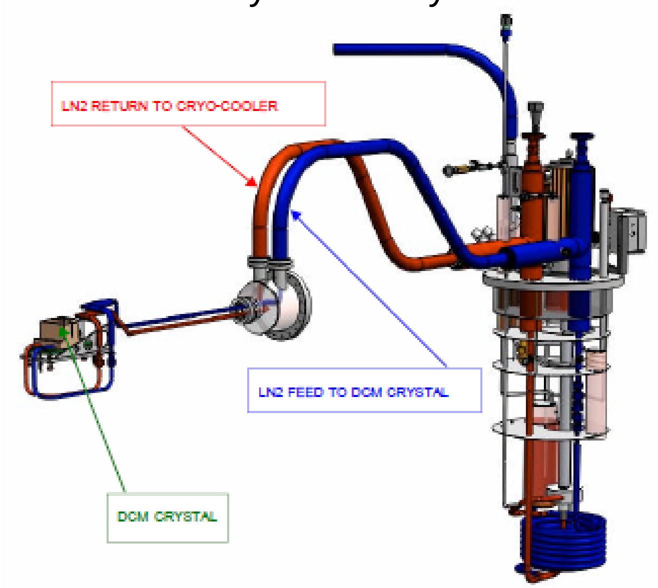
„figure of merit“ α/κ

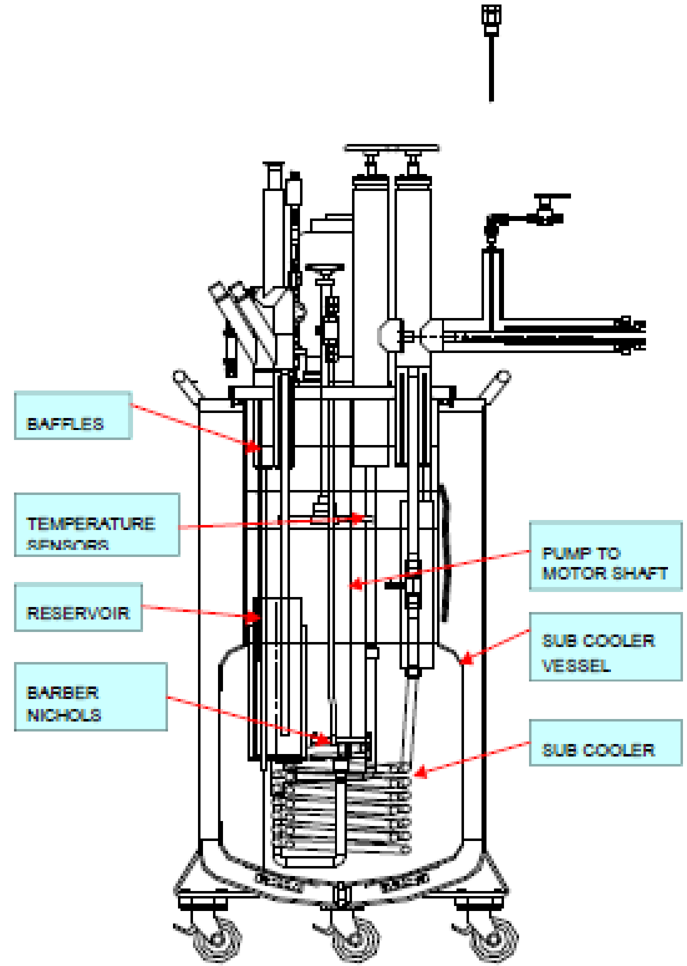


Heatload Issues: LN2 Systems



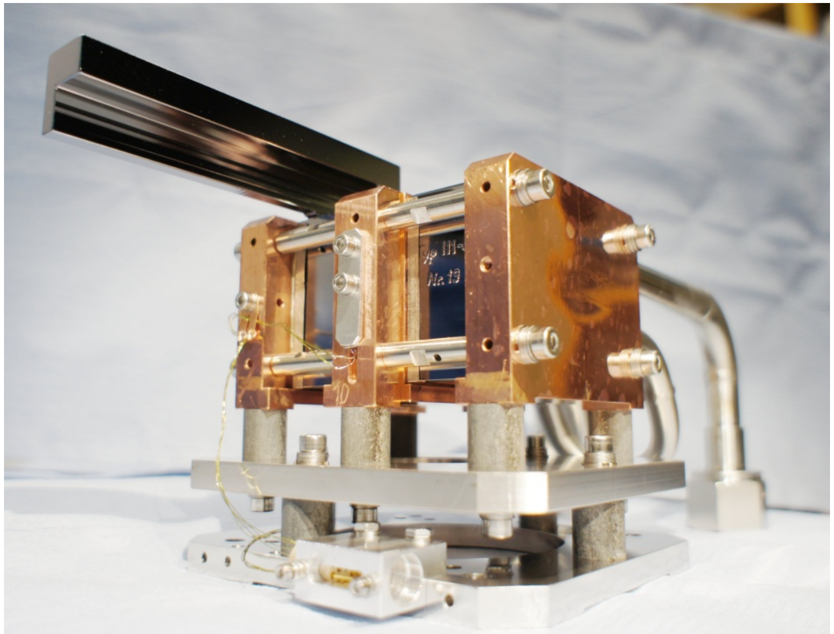
Indirectly cooled crystal sets



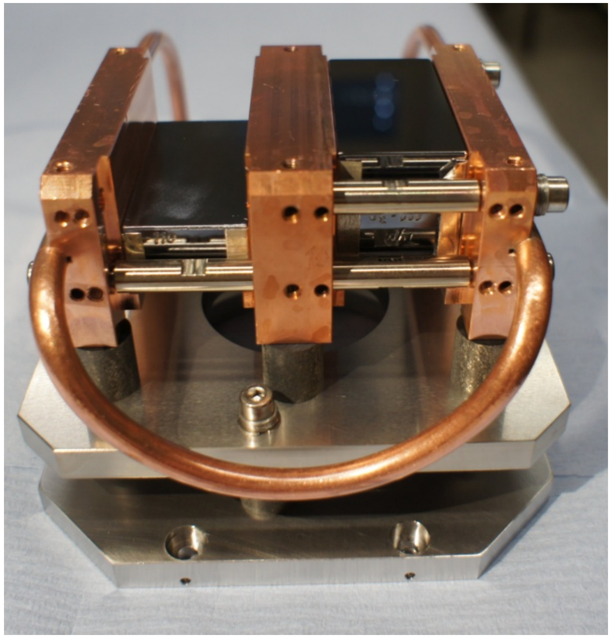


FMB-Oxford Model D cryocooler, cryo-loop and vessel (from manual)

Heatload Issues: LN2 Systems: Photon Beam Stability



first crystal set



second crystal set

Channel-Cut crystal system integrated into the high heatload fixed exit design.

