VUV & SX Beamline Design

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Outline

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 - 1.1. energy region
 - 1.2. resolution & intensity
 - 1.3. some hints for the choice
 - 1.4. examples for soft X-ray monochromator
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 - 2.3. ray-tracing simulation
- 3. Beamline installation
 - 3.1. alignment
 - 3.2. optical adjustments using SR
 - 2.3. experimental estimation of beamline performance

1.1. energy region

- High-energy region (>~150 eV)
 Grazing incidence (>~85 deg) monochromator is inevitable
 *except for multilayer grating
- 2. Low-energy region (<~50 eV)

 (Near) normal incidence monochromator is also available
 - *Medium incidence monochromator?

 Strongly affects the polarization
- 3. Wide-energy beamline (e.g. 30 eV 1500 eV)
 - (a) Combination of grazing and normal incidence monochromators
 - (b) Variable included angle monochromator
 - (c) Interchangeable gratings



1.2. resolution & intensity

Energy resolution depends on...
 Dispersion & Focus

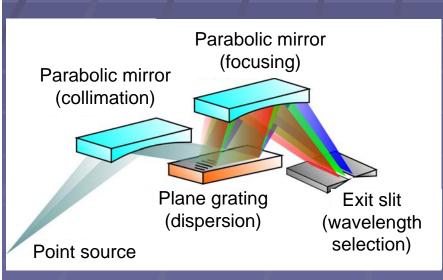
Focus size depends on...

Source size, demagnification, aberration, slope error,...

Some of them drastically change according to technical progress

No absolute solution !!

e.g. aberration-free monochromator

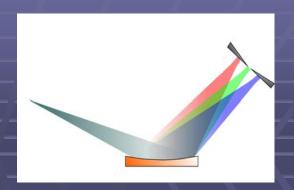


Perfect monochromator, in principle, except for the reflectivity loss

Slope errors in parabolic mirrors are large Use of cylindrical mirrors ⇒ large aberration

Recent progress in SR sources;

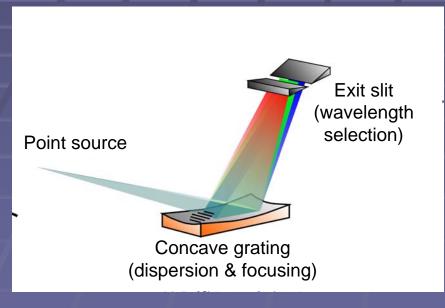
Small divergence ⇒ negligible aberration



1.2. resolution & intensity

2. Intensity depends on...
 Number of optical elements
 Incidence angle & acceptance (* larger incidence needs larger mirror)
 Diffraction efficiency of the grating
 * High groove density ⇒ large dispersion but low efficiency

e.g. the simplest monochromator



Minimum intensity loss (no mirrors)

Focal condition depends on wavelength Aberration might be serious

We must compromise!!

Intensity, resolution, energy range,...

1.3. some hints for the choice

1. Grating shape (plane, spherical, ...)

Spherical: dispersion & focus ⇒ small number of optical elements be careful for aberrations

2. Groove density (uniform or varied)

Varied line spacing: simpler optics (or higher resolution with the same optics) be careful for precision in the groove parameters

3. Included angle (constant or variable)

Variable: higher degree of freedom ⇒ resolution & intensity in wide energy range scanning mechanism is more complicated ⇒ be careful for reproducibility

4. Entrance slit

Without slit: Source size of SR itself directly affects the resolution

Higher resolution than the source-size limit is never obtained!

With slit: Higher resolution can be achieved at the sacrifice of intensity pre-focusing optics is necessary

5. Focusing elements in monochromator (upstream, downstream, or nothing)

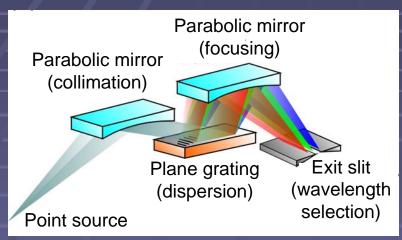
Effects of the slope errors in the focusing mirror are smaller in the upstream case

The choice depends on properties of light source, precision of mirrors, reliability of scanning mechanism, needs from applications, costs, ...

1.4. examples for soft X-ray monochromator

(1) Plane grating monochromators

Collimated light illumination



Essentially no aberration

- $\Rightarrow \alpha$ and β can be freely chosen
- ⇒ Demagnification can be controlled

Precision of parabolic mirrors is relatively poor

One can use cylindrical mirrors if divergence is small enough

Diverging light illumination (SX-700)

Plane grating & post-focusing mirror (e.g. elliptical mirror) with variable included angle

Precision of elliptical mirrors is relatively poor

One can use cylindrical mirrors if divergence is small enough

Number of optical elements is reduced compared to the collimated case

Relation between α and β must be properly chosen to keep focal condition

1.4. examples for soft X-ray monochromator

(2) Spherical (or cylindrical) grating monochromators

Rowland mount

Monochromator itself consists of a grating only

But...

