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THE RAYTRACING OF A FOCUSSING MIRROR FOR PX AND SSP STATIONS ON STORAGE RING "SIBERIA-2" (MOSCOW, USSR)

by

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The Raytracing of a Focussing Mirror for PX and SSP Stations on Storage Ring "Siberia - 2" (Moscow USSR).

by

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Abstract.

This report describes the use of the MAXRAY raytracing package /1,2/ in assessing the design of a focussing mirror for the Protein Crystallography (PX) and Solid State Physic (SSP) stations due to be constructed on the storage ring "SIBERIA - 2" in Moscow. Focussing optics are required for PX because of the large discrepancy in size of the diverging synchrotron radiation beam and a protein crystal sample (typically 0.3 x 0.3 x 0.3 mm^3). The efficiency of X - ray collection is investigated as a function of grazing angle, magnification and misalignment error for both toroidal and ellipsoidal mirror forms.

1. Introduction.

The storage ring "SIBERIA-2" is under construction at the Moscow Kurchatov Institute of Atomic Energy /3/. The main parameters of the storage ring are presented in Table 1. The Institute of Molecular Genetics (USSR Academy of Sciences) are planning several biological stations including Protein Crystallography (PX) - a full list of the planned workstations is given in Table 2. The schematic layout of the biological beamline is given in Fig 1, and includes an experiment at 29.5m from the tangent point of D24 - 2 for PX, and one at 25.5m from the tangent point for solid state physics (SSP) investigations. The raytracing investigation was required in order to determine whether these two stations could use the same focussing mirror, and to evaluate the aberrations associated with the two focussing positions (1.3:1 and 2:1). The effect of mirror misalignments was also investigated in order to simulate incorrect mirror mounting and positioning.

2. Raytracing.

The MAXRAY package was developed at Uppsala University, and has already been used at Daresbury in the study of a mirror for a PX station /4/. Each optical element is represented by a subroutine, with rays from a simulated synchrotron source distribution being traced through each element to the image plane. The output of the program therefore consists of a predicted two dimensional intensity distribution which can be integrated over an area of interest (for example, the size of a typical X - ray collimator) in order to estimate the overall efficiency of focussing. The drawback of the ray tracing approach is that the images so produced represent those from a perfectly figured mirror, unaffected by the heat load of the X - rays incident on it, and with zero surface roughness. Prior to any raytracing analysis it is important to take into account the above parameters and their likely impact on the quality of focus and reflectivity.

3. Results.

The following questions were addressed:-

a) What is the optimum length of mirror taking into account collection efficiency, beam acceptance and reflectivity, cost and difficulty of fabrication?
b) Would it be more efficient to use a small ellipsoid than a large toroid?
c) Is it possible to share a mirror between the two stations described above either by using a fixed figure mirror and changing the grazing angle, or by refocussing a toroidal mirror?
d) What is the optimum magnification to use, and how quickly does aberration begin to dominate the image when working away from this position?

The flux from the storage ring at various energies was calculated using the program due to Laundy /5/ for a stored beam of 100 mA and integrated over several vertical beam apertures corresponding to many possible combinations of mirror length and grazing angle. These fluxes were than multiplied by the calculated reflectivity of a Pt mirror with a typical (good!) surface roughness of 10Å rms. The results of these calculations are shown for various mirror lengths and the preferred grazing angle of 3 mrad in Fig 2. It can be seen that there is a decreasing return in going for longer and longer mirrors when the escalating price and difficulty of fabrication is taken into account. It was therefore deemed unnecessary to increase the mirror length beyond 60 - 80 cm.

The 3 mrad grazing angle was selected as the largest possible grazing angle (for a Pt coated mirror) to give the required wavelength spread (0.5Å - 2.0Å) for Laue crystallography.

