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RAYTRACING EVALUATION OF A TOROIDAL MIRROR FOR WIGGLER STATION 9.5

by

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1. INTRODUCTION

This note outlines the performance of a toroidal mirror as the sole focusing element of a Protein Crystallography (PX) station. The mirror is intended to be used in two ways. These are, firstly, to focus the white synchrotron radiation beam (point focused Laue mode) and, secondly, to focus a beam already monochromated by a double crystal (point focused tuneable monochromatic mode). In the latter case, the advantage of the toroid is that the focusing and monochromatising functions are separated allowing the use of a tuneable monochromator for anomalous dispersion.

In Laue mode, a shallow grazing angle is needed to restrict the power absorbed by the mirror from the wiggler beam at wavelengths shorter than the critical wavelength. In monochromatic mode, the mirror will be placed as the second optical element after the monochromator thus relaxing the power restriction.

It should be noted that (in the absence of a toroidal mirror), a beam from the wiggler of divergence 0.2 mrad × 1 mrad would give a cross section 30 m from the source of 6.4 mm × 32.0 mm compared with a sample of typically 0.25 mm × 0.25 mm (a mismatch of 3277). This is similar to the situation on 9.6 and 9.7 where (in Laue mode on both stations, and with the channel cut monochromator on 9.6) only a small portion of the beam is actually used.

Fortunately the small source size of the SRS high brightness lattice (HBL) means that a large focusing ratio is not required. This is in direct contrast to the pre-HBL horizontal source size, which demanded a 10:1 demagnification achieved on 7.2 and 9.6 by a curved assymmetrically cut crystal monochromator. Hence, for the first time, because of the SRS HBL, the use of = 1.1 imaging of the source (in both directions) is feasible for PX, and allows this role to be filled entirely by the toroidal mirror.

2. RAYTRACING

The raytracing was performed using the package compiled by D. Hubbard and E. Pantos$^{(1)}$.

The condition for minimum aberration from a toroid is given by:-

$$\frac{1}{u} + \frac{1}{v} = \frac{2}{(R_h \sin\phi)}$$

$$\frac{1}{u} + \frac{1}{v} = \frac{2 \sin\phi}{R_v}$$

where R_h = horizontal curvature of mirror (fixed)
R_v = vertical curvature (variable via bending mechanism)
ϕ = grazing angle
u and v are the object and image distances

The vertical acceptance of the mirror is the angle subtended by the projection of the mirror's tilt minus the vertical size of the source.

The horizontal acceptance of the mirror is limited by the sagittal curvature.

A complication of the wiggler is that two sources of radiation are visible from 9.5 (and 9.6, 9.7): one from the main bump of the electron beam, and the other from the deflection bump which restores the electron beam to its original orbit. These sources would, for the HBL, be well resolved. In PX this is not a worry since the focused beam is finely collimated before striking the sample. In the raytracing study, we consider only the focusing effect of the toroid on the main wiggler source (λ_c = 0.9 Å) onto the protein crystal sample.

3. MIRROR PERFORMANCE AND RESULTS OF THE TRACING RUNS

A typical trace is given in fig. 1. Traces were performed for a grazing angle of 3 mrad.

In order to get a picture of the relative efficiency of the various mirror settings, a figure of merit F is quoted with each result, where:

F = Fraction of successful rays × effective collection area
÷ beam focus area. (See for example, ref. 3.)

The fraction of successful rays is produced by the program output, as are the beam sizes (fig. 3). The figure for successful rays is produced by counting the number of source rays which miss the mirror or do not come to a focus. The former rays should be eliminated by careful choice of beam divergences, but this condition is only approximately met in the results due to rounding errors in the ray tracing program. To check the divergences used, the source was traced for a simple plane mirror, where no failed rays due to surface curvature are expected.

The effective collection area of a mirror:-

$$A_{eff} = A \times R(\lambda)$$

where A is the projected area of illumination at the source on the mirror. The R(λ) (the mirror reflectivities) are calculated using the expressions mentioned below.

For an ideal mirror with $\theta = 3$ mrad, $u = 18$ m, $v = 12$ m (1.5:1 focusing) and $R(\lambda) = 1$, $A_{eff} = 61.92\ \mathrm{mm}^2$ and image area = $0.356\ \mathrm{mm}^2$ ($F_{ideal} = 173.9$). The 1.5:1 focusing ratio and 18 m object distance were chosen because of available space in beam line 9, being the closest possible to 1:1.