Relation among α , β , r, and r must be properly chosen

"Rowland condition": $r = R \cos \alpha$, $r' = R \sin \beta$

⇒ Many optical elements and complicated scanning mechanism

DRAGON mount

Monochromator consists of a spherical (cylindrical) grating only Fixed included angle

⇒ Simple scanning mechanism

Kinds of aberration arises, but only the defocus term can be canceled by moving the exit slit

1.4. examples for soft X-ray monochromator

(3) Varied-line-spacing (VLS) plane grating monochromators

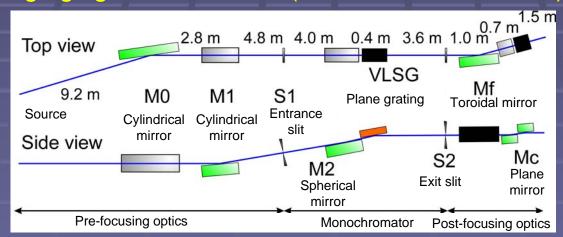
Diverging light illumination

Monochromator itself consists of a VLS plane grating only

Relation between α and β must be properly chosen

⇒ A precise variable included angle system is inevitable

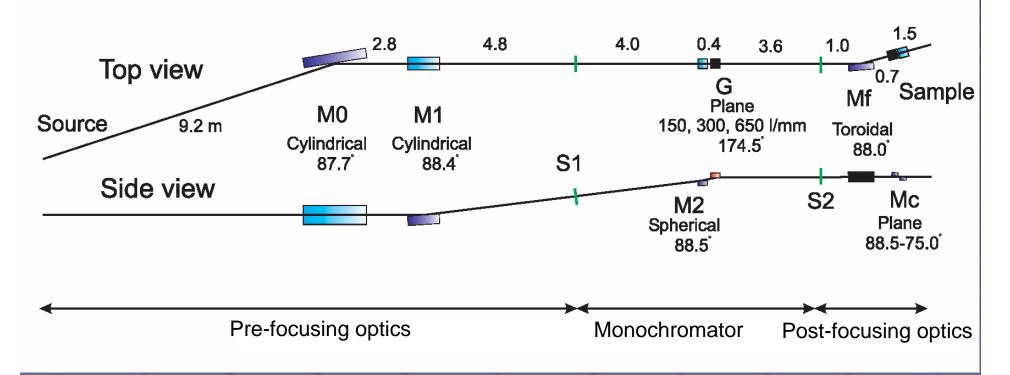
Converging light illumination (Monk-Gillieson mount)



Pre-focusing mirror upstream of VLSG

Constant included angle ⇒ Simple scanning mechanism Moderate aberration in spite of constant included angle Variable included angle system is also adopted recently

Overview of a typical soft X-ray beamline



Pre-focusing optics: focuses X rays onto the entrance slit

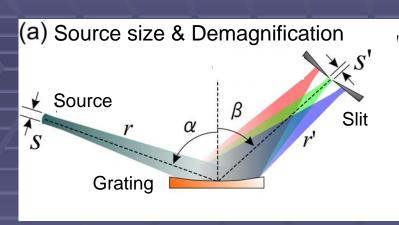
Monochromator: from the entrance slit to the exit slit

Post-focusing optics: focuses monochromatized X rays onto sample position

Higher order suppression (Mc):

utilizes energy dependence of reflectivity (or transmittance)

1. Source-size limit



Dispersion:

$$dz/d\lambda = r'nm/\cos\beta$$

Beam size at the exit slit

$$s'$$
 (lower limit) = $s r'/r$

$$\Rightarrow \lambda/\Delta\lambda \propto r/S$$

- (a) If the source size is the same, longer monochromator gives higher resolution.
- (b) If the monochromator length (r + r') is the same, longer entrance arm (r) gives higher resolution. \Rightarrow Higher demagnification factor is better!

But...

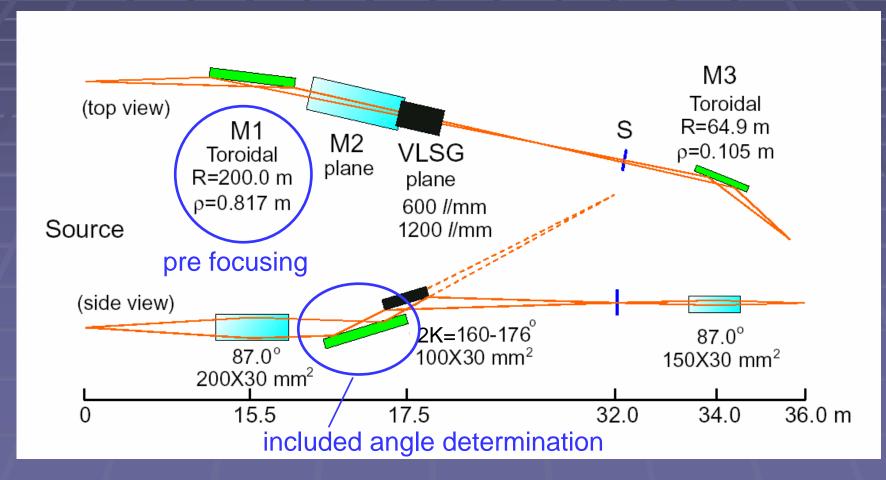
- (a') Long monochromator needs large mirrors to keep enough acceptance ⇒ higher cost, or intensity loss by reduced acceptance
- (b') High demagnification factor causes large aberration.
 - ⇒ Eventual decrease in energy resolution

Most people choose ~1:1 demagnification optics, though it might not be the best solution.

Groove density (n) and included angle are chosen, considering the balance among dispersion, demagnification, diffraction efficiency, etc.

