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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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**SCHOOL ON THE USE OF SYNCHROTRON RADIATION
IN SCIENCE AND TECHNOLOGY:
*"John Fuggle Memorial"***

3 November - 5 December 1997

Miramare - Trieste, Italy

Several beamline designs

**Daniele Cocco
Sincrotrone Trieste, Italy**

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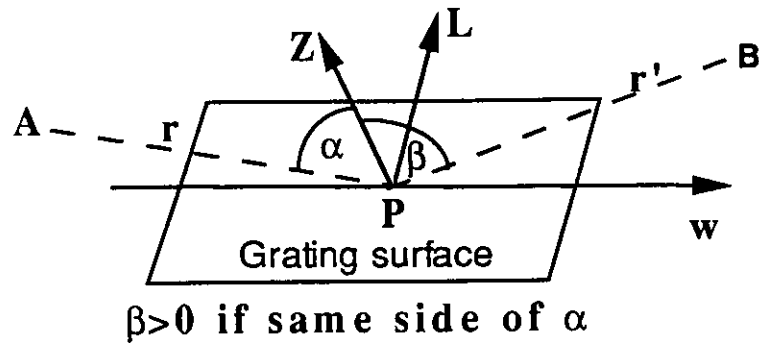
**School on the Use of Synchrotron
Radiation in Science and
Technology:
"John Fuggle Memorial"
3 November - 5 December 1997**



How to choose a Synchrotron radiation Monochromator

- 1) Working range**
 - 2) Aberration free**
 - 3) Transmission**
 - number of elements**
 - quality of optical elements**
 - mirrors and gratings efficiency**
 - 4) Resolving power**
 - 5) Large range without change gratings**
 - 6) Fixed entrance and exit direction**
 - 7) High order suppression**
 - 8) Angular acceptance**
 - 9) Fixed entrance (if there) and exit slit**
 - 10) Perfect matching to source**
 - 11) Tolerances**
 - Heat load**
 - Slope errors**
 - 12) Alignment possibility**
 - 13) Cost**
- and, of course, matching the experiments**

Geometrical Aberration Theory



Optical path function: $F = AP + PB + Nk\lambda$

Fermat's Principle $\delta F / \delta w = 0$ meridional focus
 $\delta F / \delta l = 0$ sagittal focus

Re-writing the optical path as a function of w and l one obtains:

$$F = F_{000} + wF_{100} + \frac{1}{2}w^2F_{200} + \frac{1}{2}l^2F_{020} + \frac{1}{2}w^3F_{300} + \frac{1}{2}w^2lF_{120} + \frac{1}{8}w^4F_{400} + \dots$$

or, more precisely:

$$F_{000} = r + r'$$

$$F_{100} = Nk\lambda - (\sin(\alpha) + \sin(\beta)) \quad \text{Grating equation}$$

$$F_{200} = \cos^2(\alpha)/r + \cos^2(\beta)/r' - 2a_{20}(\cos(\alpha) + \cos(\beta))$$

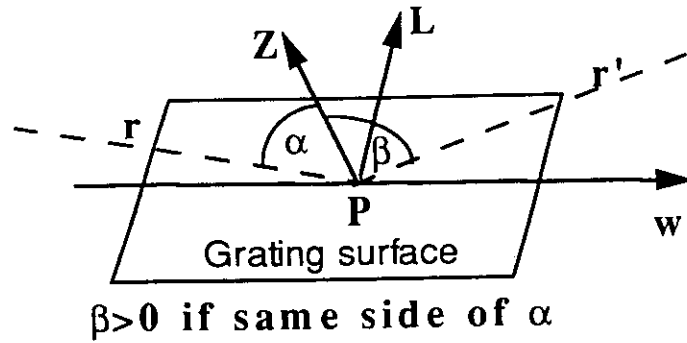
Meridional focus

$$F_{020} = 1/r + 1/r' - 2a_{02}(\cos(\alpha) + \cos(\beta)) \quad \text{Sagittal focus}$$

F_{300} Primary Coma

F_{120} Astigmatic Coma

The Toroidal/ Spherical Grating Monochromator



In the case of a spherical/ toroidal, substrate one obtain:

$$F_{100} = Nk\lambda - (\sin(\alpha) + \sin(\beta)) \quad \text{Grating equation}$$

$$F_{200} = \left(\frac{\cos^2(\alpha)}{r} - \frac{\cos(\alpha)}{R} \right) + \left(\frac{\cos^2(\beta)}{r'} - \frac{\cos(\beta)}{R} \right) \quad \text{Meridional focus}$$

$$F_{020} = \frac{1}{r} + \frac{1}{r'} - \left(\frac{1}{\rho} \right) (\cos(\alpha) + \cos(\beta)) \quad \text{Sagittal focus}$$

$$F_{300} = \left(\frac{\cos^2(\alpha)}{r} - \frac{\cos(\alpha)}{R} \right) \left(\frac{\sin(\alpha)}{r} \right) + \left(\frac{\cos^2(\beta)}{r'} - \frac{\cos(\beta)}{R} \right) \left(\frac{\sin(\beta)}{r'} \right) \quad \text{Primary Coma}$$

One particular solution is the Rowland circle geometry for which one should satisfy:

$$\cos^2(\alpha) / r = \cos(\alpha) / R$$

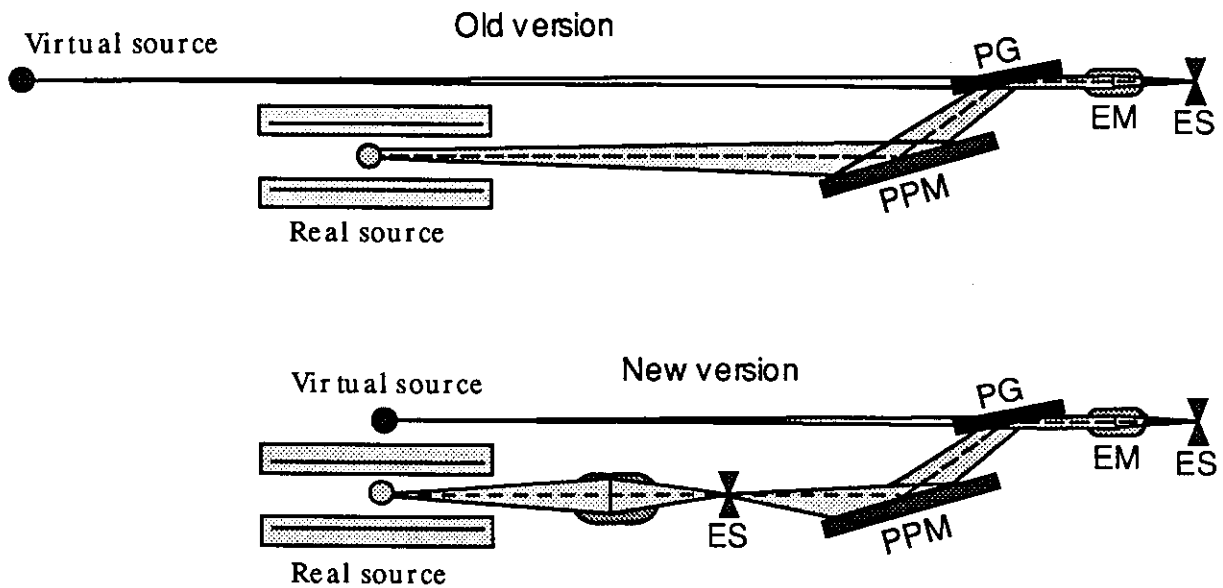
$$\cos^2(\beta) / r' = \cos(\beta) / R$$

Which means: $F_{200} = F_{300} = 0$

SX700 Plane Grating Monochromator

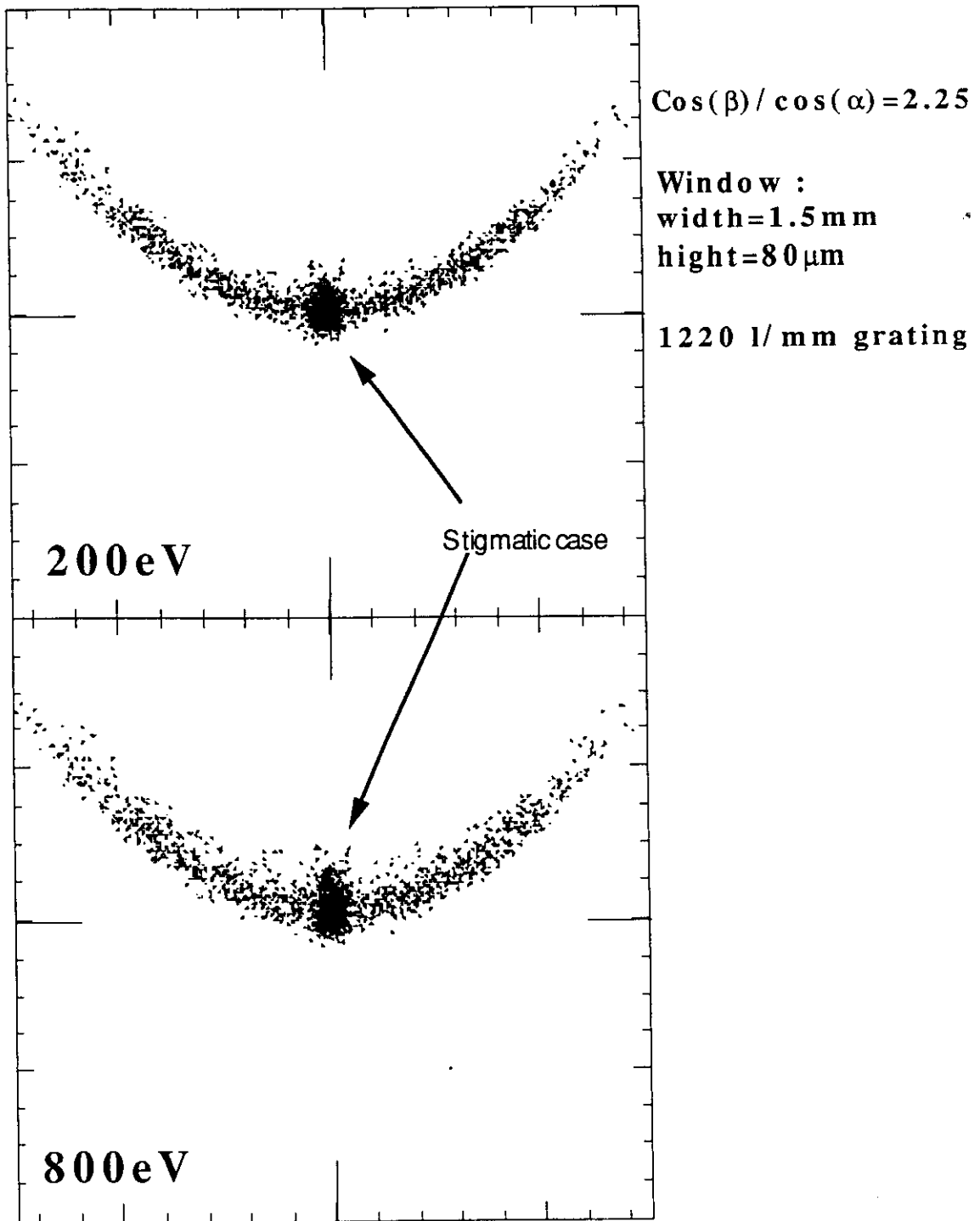
For a plane grating, the equations became:

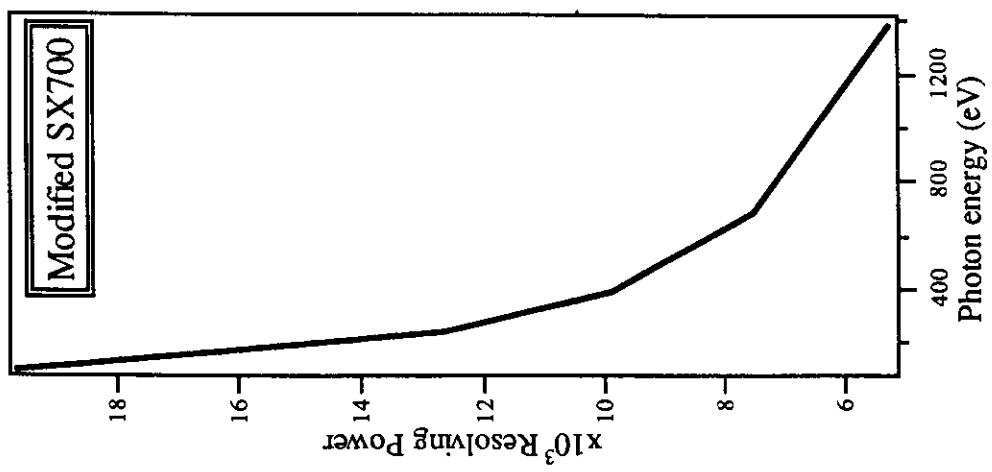
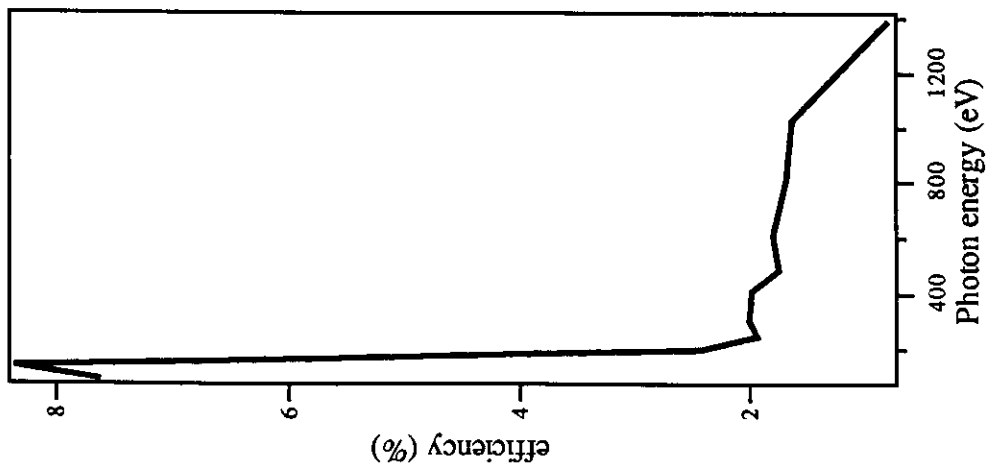
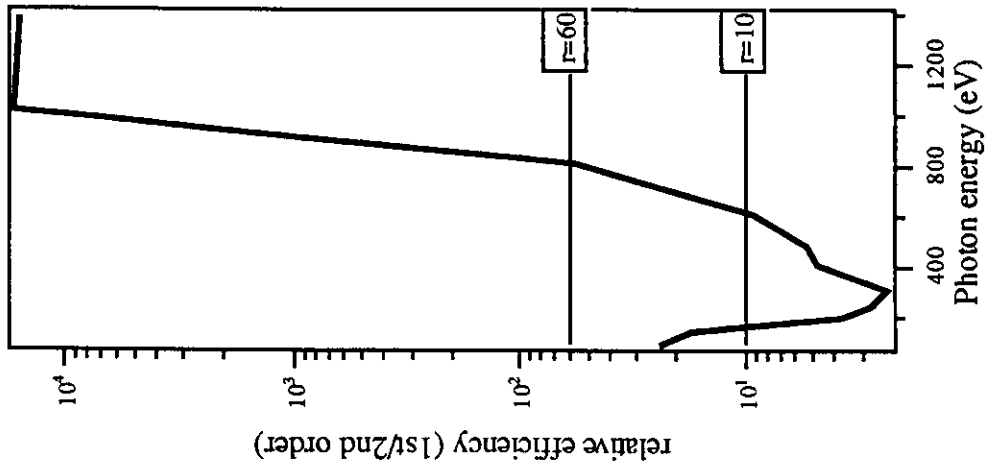
$$F_{200} = \cos^2(\alpha) / r + \cos^2(\beta) / r' = 0 \quad \longrightarrow \quad r' / r = \cos^2(\beta) / \cos^2(\alpha) = C = 2.25$$



Following the above equation, the grating change the divergence of the incoming radiation in such a way that it seems that the radiation come from a distance that is $(2.25)^2$ time greater than the original. In the old version this fact introduce an astigmatism, because only in the dispersion direction the divergence was changed. In the new configuration a pre-focusing optics create a new source at a distance from the grating that is $(2.25)^2$ the source distance. After the grating dispersion the radiation is again stigmatic and an elliptical mirror can perfectly focalise the radiation in the exit slit.

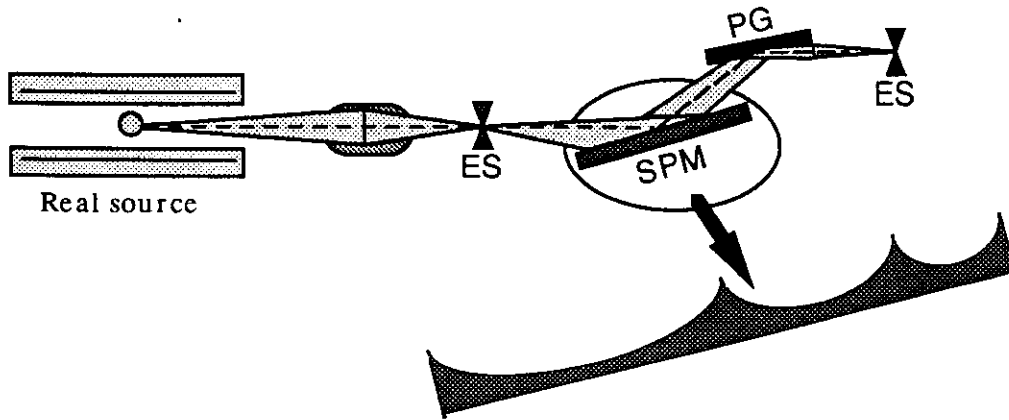
Comparison between stigmatic and astigmatic SX700





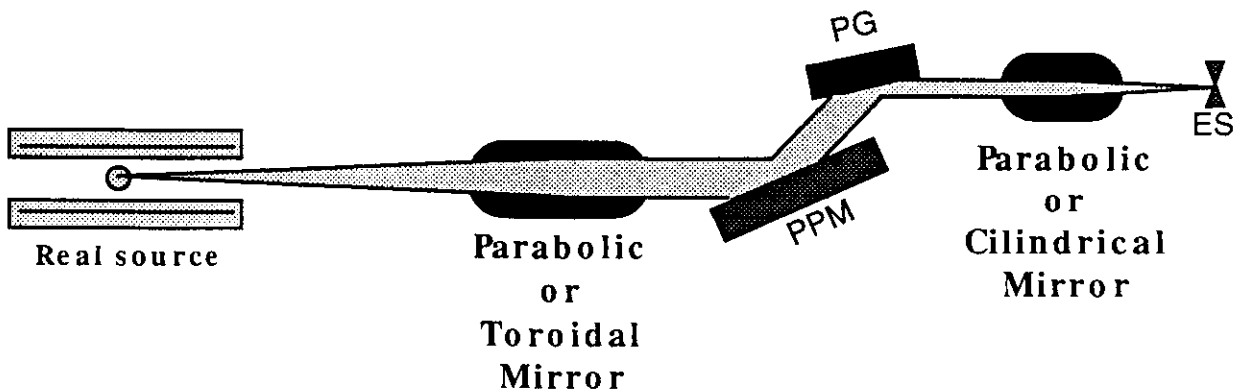
Performance of the SX700 beamline at Elettra.