The efficiency of collection of rays from the mirror was calculated by summing the rays falling within in a user selected box centred around the peak intensity. The number of rays falling within this area is expressed as a percentage of the total number of rays striking the mirror, and was calculated for square boxes with 0.3mm, 0.5mm and 0.7mm edges. This forms a sensible estimate only if a sufficiently large total number of rays are traced (thus overcoming any non - randomness due to the "seed" used to generate the starting point of the ray in the computer code).

A number of raytraces of the effects of different mirror parameters were carried out in order to model the sensitivity of various mirror misalignments.

In order to share a mirror between the SSP and PX modes of beamline D24 - 3 (distances 9m and 13m from the mirror position), the curvatures of two types of mirror (toroid and ellipsoid) were optimised for a point in between the two stations (11m) and the two systems traced at various grazing angles. The results of the calculations are presented in Table 3. The better focussing at 9m (about 50% of optimum value) is achieved for 3.4 mrad graze angle, and at 13m for 2.7 mrad - Figs 3 and 4 show the corresponding focal spots.

4. Discussion.

The raytracing for the ellipsoidal mirror shows the expected very high quality of focus. These mirrors, however, are extremely difficult to fabricate, particularly if a large (60 - 80 cm) mirror is required. Therefore, for focussing ratios close to 1:1, a toroidal mirror is used to approximate the shape of an ellipsoid.

Fig 5 shows the calculated focal spot produced by an ideal toroid for the magnification required to focus the beam at the PX station (M = 0.78). This gives approximately 30% less intensity in a 0.3mm square box than the M=1 case (Fig 6). Moreover, the efficiency of the focus of the real mirror will be critically dependent on the figure accuracy of the mirror, and (in particular) on the slope error. This is the "flatness" of the surface in the long direction of the mirror, and effectively makes the mirror appear as several mirrors at slightly different grazing angles. When the slope error is around 2 arc seconds, the vertical focus is doubled in size. These slope errors are simulated in Fig 7 by varying the graze angle by +10 and -10 arc seconds. The overall image obtained with a 20 second slope error would be the superposition of these images.

The effect on the focussing properties of changing the sagittal radius from the optimum is illustrated in Fig 8. Figs 9 and 10 show the very critical variation of yaw angle (the rotation of the mirror around an axis perpendicular to its surface) with the toroid efficiency. It is important that corrections of smaller than 0.05 mrad over the length of the mirror can be made.

An illustration of the effect of a mirror translation about the optimum position is shown in Fig 11. The effect of a mirror rotation around a longitudinal axis (roll) is given in Fig 12. The variation in the efficiency of a toroid optimised to focus at an image distance of 13m is shown in Fig13.

It should be pointed out that arguments about slope error, figure and off axis source still apply to the ellipsoidal mirror where there are similar difficulties in aligning the mirror. The opportunity of refocussing the mirror for different image distances is also lost.

<u>List of Figures.</u>

Table 1.

Main Parameters for the SIBERIA - 2 Storage Ring.

Electron Energy	2.5	GeV
Beam Current		
single bunch	100	mA
multi bunch	300	mA
Emittance		
horizontal	76.5	rad. nm
vertical	0.76*	rad. nm
Bending Magnets		
Magnetic Field	1.7	T
Bending Radius	4.9054	m
SR Critical Energy	7.1	keV

* Preliminary data.

Table 2.

The Biological Experiments Proposed for SIBERIA - 2.

