A new ray-tracing program *RIGTRACE* for X-ray optical systems

T. Yamada,[a] N. Kawahara,[a] M. Doi,[a] T. Shoji,[a] N. Tsuruoka[b] and H. Iwasaki[b]*

[a]X-ray Research Laboratory, RIGAKU Corporation, Takatsuki, Osaka 569-1146, Japan, and [b]Faculty of Science and Engineering, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan. E-mail: iwasakih@se.ritsumei.ac.jp

A new ray-tracing simulation program, *RIGTRACE*, has been developed specifically for the X-ray optics range. It traces consecutively each ray, following its path from the source to the observation plane, and treats diffraction by a monochromator crystal by adopting the Darwin–Prins theory so that it may be seen how rays of slightly different energies and incident angles reach the plane. It is also possible to treat the case of the laboratory system, in which the optical elements are disposed close to each other. Examples of the application are provided.

Keywords: ray-tracing programs; X-ray optics range; beamlines.

1. Introduction

Ray-tracing simulations are indispensable when designing beamlines for synchrotron radiation sources, and many kinds of programs have been developed during the last two decades. Among them, *SHADOW* (Lai & Cerrina, 1986; Lai *et al.*, 1988) is the one most widely used. We have developed a new program, *RIGTRACE*, specifically for the X-ray optics range, which is useful not only for designing beamlines but also for designing compact diffraction or spectroscopic systems in a laboratory. Basic techniques of simulation, *i.e.* source description, reflection process *etc.*, are similar to those adopted in *SHADOW*, but *RIGTRACE* has the following unique methods of implementation: (i) rays are traced consecutively from the source to the observation plane (sample position) keeping one-by-one correspondence through reflections and diffractions by a series of optical elements so that a ray-propagation diagram can be constructed; (ii) diffraction by the monochromator crystal is treated by adopting the Darwin–Prins theory (James, 1958) for rays differing slightly in energy and incident angle; and (iii) rays can be traced for systems in which the optical elements are disposed close to each other, often encountered in a laboratory. The present paper describes the unique methods of implementation along with some results of the application.

2. The program structure

The program *RIGTRACE* is written in NDP-Fortran-77 and runs on the personal computer DEL XPS H266. Output is displayed either in the form of a ray-propagation diagram or a spot diagram, the cross-sectional image of the radiation beam, displayed on-screen on the computer and color-printed on paper.

Sources which can be incorporated are bending magnets, in which a Gaussian-type distribution of the source points and ray directions is assumed, as in *SHADOW*. It is also possible to incorporate the source in an X-ray generator, which is necessary when designing laboratory optical systems.

RIGTRACE treats a set of optical elements as one system and simulates the propagation of rays from the source to the observation plane. It is not possible to interrupt the calculation at an optical element and restart from that point after replacing it, whereas with *SHADOW* this is possible.

Optical elements which can be incorporated are mirrors, monochromator crystals and multilayers. It is not only those elements with plane surfaces that may be treated, but also cylindrically, spherically, toroidally, ellipsoidally and paraboloidally curved mirrors and Johann-type curved monochromator crystals. Surface roughness can be taken into account in the form of the pseudo-Debye–Waller factor. Auxiliary devices such as entrance slits, divergence slits, soller slits *etc.* can also be incorporated, if necessary.

3. Consecutive tracing of rays

When a ray is emitted from the source it is reflected and diffracted by a series of optical elements and finally reaches the observation plane. *RIGTRACE* traces its whole path of propagation throughout the optical system and, by plotting the path for each ray, a ray-propagation diagram may be constructed. Fig. 1 shows an example of a beamline consisting of a toroidally curved mirror at $Z = 0$ mm and a couple of the plane-crystal monochromators in an antiparallel arrangement at $Z = 1500$ mm. An entrance slit is placed at $Z = -1000$ mm to restrict the divergent incident beam. The number of rays used to construct the diagram is 1000. Note the large difference in scale for the synchrotron radiation beamline between the direction of ray propagation and the direction perpendicular to it: in order to show the diagram in a compact form the ordinate in Fig. 1 is shown on an enlarged scale. Different colors are used to show the decrease in the weight (intensity) of rays after successive reflection and diffraction. If the number of rays is reduced, it is possible to show clearly how different rays hit different parts of the surface of the optical elements and finally arrive at the observation plane. An example will be shown in a later section (Fig. 3). The ray-propagation diagram provides information on which part of the surface of the optical element contributes most to the formation of converging rays at the central point (the focus point) of the observation plane. It is useful to determine the width of the entrance slit which protects the surface area of the element from unnecessary irradiation.

