





Synchrotron radiation beamlines in the vacuum ultraviolet and soft X-ray region

k. ito 3 JASS2002 Oct 21, 2002

Kenji ITO e-mail: kenji.ito@kek.jp Photon Factory, IMSS, KEK, Tsukuba, Ibaraki 305-0801, Japan

Introduction

Optical elements

 mirrors geometrical shape reflectivity
 grating basic understanding geometrical optics → ray tracing varied-line spacing grating

Monochromators

normal incidence type grazing incidence type

Summary

k. ito 4 JASS2002 Oct 21, 2002



What is the role of beamlines for SR usage?

- 1) conducting SR from the storage ring to the experimental stations
- 2) shaping SR beam, spatially and energetically, to meet the experimental requirements



Definition of VUV and SX

k. ito

JASS2002

Oct 21, 2002

VUV: vacuum ultraviolet EUV: extreme ultraviolet SX: soft X-ray

VUV-SX photons cannot propagate in the atmosphere!!!





VUV-SX beamlines must be Kept at ultra-high vacuum (UHV)

k. ito

JASS2002 Oct 21, 2002

1) To facilitate the propagation of the VUV-SX photons

- 2) Not to disturb the storage ring no mechanically-rigid window is available!!!
- 3) To protect the optical elements from contamination, oil-free primary pumps are recommended!!!





Construction of a VUV-SX beamline

k. ito 7 JASS2002 Oct 21, 2002

What kinds of measurements are required?

Photon energy range Photon flux Beam size Photon band width Polarization Purity Coherence

Beamline optics pre-focusing mirrors monochromator post-focusing mirrors

Light source bending magnet undulator multipole wiggler

This procedure does not work for a multipurpose beamline.



k. ito 9 JASS2002 Oct 21, 2002

Optical elements used in the VUV-SX beamlines

1) reflection mirrors as a focussing tool

2) diffraction gratings, zone plates, multilayered mirrors, filters and crystals as dispersion tools

monochromators as a beamline system



Mirrors for SR use

 focusing of VUV-SX light by various shapes of mirror: sphere, cylinder, parabola, paraboloid, ellipse, ellipsoid, toroid, etc

k. ito

JASS2002 Oct 21, 2002

2) for better reflectivity in the VUV-SX region: substrate: SiC, Si, SiO₂, metal, other glass coating materials: Au, Pt, Os,...

> with modern technology: 1-m long mirrors available surface roughness < 0.5 nm in rms slope error < 1 µrad → beamspot size









For 2D focusing: ellipsoidal shape mirrors

k. Ito

JASS2002 Oct 21, 2002

14









Henke et al., Atomic and Nuclea Data Tables, **54**, 181 (1993)





k. ito 20 JASS2002 Oct 21, 2002

Gratings as dispersion elements

Diffraction grating Zone plate Multi-layered mirror Filters Crystals

Introduction
 Efficiency
 Geometrical optics → ray tracing
 Varied-line spacing grating







Diffraction efficiency can be calculated by the scalar theory for $\lambda/d \ll 1$. Rigorous numerical calculations based on Maxwell equations gives solutions with much better precision. Note that the efficiency strongly depends on the polarization of incident radiation.



Calculated by M. Neviere

 $\theta = 85^{\circ}$ $\alpha = 1.624^{\circ}$

TE

TM

30

40

k. ito 24 **JASS2002** Oct 21, 2002





k. ito 26 JASS2002 Oct 21, 2002

When the path difference between 1 and 2 is equal to $\lambda/2$, destructive interference occurs.

 $h(\sin i + \sin \theta) = \lambda/2$ normal incidence: $\lambda = 4h$ grazing incidence: $\lambda = 2h(i+\theta)$

Suppression of 2nd order!!!

Geometrical optics of diffraction gratings(1)

k. ito 27 JASS2002 Oct 21, 2002



Fermat's principle: the pathlength of an actual ray traveling from a point A to a point B takes an extremal or stationary value.

 $\delta F=0$, where *F* is the pathlength from A to B. *F*: light path function The red ray meets the grating at a point P(ξ ,w,l) on the *n*th groove, the zeroth groove being assumed to pass through O. Two rays diffracted from the zeroth and *n*th grooves are reinforced when their path difference is equal to $nm\lambda$.