2. Monochromator parameters (mirror radius, groove parameter, etc.)- highly depends on the type of monochromator

Design example: Variable-included-angle Monk-Gillieson mount varied-line-spacing (VLS) grating monochromator

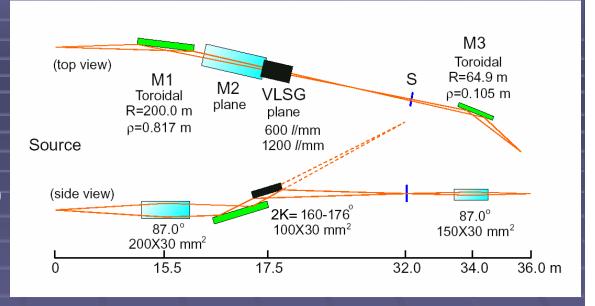


Parameters:

p (sagittal radius of M1)

Groove parameters of VLSG

$$N = N_0 (1 + a_1 w + a_2 w^2 + a_3 w^3)$$



K. Amemiya & T. Ohta, J. Synchrotron Rad. 11 (2004) 171.

- 1. Choose two energies (E₁ and E₂) and respective included angles (K₁ and K₂)
- 2. Optimize ρ and a_1 so that the defocus vanishes at (E_1, K_1) and (E_2, K_2)
- 3. For other energies, included angles are set so that the defocus vanishes
- 4. Choose an energy (E_3) and optimize a_2 so that the coma aberration vanishes
- 5. Choose E₄ and optimize a₃ so that the spherical aberration vanishes

pA(S-FM) qA(FM-G) rB Incidence angle of FM R (radius of FM)	21 1.5 15.5 88 390	
N0(I/mm) Included angle @E1 Included angle @E2 Included angle @E3 Included angle @E4	600 168 175 170.0075871 170.0075871	1200 168 175 170.0075871 170.0075871
E1(eV)[defocus=0]	50	100
E2(eV)[defocus=0]	500	1000
E3(eV)[coma=0]	100	200
E4(eV)[spherical=0]	100	200
λ1(Å)	247.97	123.985
λ2(Å)	24.797	12.3985
λ3(Å)	123.985	61.9925
λ4(Å)	123.985	61.9925

α 1(deg) β 1(deg) α 2(deg) β 2(deg) α 3(deg) β 3(deg) α 4(deg) β 4(deg)	88.08108609 -79.9189139 88.4772024 -86.5227976 87.45160484 -82.5559822 87.45160484 -8.2556E+01	88.08108609 -79.9189139 88.4772024 -86.5227976 87.45160484 -82.5559822 87.45160484 -8.2556E+01
rA(m)	-14.9820	-14.9820
n20(mm-2)	-7.6699E-02	-1.5340E-01
n30(mm-3)	4.8778E-06	9.7556E-06
n40(mm-4)	-1.3394E-09	-2.6789E-09
ρ(m)	6.4455E-01	6.4455E-01
a1(mm-1)	-1.2783E-04	-1.2783E-04
a2(mm-2)	1.2195E-08	1.2195E-08
a3(mm-3)	-1.1162E-12	-1.1162E-12