LN2 Distribution Systems

central storage, central phase separator, and LN2 distribution systems installed at PETRA III

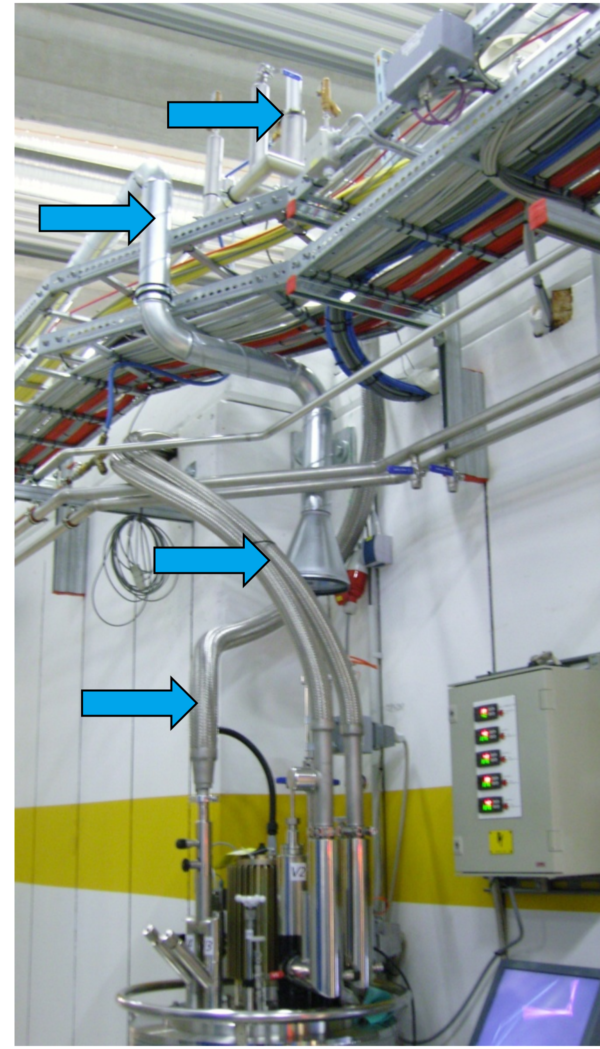
heat transfer capacity of up to 2000 Watt for each monochromator

ln2 refill valve

gas exhaust

high pressure lines to monochromator

ln2 refill

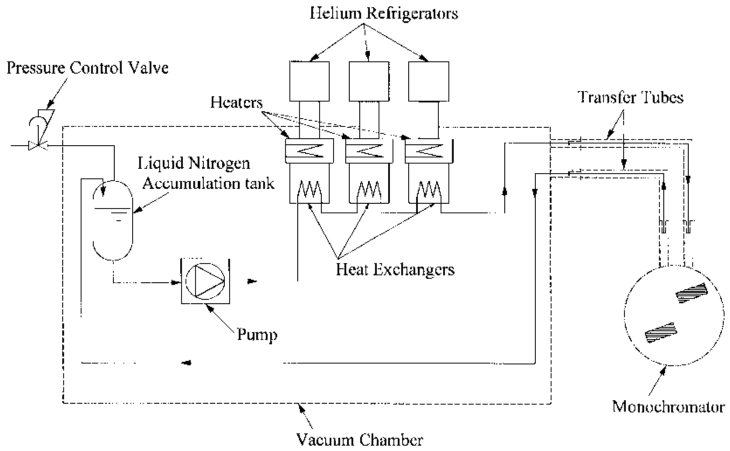


DESY

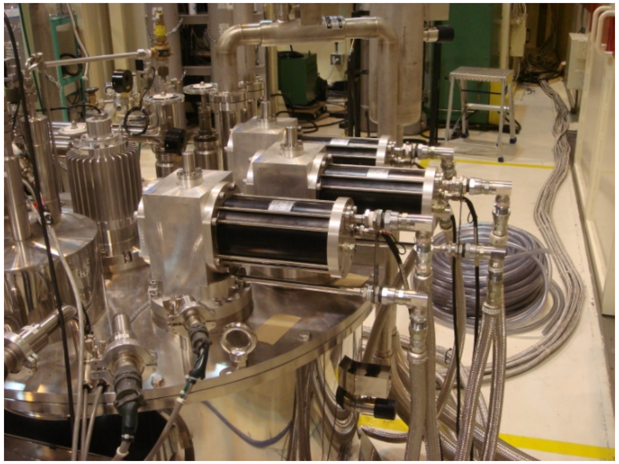
LN2 Distribution Systems

local storage and helium refrigeration systems installed at Spring8

heat transfer capacity of 500 Watt for each monochromator



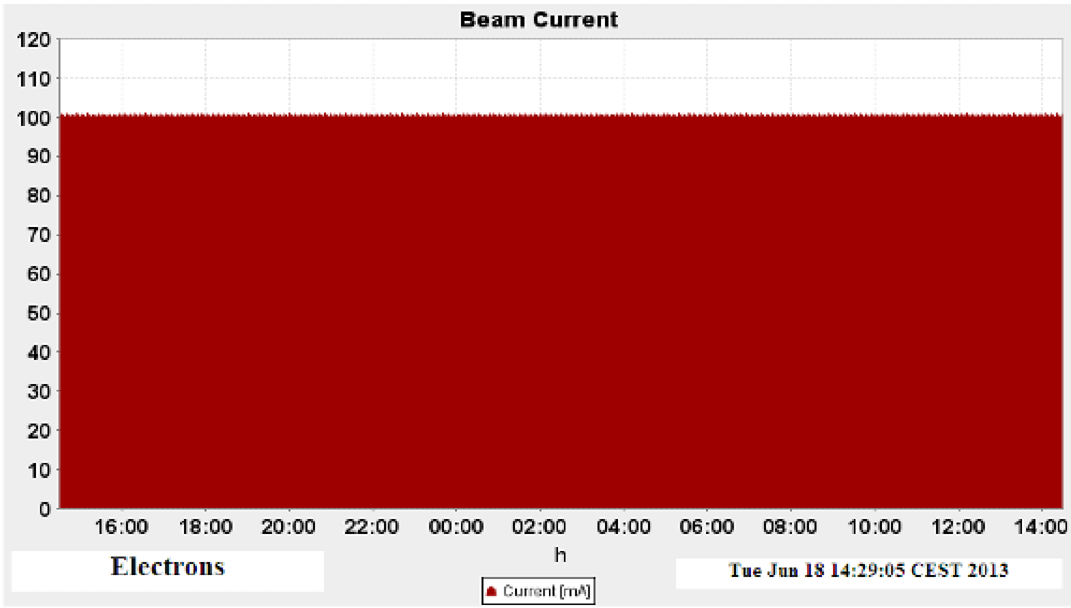
Cryogenic cooling monochromators for the SPring-8 undulator beamlines
T. Mochizuki et al. / Nuclear Instruments and Methods in Physics Research A 467–468 (2001) 647–649



Photos
H. Schulte-Schrepping

Top-Up Operation: Stable Power Load on Optics

PETRA Energy: 6.084 GeV Lifetime: 12.04 h Current: 100.87mA



Und.	Gap	Status
PU01a	25.42	
PU01b	25.61	
PU02	10.00	
PU03	10.21	
PU04	22.19	
PU05	11.22	
PU06	11.46	
PU07	10.31	
PU08	11.82	
PU09	18.80	
PU10	10.96	
PU11	15.68	
PU12	20.05	
PU13	101.00	
PU14	11.01	