4. Diffraction by a monochromator crystal

Diffraction by a monochromator crystal is represented by the Darwin–Prins curve. It shows that there is a range of energy (wavelength) and incident angle for diffracted X-rays and, in addition, the reflectivity is not necessarily unity over the range owing to absorption. *RIGTRACE* treats, according to this curve, the diffraction of rays incident to the monochromator crystal with some degree of divergence and spread in energy, assigning weights of less than unity when they are diffracted under the condition represented by the 'shoulder part' of the curve. Examples have been shown in Figs. 1(*a*) and 1(*b*) for rays diffracted by a couple of the Si(111) crystals. The rays whose weights are lower than a pre-fixed value may be eliminated from further tracing.

It is desirable to observe how rays having slightly different energies reach the final observation plane. Figs. 2(*a*)–2(*e*) show a series of spot diagrams on the observation plane for those rays. A couple of plane Si(111) crystals are set to satisfy the Bragg condition for rays of energy 5000 eV. The divergence of the incident beam has been assumed to be 1 mrad in the vertical plane and 10 mrad in the horizontal plane. The number of rays used is 25 000 for each diagram. It is seen that the majority of rays reaching the central part of the observation plane are those of energy 5000 eV, but there are contributions by rays of different energies. It may also be seen that the cross-sectional image of the beam is appreciably different for rays of different energies. By adding the contributions from all the rays, the diagram shown in Fig. 2(*f*) has been obtained. It can be used to estimate the energy resolution of the optical system of the beamline. It is not possible to make these kinds of observations using *SHADOW*.

5. Ray tracing for the optical system on a laboratory source

In diffraction or spectroscopic systems on a laboratory X-ray source, the optical elements such as crystal monochromator, multilayer monochromator and mirror are placed close to the source and to each other. The divergence of the radiation beam is quite large both in the vertical and horizontal planes. There are cases in which one optical element interrupts part of the incident rays to the neighboring element and reduces the effective beam divergence. An example may be found in the channel-cut type of monochromator. *RIGTRACE* simulates the propagation of rays for those cases by detecting the position of the obstacle and finding actual beams that hit the neighboring element. Fig. 3 shows a ray-propagation diagram for the system consisting of a couple of the closely spaced cylindrical W/C multilayers on the laboratory X-ray source. The rays diverging from the source are reflected twice by the multilayers and converge at a point denoted by the letter *F*. It is seen that there are non-negligible components of the rays reflected four times, which pass through the point near *F*.

6. Examples of the application

RIGTRACE has been used to design X-ray beamlines BL-3 and BL-10 on the compact synchrotron radiation source at Ritsumeikan University (Iwasaki *et al.*, 1998). Both consist of a prefocusing toroidally curved mirror and a couple of the plane-crystal monochromators. The small radius, 0.5 m, of the electron orbit in the ring allows the optical elements to be placed close to the radiation source so that the total length of the beamline is approximately 9 m, smaller than that at the large storage ring.