 $N = N_0 (1 + a_1 w + a_2 w^2 + a_3 w^3)$

2.2.analytical estimation of energy resolution

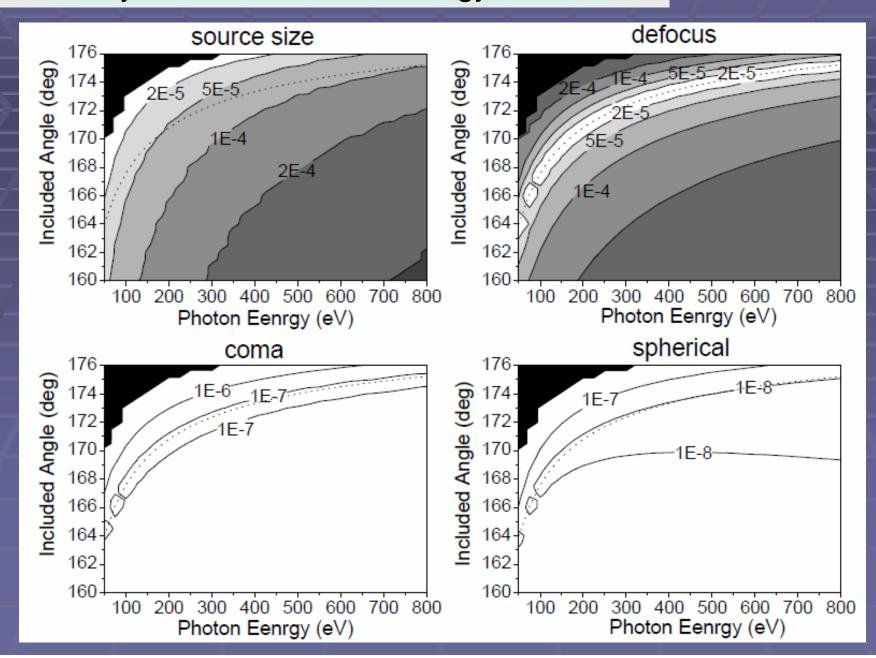
N0(I/mm)	600					un	dulator le	ngth(m)=	4.5								
rA(m)	-14.9820		pA(m)	21		electron d	liv.hor./ve	er.(urad)=	20.00	5.00							
rB(m)	15.5		qA(m)	1.5		electron s	size.hor./	ver.(um)=	350.00	20.00							
n20(mm-2)	-0.0767		ρ (m)	0.6445													
n30(mm-3)	4.88E-06	Incide	nce angle	88													
n40(mm-4)	-1.3E-09	R (i	radius of l	390													
error (μ rad)	0.48	grati	ng length	100													
Included	_	1/8)	- ()				-		-	0	()	1 1 00 / 1	A 1 00 / 1	1 10/1	A 1 / 1	A 1 1/1	/ /
angle (deg)	Energy	λ(Å)	σp(um)	Σh(um)	Σ v(um)	σp'(urad)	Σh'(urad)	∑ v'(urad)	α	β	w(m)	Δ λ 20/ λ	Δ λ 30/ λ	$\Delta \lambda 40/\lambda$	Δ Λ so/ Λ	Δ Λ sl/ Λ	total(w/o sl total
									α	β							
168	50	247.97	26.58	351.01	33.27	74.23	76.88	74.40	88.081	-79.92	0.037481	5.68E-17	2.61E-07	6.20E-08	1.05E-05	1.83E-05	1.05E-05 2.11E-05
169.0155705	75	165.31	21.70	350.67	29.51	60.61	63.82	60.82	87.478	-81.54	0.026383	2.46E-17	4.82E-08	7.32E-09	1.83E-05	2.58E-05	1.83E-05 3.16E-05
170.0075871	100	123.99	18.80	350.50	27.45	52.49	56.17	52.73	87.452	-82.56	0.022637	3.34E-17	0.00E+00	0.00E+00	2.29E-05	3.17E-05	2.29E-05 3.91E-05
170.8042113	125	99.188	16.81	350.40	26.13	46.95	51.03	47.21	87.529	-83.27	0.020908	0.00E+00	2.00E-08	1.49E-09	2.65E-05	3.67E-05	2.65E-05 4.53E-05
171.4465431	150	82.657	15.35	350.34	25.21	42.86	47.29	43.15	87.629	-83.82	0.019908	7.20E-17	3.10E-08	1.68E-09	2.94E-05	4.12E-05	2.94E-05 5.06E-05
171.9748591	175	70.849	14.21	350.29	24.53	39.68	44.43	39.99	87.728	-84.25	0.019257	1.34E-16	3.80E-08	1.49E-09	3.20E-05	4.53E-05	3.20E-05 5.55E-05
172.4179974	200	61.993	13.29	350.25	24.01	37.12	42.16	37.45	87.821	-84.6	0.018801	4.46E-17	4.29E-08	1.18E-09	3.43E-05	4.91E-05	3.43E-05 5.99E-05
172.7960709	225	55.104	12.53	350.22	23.60	34.99	40.31	35.35	87.906	-84.89	0.018466	5.98E-17	4.65E-08	8.52E-10	3.65E-05	5.26E-05	3.65E-05 6.40E-05
173.1233189	250	49.594	11.89	350.20	23.27	33.20	38.76	33.57	87.983	-85.14	0.01821	1.35E-16	4.93E-08	5.35E-10	3.85E-05	5.59E-05	3.85E-05 6.78E-05
173.4100546	275	45.085	11.33	350.18	22.99	31.65	37.44	32.05	88.053	-85.36	0.018009	3.85E-17	5.15E-08	2.41E-10	4.03E-05	5.90E-05	4.03E-05 7.15E-05
173.6639224	300	41.328	10.85	350.17	22.75	30.31	36.31	30.71	88.117	-85.55	0.017848	4.79E-17	5.33E-08	2.94E-11	4.21E-05	6.20E-05	4.21E-05 7.49E-05
173.8907098	325	38.149	10.43	350.16	22.55	29.12	35.32	29.54	88.176	-85.71	0.017717	1.53E-16	5.49E-08	2.75E-10	4.38E-05	6.48E-05	4.38E-05 7.82E-05
174.0948831	350	35.424	10.05	350.14	22.38	28.06	34.46	28.50	88.23	-85.87	0.017609	8.99E-17	5.62E-08	4.99E-10	4.55E-05	6.75E-05	4.55E-05 8.14E-05
174.2799478	375	33.063	9.71	350.13	22.23	27.11	33.69	27.56	88.279	-86	0.017519	4.47E-17	5.73E-08	7.03E-10	4.70E-05	7.01E-05	4.70E-05 8.44E-05
174.4486972	400	30.996	9.40	350.13	22.10	26.25	33.00	26.72	88.325	-86.12	0.017444	5.56E-17	5.83E-08	8.89E-10	4.86E-05	7.26E-05	4.86E-05 8.74E-05
174.6033869	425	29.173	9.1177	350.12	21.98	25.461	32.377	25.948	88.367	-86.24	0.01738	1.59E-16	5.92E-08	1.06E-09	5.00E-05	7.51E-05	5.00E-05 9.02E-05
174.7458606	450	27.552	8.86	350.11	21.87	24.74	31.82	25.24	88.406	-86.34	0.017326	1.46E-16	6.00E-08	1.22E-09	5.14E-05	7.74E-05	5.14E-05 9.30E-05
174.8776414	475	26.102	8.6245	350.11	21.78	24.084	31.306	24.598	88.443	-86.43	0.01728	1.26E-16	6.07E-08	1.36E-09	5.28E-05	7.97E-05	5.28E-05 9.56E-05
175	500	24.797	8.41	350.10	21.69	23.47	30.84	24.00	88.477	-86.52	0.01724	1.22E-16	6.14E-08	1.50E-09	5.42E-05	8.20E-05	5.42E-05 9.82E-05
175.1140057	525	23.616	8.2035	350.1	21.617	22.909	30.411	23.448	88.509	-86.6	0.017206	4.74E-17	6.20E-08	1.62E-09	5.55E-05	8.41E-05	5.55E-05 1.01E-04