Light path function $F = AP + PB + nm\lambda$

$$AP = \sqrt{(\xi - x)^{2} + (w - y)^{2} + (l - z)^{2}}$$
$$PB = \sqrt{(x' - \xi)^{2} + (y' - w)^{2} + (z' - l)^{2}}$$

Expansion of
$$F$$
 for $z=0$ and $n=1/d$
F = $F_{00} + F_{10}w + \frac{1}{2}F_{20}w^2 + \frac{1}{2}F_{02}I^2 + \frac{1}{2}F_{30}w^3 + \frac{1}{2}F_{12}wI^2 + \frac{1}{8}F_{40}w^4 + \frac{1}{4}F_{22}w^2I^2 + \frac{1}{8}F_{04}I^4 + \dots$
spherical aberration
F₀₀ = $r + r_0$
F₁₀ = $-\sin \alpha - \sin \beta_0 + \frac{m\lambda}{d}$ grating equation
F₂₀ = $\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} + \frac{\cos^2 \beta_0}{r_0} - \frac{\cos \beta_0}{R}$ defocus in y-direction
F₀₂ = $\frac{1}{r} - \frac{\cos \alpha}{R} + \frac{1}{r_0} - \frac{\cos \beta_0}{R}$ defocus in z-direction
F₃₀ = $\frac{\sin \alpha}{r} \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) + \frac{\sin \beta_0}{r_0} \left(\frac{\cos^2 \beta_0}{r_0} - \frac{\cos \beta_0}{R} \right)$ comma







Geometrical optics of diffraction gratings(5)

k. ito 31 JASS2002 Oct 21, 2002

Equation of image plane: $x'\cos(\beta_{0} + \phi) + y'\sin(\beta_{0} + \phi) = r_{0}'\cos\phi$ where $x' = \xi + L'd \qquad y' = w + M'd \qquad z' = l + N'd$ $d = \frac{r_{0}'\cos\phi - \xi\cos(\beta_{0} + \phi) - w\sin(\beta_{0} + \phi)}{L'\cos(\beta_{0} + \phi) + M'\sin(\beta_{0} + \phi)}$



YZ-coordinate on Σ -plane $Y = (y' - r_0' \sin \beta_0) \sec(\beta_0 + \phi)$ Z = z'

$$Y = r_0' \sec \beta_0 \sec \phi \times \left[wf_{100} + w^2 f_{200} + l^2 f_{020} + lzf_{011} + z^2 f_{002} + w^3 f_{300} + wl^2 f_{120} + wlzf_{111} + wz^2 f_{102} + O(w^4 / R^3) \right]$$

$$Y = r_0' \left[zg_{001} + \lg_{010} + w \lg_{110} + wzg_{101} + w^2 \lg_{210} + w^2 zg_{201} + l^3 g_{030} + l^2 zg_{021} + lz^2 f_{012} + z^3 f_{003} + O(w^4 / R^3) \right]$$



By ray-tracing, it is possible to see1) how the beam is focused on the slits and at F,

- 2) how it spreads on the grating,
- 3) the geometrical through-put.





Geometrical optics of diffraction gratings(7)

k. ito 33 JASS2002 Oct 21, 2002

Analytical expression for spot diagrams

$$Y = r_0' \sec \beta_0 \sec \phi \times \left[w f_{100} + w^2 f_{200} + l^2 f_{020} + lz f_{011} + z^2 f_{002} + w^3 f_{300} + w l^2 f_{120} + w lz f_{111} + w z^2 f_{102} + O\left(\frac{w^4}{R^3}\right) \right]$$

 $Z = r_0' \left[zg_{001} + \lg_{010} + w \lg_{110} + wzg_{101} + w^2 \lg_{210} + w^2 zg_{201} + l^3 g_{030} + l^2 zg_{021} + lz^2 f_{012} + z^3 f_{003} + O\left(\frac{w^4}{R^3}\right) \right]$

Analytical merit function: Q

$$Q = \sum_{i} Q(\lambda_{i})$$

= $\sum_{i} \left[\frac{1}{WLH} \iiint (Y - \overline{Y})^{2} dw dl dz + \frac{\mu}{WLH} \iiint Z^{2} dw dl dz \right]$

Optimization of design parameters so as to minimize Q, where μ is a weight function. Triple integrals have to be done over the grating surface. Note that Y and Z are dependent on λ_i (*i*=1, 2, ...,*N*).