The F's quoted in Table 1 are normalised to the ideal values, so that the performance of an ideal mirror gives F = 1. Also quoted is the gain (G) over an unfocused beam at the sample.

The reflectivity is calculated assuming a Pt-coated mirror, and is used at two different wavelengths on either side of the Pt L absorption edges. The reflectivity is given by(2):

$$R(\theta,\lambda) = \frac{(\theta - a)^2 + b^2}{(\theta + a)^2 + b^2}$$

$$\text{where } 2a^2 = \sqrt{[(\theta - 2\delta)^2 + 4\beta^2]} + \theta^2 - 2\delta$$

$$2b^2 = \sqrt{[(\theta - 2\delta)^2 + 4\beta^2]} - \theta^2 + 2\delta$$

$$\text{with} \quad \beta = \mu\lambda/(4\pi) \text{ and } \delta = \frac{NZ\rho e^2\lambda^2}{2\pi\ Amc^2} .$$

μ = mass absorption coefficient, N = Avogadro's number
λ = wavelength, Z = atomic number
m = classical electron mass, A = atomic weight.

The quantity NZρ/A is an approximation for the number of scattering electrons per cm^3 - a more rigorous approach (such as that used by Henke et al., ref. 4) uses the real and imaginary parts of the structure factor. Since the most useful wavelengths for PX lie close to the Pt absorption edges (Table 2), this approximation for the reflectivity is not good. To that end measurements of the reflectivity of a Pt-coated mirror used on 9.6 around the absorption edges should be made. These will be reported in a later paper.

The aberrations of the mirror dominate the quantity F, since the focused beam area is typically four times that obtained for an ideal 1.5:1 focus. The spot sizes produced are quite reasonable, however. The results show little improvement in slitting down the vertical divergence, but great improvement by restricting the horizontal. Notice in particular the considerable improvement betwen accepting 1.2 mrad and 1.0 mrad horizontal. This shows that the most intense portion of the beam is in the centre. This is further illustrated by the intensity plot in fig. 1 which is simply the plot of the integrated number of rays in 40 equal 'bins' across the image. The mirror dimensions calculated for use on proposed station 9.5 are given in Table 2.

Toroids only produce their best focus at one position. In order to determine the effect on the focus of mis-setting the toroid critical angle, traces at grazing angles 0.5 mrad on either side of the true angle were performed. The results of these traces show a rapid deterioration of the image, but even in these conditions there is still a factor of ten gain on the unfocused beam. The plot for a 3.5 mrad grazing angle is presented in fig. 2.

The toroidal mirror is designed to accept one-fifth of the horizontal aperture of the 9.6 mirror (ref. 5), and operates at the same grazing angle. The 9.6 mirror has operated in the white wiggler beam for almost 2 years with no observable deterioration in performance. The heat loading on the toroid is then unlikely to cause any rapid surface deterioration.

CONCLUSION

We conclude that, within the constraints of the accuracy of the raytracing package, a reasonable focus can be achieved from a toroid even at a grazing angle of 3 mrad whilst accepting 0.1 mrad × 1 mrad of wiggler beam. The main difficulty in implementing this design will be the mechanical arrangement used to achieve a controlled bending radius of curvature of 4.8 km.

REFERENCES

1. D. Hubbard and E. Pantos, Raytracing Facilities at Daresbury Lab., Nucl. Instrum. Meth. 208 (1983) p.319.
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3. B. Aschenbach, Rep. Prog. Phys. 48 (1985) p.579.
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TABLE 1

COMPARISON OF RAYTRACING RESULTS

% GOOD RAYS	σ_v'	σ_h'	H	V	F 0.8 Å	F 1.5 Å	G 0.8 Å	G 1.5 Å
72.5	0.08	1.418	0.95	0.73	0.25	0.28	110	118
80.0	0.08	1.2	0.97	0.73	0.24	0.27	101	114
86.9	0.08	1.0	0.79	0.72	0.27	0.31	115	130
66.6	0.103	1.418	1.03	0.75	0.26	0.29	113	127
73.0	0.103	1.2	0.99	0.74	0.25	0.22	112	126
83.8	0.103	1.0	0.79	0.73	0.32	0.35	137	154
	1.5:1, 3.5 mrad Grazing Angle							
65.5	0.124	1.0	0.69	2.95	0.08	0.09	40	36
	1.5:1, 2.5 mrad Grazing Angle							
92.3	0.082	1.0	1.29	3.41	0.04	0.04	18	16

σ_v' = vertical divergence (mrad)
σ_h' = horizontal divergence (mrad)
H = horizontal focus size (mm)
V = vertical focus size (mm)

(Both the vertical and horizontal focus sizes are for the whole focal spot. Examination of fig. 1 shows that the main intensity is concentrated at the centre of the spot, and the FWHM spot size is ≈ 0.22 mm in all cases.)

