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A Comparison of Three Different Ray Trace Programs for X-ray and Infrared Synchrotron Beamline Designs

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Abstract

There are a number of ray trace programs currently used for the design of synchrotron beamlines. While several of these programs have been written and used mostly within the programmer's institution, many have also been available to the general public. This paper discusses three such programs. One is a commercial product oriented for the general optical designer (not specifically for synchrotron beamlines). One is designed for synchrotron beamlines and is free with restricted availability. Finally, one is designed for synchrotron beamlines and is used primarily in one institution.

The wealth of information from general optical materials and components catalogs is readily available in the commercial program for general optical designs. This makes the design of an infrared beamline easier from the standpoint of component selection. However, this program is not easily configured for synchrotron beamline designs, particularly for a bending magnet source. The synchrotron ray trace programs offer a variety of sources, but generally are not as easy to use from the standpoint of the user interface. This paper shows ray traces of the same beamline using Optikwerks, SHADOW, and RAY, and compares the results.

Introduction

In the past many commercial raytrace programs were not able to model the unconventional light sources found in synchrotrons. Also, grazing incidence configurations and reflection gratings were not able to be modeled without producing inaccurate results. Thus synchrotron beamline designers created their own programs which, over the years, have become quite sophisticated in the variety of sources and beamline components that they can model.

With the advance of personal computers many commercial raytrace programs have also become more sophisticated. Can they now model synchrotron beamlines? The answer to this is "yes", to a degree. This is demonstrated with Optikwerks, which was chosen because of its cost and ease of use. Other commercial programs may be comparable in ability; this depends largely on the cost of the program.

A typical soft X-ray beamline is used for raytracing on three programs: RAY¹ (developed at BESSY, Berlin, Germany), SHADOW² (developed at CXrL, University of Wisconsin), and Optikwerks³ (a commercial program from Optikwerk, Inc.). The beamline PM5 at BESSY was chosen because it uses separate components for decoupled horizontal and vertical beam shaping and photon energy dispersion. The same basic design is used on all three programs, with two

parameters being changed (to give a matrix of four combinations) in the same way for all three programs. Then an infrared beamline is raytraced for SHADOW and Optikwerks. The authors show how the raytrace programs compare in predicting illumination in the output plane. Ease of entering design parameters is briefly discussed.

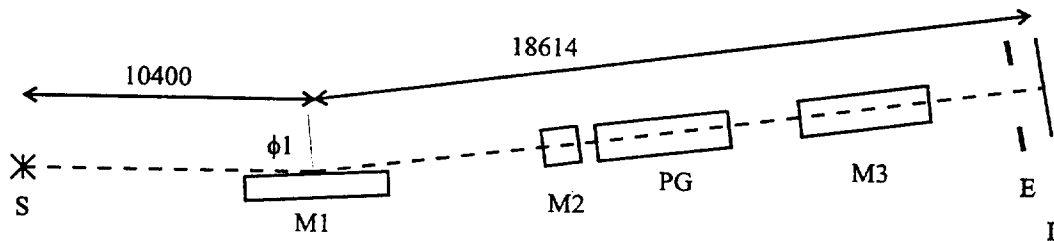
The PM5 beamline at BESSY

The BESSY PM5 beamline (Petersen monochromator beamline nr. 5) operates between 20 and 2000 eV. The design, whose schematic is shown in Figure 1, is straightforward, using the least number of components to get reasonable spectral resolution with small aberrations. Synchrotron light comes from a bending magnet and has the characteristics shown in Table 1. The first component, mirror M1 with radius of curvature 263000 mm, horizontally deflects and focuses the beam at the output plane I, which is at the experimental station. Thus M1's tangential dimension determines the system horizontal divergence. This is the only horizontal action in the system. M2 is a plane mirror. The position and angle of M2 are determined so that the dispersed beam coming out of the grating PG has its axis parallel to the input beam from source S. The plane grating PG has straight grooves at 1200 grooves/mm. Mirror M3 focuses the beam onto the exit slit E. The plane grating PG has straight grooves at 1200 grooves/mm. Mirror M3 focuses the beam onto the exit slit E.