Spherical pre-mirrors Plane Grating Monochromator



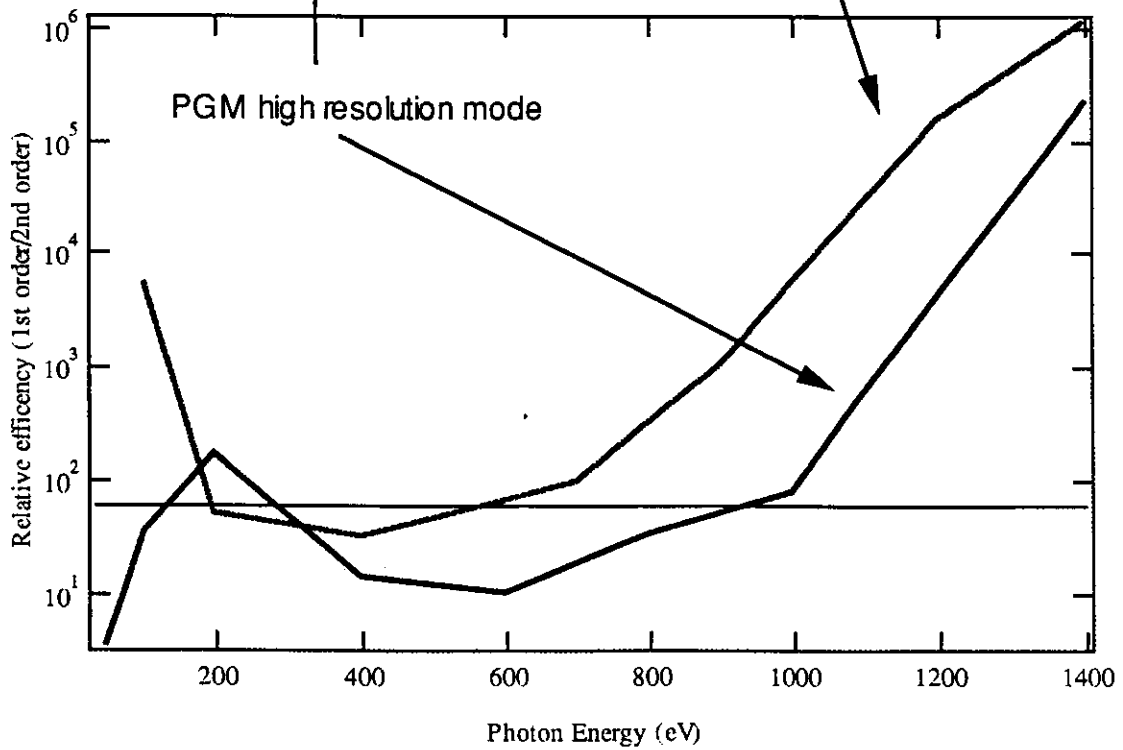
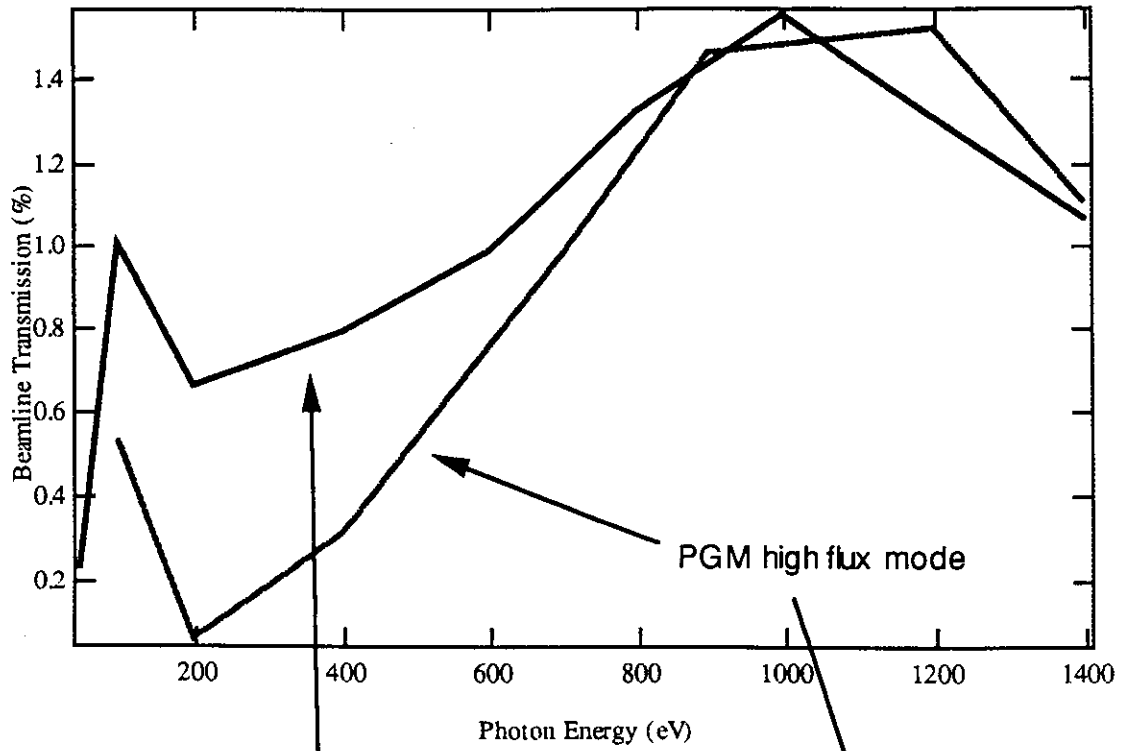
This plane grating monochromator has a spherical pre-mirror. This spherical surface is rotatable and the combination of the focussing propriety of the mirror and the dispersion effect of the grating, focalise the desired radiation in the exit slit. The performance are very similar to that of the SX700, but this solution do not use aspherical surface.

Collimated light Plane Grating Monochromator

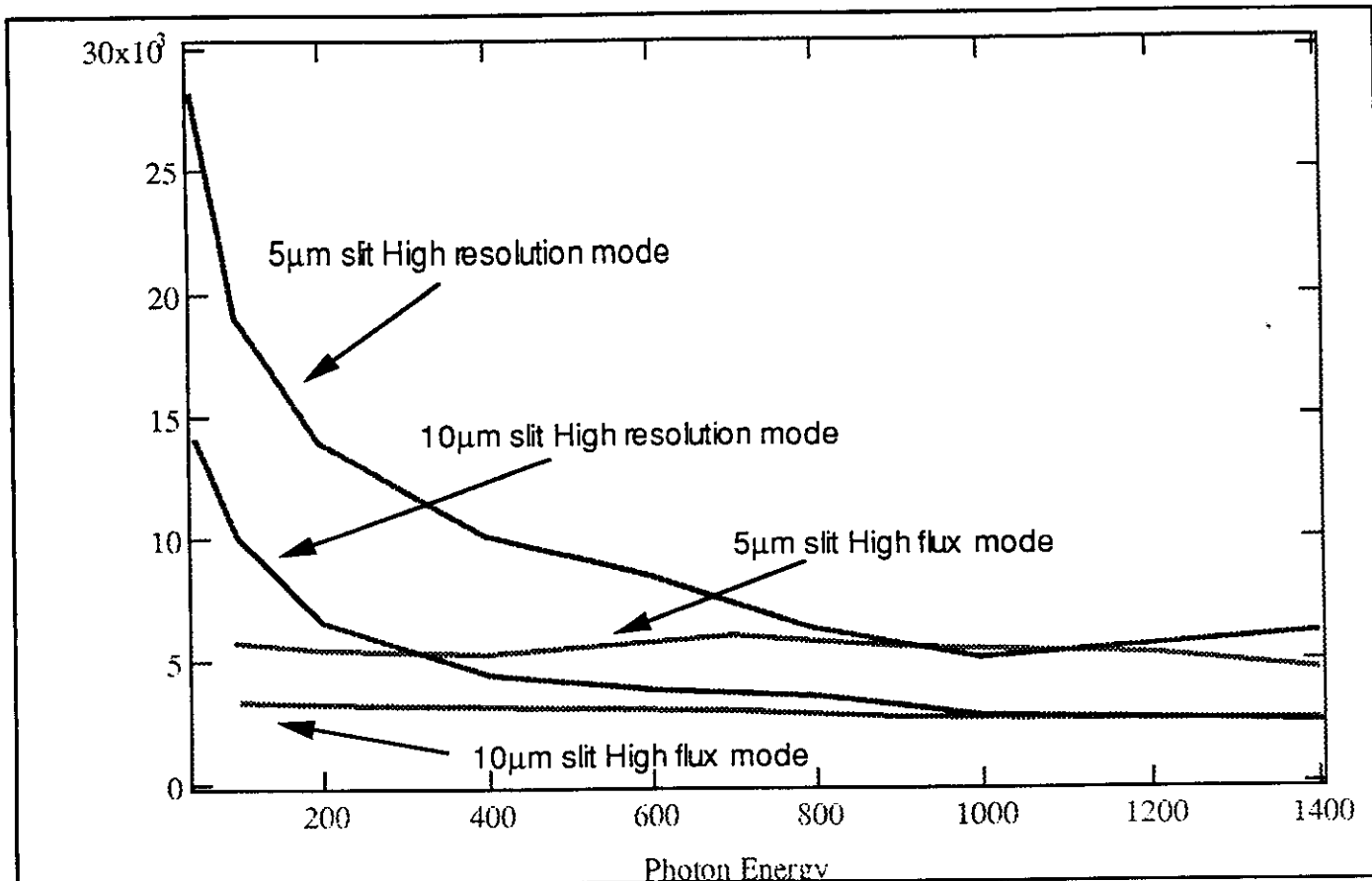


This solution use a parabolical miro, which create a collimated beam of photons. In this way there is no other restriction on the angle of the grating except the grating equation (F100). The main problem of f this solution is the use of aspherical components, which are very hard to produœ. There is two main working condition: High flux and High resolution. In the firs case one work always on blaze, condition of maximum efficiency of the grating. In the high resolution mode the incidence angle is fixed.