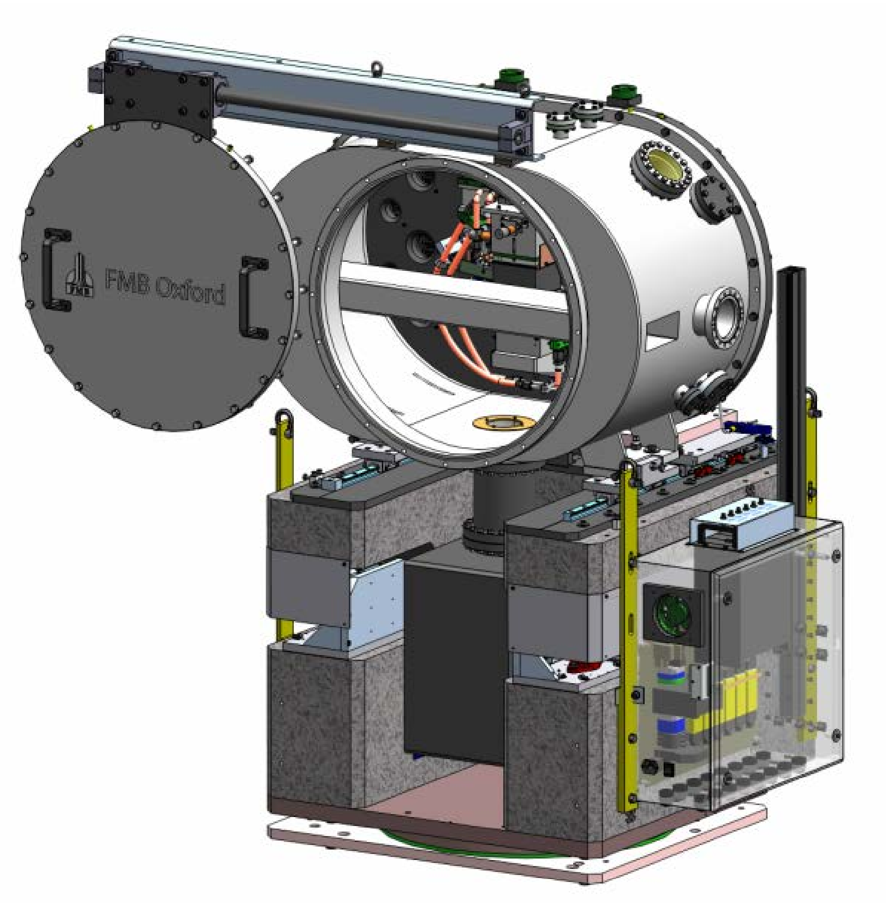
Number of Bunches: 960 Mean Vacuum Pressure: 1.529E-08 mbar

Orbit Control: On Top-Up Operation: 1.02 mA (Max-Min)