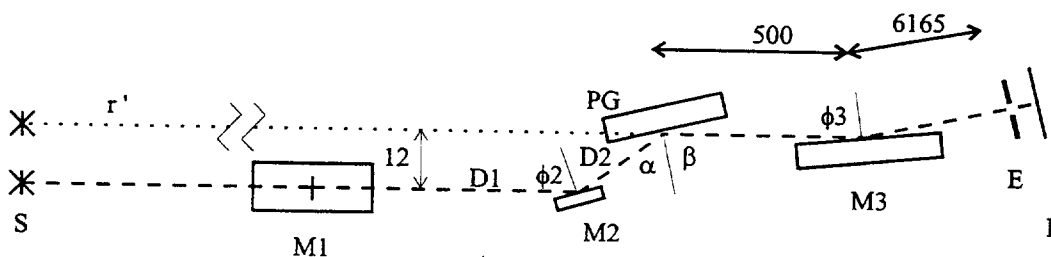
Distances D1 and D2 and angle ϕ_2 depend on the configuration value c_{ff} . The parameter c_{ff} is physically related to the ratio of cross sectional width of the beam leaving the grating to the cross sectional width of the beam going into the grating, and this is related to the demagnification of the source size by the grating. It is defined as

$$c_{ff}^2 = r'/r \tag{1}$$

where r is the real source distance (S to PG), and r' is the virtual source distance. The system layout is affected by c_{ff} as a



(a) Horizontal plane (top view)



(b) Vertical plane (side view)

Figure 1. PM5 beamline layout. All distances are in mm. Incidence angles ϕ_1 and ϕ_3 are each 88 degrees.

change in the position and angle of plane mirror M2, which changes the real source distance a small amount; but this changes the virtual source distance very much. As a result, the input angle α of the grating is quite different for the two configurations for a given photon energy. The quantities shown in Figure 1 that change with c_{ff} are given in Table 2.

Electron energy	0.8 GeV
Bending radius	1779 mm
Horizontal emittance	5 e-8 π m rad
Vertical emittance	2 e-9 π m rad
Horizontal divergence	4 e-3 rad
Central photon energy	400 eV
Other photon energies	399.5, 400.5 eV (for dispersion analysis)

Table 1. Source and immediate system characteristics for the PM5 beamline.

	<u>$c_{ff} = 1.2$</u>	<u>$c_{ff} = 12.0$</u>
Virtual distance r'	18500 mm	1800500 mm
Distance D1	2059.13 mm	1972.43 mm
Incident angle ϕ_2	81.8187 deg	87.3131 deg
Distance D2	42.596 mm	128.132 mm
Grating incident angle α	82.5675 deg	89.5871 deg
Grating diffracted angle β	81.0699 deg	85.0395 deg
M3's radius of curvature R3	265000 mm	352095 mm

Table 2. Quantities that change with c_{ff} .

The two parameters that are changed to give a matrix of four raytrace results are the configuration value c_{ff} and the root-mean-square slope variation v_{rms} of M3. These are listed in Table 3.

	<u>$v_{rms} = 0.235$ arcsec</u>	<u>$v_{rms} = 0.705$ arcsec</u>
<u>$c_{ff} = 1.2$</u>	Case A	Case B
<u>$c_{ff} = 12.0$</u>	Case C	Case D

Table 3. Parameters that are adjusted to give four raytrace results.

Figures 2 through 13 below allow the designer to subjectively determine spatial and spectral distributions. A histogram of the ray intercepts in the output plane in the dispersion dimension is often helpful, because the spectral resolution of the monochromator can be determined quantitatively. Figure 14 gives an example of SHADOW and RAY histogram outputs which correspond to Case B above. It is possible to get a histogram from Optikwerks also, but not without considerable additional effort.

Case A: $c_{ff} = 1.2$, $v_{rms} = 0.235$ arcsec

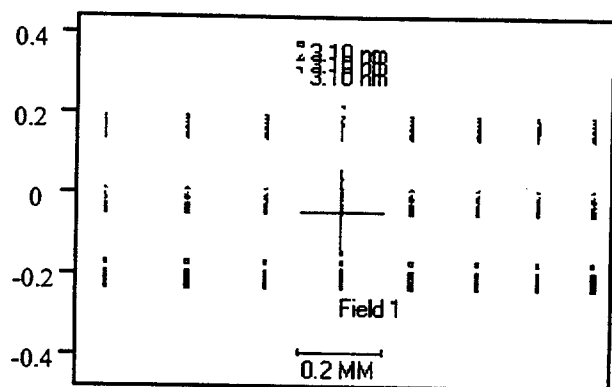


Figure 2.