PGM collimated light performances



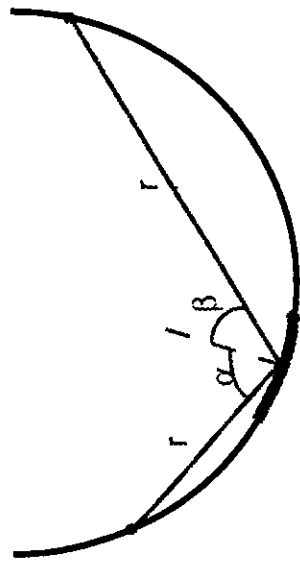
PGM collimated light resolving power



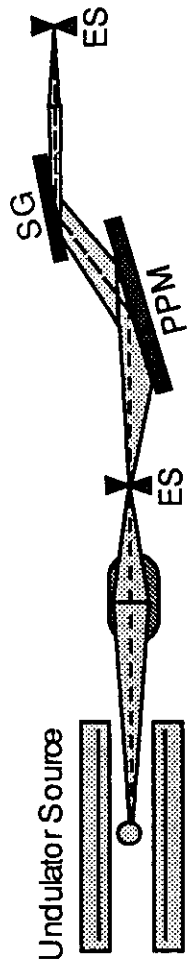
Spherical Grating Monochromators

$$\cos^2(\alpha) / r = \cos(\alpha) / R \quad \rightarrow \quad F_{200} = F_{300} = 0$$

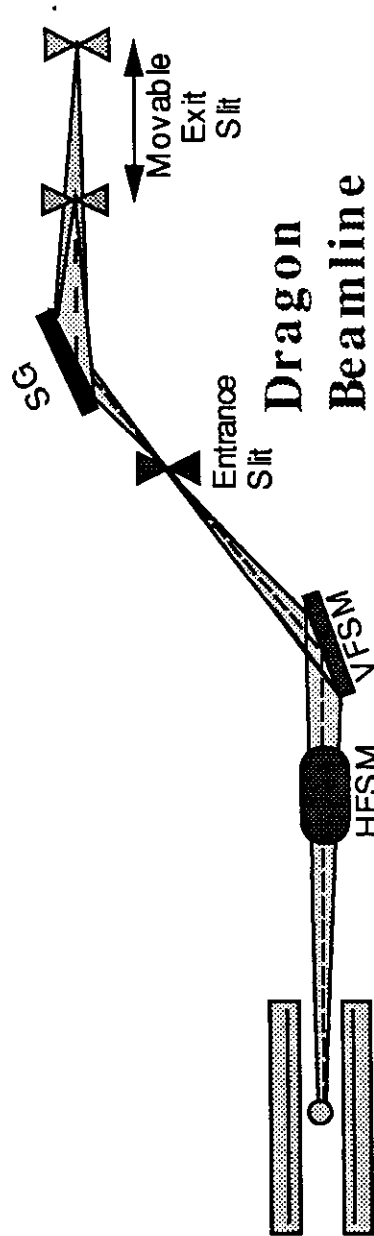
$$\cos^2(\beta) / r' = \cos(\beta) / R$$



Rowland circle configuration

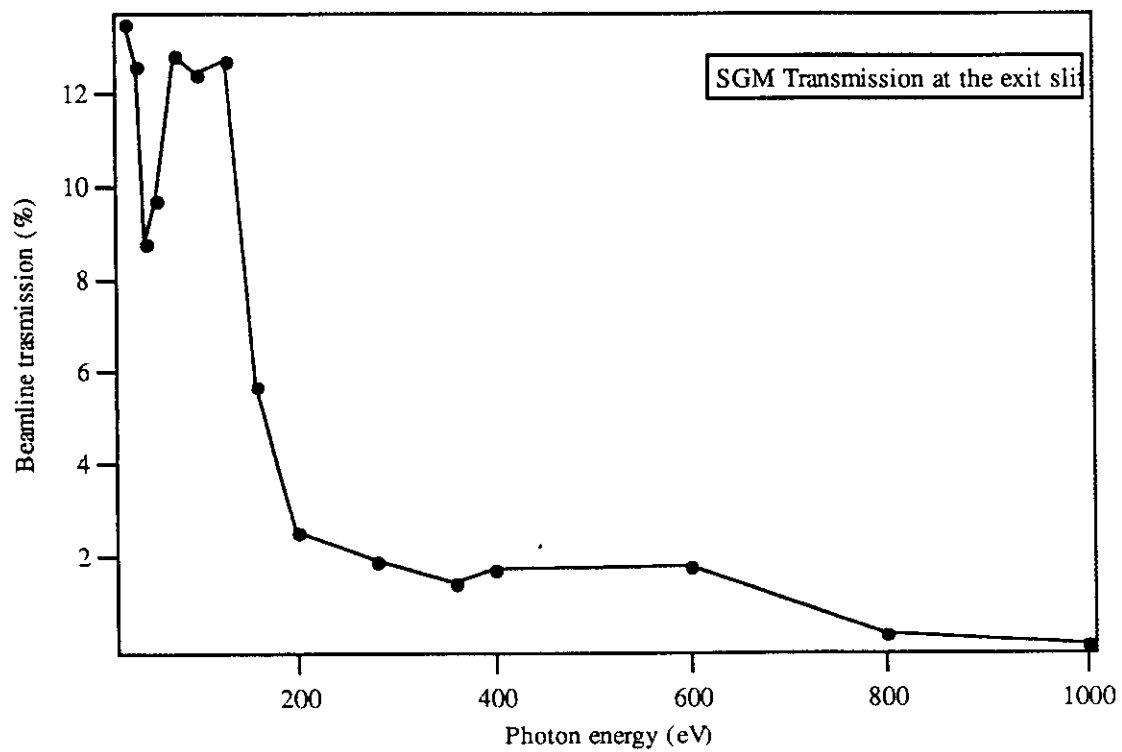
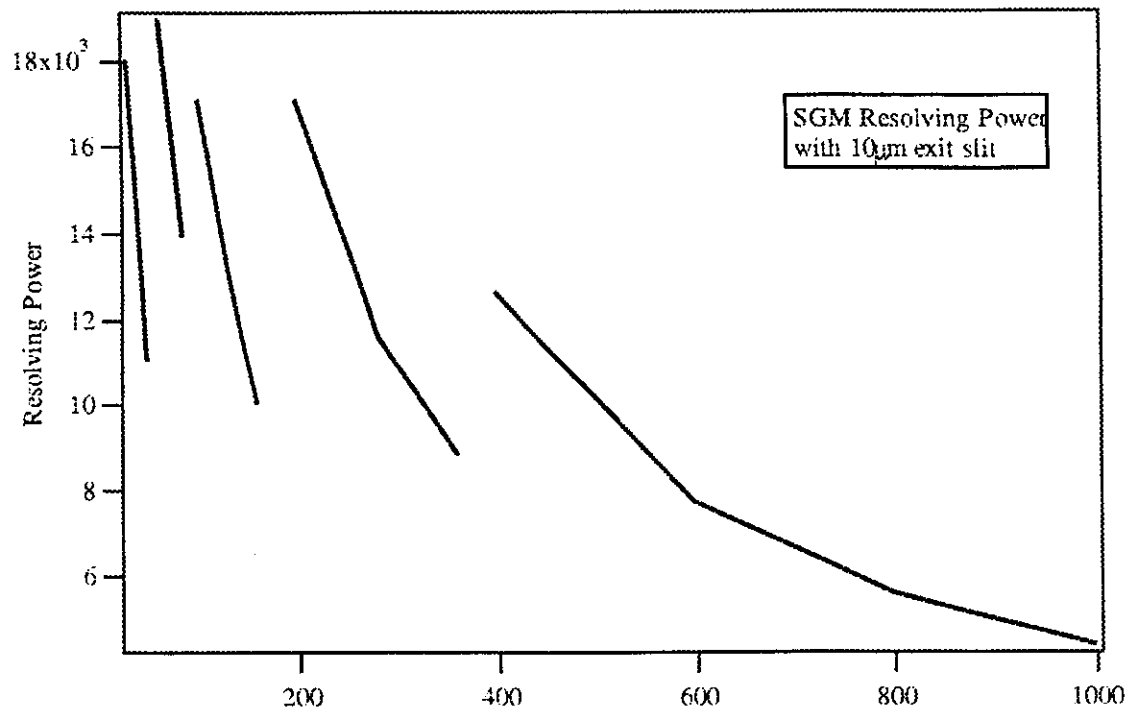


Variable included angle SGM



Dragon Beamline

SGM resolving power and transmission



An SGM Beamline description (BACT)

This beamline is design to perform dichroic absorption and scattering experiments on a wider spectral range, i.e. from ≈ 35 eV up to ≈ 1400 eV, with high energy resolution, efficiency and a significant suppression of the undulator higher order harmonics. The photon dispersion, based on a spherical grating monochromator with fixed entrance and exit slits, is similar to that proposed by Padmore [1] and it can allocate a maximum of five gratings. For the actual purposes three gratings are designed. Two optimized for high energy resolution, in the 100-200 eV and 500-1000 eV regions and, the third with a relatively low dispersion power to obtain a high brilliance suitable for scattering experiments. In addition, the two grating with high resolving power are designed to suppress the higher order harmonics. The optics of the line presents two physically separated focal points for dichroic and scattering experiments.