defocus

Source size

slope error

2.2.analytical estimation of energy resolution



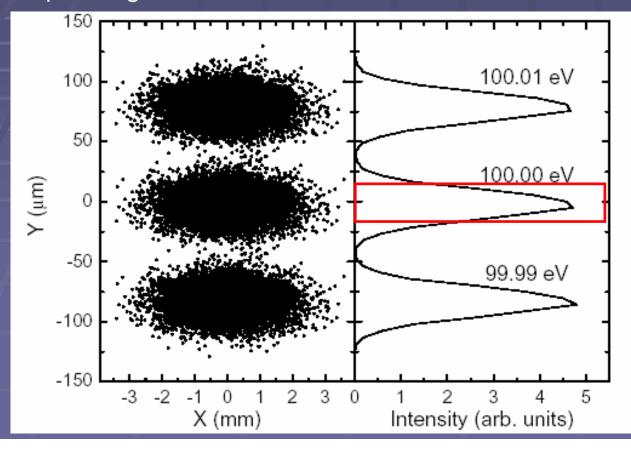
Source parameters:

 $\sigma_x = 350 \ \mu\text{m}, \ \sigma_y = 20 \ \mu\text{m}, \ \sigma_x' = 20 \ \mu\text{rad}, \ \sigma_y' = 5 \ \mu\text{rad}, \ 4.5 \ \text{m} \ \text{undulator}$

Optimization conditions for $N_0 = 600 \text{ l/mm}$:

$$E_1 = 50 \text{ eV}, E_2 = 500 \text{ eV}, K_1 = 164^{\circ}, K_2 = 174^{\circ}, E_3 = E_4 = 100 \text{ eV}$$