Output plane spot diagram from Optikwerks

Case B: $c_{ff} = 1.2$, $v_{rms} = 0.705$ arcsec

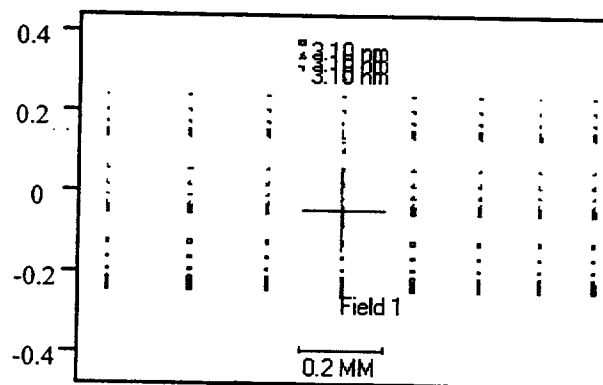


Figure 5.

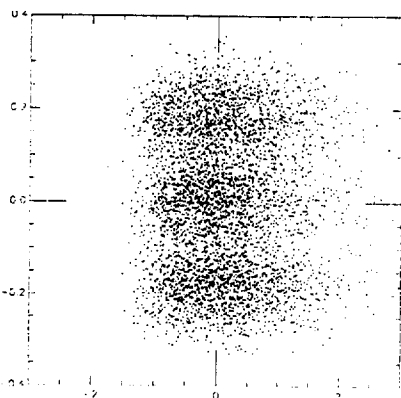


Figure 3.

Output plane spot diagram from SHADOW

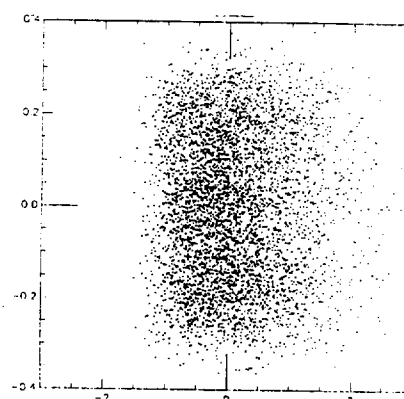


Figure 6.

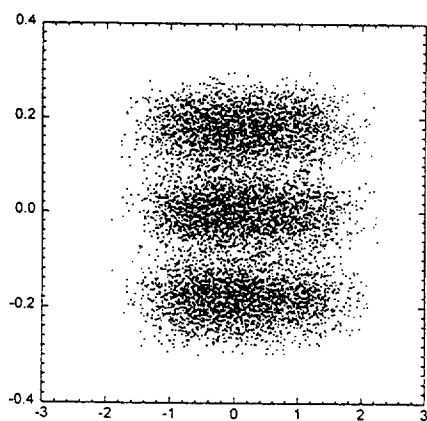


Figure 4.

Output plane spot diagram from RAY

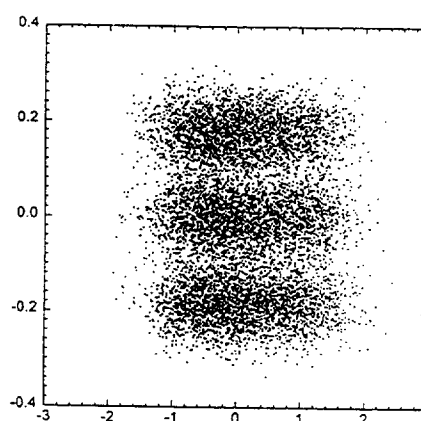


Figure 7.