Before to describe the optical layout of the beamline it is necessary to remaind that the use of two undolators will results in two focal points on the \mathbf{K} vector direction (direction of propagation) of the photon beam. By adjusting the incidence angle on the gratings it is possible to overlap the the vertical focus (dispersion direction) on the exit slit, whereas on the orizontal plane the two focus are about 0.2 m apart. This effect implies an orizontal size of the spot, into the experimental chamber, larger of $\approx 5\%$ ($\approx 10 \mu\text{m}$) than that expected in the beam wist.

The beamline layout is reported in Fig.1. A spherical pre-mirror (SM1), located 19.2 m from the middle point (S1) of the straight section (intermediate point between the two Sasaki undulators), having a radius of 179.2 m and operating at 1.75° grazing incidence angle, focuses the radiation vertically 3.2 m behind, in the entrance slit. In this way a new virtual source, six time smaller then real one, is formed in the diffraction plane.

A second spherical mirror (SM2), 21.2 m from source, with a radius of 404.1 m and operating at 2° grazing incidence angle, focuses horizontally the radiation directly into the exit slit located 10.6 m after SM2.

The spherical grating monochromator, SGM, covers a photon energy range between 35 to 1600 eV. The ideal solution should involve 3 inter-changeable gratings. Nevertheless, an accetable compromise is represented by two gratings working abberation free form 50 eV to 1600 eV. In this case the extention of the lower photon energy limit down to 35 eV will results in an accetable reduction of the performances (Fig 2 and Fig.3a) [2].

To achieve the best arrangement among flux, resolution and high order suppression, the following parameters are chosen. The entrance arm (distance from entrance slit to the grating) is 7 m, the exit arm (grating-exit slit) is 2.4 m. The low

energy grating (SG1) has a radius of 30 m and 1200 l/mm of groove density. The laminar shape, with a ratio between ruled and unruled area of 0.576 and a groove depth of 11 nm. On the basis of these parameters a significant high order suppression and a high efficiency are achieved, Fig 3a and Fig.3b. In Fig.3b the efficiency and high order suppression are reported considering the overall optical behaviour of the beamline. For the higher photon energy range a grating with a radius of 70 m with 1200 l/mm of groove density is chosen. This grating a blaze shape and it is optimised for the 500-1000 eV photon energy region. The results reported in Fig.3, in agreement with the requirements [3], are obtained using a blaze angle of 3.76° and 175.7° of apex angle. By coupling the grating with a plane pre-mirror (PM) it is possible to focus stigmatically the radiation, for all the photon energies, on the fixed exit slit. To reduce possible errors and to have a fixed exit direction, the incoming radiation has to hit the gratings always at his pole. As a matter of fact by a proper choice of the rotation axis parameters it is possible to minimise for different photon energies the displacement of the beam from the grating pole, hance reducing the angular error to negligible values with respect to the radiation divergence.

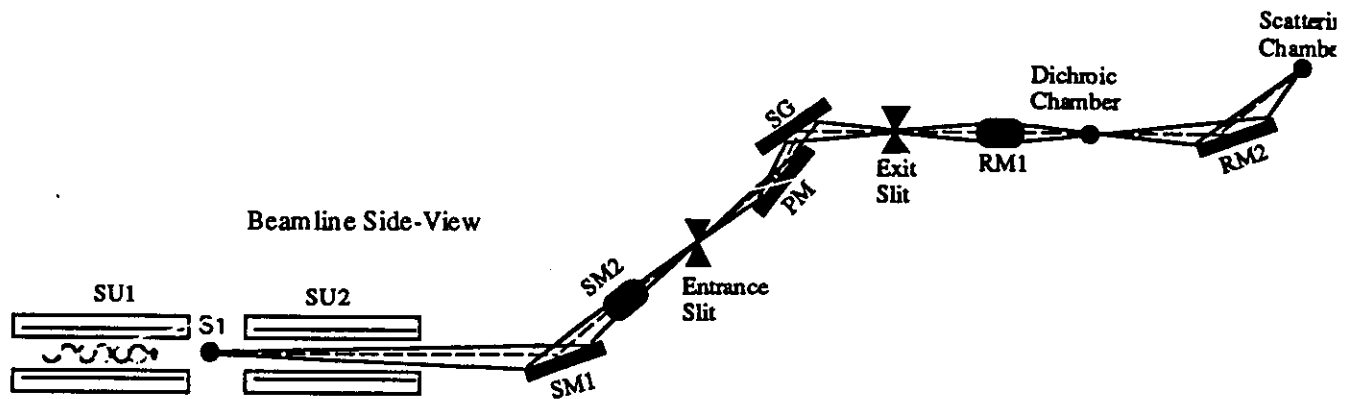
A refocusing mirror RM1 (thoroidal with major radius of 45.86 m and the minors of 5.58 cm) re-focalises the beam into the first experimental chamber (dichroic measurements), whit a spot size of about $10 \times 160 \mu\text{m}^2$, as shown in Fig.4. The expected photon flux are given on Tab.I for both SG1 and SG2.

In order to obtain a high brilliance spot to perrforme inelastic scattering experiments it is necessary to use a grating (SG3) with a lower dispersion power, with respect to SG1 and SG2 and a re-focusing mirror after the first experimental chamber, indicated in Fig.1 as RM2. SG3 has a laminar grating with grove density of 400 l/mm and a radius of 75 m. The behaviour of this grating is reported in Fig. 2 and Fig.3a/b. The photon transport from SG3 up to the first experimental chamber remain essentially the same as described before. Being the first experimental chamber "transparent" to the photon beam a second refocusing mirror (RM2, elliptical, placed horizontally to permit an easier beam alligement) placed 3.6 m after the focus of RM1, re-focalize the spot 1.2 m apart into the scattering chamber. In this case the calculated spot size is $\approx 10 \times 50 \mu\text{m}^2$, as shown in Fig.5, while the photon flux is reported in Tab.I .

Another problem to consider is the diferent efficiency of the gratings and of the mirrors in the case of s-polarized and p-polarized light. In our case, using small grazing angle of incidence, the trasmission of the two components is almost the same at every photon energy. This is shown in figure 6, where the plotted relative efficiency is calculated for the light in the experimental chamber for SG1 and SG2 and in the scattering chamber for SG3.

[2] Ray tracing performed with the program SHADOW by F. Cerrina

[3] The grating efficiency calculation was performed with the program LUMNAB by M. Neviere



- SU1,2= Sasaki section for the 1) lower photon energy, and 2) higher photon energy
- S1= Straight section middle point
- SM1= Vertical Prefocussing Mirror (Spherical 179.2 m Radius 1.75 incidence angle)
- SM2= Horizontal Prefocussing Mirror (Spherical 404.1 m Radius 2.0 incidence angle)
- PM= Plane pre-mirror
- SG= Spherical Gratings (SG1: low energy (35-400 eV) 1200 l/mm 30 m radius
SG2: high energy (300-1600 eV) 1200 l/mm 70 m radius
SG3: high flux (100-1200eV) 400 l/mm 75 m radius)
- RM1= Toroidal Refocussing mirror (R=4584.6cm ρ =5.58cm 2.0 incidence angle)
- RM2= Elliptical refocussing mirror (r =3.6mt r' =1.2mt 2.0 incidence angle)

Fig. 1 Scheme of the beamline.

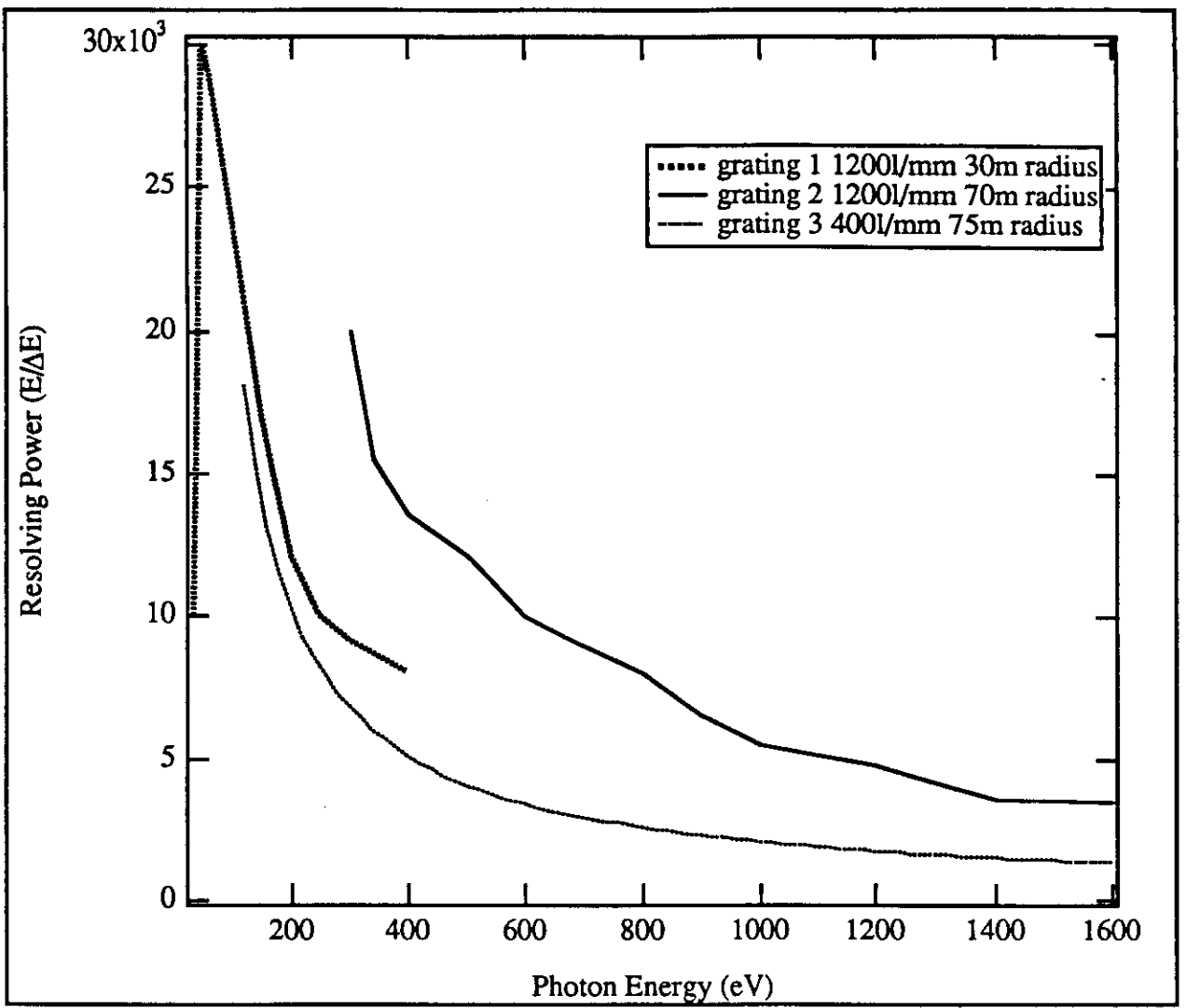


Fig. 2 Resolving power ($E/\Delta E$) for the two gratings.