BEAM LINE	D24 - 1^+	D24 - 2^+	D24 - 3	W1 - 1^*	W1 - 1^*
SOURCE	BENDING MAGNET	BENDING MAGNET	BENDING MAGNET	WIGGLER	WIGGLER
EXPERIMENT	ISOMORPHOUS REPLACEMENT	POLYCHROMATIC X - RAY DIFFRACTION	MAD, EXAFS	LAUE	TIME RESOLVED LAUE
WAVELENGTH [Å]	1	0.5 - 3.0	0.5 - 3.0	0.2 - 3.0	0.2 - 3.0
$\frac{\delta\lambda}{\lambda}$	10^{-3}	10^{-2} - 10^{-3}	$<10^{-4}$	10^{-1}	10^{-1}
EXPECTED FOCAL SPOT SIZE [MM X MM]	1 x 1	1 x 1	0.3 x 0.3	UNFOCUSSED	UNFOCUSSED
MONOCHROMATOR	BENT TRIANGLE	BENT TRIANGLE	TWO CRYSTAL	n/a	n/a
MIRROR	CYLINDRICAL	CYLINDRICAL	TOROIDAL	n/a	n/a
DETECTOR	MWPC	FILM	MWPC	FILM	FILM

Note that $^+$ and * represent shared stations.

Table 3.

Efficiency of Toroid vs Ellipsoid

The efficiency (as a percentage of total number of rays traced) of a simulated toroid and ellipsoid are given for image collection at 9m (SSP station) and 13m (PX station) from the mirror for beam line D24 - 3. The figure