Case C: $c_{ff} = 12.0$, $v_{rms} = 0.235$ arcsec

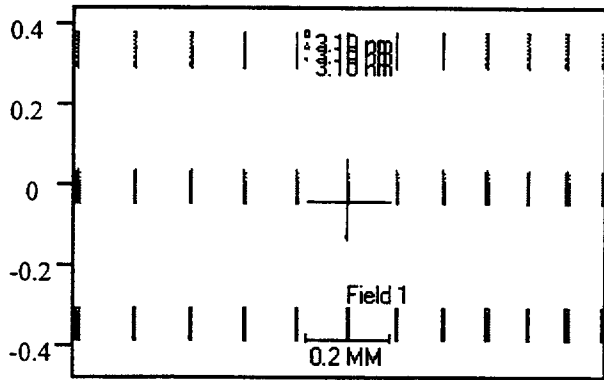


Figure 8. Output plane spot diagram from Optikwerks

Case D: $c_{ff} = 12.0$, $v_{rms} = 0.705$ arcsec

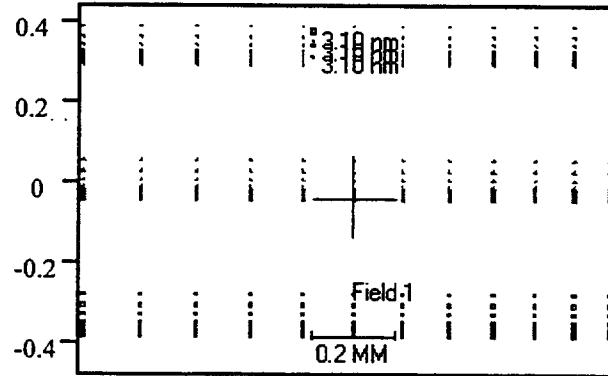


Figure 11.

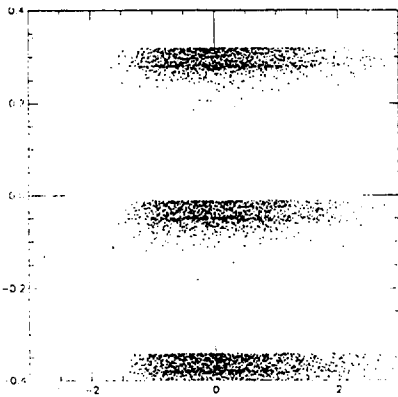


Figure 9. Output plane spot diagram from SHADOW

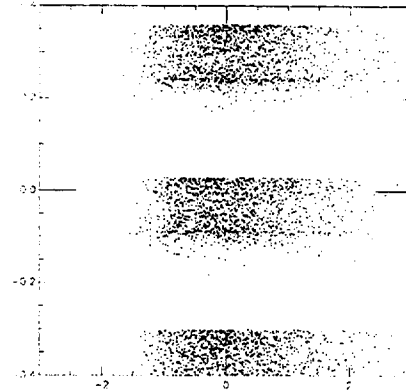


Figure 12.

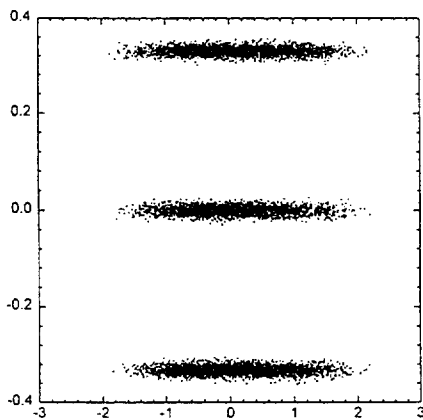


Figure 10. Output plane spot diagram from RAY

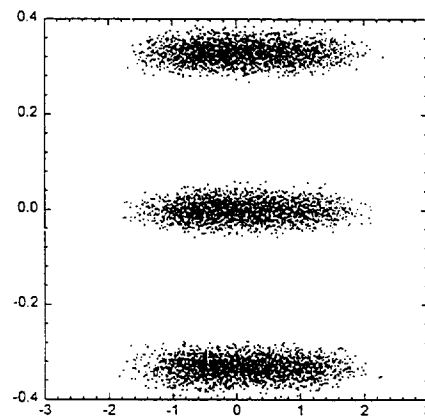


Figure 13.