User Operations->Experiments

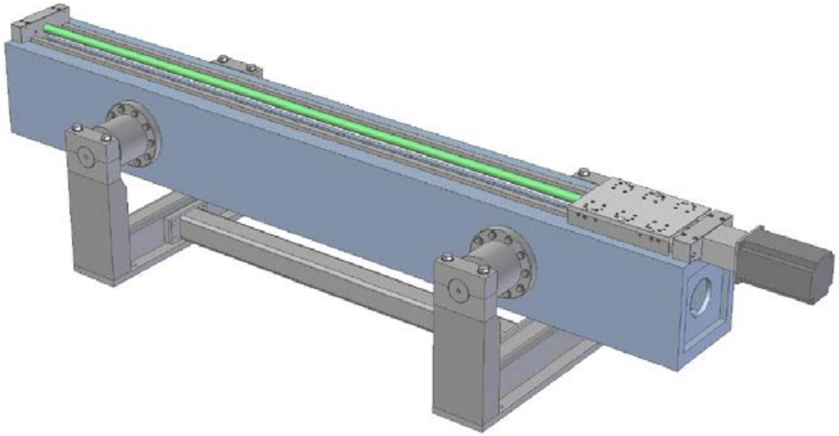
User run, 960 bunches, 100 mA

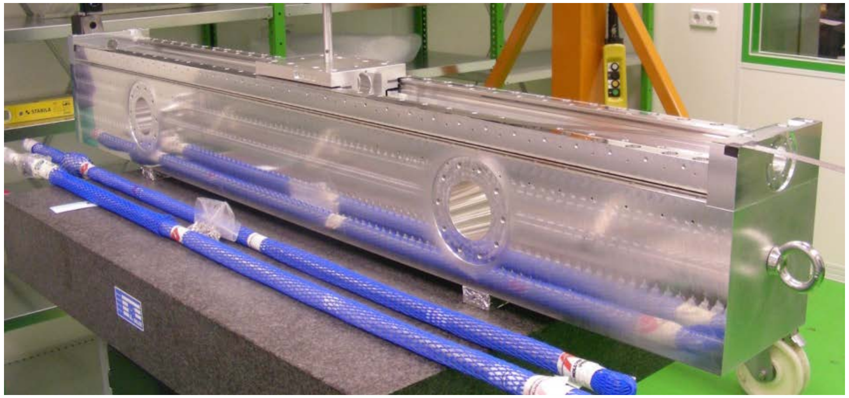
High Heatload Monchromators

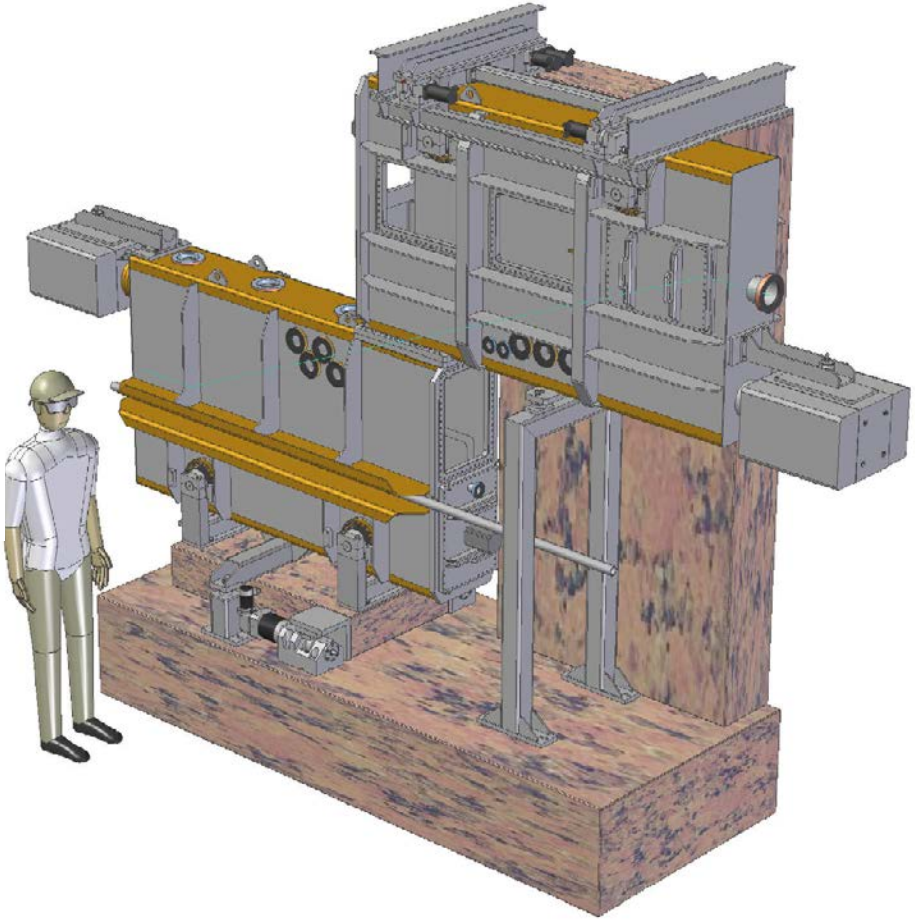


Monochromator systems for canted undulator sectors at PETRA III

Large Offset Monochromator LOM1250 for P08





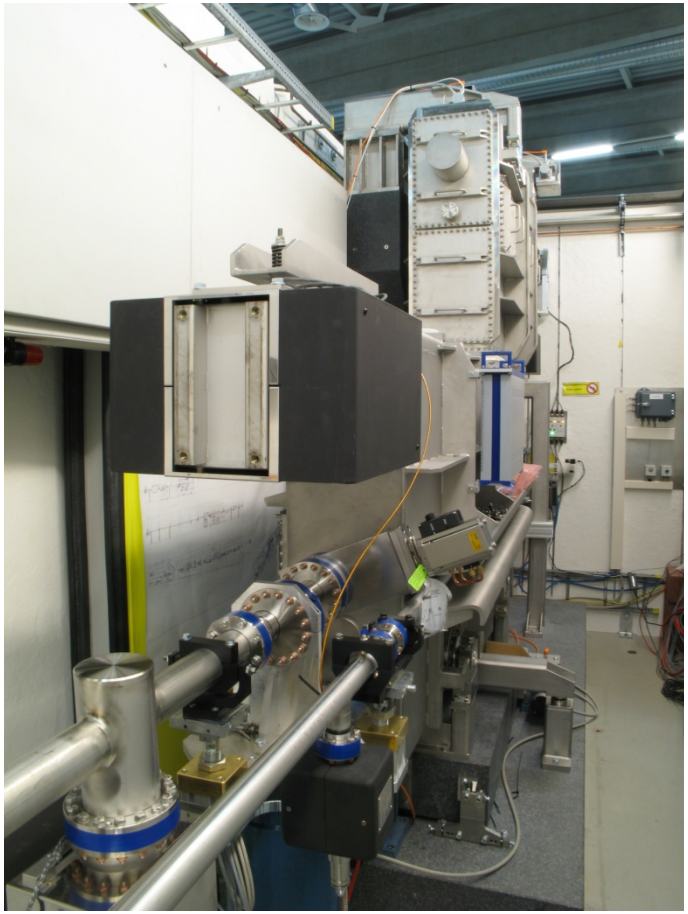


Vertical offset of a monochromatic beam = +1.25m

2 * 1.5m crystal translation, two separate vessels with granite support

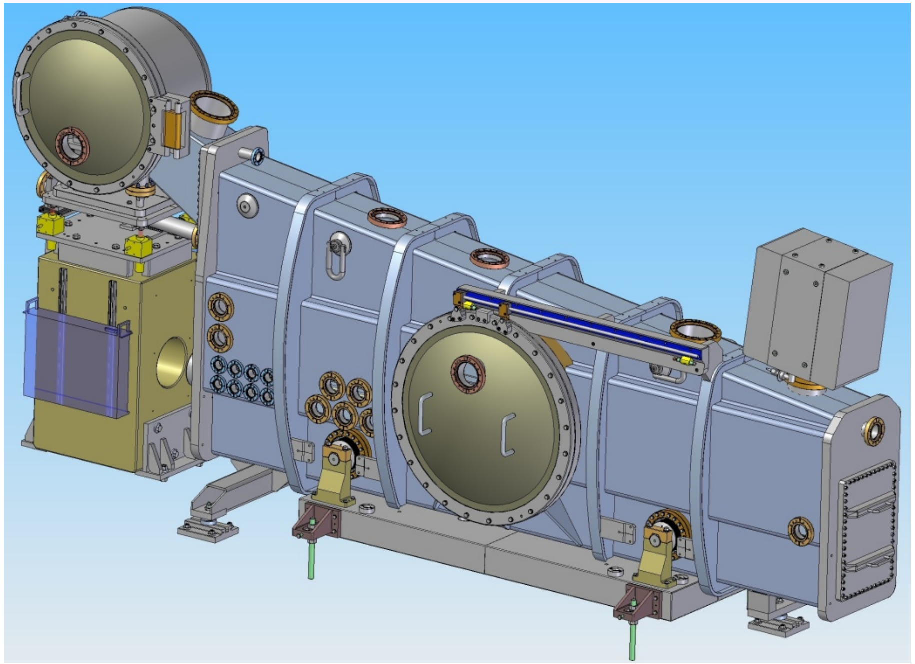
Large Offset Monochromator

Both vessels with mounted translation



Installed system in P08 hutch

Large Offset Monochromator LOM500 for P03



4.5m

Monochromatic beam with Multilayer option, high heat load design , LN2 cooled

Vertical offset = - 0.5 m

One 2.4m long translation for second crystal/multilayer system

Beamline-Technology Infrastructure

Local infrastructure for the maintenance, on-site repair and modification of user experiments, and for the preparation of samples :

- **mechanical workshop**
- **chemistry laboratories**
- **vacuum group infrastructure support**
- **crystal/sample preparation laboratory**

Mechanical Workshop

Chemistry Laboratories

Beamline-Technology Infrastructure

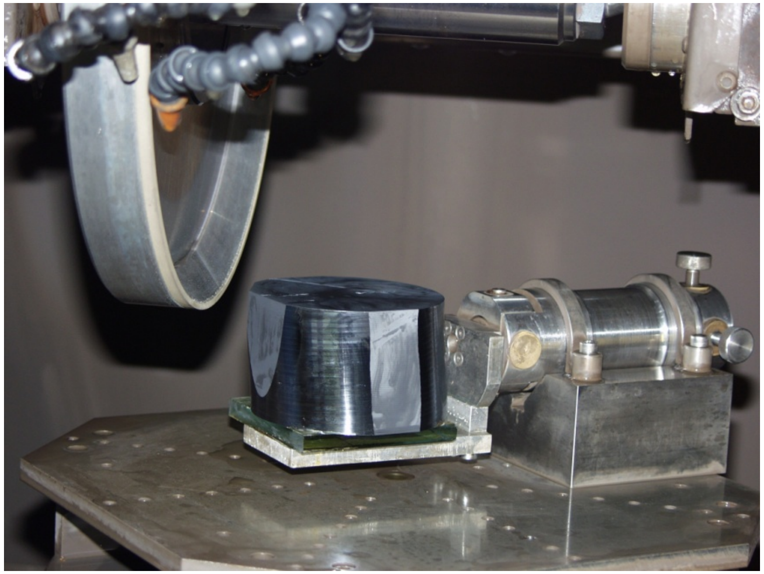
Vacuum group facilities

- Cleaning facilities for UHV parts
- Assembly and test of vacuum components in clean room environment
- Leak testing, UHV mass-spectrometry