TABLE 2

LIKELY OPERATING PARAMETERS OF MIRROR FOLLOWING FROM THE RESULTS SHOWN IN TABLE 1

Beam size (HBL magnets) 2 mm horiz. × 0.44 mm vert. (2.3 σ)
Mirror length 75 cm
Mirror width = 9.0 cm
Saggital radius of curvature 4.8 km
Meridional radius of curvature 4.3 cm
Distance from source 18 m
Focal length 12 m
Grazing angle 3 mrad
Pt L_1 = 0.892 Å
Pt L_2 = 0.932 Å
Pt L_3 = 1.07 Å
Critical angle = 0.0068λ Rad (where λ is given in Å)

FIGURE CAPTIONS

Fig. 1 1.5:1 trace, 1 mrad horizontal acceptance, 0.08 mrad vertical.

Fig. 2 1.5:1 trace. The mirror parameters were calculated for a 3 mrad grazing angle, the trace is for a 3.5 mrad angle. Note that the image has blown up to 3.5 times its previous size.

Fig. 3 Typical program output.

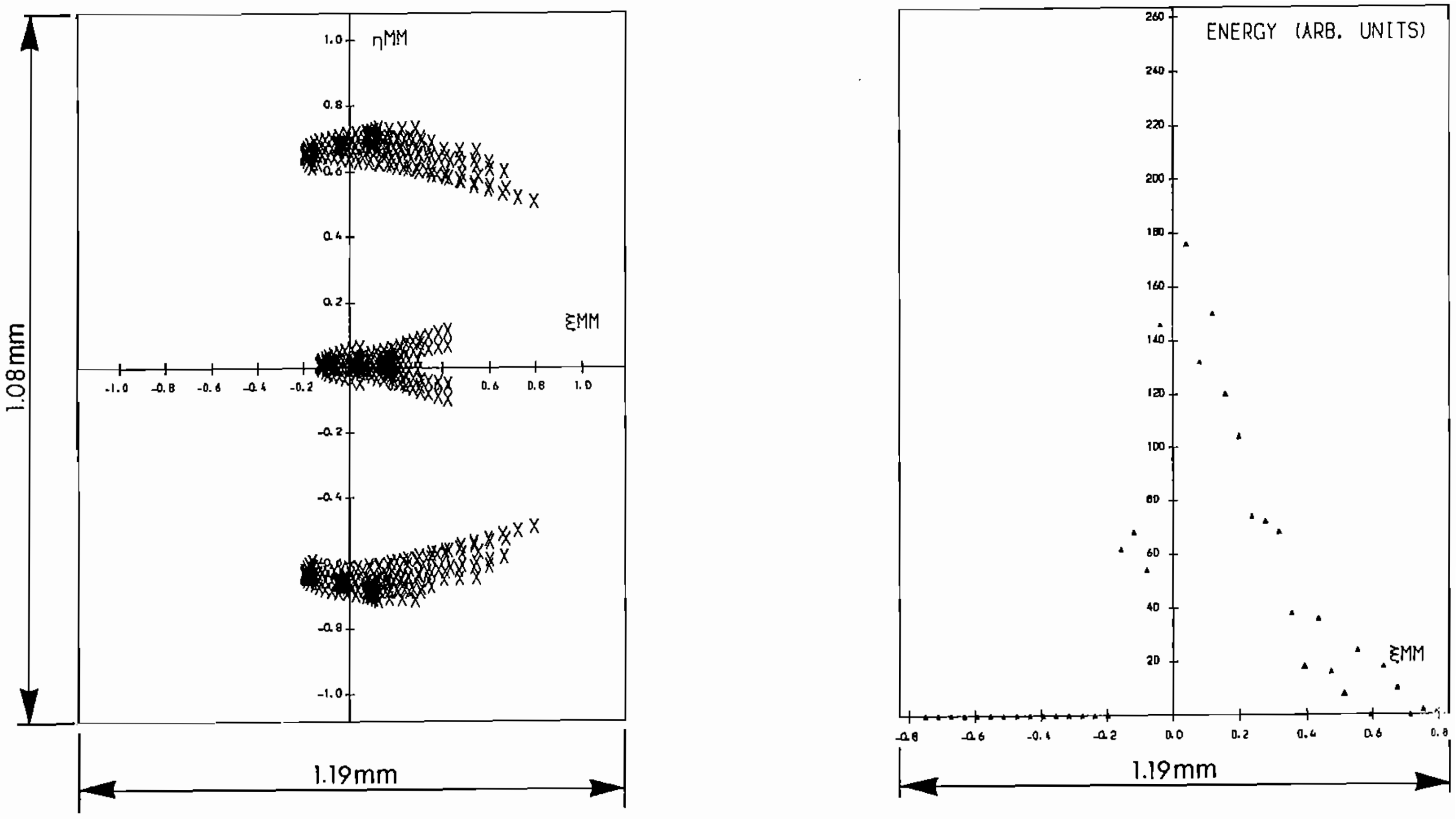
1.08mm
ηMM
1.0
0.8
0.6
0.4
0.2
ξMM
-1.0
-0.8
-0.6
-0.4
-0.2
0.6
0.8
1.0
-0.2
-0.4
-0.6
-0.8
-1.0
1.19mm
ENERGY (ARB. UNITS)
260
240
220
200
180
160
140
120
100
80
60
40
20
ξMM
-0.8
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.6
0.8
1.19mm