Fig. 4 shows a spot diagram of the rays at the observation plane at BL-3 (Saisho, 2000) for energies of 3000, 5000 and 7000 eV, with allowances being made for the divergence of the primary beam, 1 mrad in the vertical and 10 mrad in the horizontal, and for the spread in energy. The mirror is platinum-coated with radii of

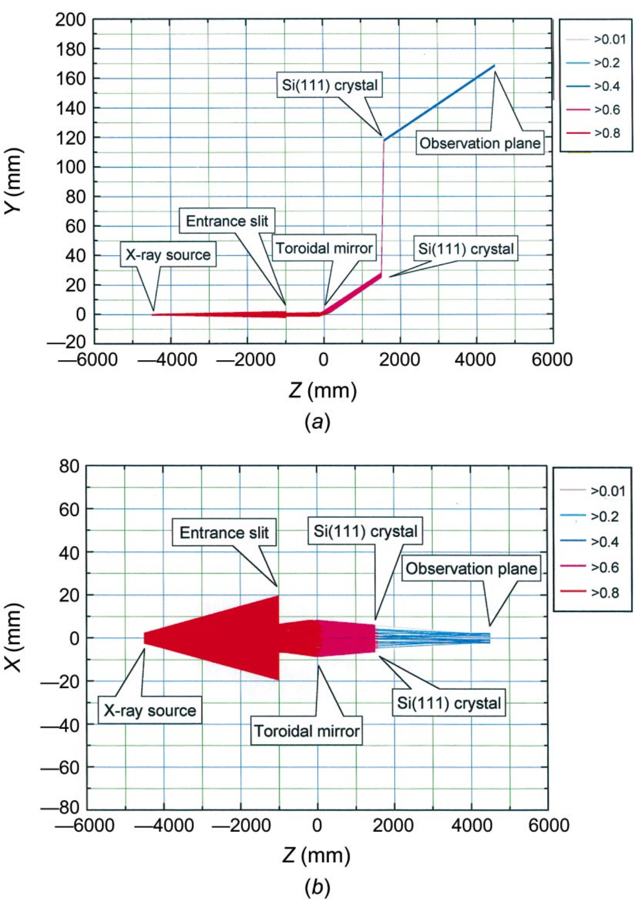

Figure 1
Ray-propagation diagram for the X-ray optical system consisting of a pre-focusing toroidal mirror and a couple of the plane Si(111) monochromator crystals. (*a*) Side view, (*b*) top view. The X-ray energy is 5000 eV. The color of the rays represents their 'weight', showing the gradual decrease in intensity after reflection and diffraction. Note that the ordinate is on an enlarged scale compared with the abscissa.

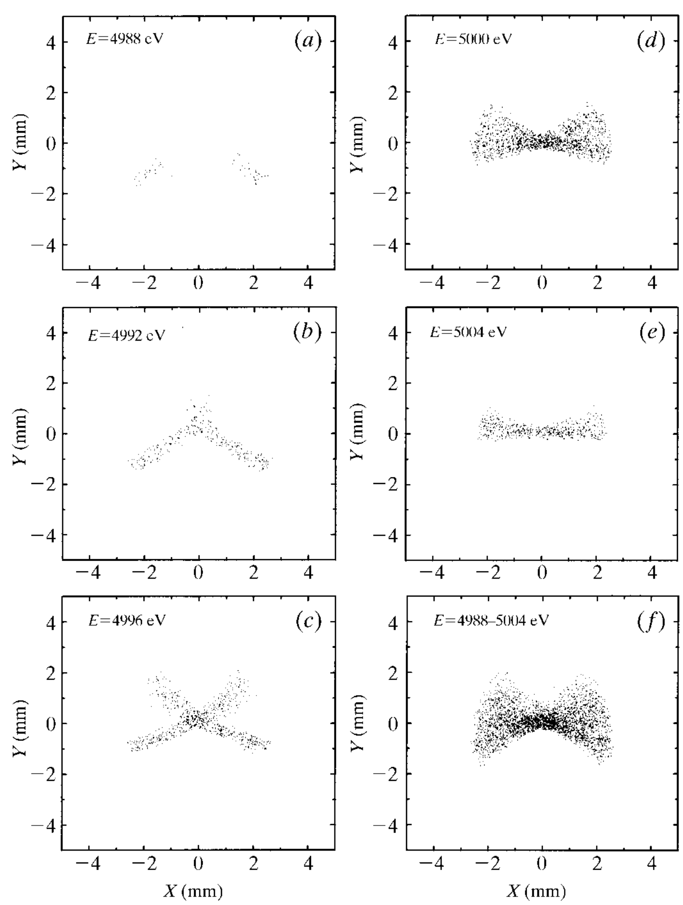

Figure 2
Spot diagram on the observation plane of the X-ray optical system consisting of a pre-focusing toroidal mirror (platinum-coated) and a couple of the plane Si(111) crystals, the bending-magnet source in the storage ring at Ritsumeikan University being assumed. (*a*)–(*e*) are the diagrams for slightly different X-ray energies. (*f*) is the diagram in which the contributions from the rays of different energies are added.