Crystal/sample preparation

Specialized tools and procedures for

- Crystal alignment, cutting, etching, polishing
- Sample preparation

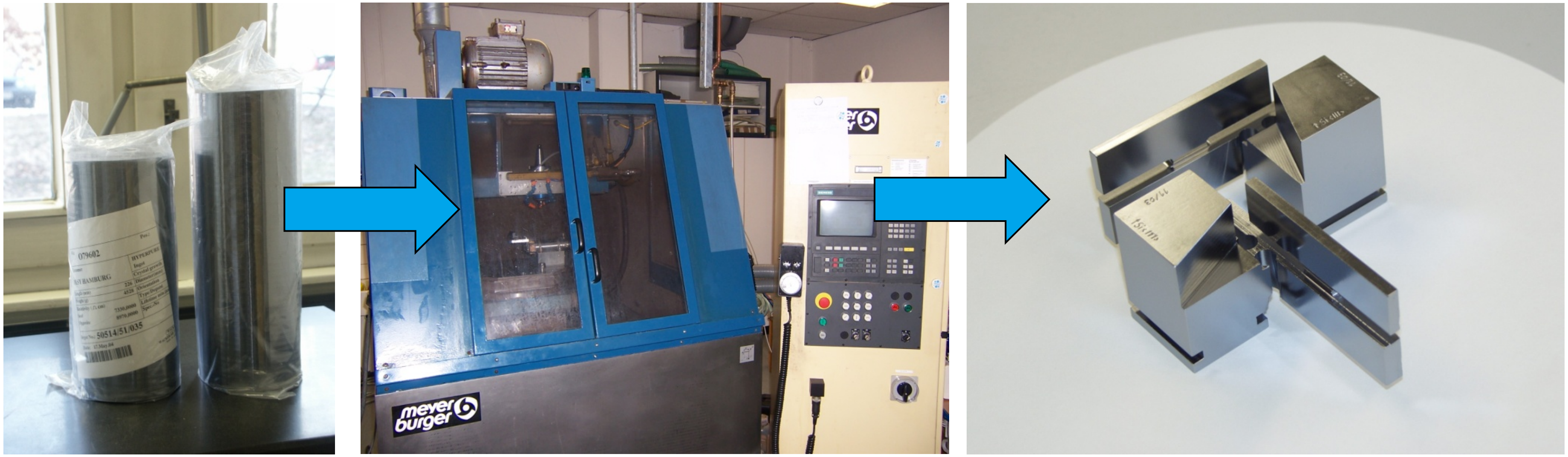


Crystals Optics: Silicon

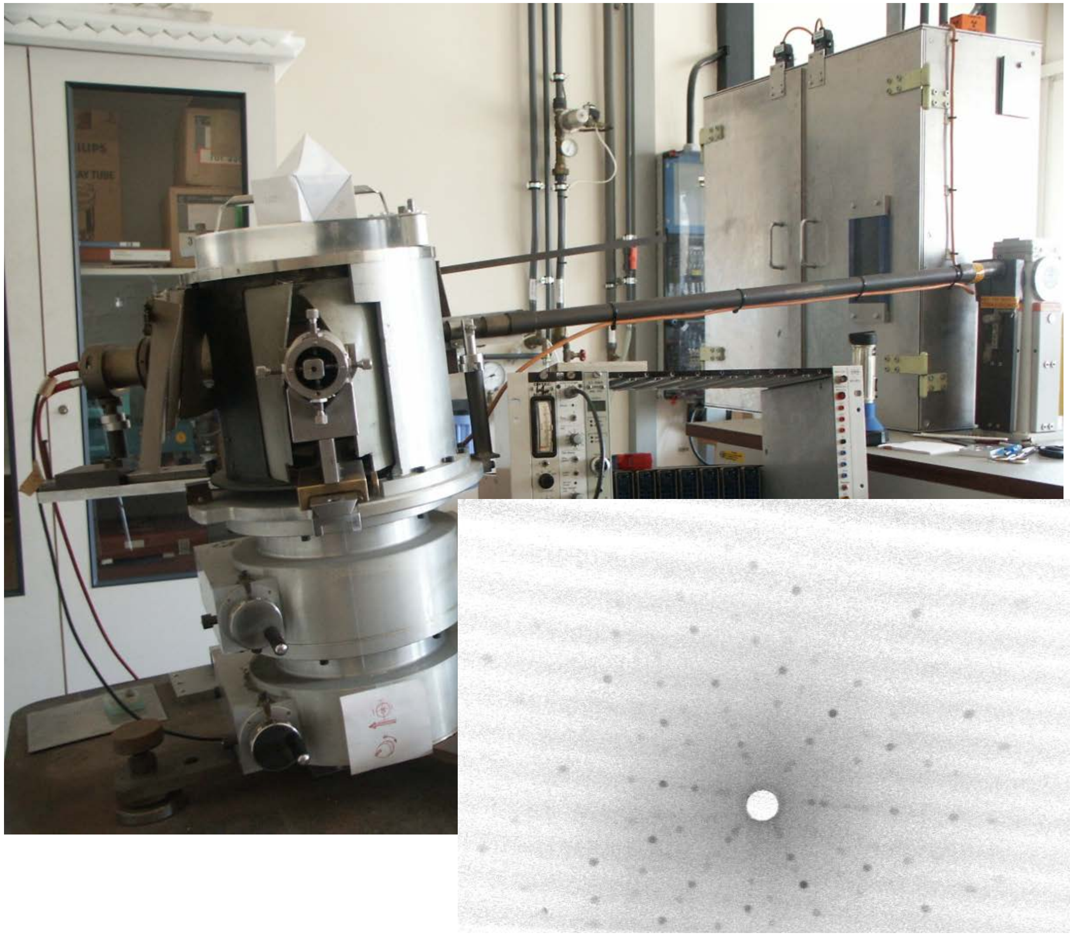
silicon based monochromators

(111),(110),(100),(311),(511) ,…..with arbitrary crystal lattice orientation

in Bragg and Laue Configuration available due to locally available processing technology



Crystal Optics: Crystal Orientation



Silicon single crystal ingots
4inch dia., length 25cm-30cm

Crystal orientation unit and Laue camera at fixed anode Mo X-ray tube. Image plates and scanner for Laue camera

DESY

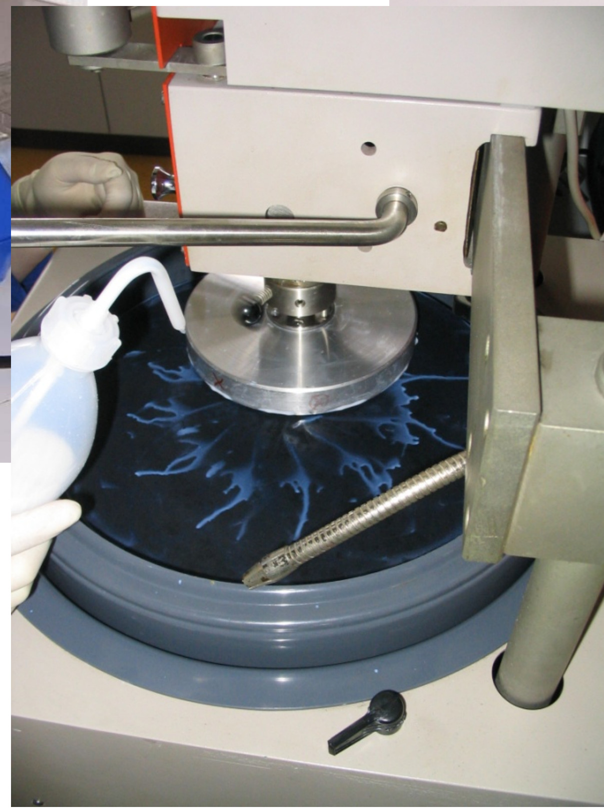
Crystals Optics: Cutting and Dicing

Wire-saw for coarse cutting of large Si pieces and special (hard) materials, i.e. tungsten, molybdenum

NC-controlled cutting with rotating blade or optional high speed milling tool, max thickness of work piece of 4 inch