Fig.1

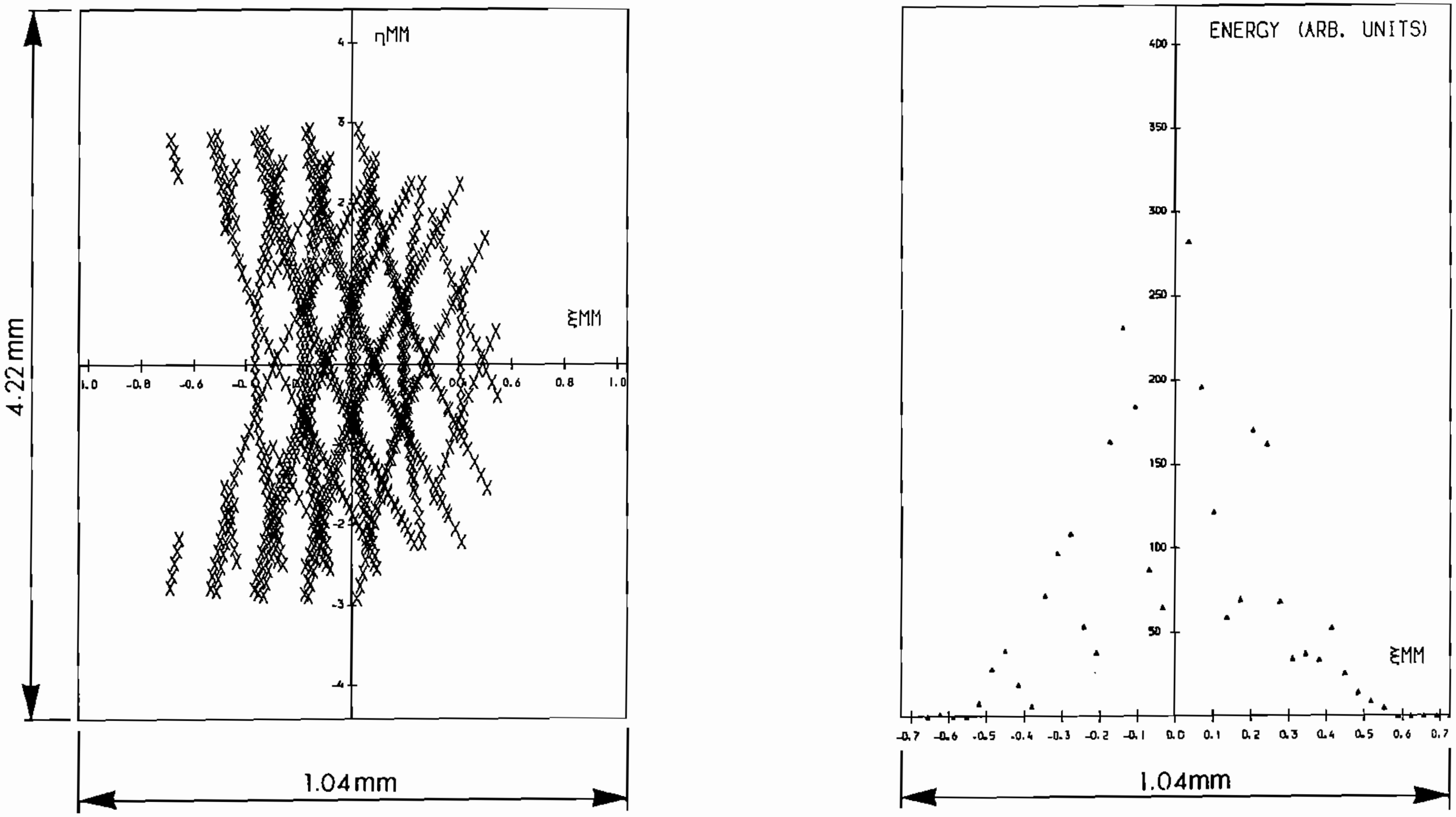
4.22 mm
ηMM
ξMM
4
3
2
-2
-3
-4
-1.0
-0.8
-0.6
0.6
0.8
1.0
1.04mm
ENERGY (ARB. UNITS)
400
350
300
250
200
150
100
50
ξMM
-0.7
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
1.04mm