curvature of 39 mm and 528 m, and the monochromator is a plane Si(111) crystal. Fig. 5 shows the cross-sectional images of the radiation beam, recorded using photo-sensing paper, at the sample position for rays of different energies. Agreement is generally good.

For beamline BL-10 (Handa *et al.*, 1999), the ray-propagation diagram was constructed in order to find the most effective surface area of the mirror and the results were used to determine the optimum sizes of the entrance slit for the mirror.

RIGTRACE was also used for designing the total reflection X-ray fluorescence system on the laboratory X-ray source. The system consists of a couple of the W/C multilayers, and the $L\beta_1$ radiation (9670 eV) from the tungsten target is used as an excitation radiation. The X-ray reflectivity of the multilayer was calculated using the method proposed by Underwood & Barbee (1981). An optimum condition for eliminating contamination in the spectrum by the $L\alpha$ radiation could be found by adjusting the setting parameters and observing the results of the ray-tracing simulation (Yamada *et al.*, 1999).

Access to the program can be made by visiting the web site http://www.rigaku.co.jp/xrl/xrf/. One may be asked to provide information on the type of source and optical elements with appropriate parameters. The calculation is made by the authors and the results are sent *via* the internet or by other means, *e.g.* by fax.

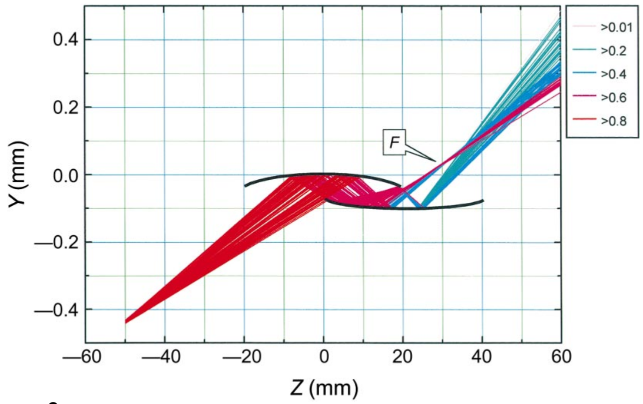

Figure 3
Side view of the ray-propagation diagram for the X-ray optical system consisting of a couple of the closely spaced cylindrical W/C multilayers on the laboratory X-ray source. The X-ray energy is 5000 eV.