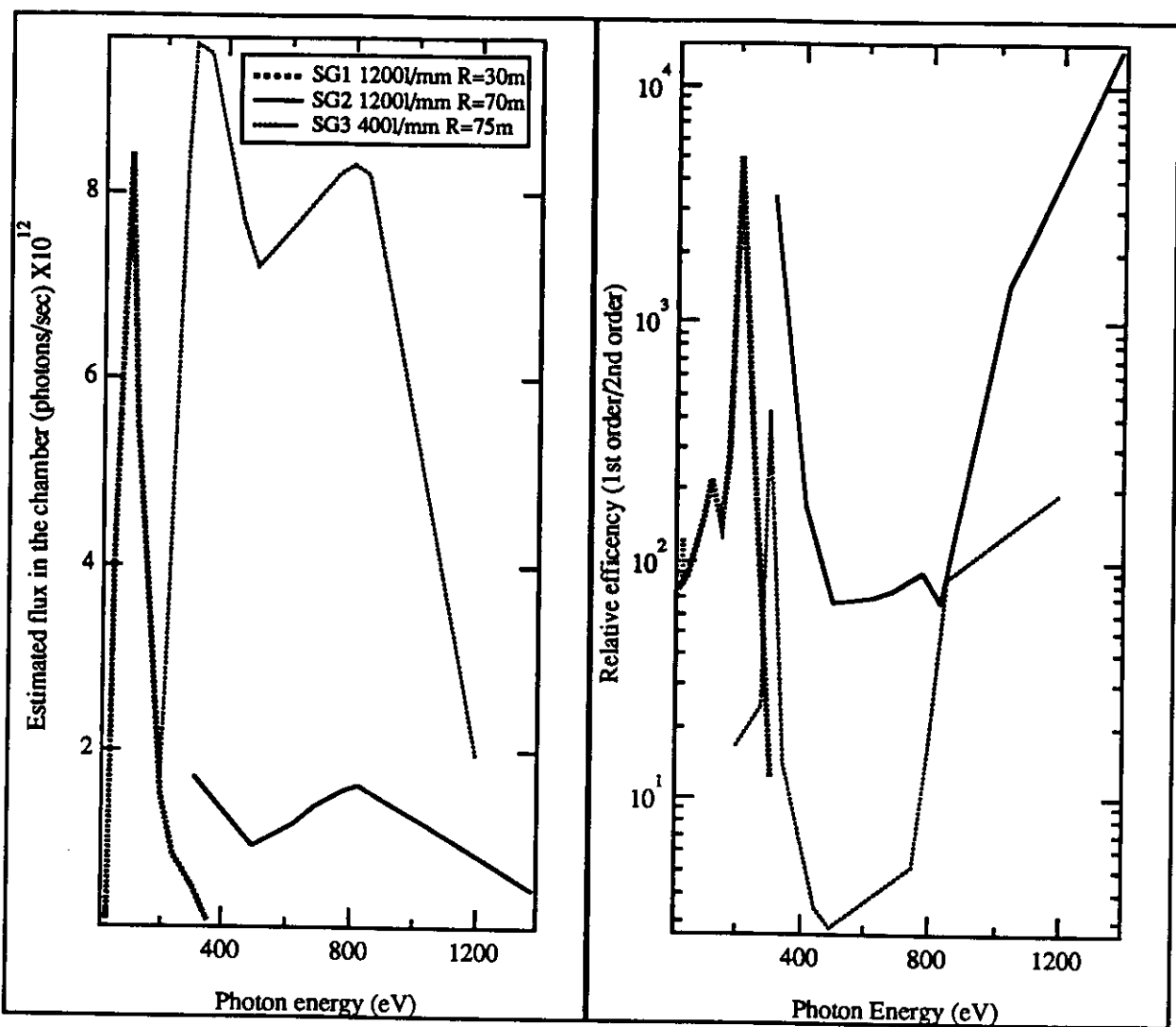


Fig. 3a Estimated photon flux of the beamline, including mirrors reflectivity and grating efficiency.

3b : Ratio between the first and second order efficiency of the beamline.

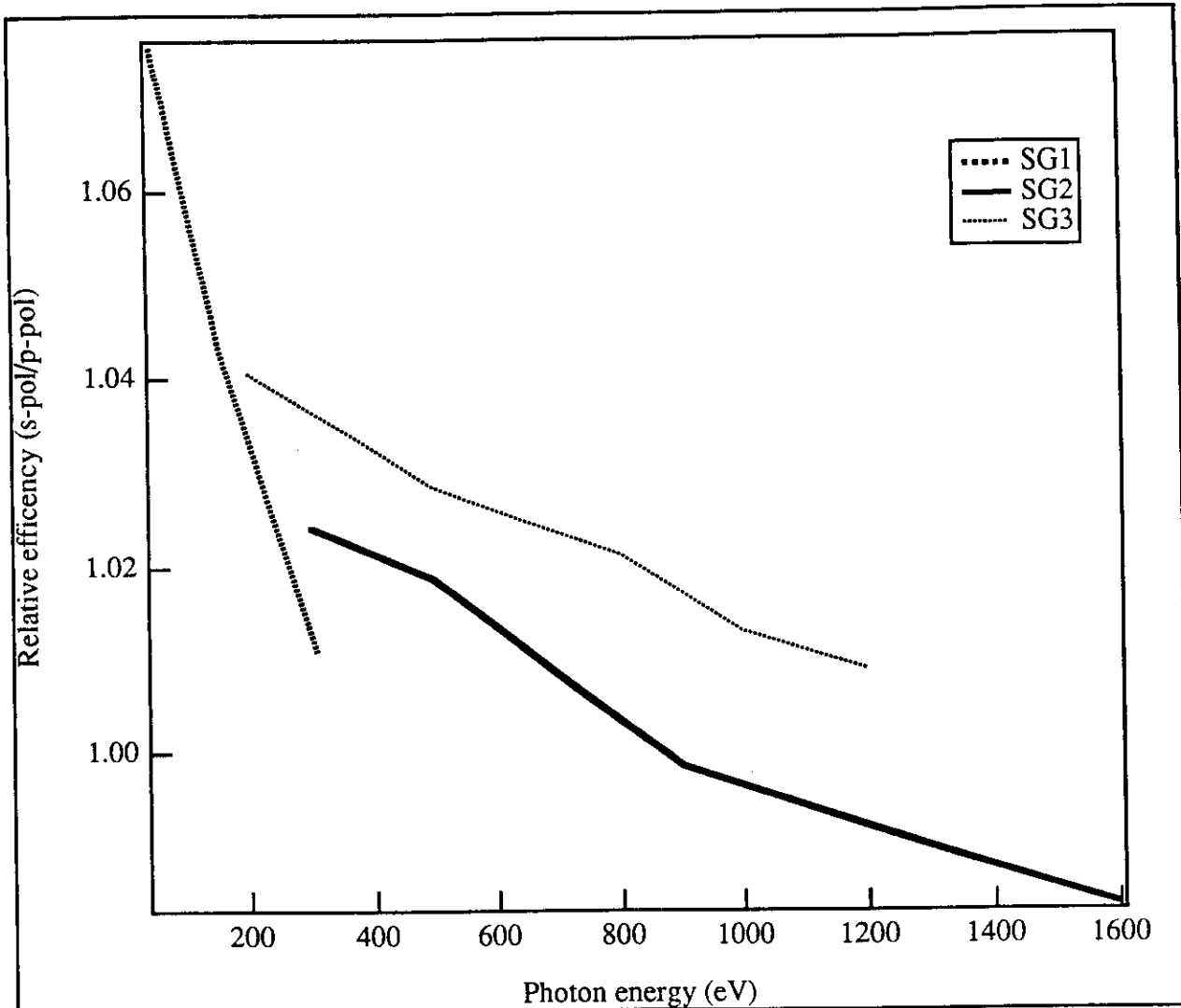


Fig. 6: Relative efficiency of the beamline transmission for the s and p-polarized light for the three different gratings. For SG1 and SG2 the calculation was made for the light in the experimental chamber, for SG3 in the scattering chamber.

