A comment on 'A new ray-tracing program *RIGTRACE* for X-ray optical systems' [*J. Synchrotron Rad.* (2001), 8, 1047–1050]

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Some points concerning the characteristics of the X-ray simulation code *SHADOW* [Welnak *et al.* (1994). *Nucl. Instrum. Methods*, A**347**, 344–347] are clarified which are not correctly mentioned by Yamada *et al.* [*J. Synchrotron Rad.* (2001), **8**, 1047–1050]. It is shown that, contrary to the authors' statement, some functionality of their new program is not original. In particular, we show that *SHADOW* can deal correctly with crystal monochromators.

Keywords: ray-tracing; X-ray optics.

1. Introduction

The unique characteristics of the X-ray *RIGTRACE* program, as stated by Yamada *et al.* (2001), are the following: (i) consecutive tracing of the rays from one optical element (OE) to the other, thus keeping one-to-one correspondence between the OEs; (ii) use of the Darwin–Prins theory, thus taking into account the different weight of rays having slightly different energy and angle; (iii) rays are traced for elements which are close to each other, thus allowing the simulation of compact laboratory instruments. We will show that these characteristics are not exclusive to the *RIGTRACE* program or that they are not pointedly different from those of existing programs such as *SHADOW*.

2. *SHADOW*: bending-magnet source, consecutive tracing of rays and crystal diffraction

The first step in simulating an optical device with a ray-tracing code is the generation of the source. *SHADOW* includes models for synchrotron [bending magnet (BM), wiggler and undulators] and geometric sources, where the shape and divergence are modeled using a given distribution (box, Gaussian *etc.*). A detailed discussion of *SHADOW*'s source models can be found by Cerrina (1989). Concerning the implementation of the BM source, its geometrical shape is calculated using the characteristics of the electron beam (sizes and divergences), its trajectory (an arc of a circle), as well as the natural divergence of the emitted photons. The resulting divergence has a more or less flat distribution in the horizontal (when considering that the trajectory arc is much larger than the horizontal divergence of the electrons), and it is approximately Gaussian in the vertical in the case when the photon emission has wavelengths of the order or less than the critical energy. Therefore, contrary to the authors' words, *SHADOW* does not use a "Gaussian-type distribution of the source points and ray directions". Moreover, the authors do not specify how *RIGTRACE* calculates the spectra of BM and X-ray tubes sources.

In *SHADOW*, each optical element (OE) can be placed in any desired position downstream of the previous one. All rays are traced sequentially from one OE to the following one. The rays are dumped into files at the screen and OE positions. The rays are numbered and all their related quantities (electric field components, energy, weight and others) are preserved during propagation from one OE to the other. In other words, the files mentioned above contain all the necessary information about every ray. Up to ten screens, with or without apertures, can be traced for each OE. By defining additional screens, the beam properties can be analysed at any desired position of the instrument. This means that (*a*) the beam physical quantities calculated by *SHADOW* can be viewed using the graphical utilities implemented in the program, and (*b*) the history of each ray is known so that a ray-propagation diagram is possible, as implemented in the program *BLViewer* (Sanchez del Rio, 2001).

The use of the Darwin–Prins formula for the reflectivity of a perfect crystal monochromator cannot be considered as a 'unique method of implementation', as stated in point (ii) of §1. There is only minimal difference in the diffraction profile obtained using the Darwin–Prins formalism when compared with the more frequently used Ewald formula (Zachariasen, 1945; Pinsker, 1978). 'Weighting' the rays impinging on the crystal monochromator according to their energy and deviation from the nominal Bragg position is a very commonly used method in ray-tracing. In *SHADOW* we used the formalism described by Zachariasen (1945). An important technical detail to be considered is the correct choice of the variable related to the deviation of the incident ray with respect to the Bragg angle. The non-approximated formula [see equation (3.114*b*) on p. 118 of Zachariasen (1945)] should be used instead of the most commonly employed approximated formula in equation (3.116), in order to be able to simulate some important cases for synchrotron radiation monochromators, like the normal-incidence and inclined monochromators.

3. Examples

In Fig. 1 we report the *SHADOW* results for a system similar to that used in §4 of Yamada *et al.* (2001). A BM source using 3.8 T magnets placed in a 575 MeV storage ring emits rays in the energy range 4990–5015 eV. The beam, after passing through a slit, impinges on a toroidal mirror with an average grazing angle of 0.573°. The mirror is placed at P = 450 cm downstream from the source and focuses the beam at Q = 450 cm (magnification = 1). An Si(111) double-crystal monochromator is placed 150 cm away from the mirror. In addition to the intensity map at the image plane, we show that, contrary to the authors' statement, the contribution of the monochromatic components to the focal intensity can be calculated using *SHADOW*.