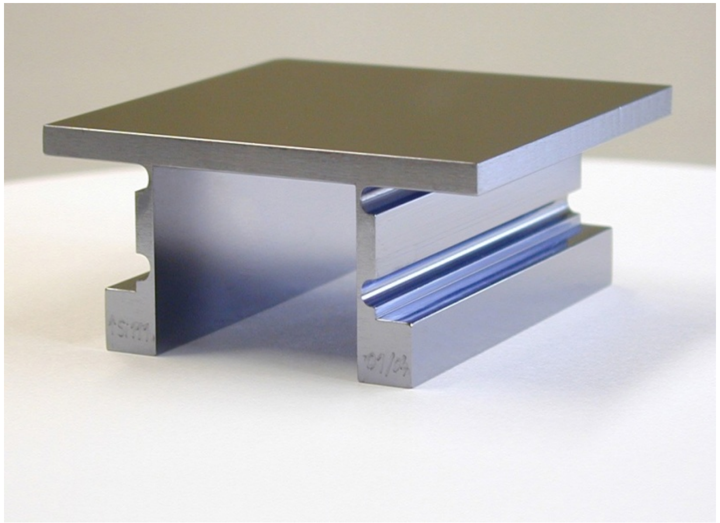
Crystals Optics: Surface Treatment

motor and ultrasonic driven handheld tools

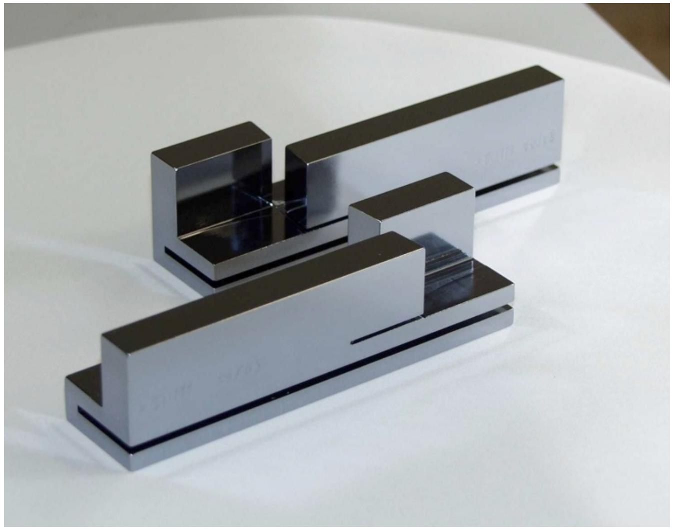


several grinding, lapping, and polishing tools
mechanical and mechanical/chemical (Syton®) surface treatment

Gallery of Silicon Art

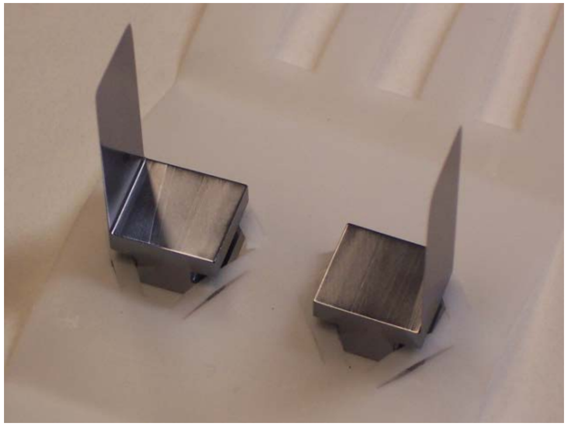


Torii crystals: W1, BW1, BW2, BW4, BW6



Bartels type channel cut

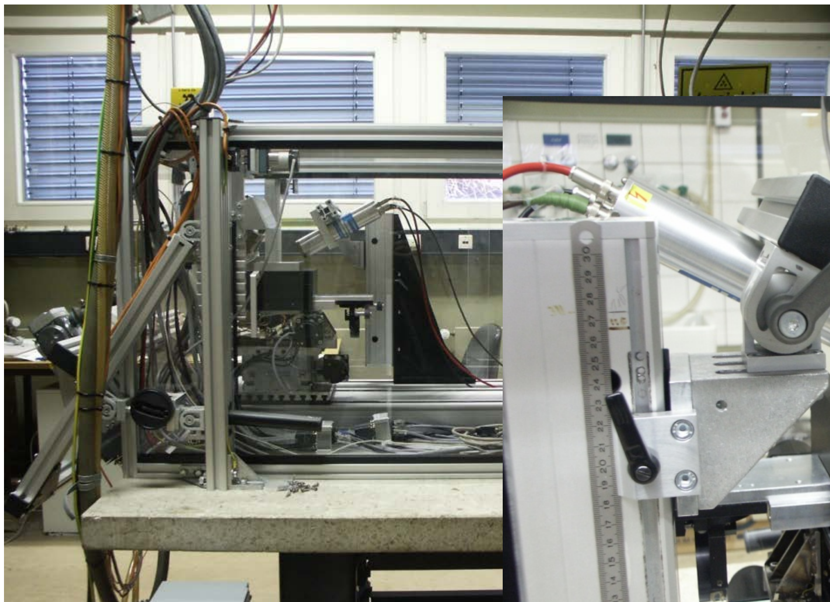
Laue case wideband focusing, 100mm wide: HARWI-II



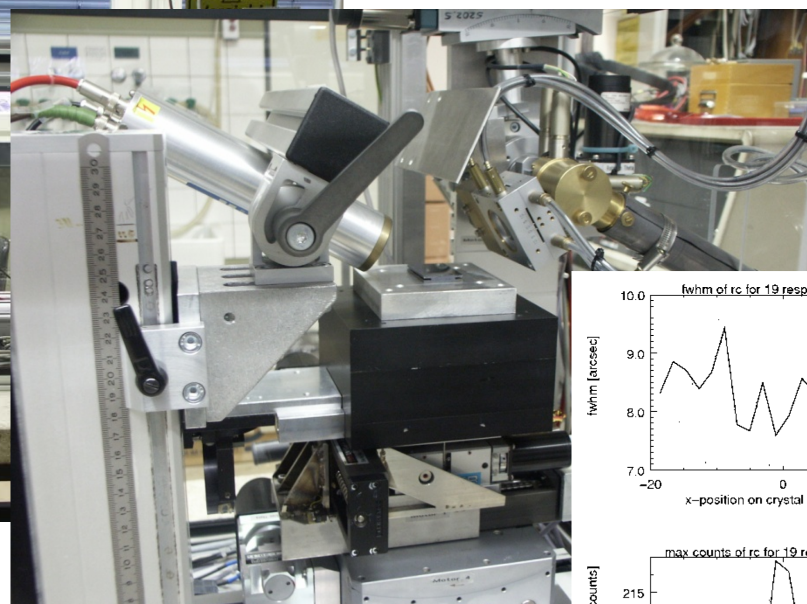
Laue case delay line crystal pair, wedge thickness from 200µm to 20µm over 20mm lamella height.

Crystals Optics: Metrology of Rocking Curves

High resolution rocking curve scans along a 100mm long line inside a 100*100mm^2 surface area.
Large system volume allows for full crystal systems with a height up to 220mm, i.e due to heat exchangers.
Automatic data evaluation provides height profiles from integrated rocking curve shifts.