of the two mirrors is optimised for a focus between the two stations i.e. at 11m from the mirror. The grazing angle of the two mirrors is adjusted to achieve better focussing, but the curvatures of the surfaces remain fixed. The optimum focus (at 11m) of the two mirrors is also given.

	Graze Angle [mrad]	0.3 mm collimator	0.5 mm collimator	0.7 mm collimator	Distance [m]
TOROID	2.6	6.5	12.8	19.6	13m
	2.7	16.8	35.2	48.5	13m
	2.8	9.6	26.7	50.1	13m
	3.3	10.6	25.9	44.1	9m
	3.4	22.8	43.2	67.4	9m
	3.5	9.9	20.7	33.2	9m
OPTIMUM	**3.0**	**44**	**58.2**	**69.3**	**11m**
ELLIPSOID	2.6	5.1	11.1	18.8	13m
	2.7	24.6	49.1	68	13m
	2.8	9.3	15	25.7	13m
	3.3	14.3	27.2	48.5	9m
	3.4	35.3	62.4	90.4	9m
	3.5	8.7	21	36.3	9m
OPTIMUM	**3.0**	**88.9**	**99.5**	**100**	**11m**

References.

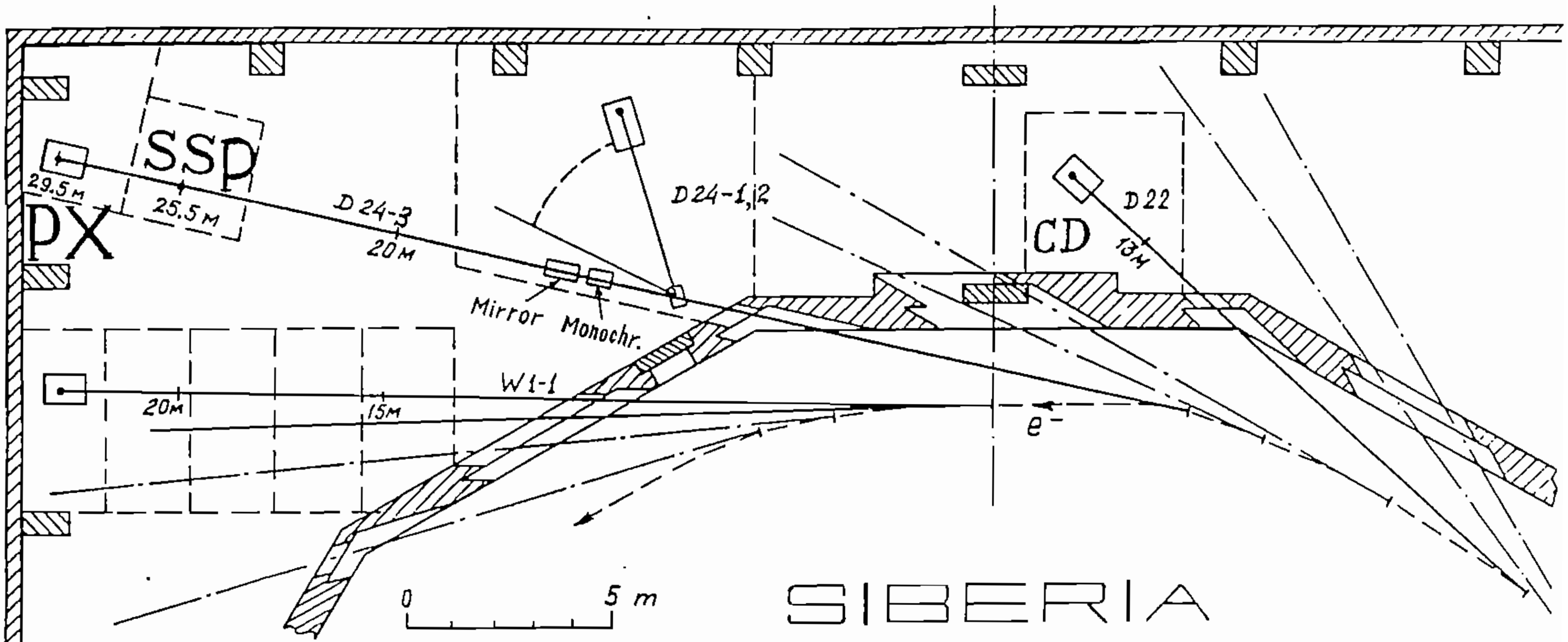
[1] S. Svensson and R. Nyholm. Uppsala University Institute of Physics Report UUIP - 1139 (1985).

