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
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 - 2.1. optimization of parameters
 - 2.2. analytical estimation of energy resolution
 - 2.3. ray-tracing simulation
- 3. Beamline installation
 - 3.1. alignment
 - 3.2. optical adjustments using SR
 - 2.3. experimental estimation of beamline performance ²

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
- 1. 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 \Rightarrow 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 (* more grazing needs larger mirror) Diffraction efficiency of the grating

* High groove density \Rightarrow 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 \Rightarrow resolution & intensity in wide energy range scanning mechanism is more complicated \Rightarrow 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 of G, 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, ... 6



(1) Plane grating monochromators

Collimated-light illumination

Parabolic mirror (focusing) Parabolic mirror (collimation) Exit slit Plane grating (wavelength (dispersion) selection) is small enough Point source refocussing mirror (ellipsoid) refocussing Focusing uirrar (tarai) sample (ARPES) mirror Grating 19'860 Collimating 8'860 mirror apertures pre 5'960 16'860 3'010 so ur ce included angle determination

> 7 http://sls.web.psi.ch/view.php/beamlines/adress/optics/index.html

Essentially no aberration

 $\Rightarrow \alpha$ and β can be freely chosen

 \Rightarrow Demagnification can be controlled

Precision of parabolic mirrors is relatively poor

One can use cylindrical mirrors if divergence

1.4. examples for soft X-ray monochromator (1) Plane grating monochromators Diverging light illumination (SX-700)

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

Precision of elliptical mirrors was essential due to high demagnification factor

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...



Spherical grating (dispersion & focusing)

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

- \Rightarrow Simple scanning mechanism
- Kinds of aberration arises, but only the defocus term can be canceled by moving the exit slit

"Active grating" (variable radius) is developed to achieve fixed exit slit 9

- 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



1.4. examples for soft X-ray monochromator

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

Converging light illumination (Monk-Gillieson mount)



Pre-focusing mirror upstream of VLSG Constant included angle \Rightarrow Simple scanning mechanism Moderate aberration in spite of constant included angle Variable included angle system is also adopted recently

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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

 $\Rightarrow \lambda/\Delta\lambda \propto nmr/s\cos\beta$

- (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. ⇒ 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.
 - \Rightarrow Eventual decrease in energy resolution

Most people choose $\sim 1:1$ ($r \sim r'$) 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. ¹⁴

- 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 (E_1 and E_2) and respective included angles (K_1 and K_2)

- 2. Optimize ρ and a_1 so that the defocus vanishes at (E₁, K₁) and (E₂, K₂)
- 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 E_4 and optimize a_3 so that the spherical aberration vanishes

pA(S-FM)	21		α 1(deg)	88.08108609	88.08108609				
qA(FM-G)	1.5		β 1(deg)	-79.9189139	-79.9189139				
rB	15.5		$\alpha 2(deg)$	88.4772024	88.4772024				
Incidence angle of FM	88		$\beta 2(deg)$	-86.5227976	-86.5227976				
R (radius of FM)	390		α 3(deg)	87.45160484	87.45160484				
			β 3(deg)	-82.5559822	-82.5559822				
N0(I/mm)	600	1200	$\alpha 4(deg)$	87.45160484	87.45160484				
Included angle @E1	168	168	$\beta 4(deg)$	-8.2556E+01	-8.2556E+01				
Included angle @E2	175	175							
Included angle @E3	170.0075871	170.0075871	rA(m)	-14.9820	-14.9820				
Included angle @E4	170.0075871	170.0075871	n20(mm-2)	-7.6699E-02	-1.5340E-01				
			n30(mm-3)	4.8778E-06	9.7556E-06				
E1(eV)[defocus=0]	50	100	n40(mm-4)	-1.3394E-09	-2.6789E-09				
E2(eV)[defocus=0]	500	1000	$\rho(m)$	6.4455E-01	6.4455E-01				
E3(eV)[coma=0]	100	200							
E4(eV)[spherical=0]	100	200	a1(mm-1)	-1.2783E-04	-1.2783E-04				
3 4 (8)	047.07	100.005	$a^{2(mm-2)}$	1,2195E-08	1.2195E-08				
$\lambda 1(A)$	247.97	123.985	$a_{3(mm-3)}$	-1 1162E-12	-1 1162E-12				
$\lambda 2(A)$	24.797	12.3985		1.11022 12	1.11022 12				
λ 3(A)	123.985	61.9925		_					
λ4(A)	123.985	61.9925	$N = N_0 (1 + a_1 w + a_2 w^2 + a_3 w^3)$						
				· · · ·					