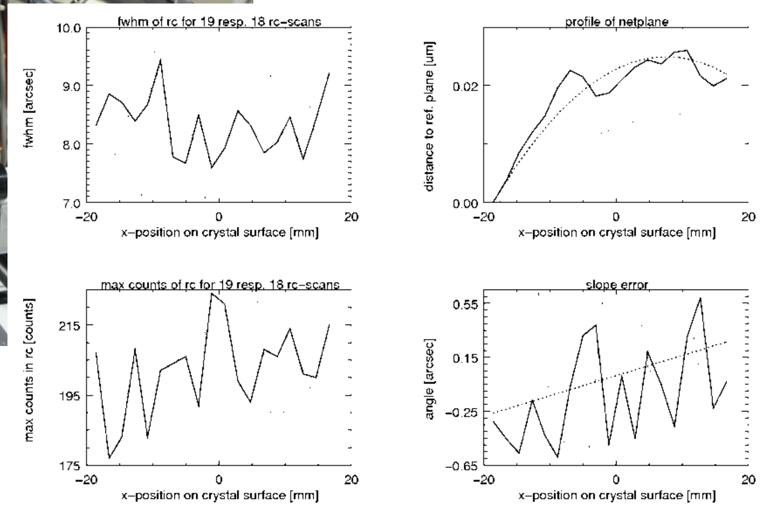


System with shielding enclosure on optical table



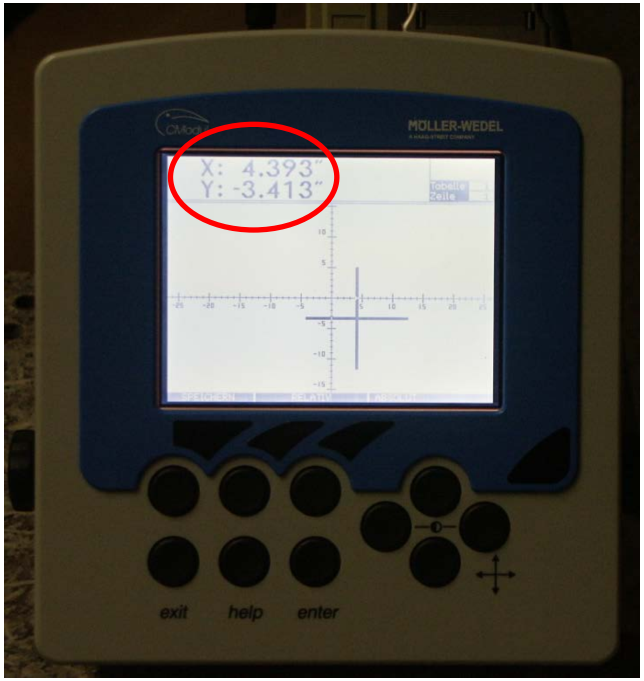
X,Y,Z,Ө stages, detector

Data evaluation



Mechanical Metrology: Autocollimation Systems

High precision simultaneous determination of 2 rotational degrees of freedom.
Two autocollimation systems with 0.1 and 0.01 arcsec accuracy
Granite benches in sand-boxes and on decoupled base structure.



Elcomat 2000, 0.1 arcsec accuracy

Elcomat HR, 0.01 arcsec accuracy

Crystals Optics: Diamond

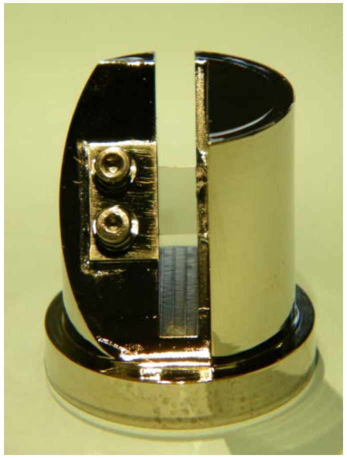
diamond based monochromators, phase plates

mostly (100) and rarely (111),(110) are the only symmetric faces available

(100) highly oriented, the others within a (few) 0.1 to 1 degree region of miscut

Few local etching and polishing tests

Aquire



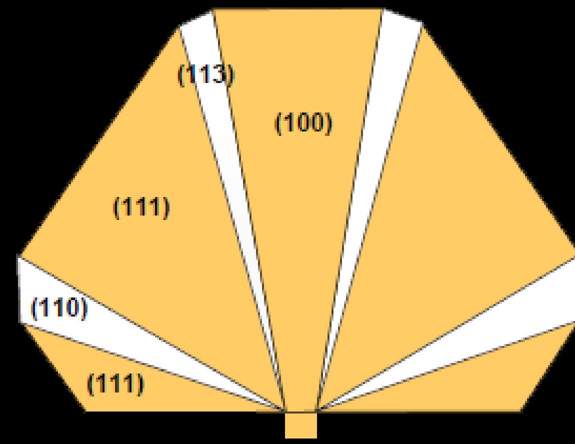
P02.1 Diamond

Mounted (100) E6-Diamond crystal, Laue case (111), indirect water cooling.

6.5mm x 6.5mm x 0.4mm

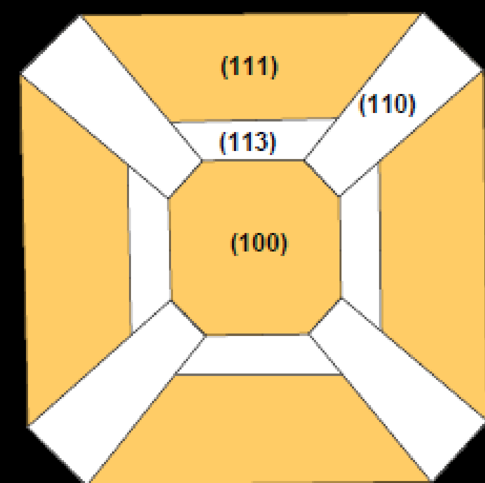
Diamonds: Growth Issues

HPHT Diamond



Growth sector dependence of
N concentration,
[111]>[100]>[113]>[115]>[110]

B concentration,
[111]>[110]>[100]=[113]>[115]



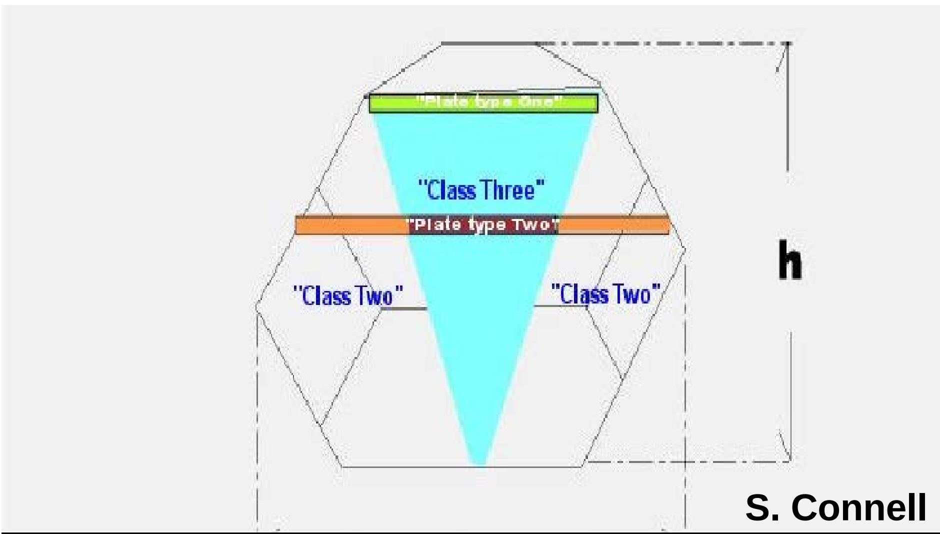
Cube growth sectors have
A high density of perp.
dislocations

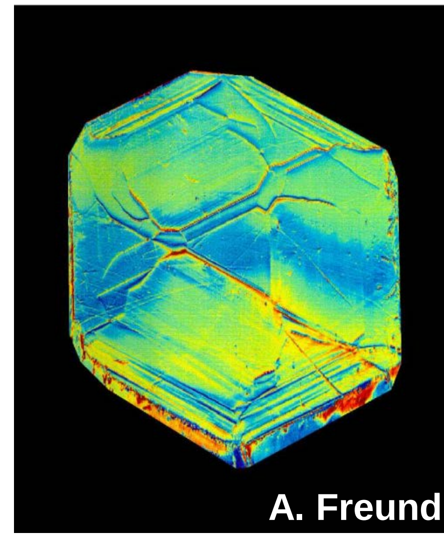
Simon Connell, Wits

Diamonds: Classification

High thermal conductivity and low thermal expansion

Monochromator applications require perfect and large (few mm²) diamond plates





Classification scheme for a diamond HPHT (100) diamond crystal for synchrotron applications:

Top plate: highest quality

Type Two plates with smaller perfect area, but larger support area

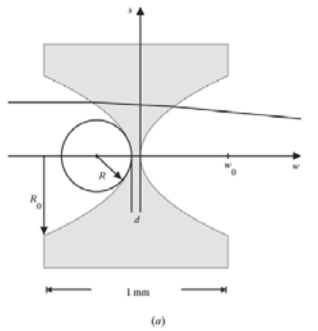
Special Optical Elements: Lenses

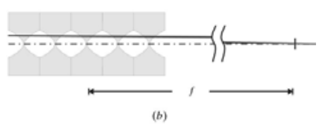
lenses	zone-plates	Bragg-Fresnel zone-plates
refraction	diffraction	diffraction
transmission	transmission	reflection by θ_B
$\delta \approx 10^{-6}$	$\Delta r_n = 30$ - 100nm	
	functions	
focusing	focusing	monochromatization and focusing