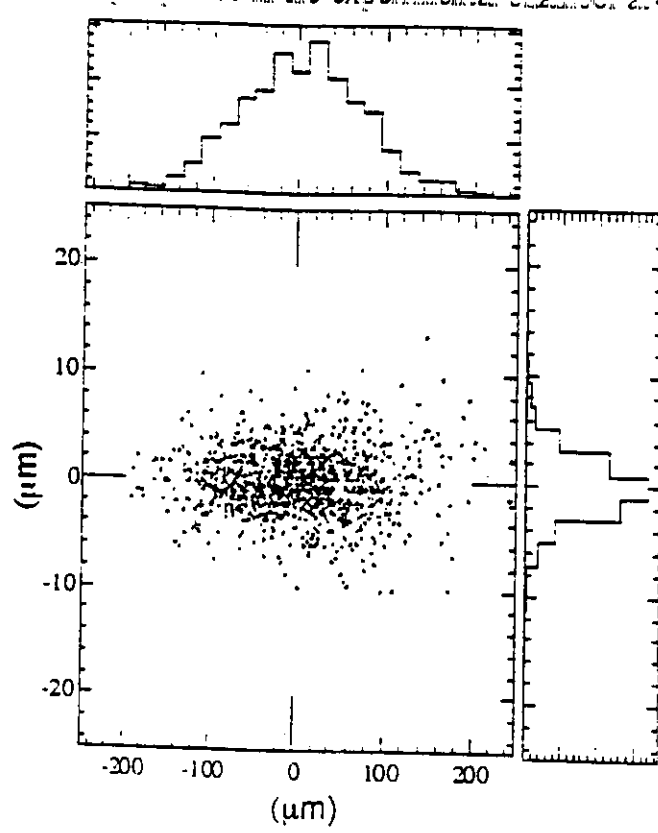


Fig. 4: Spot profile in the Experimental chamber, calculated at 400eV with SG2.

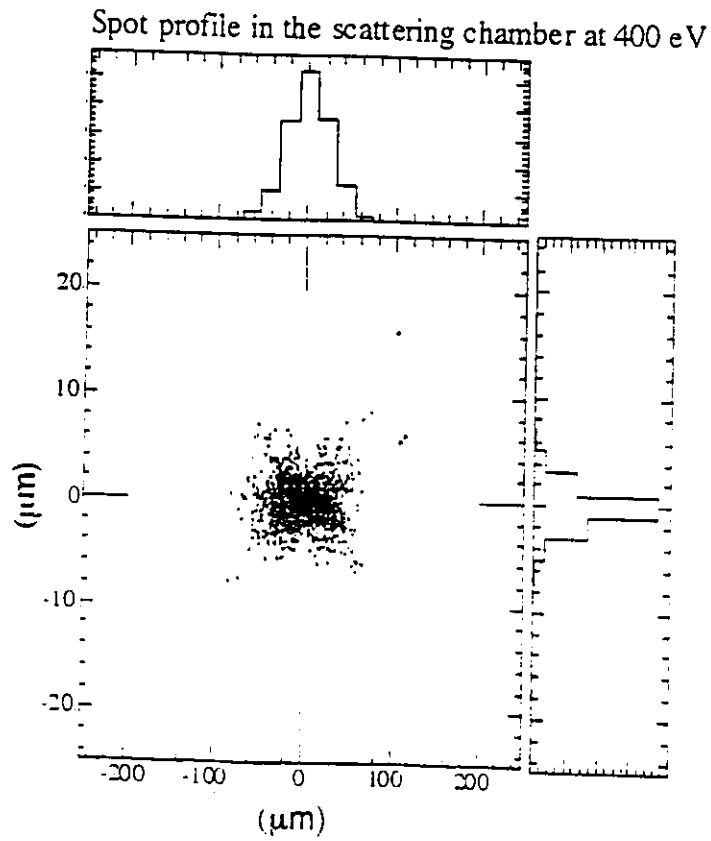


Fig.5 Spot profile in the scattering chamber, calculated at 400 eV with SG3.

Available photon flux at the BACH beamline

Low energy grating (SG1) (1200 l/mm R=30 m)

Photon Energy (eV)	Photon flux in the experimental chamber (ph/sec) at maximum resolution available
35	0.15×10^{12}
100	8.4×10^{12}
200	1.5×10^{12}

High energy grating (SG2) (1200 l/mm R=70 m)

Photon Energy (eV)	Photon flux in the experimental chamber (ph/sec) at maximum resolution available
500	0.96×10^{12}
800	1.6×10^{12}
1400	0.5×10^{12}

High flux grating (SG3) (400 l/mm R=75 m)

Photon Energy (eV)	Photon flux in the scattering chamber (ph/sec) at maximum resolution available
200	1.7×10^{12}
500	7.2×10^{12}
800	8.3×10^{12}

Tab 1: Calculated available photon flux at this beamline in the condition of maximum resolution (10 micron exit slit) with 400mA ring current.

Toroidal Grating Monochromator

$$F_{100} = Nk\lambda - (\sin(\alpha) + \sin(\beta))$$

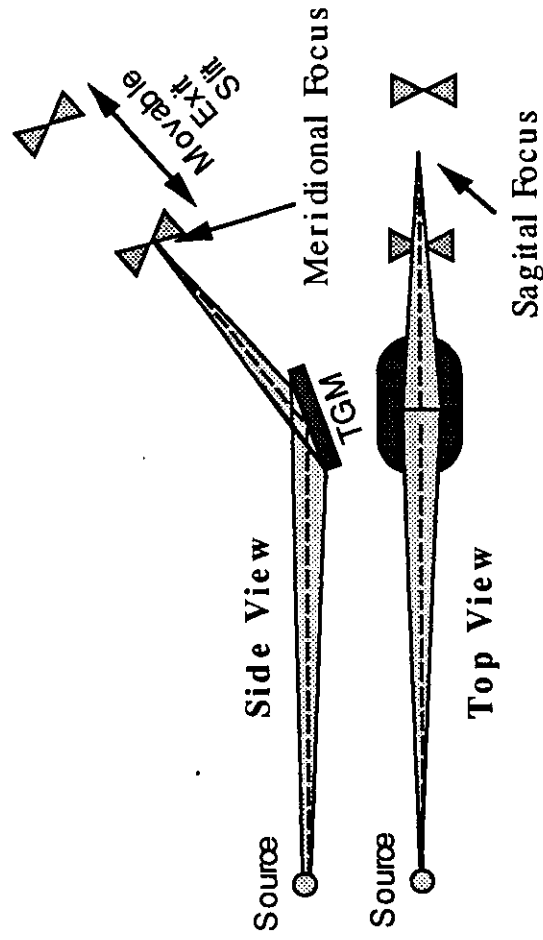
Grating equation

$$F_{200} = \cos^2(\alpha) / r + \cos^2(\beta) / r' - 1 / R(\cos(\alpha) + \cos(\beta))$$

Meridional focus

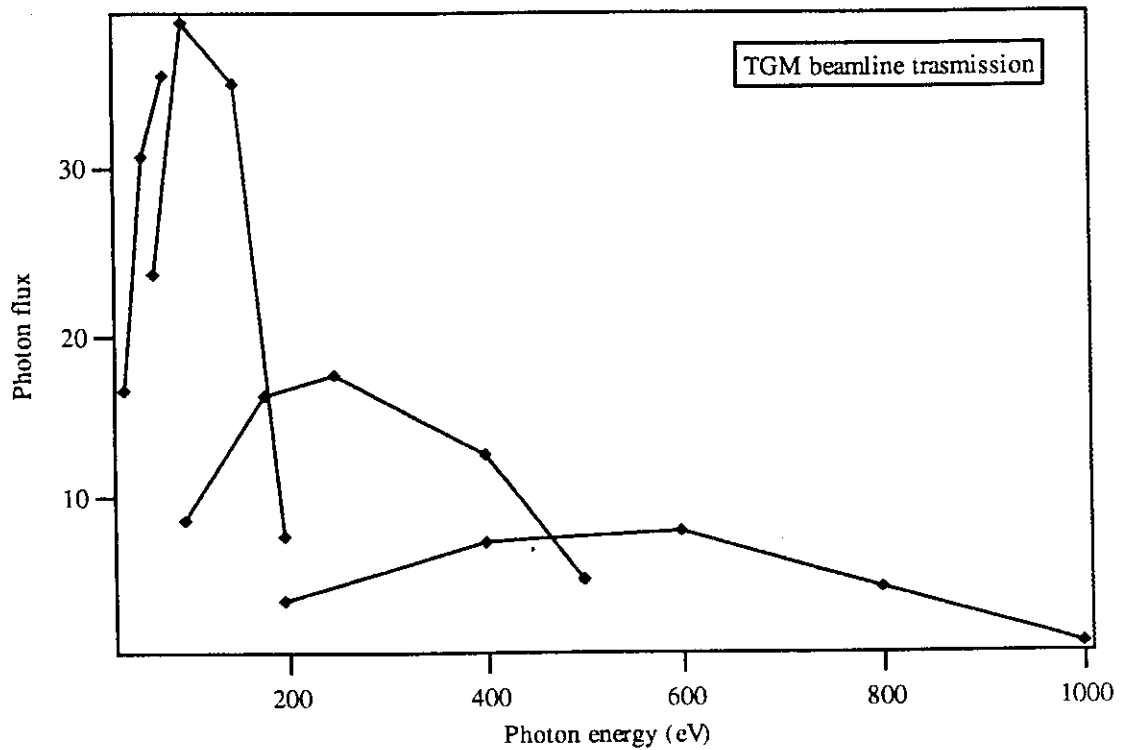
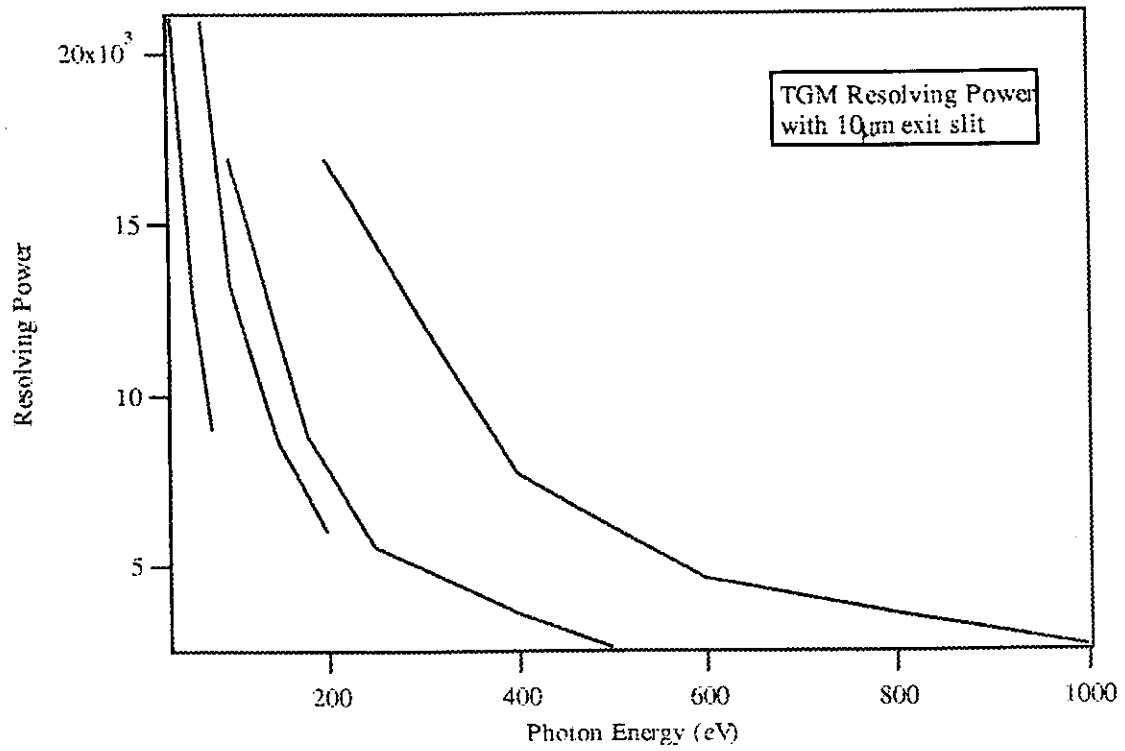
$$F_{020} = 1 / r + 1 / r' - 1 / \rho(\cos(\alpha) + \cos(\beta))$$