In *SHADOW* the ray distribution can be observed as a scatter, contour or histogram plot as a function of position, direction cosines, electric field components, energy, lost ray flag and others. In the case of the contour or histogram plots the ray distribution can be weighted by the ray probability. This is an important point because the ray distribution, usually represented in the scatter plot, does not correspond to the intensity distribution that is obtained by weighting the rays and is viewed as a contour plot. This is particularly evident in the dispersive set-ups, *i.e.* in Laue or asymmetric Bragg geometry.

In conclusion, we have clarified some points regarding the ray-tracing code *SHADOW*. In particular, we have shown that *SHADOW* is able to compute crystal monochromators at the same level of accuracy as *RIGTRACE*. Other aspects, like the simulation of

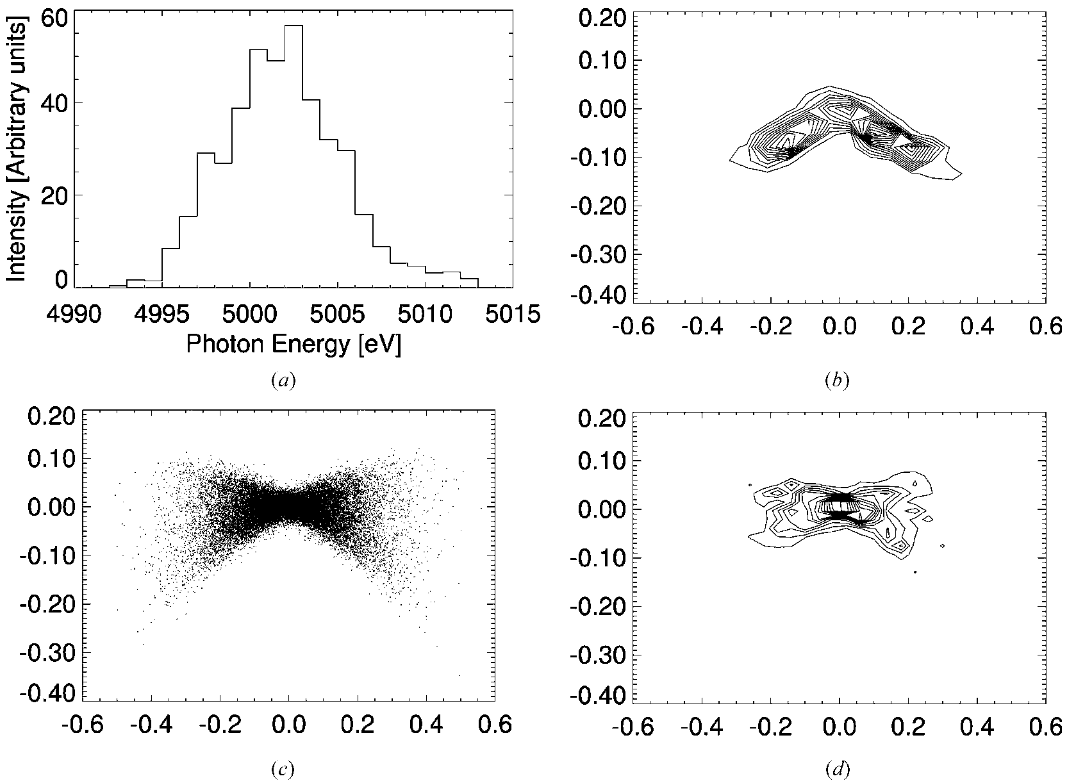

Figure 1
(*a*) Intensity distribution *versus* photon energy. The width of this histogram gives the energy bandpass of the simulated beamline, consisting of a toroidal mirror and a double-crystal monochromator. (*b*) Intensity distribution of a monochromatic component (E = 5008 eV) at the image plane. A monochromatic source has been used to create this plot. (*c*) Ray distribution at the image plane. The source contains rays in the energy interval 4990–5015 eV. (*d*) Intensity distribution at the image plane. This plot has been calculated by weighting the rays shown in (*c*) with their intensity after being diffracted by the double-crystal monochromator. Plots units are cm [except for in (*a*)].

compact instruments, full beamline visualization *etc*., can also be addressed using *SHADOW*.

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