Lenses: Refractive Optics

Complementary design route to high precision mirror developments

Optical elements based on refraction : X-ray refractive lenses

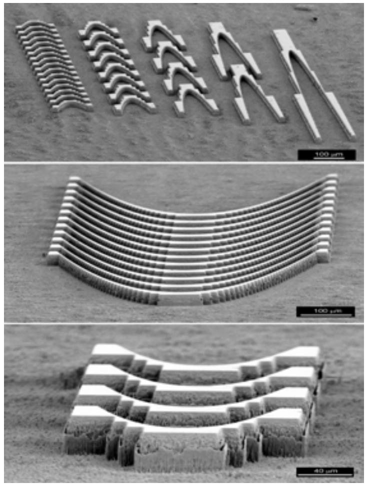




- lens maker formula 1/f=2(n-1)/R
- small R, e.g. 180µm and many lenses
- low absorption material and small d, e.g. 150 µm
- $2R_0$ energy dependent, e.g. at 8 keV ~ 1.2 mm

Be X-ray lens by B.Lengeler, Ch. Schroer

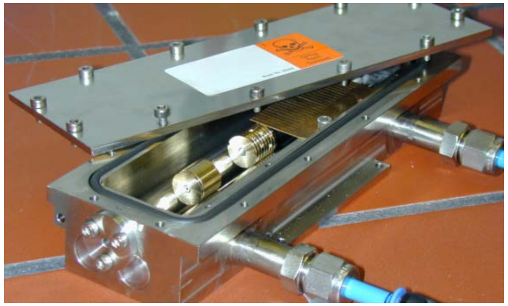
- choice of materials: Al, **Be, C**, B_4C
- KB-like decoupled planar devices: **Si, C**



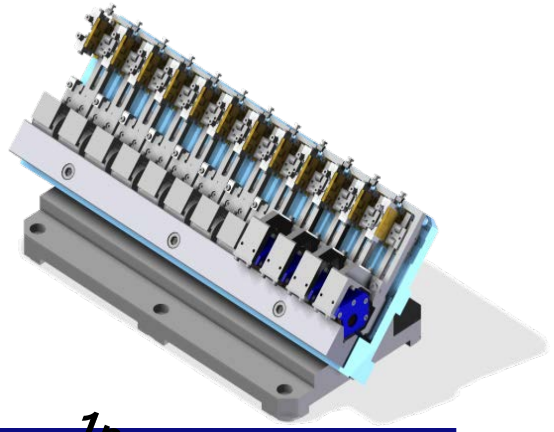
diamond planar refractive lenses for third and fourth-generation X-ray sources:
B. Nöhammer, J. Hoszowska, A.K.Freund, Ch. David, J. Synchrotron Rad. (2003). **10**, 168-171

Development of Refractive Optics Systems at PETRA III

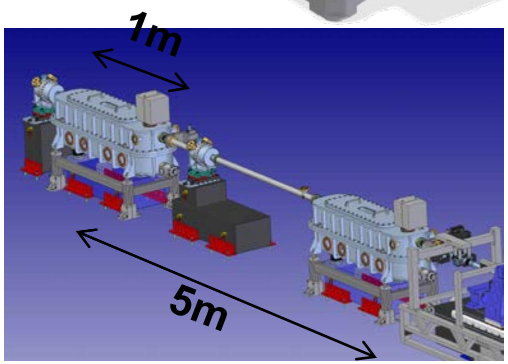
From stacking lenses to automated systems and Transfocators



Original manual stacked parabolic lenses as used in monochromatic and white beams at ESRF (C.Schroer et.al.)



Mixed 1D and 2D lenses Transfocator at the PETRA III coherence beamline P10. (M.Sprung et.al.)



Remotely stackable and moving lens system at PETRA III MINAX beamline P03 (S.Roth et.al.)

Special Optical Elements: Zone-Plates

lenses	zone-plates	Bragg-Fresnel zone-plates
refraction	diffraction	diffraction
transmission	transmission	reflection by θ_B
$\delta \approx 10^{-6}$		$\Delta r_n =$ 30 - 100nm
	functions	
focusing	focusing	monochromatization and focusing

Multilayer Laue Lens

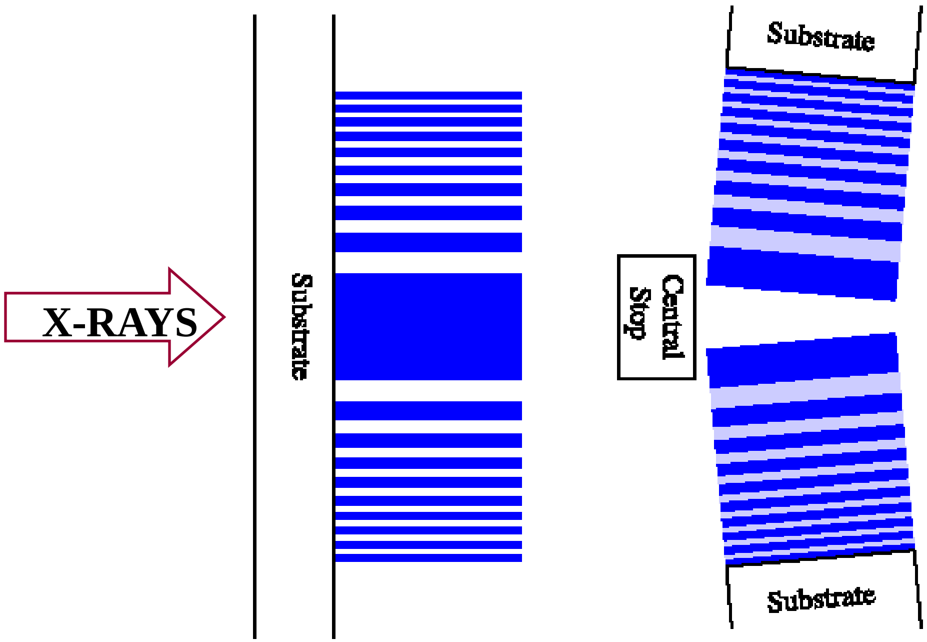
focal spot size **d = λ/2N.A.**

Zone plate structures for hard x-rays must be several microns thick to achieve high efficiency

Small focal spot sizes require small zone widths, which implies high aspect ratios (~100)

It is difficult to produce such high aspect ratio structures using lithography

Sectioning of multilayers allows very high aspect ratios to be produced



Standard lithographically fabricated hard x-ray zone plate

Transmission multilayers fabricated by deposition and sectioning

J. Maser, Ph.D. Dissertation, Gottingen, 1993;
J. Maser, G.B. Stephenson, S. Vogt, W. Yun, A. Macrander, H.C. Kang, C. Liu, R. Conley, Proc. SPIE, Denver Annual Meeting, 2004.

Links

XOP

http://www.esrf.eu/Instrumentation/software/data-analysis/xop2.3

(Including SHADOW)

SPECTRA

http://radiant.harima.riken.go.jp/spectra

PHASE

http://www.helmholtz-berlin.de/forschung/grossgeraete/undulatoren/arbeitsgebiete/phase_en.html

X-Ray Interactions with Matter

http://henke.lbl.gov/optical_constants/

X0h: X-ray dynamical diffraction data on the web

http://sergey.gmca.aps.anl.gov/x0h.html/

Thank you