[2] R. C. Brammer. Raytracing with MAXRAY and the Design of PX Station 9.5. Daresbury Lab. Technical Memorandum DL/SCI/TM56E (1987).

[3] S. D. Fanchenko. Synchrotron Radiation News **3** (1990) 6 - 9.

[4] R. C. Brammer et Al. **NIM** A271 (1988) 678 - 687.

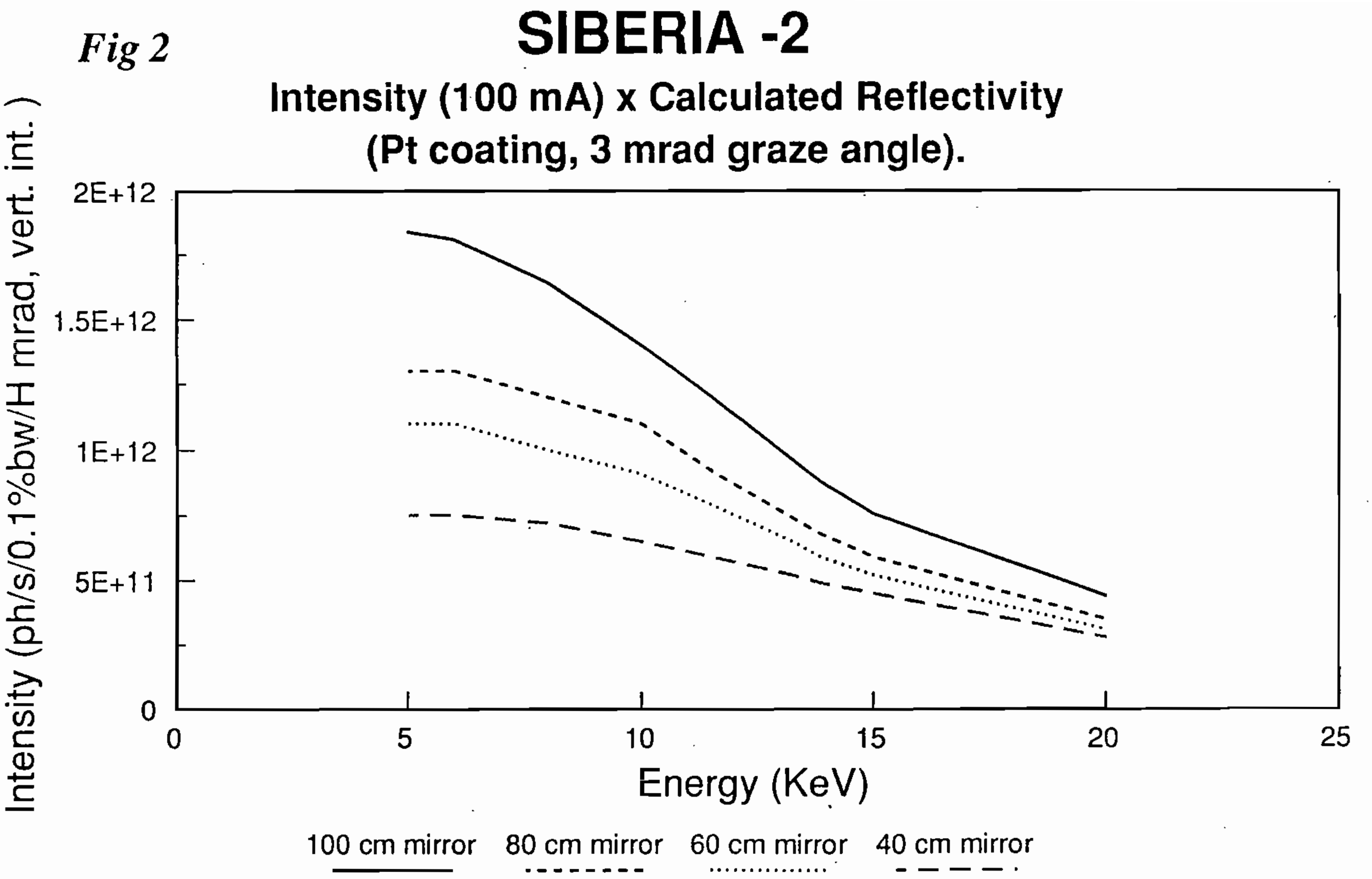
[5] D. Laundy et Al. DL/SCI/P683E Submitted to **NIM** March 1990.



SSP
PX
29.5 м
25.5 м
D 24-3
20 м
D 24-1,2
D 22
CD
13 м
Mirror
Monochr.
W1-1
20м
15м
e⁻
0
5 m
SIBERIA