Fig. 2

```
***   SYSOUT=A   DDNAME=F106F001


>>> SRL PGM RAYMOD - RAYTRACES ELLIPSOIDS I.E. A#B#C
>>> RAYTRACE PROCEDURE STARTING

>>> INPUT DATA IN NAMELIST FORMAT
BL.1.S:1.V 3 MRAD
SOURCE DIMENSIONS:     0.10000(H)  X      0.02000(V)  X      0.00000(D)
BEAM DIVERGENCES (RAD)   0.50000E-03(H)   0.40000E-04(V)
NO OF ELEMENTS   1
NO OF GRATINGS   0 WAVELENGTH  0.10000E-04
ELEMENT 1.
ORDER          :    0
CURVATURE      : MERIDIAN   -0.2083000E-05 SAGGITAL   -0.2314800E+00
ECCENTRICITY:      "         0.0000000E+00     "        0.0000000E+00
DIMENSIONS     :   "         0.3750000E+02     "        0.4320000E+01

IMAGE PLANE     1:
ANGLE OF INCIDENCE          : -0.1567800E+01
DISTANCE FROM SOURCE        :    0.1800000E+04

IMAGE PLANE 2.
ANGLE OF INCIDENCE          :  0.0000000E+00
DISTANCE FROM ELEMENT   1:  0.1200000E+04

SELECT SOURCE TYPE: ISOTROPIC OR GAUSSIAN
IS A DENSE DISTRIBUTION OF POINTS ACROSS THE SOURCE
HORIZONTAL DIRECTION REQUIRED?
DO YOU WISH TO SET THE IMAGE SCALE
DO YOU WISH TO RAYTRACE TO A FLAT FIELD IMAGE PLANE
>>> OUTPUT DEVICE: VERSATEC
>>> RAYTRACING GAUSSIAN SOURCE

RANGE VALUE   1.
AREA TRACE FLAG   0
WAVEFRONT FLAG   0
SOURCE POINTS FLAG   0
FLAT FIELD FLAG   0
DIFFRACTED ANGLE =   -0.1567800E+01
SIG(ROTATION) = -0.1567800E+01
DIRECTION COSINES BEFORE ROTATION = -0.3999998E-04 -0.4999998E-03  0.1000000E+01
ELLIPSE PARAMETERS:  -0.5600000E-01 -0.9000000E+03
SURFACE NORMAL DCS =  -0.1674269E-04  0.2305238E+00 -0.9730668E+00
XSPR : YSPR : ZSPR ARE   ; -0.1411771E+00 -0.9958695E+00 -0.1208260E+04
DCS OF RAY ARE ;  0.1625221E-03  0.8719105E-03  0.9999997E+00
TOTAL NO OF RAYS TRACED:     703
RAY FAILURE AT TOROIDAL SURFACES DUE TO COMPLEX DISTANCES:      0
RAY FAILURE AT NON-TOROIDAL SUBSTRATES:      0
IMAGE SCALE=    1.18705(MM)  X     1.08333(MM)
TOTAL RAY FAILURE FOR EACH ELEMENT:    92
CPU TIME FOR RAYTRACE:       0.750 SECONDS
CPU TIME FOR SPOT DIAGRAM PLOT:       1.420 SECONDS
```

Fig. 3