Sagittal focus

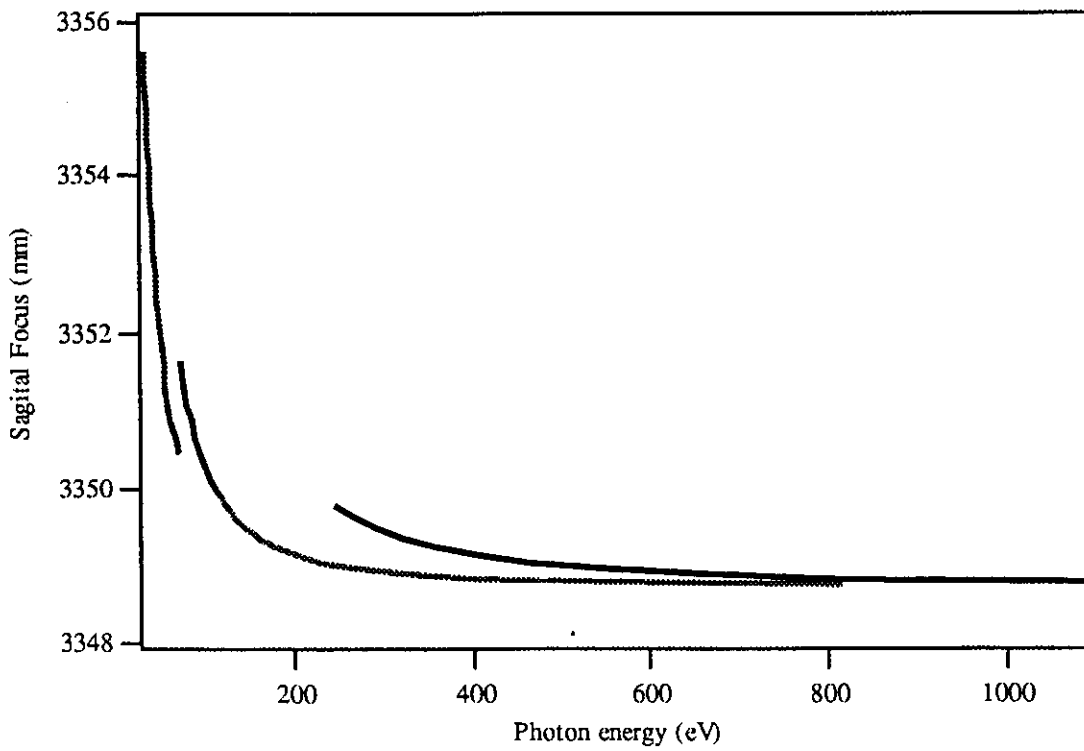
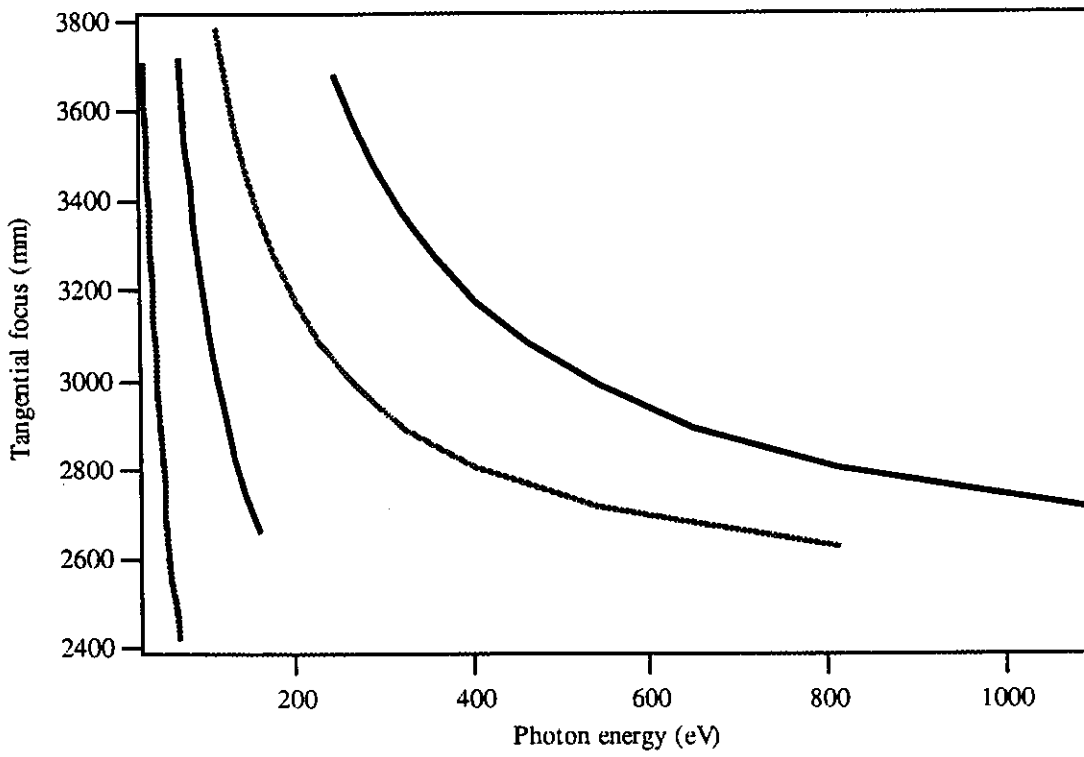


One grating, toroidal shape, is enough to focalise in both direction the radiation. This beamline is usefull with sources with low brillance, due to the fact that the grating recive directly the synchrotron radiation. To scan the energies, is necessary to move the exit slit. Typical displacement are of the order of 1 m.

TGM Performances



The flux and the resolving power of a TGM are quite good. The great problem are related to the difficulty to maintain the calibration and the necessity to use different grating to cover the whole range.



Displacement of the Tangential and sagittal focus of the TGM with the energy.

Possible future Monochromators

Variable Line Space Gratings

Plane focussing Grating

Reduction of third order aberation

Reduction of the Rowland circle exit arm variation

Conical Diffraction Mounting

High efficiency

Adjustable Radius Mirror and Grating

Single grating SGM

Always in Rowland circle condition

New coating materials

Increase the reflectivity

Increase the range of utility of mirrors and gratings

Improvements of surface quality

Make use of aspherical surface without increase the slope errors problems

Summary of the performances

	Very good	Good	Normal	Poor
Working range (involving one or more gratings)		SX700		
				SGM
	CL-PGM			DRAGON
				TGM
Aberration (how much is it sensible and/or how much are the residual aberrations)		SGM		SX700
	DRAGON			
			CL-PGM	
			TGM	
Transmission (efficiency of the mirrors and gratings and geometrical transmission)		SX700		
		SGM		
		DRAGON		
	TGM	CL-PGM		
Resolving Power		SX700		
	SGM			
	DRAGON			
		CL-PGM		
	TGM			
High Order Suppression				SX700
		SGM		
			DRAGON	
		CL-PGM		
		TGM		
Angular acceptance				SX700
		SGM		
		DRAGON		
			CL-PGM	
			TGM	
Tolerances (on the pre-mirror and grating movement)		SX700		
			SGM	
		DRAGON		
		CL-PGM		
	TGM			
Alignment (easy to do, number of optical element in the mono)				SX700
		SGM		
		DRAGON		
		CL-PGM		
	TGM			
Cost				SX700
			SGM	
			DRAGON	
				CL-PGM
	TGM			