Masui and Namioka, JOSA, **16**, 2253 (1999)



Geometrical optics of diffraction gratings(8)

k. ito 34 JASS2002 Oct 21, 2002

Hybrid design method : Koike and Namioka, JESRP, 80, 303 (1996)

$$Y_n(w_n, l_n, z_n) = \sum_n f_{ijk} w_n^i l_n^j z_n^k$$
$$Z_n(w_n, l_n, z_n) = \sum_n g_{ijk} w_n^i l_n^j z_n^k$$

Ray-tracing of 18 rays determines f_{ijk} 's and g_{ijk} 's by solving simultaneous equations. Optimization process using the merit function in the same manner as before.

Ray-tracing program is available at http://www.xraylith.wisc.edu/shadow/shadow.html



Varied line spacing gratings (1)

Groove function $n(w,l)\sigma = w + \Gamma \left[\frac{1}{2} \left(n_{20} w^2 + n_{02} l^2 + n_{30} w^3 + n_{12} w l^2 \right) + \frac{1}{8} \left(n_{40} w^4 + 2n_{22} w^2 l^2 + n_{04} l^4 \right) + \dots \right]$

Effective grating constant

$$\sigma \equiv 1 / \left[\frac{\partial n(w, l)}{\partial w} \right]_{w=l=0}^{\infty}$$

 $\Gamma=1$ for mechanically ruled grating $\Gamma=\sigma/\lambda_0$ for holographic grating



k. ito 35 JASS2002 Oct 21, 2002



Monochromators in the VUV-SX region for SR use (1)

Normal incidence monochromators

M. Koike, "Normal incidence monochromators and spectrometers" in J.A.R. Samson and D.L. Ederer Eds., "Vacuum Ultraviolet Spectroscopy II in Experimental Methods in Physical Sciences" Vol. 32, (Academic Press, New York, 1998, Chapter 1, pp. 1-20 review

(A) Seya-Namioka type monochromator

(B) Pseudo Rowland mount monochromator

K. Ito, Y. Morioka, M. Ukai, N. Kouchi, Y. Hatano and T. Hayaishi, RSI, 66, 2119 (1995)

(C) Eagle type monochromator

1) 6.65-m Eagle at BL-12B of the Photon Factory

K. Ito, T. Namioka, Y. Morioka, T. Sasaki, H. Noda, K. Goto, T. Katayama and M. Koike, Appl. Opt., 25, 837-847 (1986)
K. Ito and T. Namioka, Rev. Sci. Instr., 60, 1573-1578 (1989)
K. Ito, K. Maeda, Y. Morioka and T. Namioka, Appl. Opt., 28, 1813-1817 (1989)
2) undulator based 6.65-m Eagle at BL9.02 of ALS
M. Koike, P. Heimann, A. Kung, T. Namioka, R. DiGennaro, B. Gee and N. Yu, NIM, A347, 282 (1994)
A.G. Suits, P. Heimann, X. Yang, M. Evans, C.W. Hsu, K. Lu, Y.T. Lee and A.H. Kung, RSI, 66, 4841 (1995)
D.A. Mossessian, P. Heimann, E. Gullikson, R.K. Kaza, J. Chin and J. Arke, NIM, A347, 244 (1994)
3) 6.65-m Eagle with varibale polarization undulator at SU5 of LURE
L. Nahon, B. Lagarde, F. Polack, C. Alcaraz, O. Dutuit, M. Vervloet and K. Ito, NIM, A404, 418-429 (1998)
K. Ito, B. Lagarde, F. Polack, C. Alcaraz and L. Nahon, J. Synchrotron Rad., 5, 839-841 (1998)
L. Nahon, C. Alcaraz, J-J. Marlats, B. Lagarde, F. Polack, R. Thissen, D. Lepere and K. Ito, RSI, 72, 1320 (2001)





Seya-Namioka monochromator (2)

k. Ito 39 JASS2002 Oct 21, 2002

(3)

1000 rays, generated from the entrance slit 10mm long, hitting the 1800-grooves/mm grating with 100(W)×60(H) mm² : from Koike's review





K. Ito, Y. Morioka, M. Ukai, N. Kouchi, Y. Hatano and T. Hayaishi, RSI, 66, 2119 (199









Koike, Heimann, Kung, Namioka, DiGennaro, Gee and Yu, NIM, A347, 282 (1994)





Monochromators in the VUV-SX region for SR use (2)

Grazing incidence monochromators

(A) Spherical grating monochromator (SGM) or Dragon C.T. Chen, NIM, A256, 595 (1987); C.T. Chen and F. Sette, RSI, 60, 1616 (1989).