2.2. analytical estimation of energy resolution

N0(I/mm) rA(m) rB(m) n20(mm-2) n30(mm-3) n40(mm-4) error (μrad)	600 -14.9820 15.5 -0.0767 4.88E-06 -1.3E-09 0.48	Incider R (i grati	pA(m) qA(m) ρ(m) nce angle radius of ing length	21 1.5 0.6445 88 390 100	undulator length(m)= electron div.hor./ver.(urad)= electron size.hor./ver.(um)=				4.5 20.00 350.00	5.00 20.00		F	From light path function						
Included angle (deg)	Energy	λ(Å)	$\sigma p(um)$	Σh(um)	Σv(um)	σ p'(urad)	Σh'(urad)	Σv'(urad)	α	β	w(m)	Δ λ 20/ λ	Δ λ 30/ λ	Δ λ 40/ λ	$\Delta \lambda so / \lambda$	$\Delta \lambda sl/\lambda$	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	4.4/E-1/	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	
1/4./458606	450	27.552	8.86	350.11	21.87	24.74	31.82	25.24	88.406	-86.34	0.01/326	1.46E-16	6.00E-08	1.22E-09	5.14E-05	7.74E-05	5.14E-05	9.30E-05	
1/4.8//6414	4/5	26.102	8.6245	350.11	21.78	24.084	31.306	24.598	88.443	-86.43	0.01728	1.26E-16	6.0/E-08	1.36E-09	5.28E-05	7.97E-05	5.28E-05	9.56E-05	
175 1140057	500	24.797	8.41	350.10	21.69	23.47	30.84	24.00	88.477	-86.52	0.017206	1.22E-10	6.14E-08	1.50E-09	5.42E-05	8.20E-05	5.42E-05	9.82E-0	
175.1140057	929	23.010	0.2030	350.1	21.017	22.909	30.411	23.440	66.009	-80.0	0.017200	4./4E-1/	0.20E-08	1.02E-09	5.55E-05	6.41E-05	5.55E-05	1.01E-04	
									/										
									defocus		Source size		slope error		r				
	F :	$= p_A$	+q	$A_A +$	r_B														
		+	M_{10}	w +	$(M_{20}$	$w^{2} - w^{2}$	$\vdash M_0$	$_{2}l^{2} +$	- M ₃	$_0w^3$	$+ M_{12}$	$_{2}wl^{2})/2$	2						
		+	(M_4)	w^{4} -	+M	$w^{2}l$	$^{2} +$	$M_{04}l$	4)/8	+.									

+ $[n_{10}w + (n_{20}w^2)/2 + (n_{30}w^3)/2 + (n_{40}w^4)/8 + ...]m\lambda$,

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2.2.analytical estimation of energy resolution



2.3. ray-tracing simulation

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 $N_0 = 600$ 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



2.3. ray-tracing simulation

Simultaneous scan mode

Included angle is scanned simultaneously with the grating



Source size or slope error limited resolution ²¹

2.3. ray-tracing simulation

Fixed included angle mode



* Analytical estimation is consistent with ray tracing simulation



Comparison with diverging illumination optics

Monk-GIllieson

converging X rays illuminate VLSG

non Monk-GIllieson

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diverging X rays illuminate VLSG
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3.1. alignment





Grating adjustment (roll and yaw) Mirror adjustment

Adjusted by using diffraction of Laser light

Adjusted by using a dummy mirror and Laser light

3.2. optical adjustments using SR

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]



This coincides with the inspection report!





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 !? ³¹







3.2. optical adjustments using SR





3.3. experimental estimation of beamline performance Absorption spectrum for N₂ gas



3.3. experimental estimation of beamline performance Absorption spectrum for Ar gas



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

3.3. experimental estimation of beamline performance

Photon Flux: photodiode is available



3.3. experimental estimation of beamline performance

Beam size: knife-edge scan

Light intensity is monitored at downstream of the knife edge





Horizontal Size





Thank you for your attention !