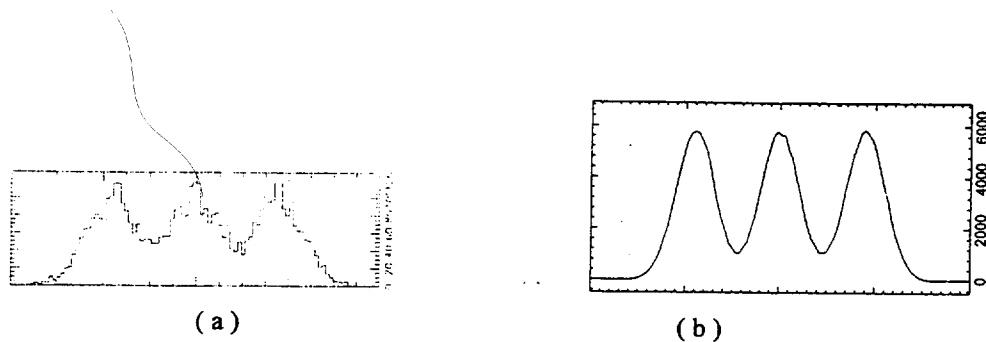


Figure 14. Histogram of spots in the dispersion dimension for (a) SHADOW (corresponding to Figure 3) and (b) RAY (corresponding to Figure 4).

PM5 raytrace results

Spot diagrams are not the only form of analysis a designer should use. Optikwerks provides paraxial analysis which is helpful in roughing in a system design and ray fan diagrams which are more useful for systems that have smaller $f/\text{numbers}$. Spot diagrams are given here because this compact form of data is easily displayed in a review paper, and it is one of the first results that a designer looks for.

Some characteristics of Optikwerks make it easy and quick for entering optical component data. While SHADOW requires only one floating point number for characterizing the surface figure error as a sinusoid, Optikwerks requires three such numbers. In Optikwerks these numbers are coefficients of a polynomial that must be externally calculated in order to represent a sinusoidal figure error. Once these numbers have been calculated, it is easy to change them in Optikwerks: it requires six keystrokes and mouse clicks plus 9 or 10 keystrokes for each floating point number, totaling 32 hits to change the figure error and see the resulting spot diagram. In SHADOW (UNIX version 2.1), however, it takes over 100 keystrokes to make the change for figure error and see the plotted results. RAY requires about 50 keystrokes for changing a single number which represents a gaussian distribution.

As seen in Figures 9 and 12, the sinusoidal figure error gives a characteristic structure to the spot diagram. A gaussian figure error may be used in SHADOW, but with considerable additional effort. Unless the form of the figure error is actually known, it is arbitrary whether a gaussian or sinusoidal error is selected. In SHADOW either a grid (various shapes) of rays or a random set of rays may be generated at the source and traced through the system. Optikwerks generates a square grid of rays, but a random set of rays may be generated with considerable additional effort. The effect of figure error agrees well among the three programs for $c_{ff} = 1.2$, but for $c_{ff} = 12.0$ Optikwerks shows some discrepancy. RAY and SHADOW have no problem modeling a beam with very little vertical divergence. However, Optikwerks requires a minimum vertical divergence when tracing rays through a component that contains figure error. The extreme grazing condition for $c_{ff} = 12.0$ and reduction of the vertical divergence of the source beam causes some of the rays to not be displayed in Figure 11.

Of greater importance is the spatial and spectral placement of the spots in the output plane. If RAY is used as a standard for comparison (because it agrees well with experimental observation), then there is good agreement among all three programs on the effect of spectral dispersion. That is, the histogram peaks are spaced 0.2 mm for $c_{ff} = 1.2$ and spaced 0.3 mm for $c_{ff} = 12.0$ in all three programs. Optikwerks outputs (Figures 2, 5, 8, and 11 above) give a line length of 3 mm, but the above figures have been truncated in order to show the dispersion dimension clearly. (The designer cannot set scaling for individual axes in Optikwerks.) The sparseness of spots (from scaling) in a square grid is responsible for the large difference in appearance of spot diagrams between Optikwerks and the other programs. Optikwerks does, however, indicate the wavelength of each spot.

Many commercially available raytrace programs are integrated with a computer aided design feature that allows mechanical placement of components to be determined while optical performance is evaluated. Optikwerks also has this feature which quickly gives a system drawing. An area of interest may be readily magnified for detailed examination. SHADOW can give two-dimensional or three-dimensional system drawings, but with considerable effort.

The infrared beamline BL 1.4 at the ALS

The ALS BL 1.4 is an infrared beamline that operates with wavelengths from 2 to 30 μm . A bending magnet is the light source, whose characteristics are given in Table 4. Figure 15 gives a layout of this beamline, which is complicated by reflections in three dimensions. M1 is a flat mirror which directs the light upward. M2 is an ellipsoidal mirror which collects the light and focuses it at point E which is the entrance to the Mirror Box.