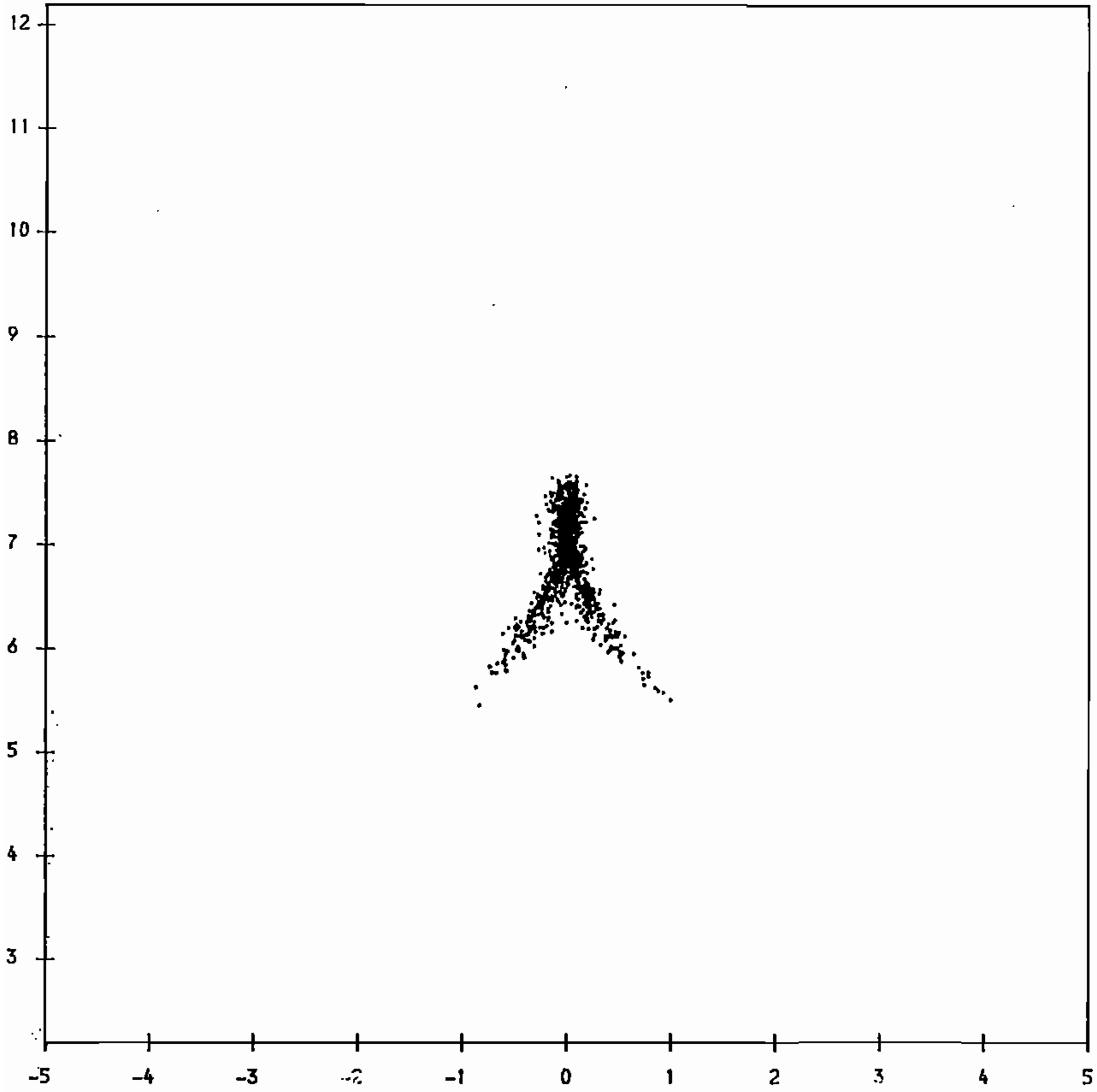
FIG - 1

Fig 2


SIBERIA -2
Intensity (100 mA) x Calculated Reflectivity
(Pt coating, 3 mrad graze angle).
Intensity (ph/s/0.1%bw/H mrad, vert. int.)
2E+12
1.5E+12
1E+12
5E+11
0
0
5
10
15
20
25
Energy (KeV)
100 cm mirror
80 cm mirror
60 cm mirror
40 cm mirror