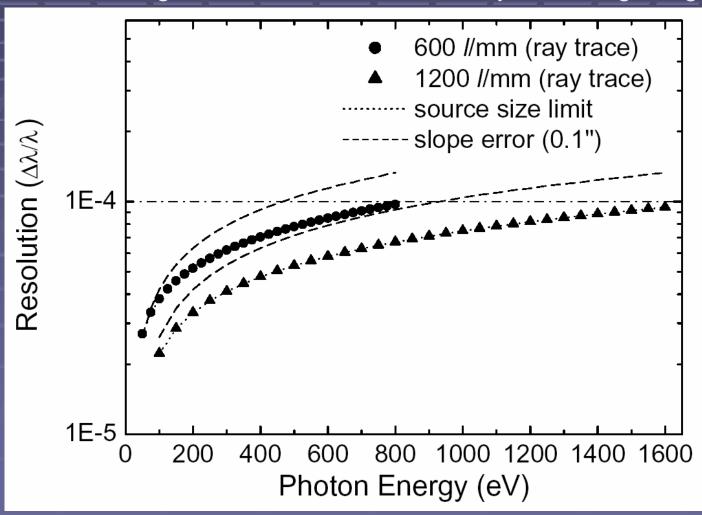
Spot diagram at the exit slit



 $=> E/\Delta E \sim 26,000$

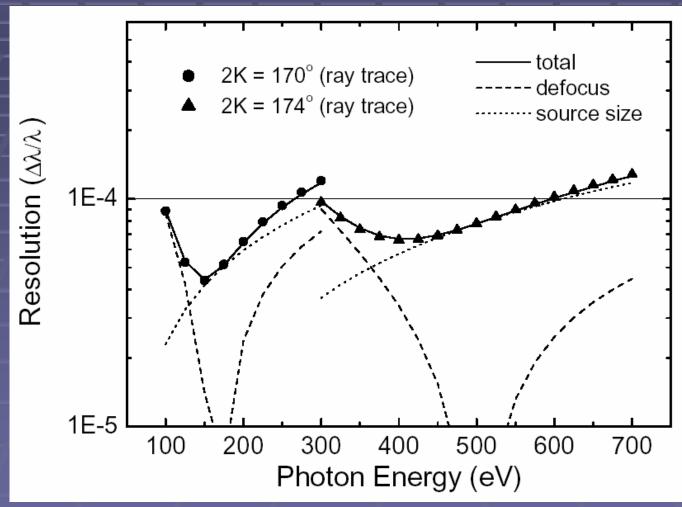
Simultaneous scan mode

Included angle is scanned simultaneously with the grating



Source size or slope error limited resolution

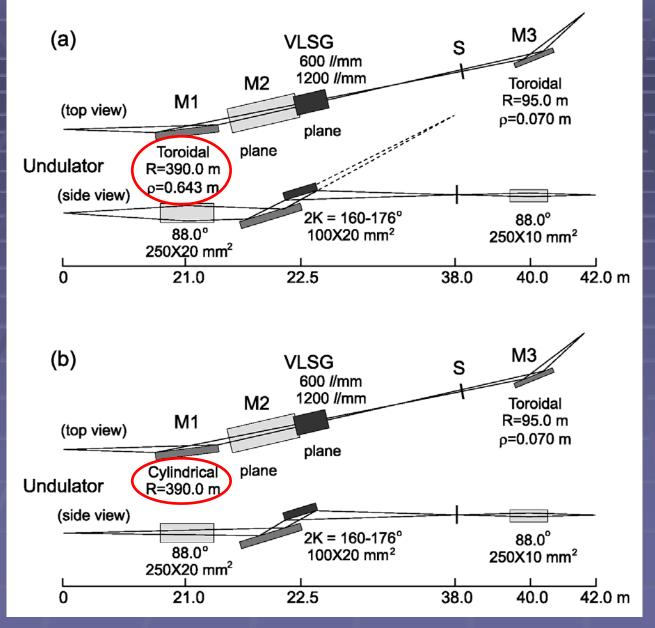
Fixed included angle mode



Relatively high resolution over wide energy range

* Analytical estimation is consistent with ray tracing simulation

Comparison with diverging illumination optics



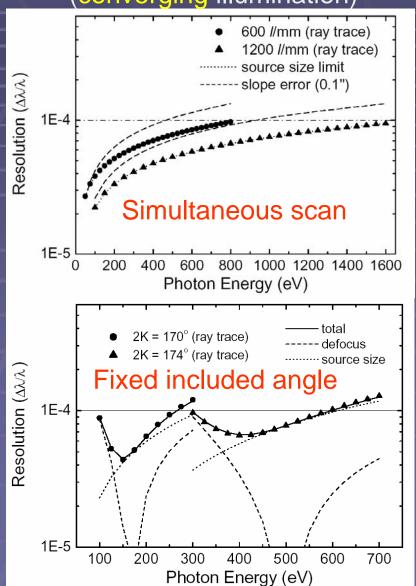
Monk-GIllieson
converging X rays
illuminate VLSG

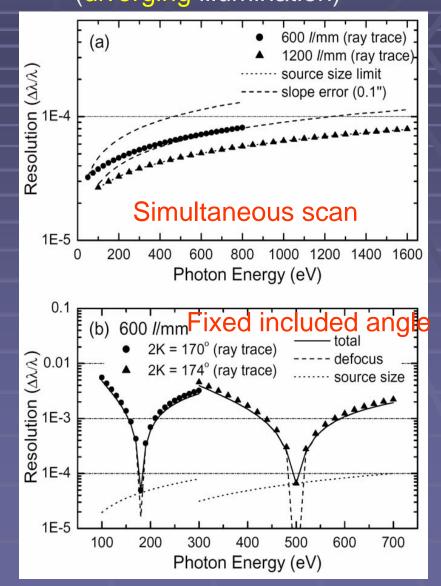
non Monk-GIllieson diverging X rays illuminate VLSG

Comparison with diverging illumination optics

Monk-Gillieson (converging illumination)

non Monk-Gillieson (diverging illumination)







Determination of beamline center



Hole on the Shield wall

to beamline

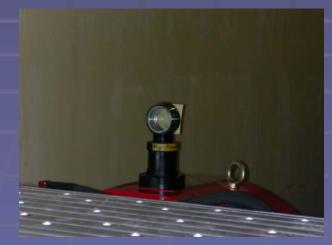


Q-magnet

Undulator

Q-magnet

Shield wall

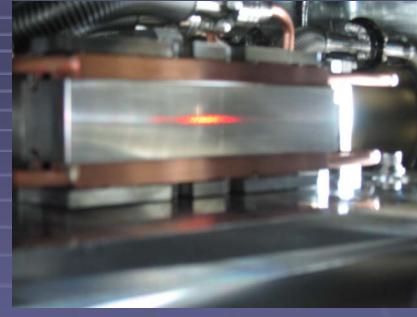


Target on the Q-magnet



3.1. alignment





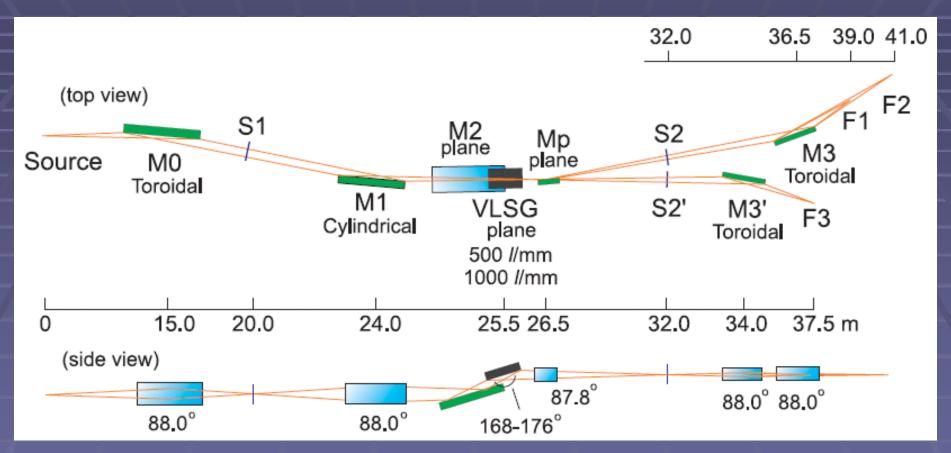
Grating adjustment (roll and yaw)