Bending radius	4.81 m
Electron energy	1.9 GeV
Horizontal emittance	6.4 e-9 m rad
Vertical emittance	6.0 e-11 m rad
Horizontal divergence	0.040 rad
Vertical divergence	0.010 rad

Table 4. Source and immediate system characteristics for BL 1.4.

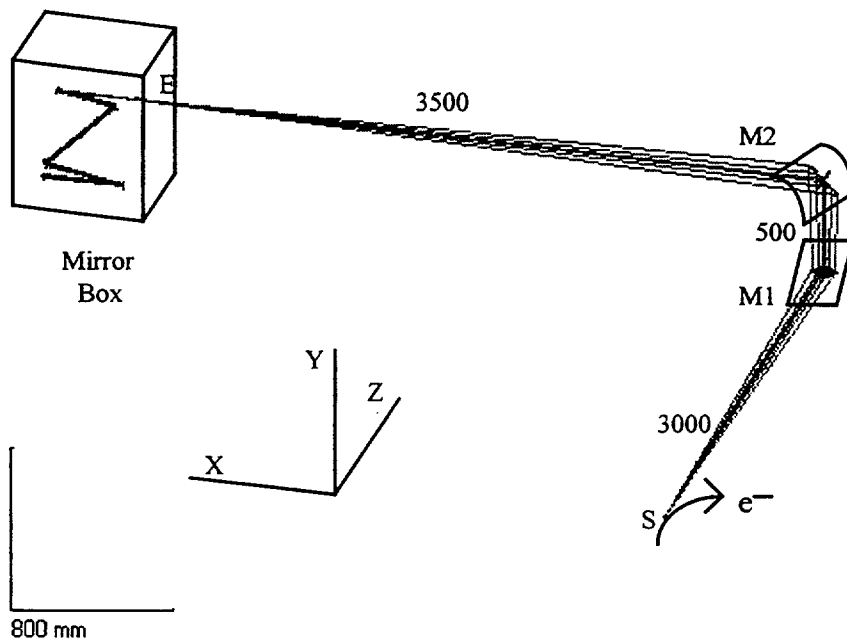


Figure 15. Layout of the BL 1.4 infrared beamline. Distances are in mm. Incidence angles for M1 and M2 are each 45 degrees.

Details of the Mirror Box are shown in Figure 16. In Figure 16, the light is collimated by cylinder mirrors M3 ($R3 = 803.056 \text{ mm}$) and M6 ($R6 = 3200 \text{ mm}$ in the opposite meridian as R3), and plane mirrors M4 and M5. Light emerges from M6 as a collimated beam and illuminates the output plane I with a square of light measuring about 15 mm X 15 mm. The spot diagrams of the output plane for a point source at S are shown in Figure 17. When a bending magnet with the characteristics in Table 4 is modeled for the source at S by SHADOW, the illumination in the output plane is a little different, as is seen in Figure 18. RAY gives a raytrace result that resembles the SHADOW raytrace in Figure 18.

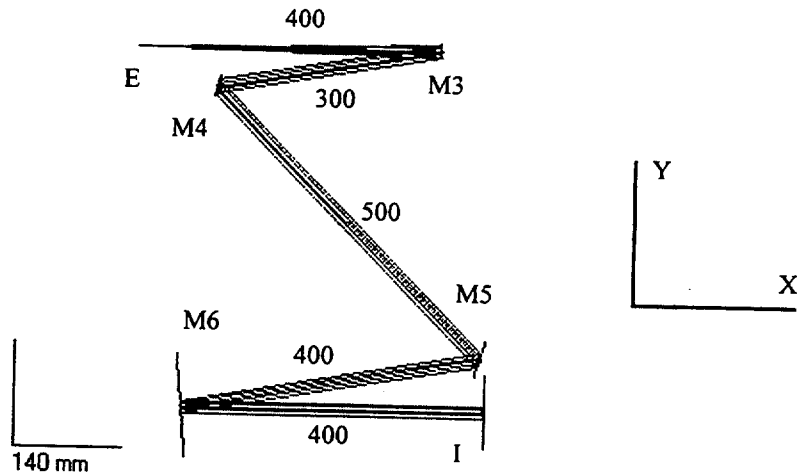


Figure 16. Details of the Mirror Box. Distances are in mm. Incidence angles for M3 and M6 are each 5 degrees. Incidence angles for M4 and M5 are each 27.5 degrees.