TOROID RAYTRACE OUTPUT

Fig 3



T.P. to mirror (m) = 16.500

T.P. to Xtal (m) = 25.500

Graze angle (mrad) = 3.400

Mer. Radius (m) =4400.000

Sag. Radius (mm) = 39.600

Yaw angle (mrad) = 0.000

Roll angle (mrad) = 0.000

Transl. error (mm) = 0.000

Total plotted rays= 1013

ftl.plot1torg34

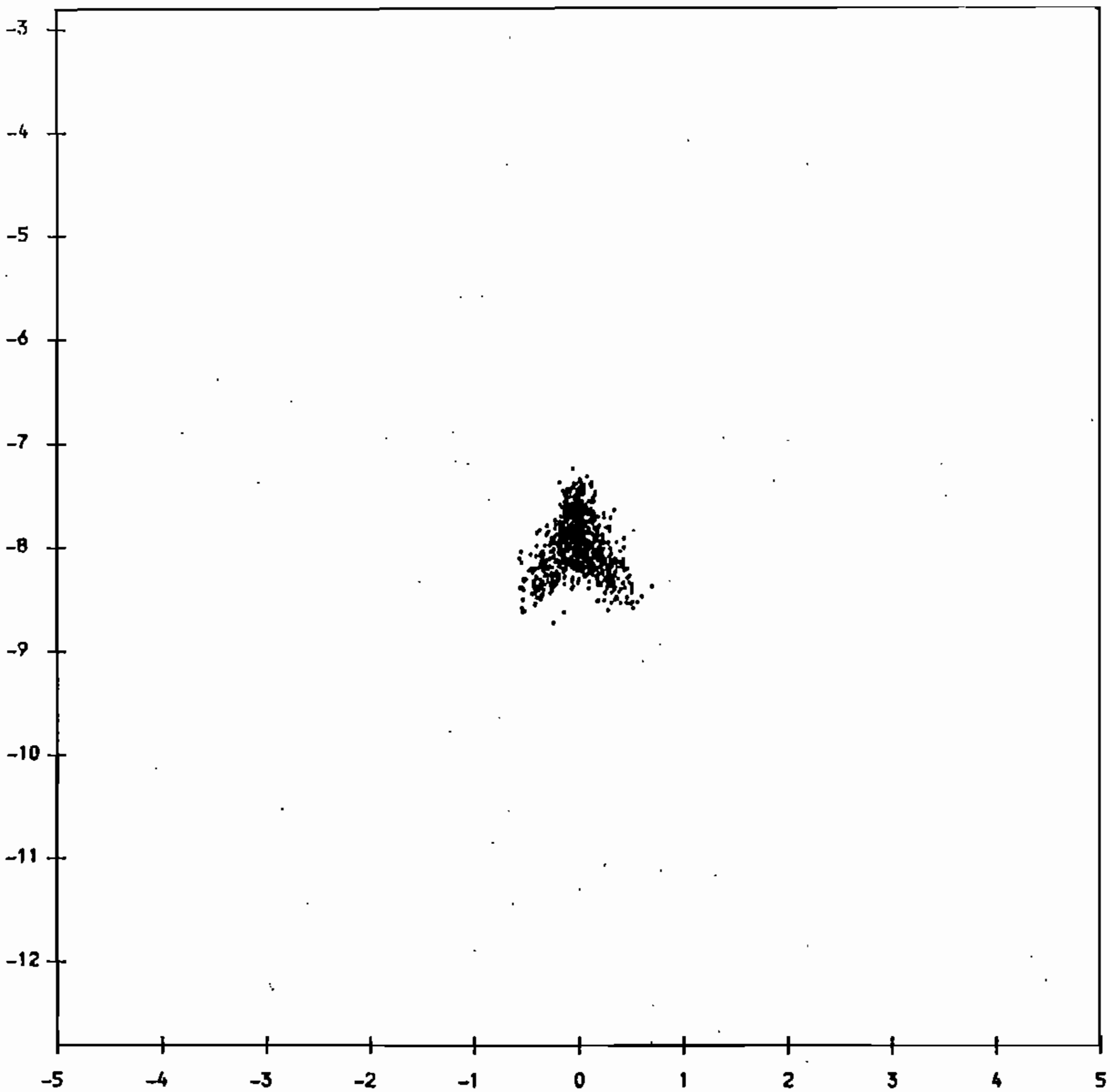