Adjusted by using diffraction of Laser light

Mirror adjustment

Adjusted by using a dummy mirror and Laser light

Example: BL-16A at the Photon Factory



M0: vertical focusing to entrance slit (S1) [r = 15 m, r' = 5 m]

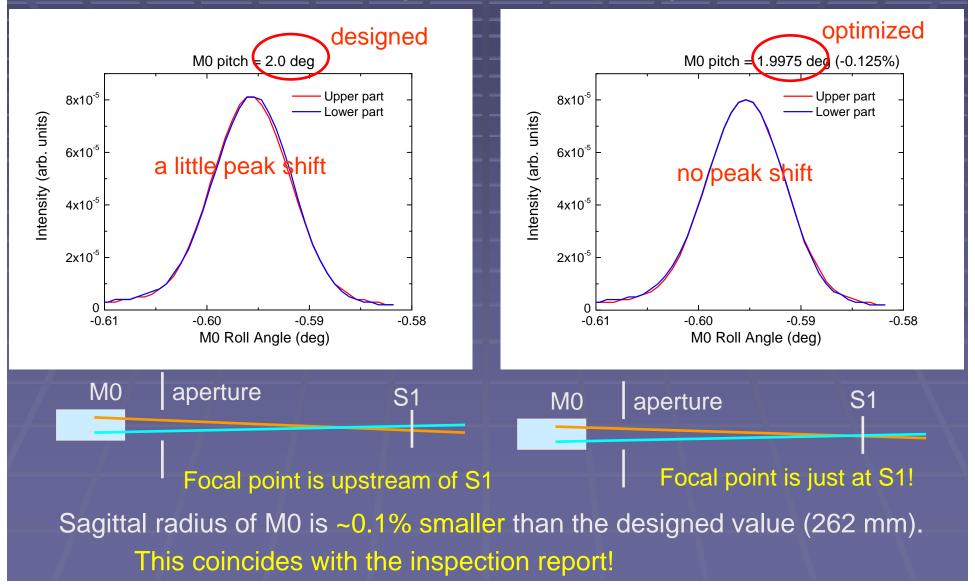
M1: vertical focusing to 90 mm upstream of exit slit (S2)

[r = 4 m, r' = 7.91 m]

(a) Vertical focusing of M0

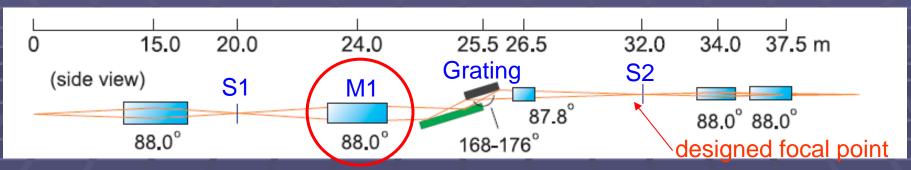
Light intensity was monitored downstream of S1 during M0 roll-angle scan.

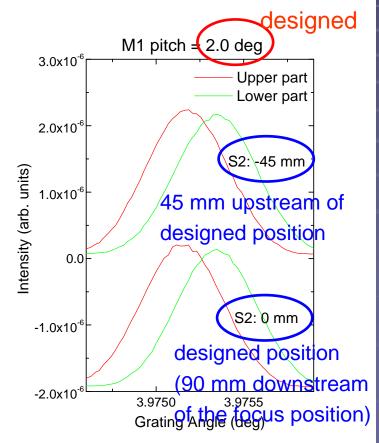
Upper and Lower parts of light were taken by using an aperture.



(2) Vertical focusing of M1

M1 is designed so that light is focused at 90 mm upstream of S2.





Zero-th order light intensity was monitored downstream of S2 during Grating angle scan.

Upper and Lower parts of light were taken by using an aperture

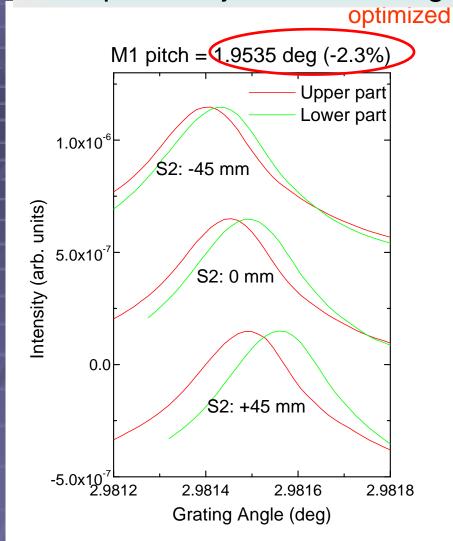
A peak shift between the upper and lower parts means that the focal position is upstream of S2.

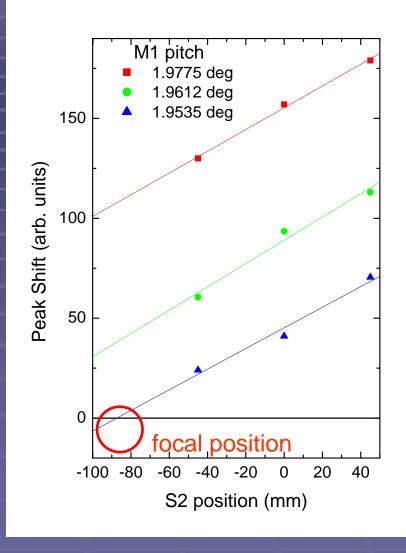
However...