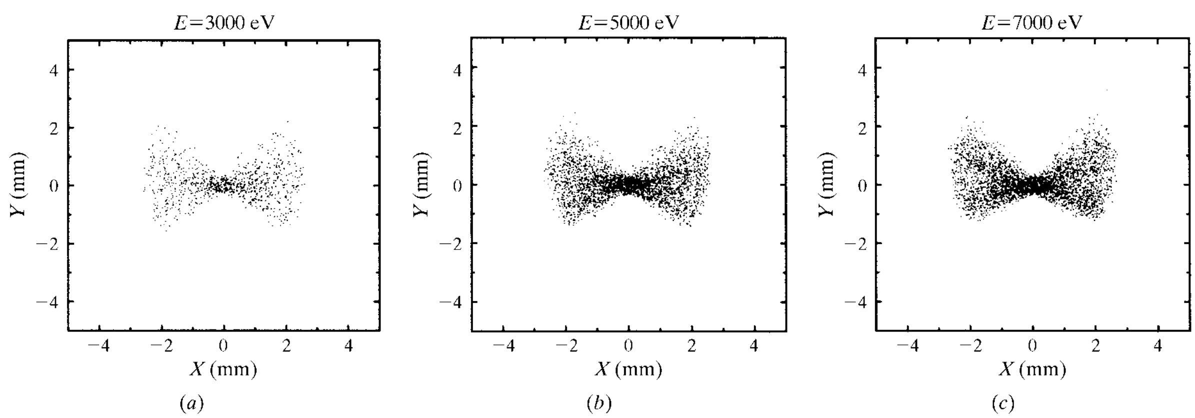

Figure 4
Spot diagram on the observation plane of the X-ray beamline BL-3 at Ritsumeikan University consisting of a pre-focusing toroidal mirror (platinum-coated) and a couple of the plane Si(111) crystals. The principal energy of the X-rays is (*a*) 3000 eV, (*b*) 5000 eV and (*c*) 7000 eV.

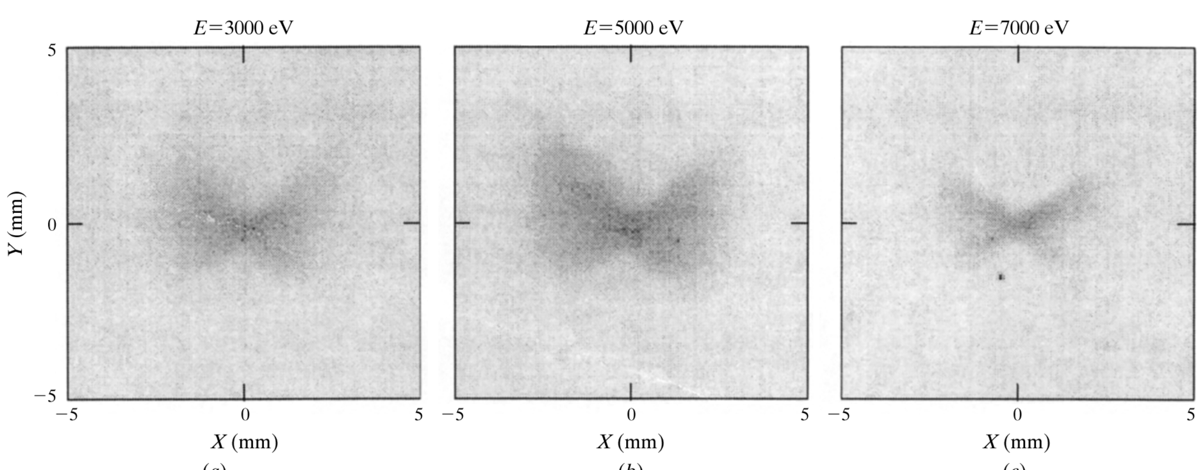

Figure 5
Cross-sectional images of the radiation beam on the observation plane of beamline BL-3 recorded on photo-sensing paper. The principal energies of the X-rays correspond to those in Fig. 4.

References

Handa, K., Sakai, I., Izuhara, O., Iwasaki, H., Yoshimura, Y., Masui, S. & Murata, T. (1999). *Jpn. J. Appl. Phys. Suppl.* **38**(1), 654–657.

Iwasaki, H., Nakayama, Y., Ozutsumi, K., Yamamoto, Y., Tokunaga, Y., Saisho, H., Matsubara, T. & Ikeda, S. (1998). *J. Synchrotron Rad.* **5**, 1162–1165.

James, R. W. (1958). *The Optical Principles of the Diffraction of X-rays*, p. 34. London: G. Bell and Sons.

Lai, B. & Cerrina, F. (1986). *Nucl. Instrum. Methods*, A**246**, 337–341.

Lai, B., Chapman, K. & Cerrina, F. (1988). *Nucl. Instrum. Methods*, A**266**, 544–549.

Saisho, H. (2000). *Mem. SR Cent. Ritsumeikan Univ.* **2**, 141.

Underwood, J. H. & Barbee, T. W. Jr (1981). *Low Energy X-ray Diagnostics-1981*, p. 170. New York: American Institute of Physics.

Yamada, T., Nisawa, A., Shoji, T. & Utaka, T. (1999). *J. Surf. Anal.* **5**, 124–127.

 Received 9 November 2000 • Accepted 9 February 2001