(B) SX700 (PGM, elliptical mirror) and modified SX700 H. Petersen, Opt. Com., 40, 402 (1982); H.A. Padmore, RSI, 60, 1608 (1989); H. Petersen et al., RSI, 66, 1777 (1995).

(C) Monk-Gillieson type monochromator M. Hettrick et al., Appl. Opt., 27, 200 (1988); M. Koike and T. Namioka, RSI, 66, 2114 (1995).

(D) Harada type monochromator (PGM)

T. Harada, M. Itou and T. Kita, Proc. SPIE, **503**, 114 (1984); M. Itou, T. Harada and T. Kita, Appl. Opt., **28**, 146 (1989).

(E) Grasshopper monochromator: Rowland mount F.C. Brown et al., NIM, **152**, 73 (1978); F. Senf et al., RSI, **63**, 1326 (1992).













Amemiya, Tsukabayashi, Ohta and Ito, JESRP, 101-103, 927 (1999).



BL-11A (2) transmission





k. ito 53 JASS2002 Oct 21, 2002

k. ito 54 JASS2002 Oct 21, 2002

slit widths vs. resolution/flux





BL-11A (3) N₂ absorption



Other important points in the construction of VUV-SX beamlines (1)

k. ito 55 JASS2002 Oct 21, 2002

Hardware design

Wavelength-scanning mechanism in monochromator: the precision of grating rotation is in the order of 1/100 sec. In-situ adjustment of optical elements, such as rotations and translation.

Enclosing the important parts in a temperature controlled booth.

Isolation of optical elements

Optical elements or optical benches are well isolated from mechanical vibrations caused by ventilators, mechanical pumps, and so on. An ideal beamline is installed on a massive concrete base.



Other important points in the construction of VUV-SX beamlines (**2**)

k. ito 56 JASS2002 Oct 21, 2002

Installing beamlines

Anticipate how to align beamlines in its design stage. Convenient tools for beamline alignment: theodolites and auto-levels with a telescope and a laser

Optical alignment

VUV-SX photons are not visible!!! Beam position monitors such as fluorescent screens, photodiodes, and wire monitors are needed.



Other important points in the construction of VUV-SX beamlines (**3**)

k. ito 57 JASS2002 Oct 21, 2002

Heat load on optical elements

Cooling system

For VUV-SX beamlines, direct cooling is difficult! In-Ga alloy is used for better thermal contact between mirrors/gratings and their water cooled holders. Entrance slits are often required to be cooled.

Thermal distortion

Selecting materials with small value for α/κ as substrate of mirrors and gratings. SiC and Si are favored.

Simulation by ANSYS



Other important points in the construction of VUV-SX beamlines (4)

k. ito 58 JASS2002 Oct 21, 2002

Specification of mirrors and gratings

Consult the makers about the micro roughness, slope error, and groove density, of optical elements, for which the beamline performance is strongly dependent.

Vacuum technology

Vacuum technology is well established to obtain 10^{-8} Pa (10^{-10} Torr). Clean vacuum is obtained by oil-free primary pumps. Contamination of optical elements. cleaning with O₂ discharge and UV-lamp.



Other important points in the construction of VUV-SX beamlines (5)

k. ito 59 JASS2002 Oct 21, 2002

Control systems of beamline

PC base control system for the monochromator including the interface boards for stepping motors and encoders Beam channel? Beamline interlock system to protect the

experimentalists from radiation hazards and to avoid vacuum problems

Characterization of beamlines

Photon flux, resolving power, purity of light, Reproducibility of the wavelength scanning Fluctuation of the beam position on the entrance slit



Other important points in the construction of VUV-SX beamlines (6)

k. ito 60 JASS2002 Oct 21, 2002

Safety

Radiation safety

Gamma-ray stopper downstream of the first mirror, which might be installed inside a cage

Flammable and toxic gases

Gas duct with a gas detection system Exhaust steam from rotary pumps