The peak shift should be reduced by ~50 % when S2 is placed at -45 mm position.

→ Focal position is far from S2!?

(2) Vertical focusing of M1

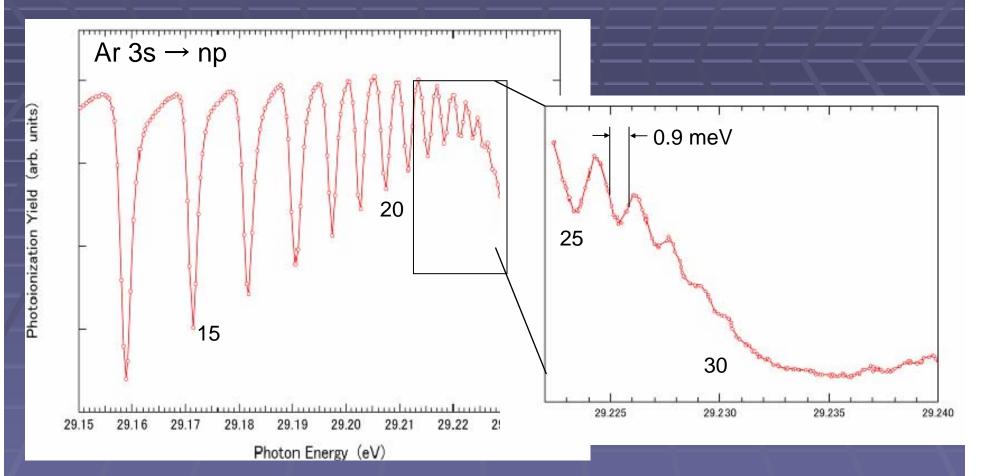




The focal point became 90 mm upstream of S2 when the pitch angle of M1 was changed to 1.9535 deg (-2.3% from the designed value).

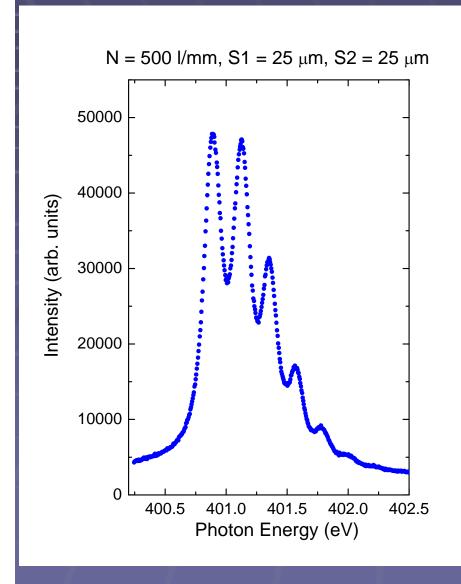
Sagittal radius of M1 is ~2.3 % smaller than the designed value !?

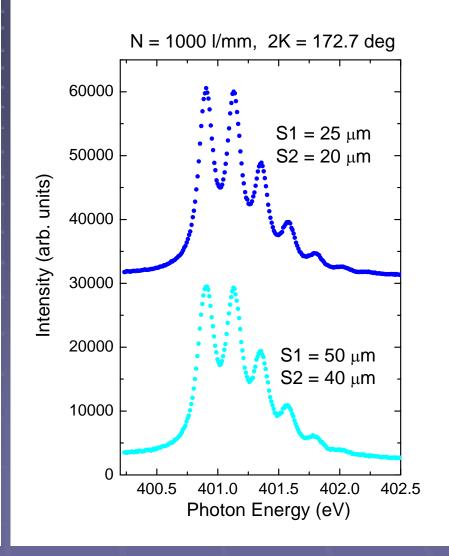
Absorption spectrum for Ar gas



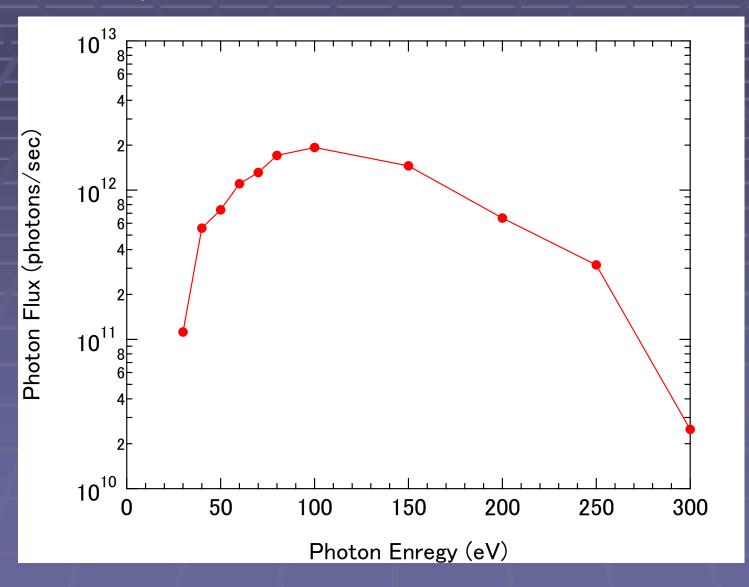
 $\lambda / \Delta \lambda > 30,000$

Absorption spectrum for N₂ gas





Photon Flux: photodiode is available



Beam size: knife-edge scan

Light intensity is monitored at downstream of the knife edge