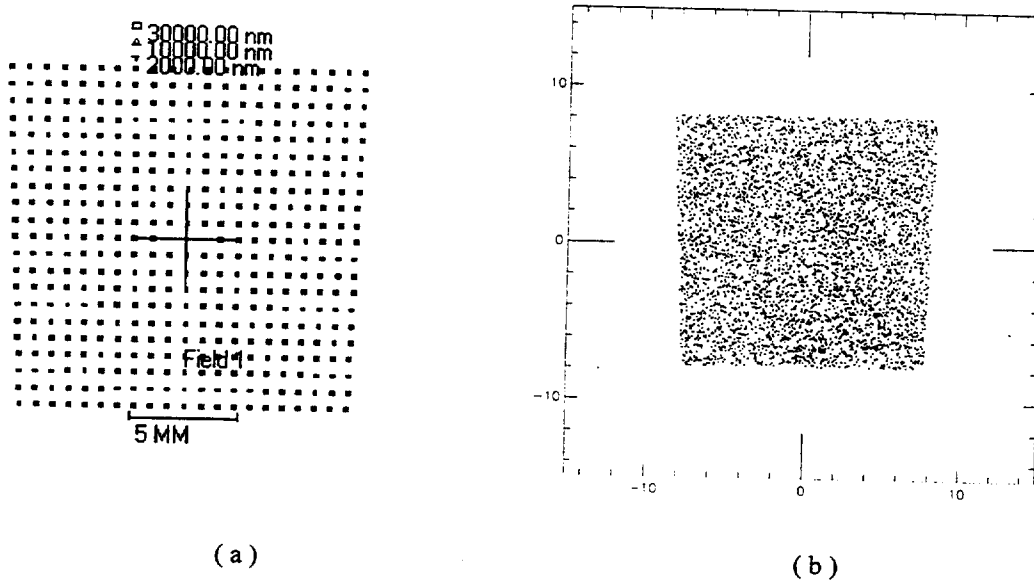


Figure 17. Spot diagrams of the output plane from (a) Optikwerk and (b) SHADOW.

BL 1.4 raytrace results

The ALS infrared beamline is easily modeled by both SHADOW and Optikwerks, except that Optikwerks could not model the bending magnet. In Optikwerks M2 was modeled as a toroidal surface with an oblate spheroid (ellipse) in one meridian and a circle in the other meridian. The spot diagrams show good agreement between Optikwerks and SHADOW when a point source is assumed. However, the finite source size, gaussian angular distribution, and changing ray angle with source depth of a bending magnet does produce a slightly different illumination.

Optikwerks has an extended source which consists of several planes within a chosen volume. The intensity of each of the pixels that make up each plane may be adjusted to represent a gaussian spatial distribution, but the principle

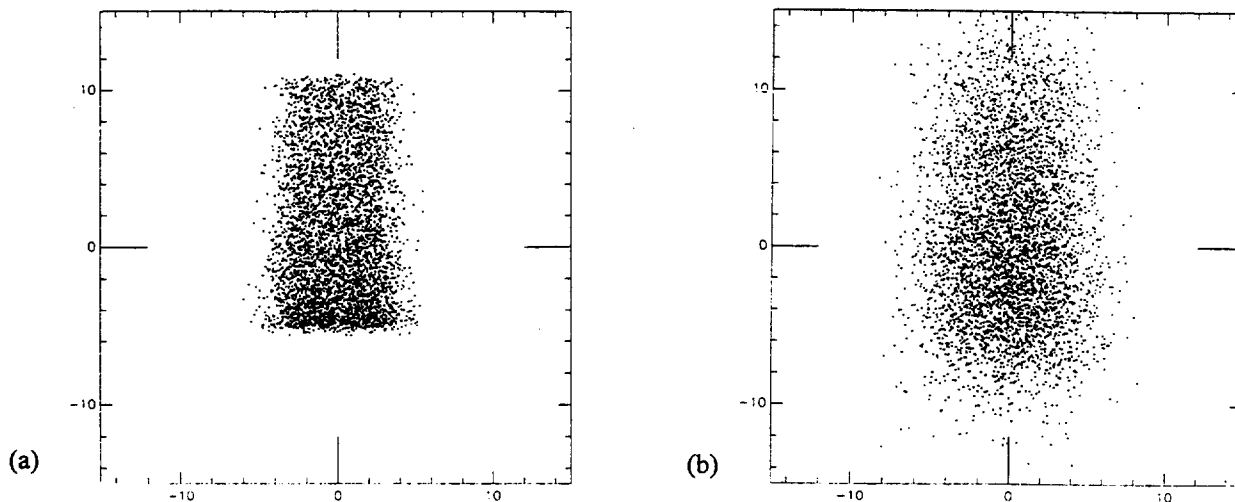


Figure 18. Illumination in the BL 1.4 output plane using a bending magnet source in SHADOW;
 (a) using the source parameters given in Table 4;
 (b) using an increased source size from an external diffraction calculation for $\lambda = 10 \mu\text{m}$.

propagation angle from each plane may not be individually adjusted. Thus the emission of rays at different angles along the bending magnet arc cannot be represented. The extended source may, however, model an undulator or a wiggler whose angular distribution of rays is approximately constant along the depth of the source.

The components in the Mirror Box took about one third the time for data entry in Optikwerks compared to SHADOW. The system diagram quickly shows the designer obvious errors in the optical system. The ellipsoid, however, took longer to model.

Conclusion

This short review of three raytrace programs primarily shows output of the programs. The different appearance of Optikwerks outputs are due partly from the fact that only square arrays of spot diagrams were displayed, but also because RAY is run on a VMS computer and SHADOW is run on a UNIX computer. Programs written for these platforms usually expect a higher resolution display than programs written for a Windows platform.

RAY and SHADOW give similar results for the PMS X-ray beamline. To first order, Optikwerks models the X-ray beamline well, including the reflection grating; using a point source for this beamline does not make a significant difference in the output plane illumination. However, in Optikwerks some rays have trouble getting through the system in the more extreme grazing configuration. In the infrared beamline design, Optikwerks models the system well for a point source, but cannot model a bending magnet source. Even with SHADOW, external calculations had to be made for determining the increased source size as a result of diffraction.

Bias is inherent in the comparison of these raytrace programs. The program that was used to design the optical system in the first place has the advantage that the designer used whatever features were available in order to get a good design. Recreating this design on a second program will expose the limitations of the second program. The X-ray beamline was designed using RAY, and the infrared beamline was designed using SHADOW. A fairer test would be to give the end requirements of a beamline to separate designers using each of the three programs.

In many cases the data entry for components in one program could have been selected so that the spot diagram would look more like that of another program. If doing this would have required a long, complicated data entry, however, an approximation was made. In the case of the X-ray beamline, a sinusoidal surface figure error was used in Optikwerks and

SHADOW instead of a gaussian surface figure error as in RAY. In the case of the infrared beamline, a toroidal ellipse-circle was used in Optikwerks instead of an ellipsoid.

A good feature of Optikwerks is that the system drawing and spot diagram are given immediately after the component icons are set up. These drawings and diagrams are compatible with Microsoft™ Object Linking and Embedding (OLE), so that they may be cut and pasted into other documents. In fact, Figures 2, 5, 8, 11, 15, 16, and 17 are Optikwerks objects. Figures 15 and 16 were then further embellished with lines and text.

Ease of use is not easily shown here. Entering the infrared beamline data for SHADOW took considerably longer as entering the data for Optikwerks. Learning to use RAY or SHADOW at the beginning takes several days to several weeks for most people who would design a system like the X-ray beamline shown here. Learning to use Optikwerks takes minutes. Typically one can start designing a system right away without using the "help" feature. One can see here the tradeoff between "user friendliness" and versatility.

These programs are constantly being improved. SHADOW can be downloaded from the CXrL Website (by employees of non-private organizations) for several platforms and includes a graphical user interface (GUI) for Windows 95 (although the GUI currently only reflects the same input/output of a UNIX system). RAY is available for a VMS platform, and continues to be improved. Optikwerks continues to add features and improve the operation based on customer response. Many such raytrace programs are available, and the authors do not endorse any particular program.

Acknowledgments

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