V. Rajko

15:35:46

//MAR/90

TOROID RAYTRACE OUTPUT

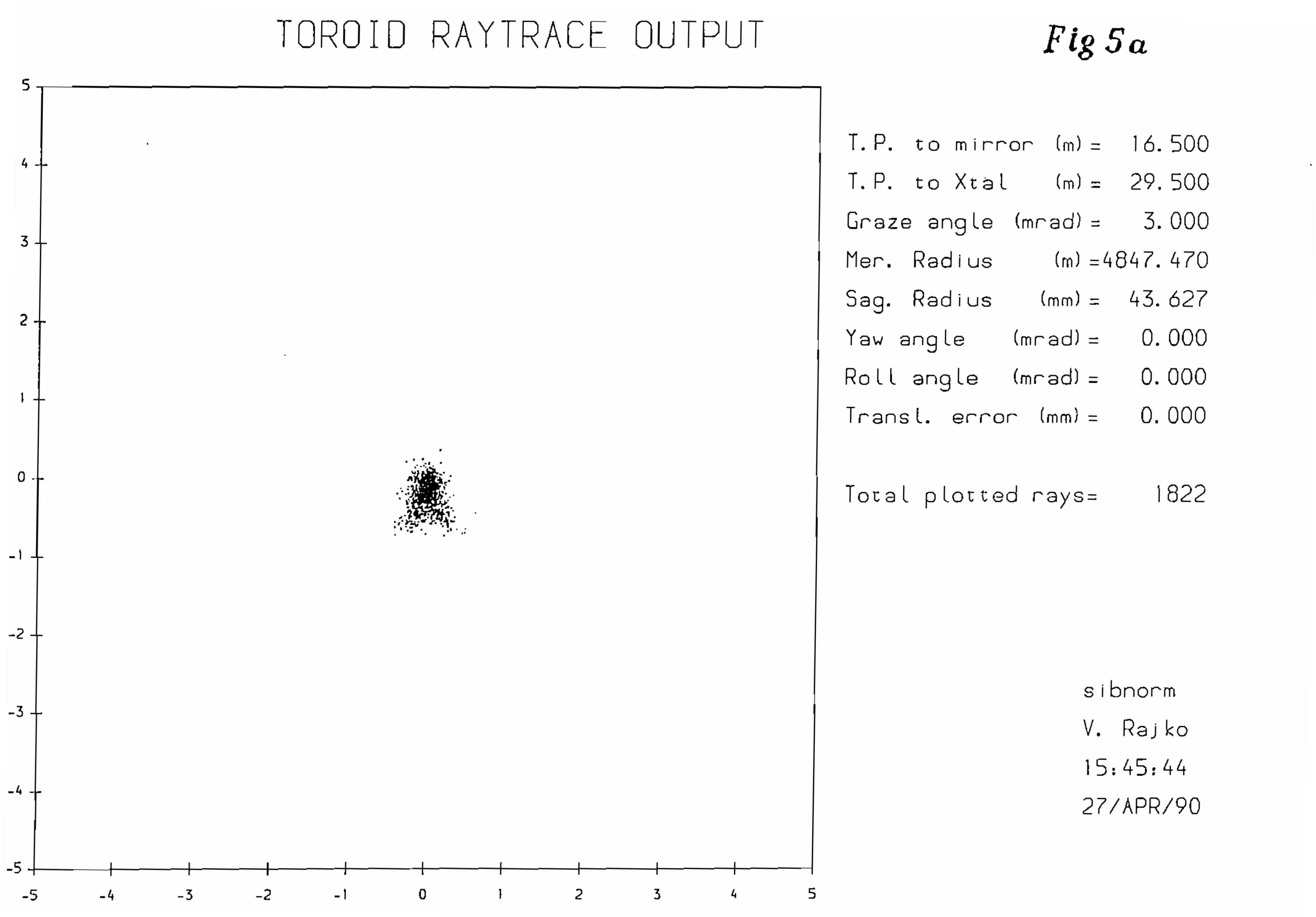
Fig 4



T.P. to mirror (m) = 16.500
T.P. to Xtal (m) = 29.500
Graze angle (mrad) = 2.700
Mer. Radius (m) =4400.000
Sag. Radius (mm) = 39.600
Yaw angle (mrad) = 0.000
Roll angle (mrad) = 0.000
Transl. error (mm) = 0.000

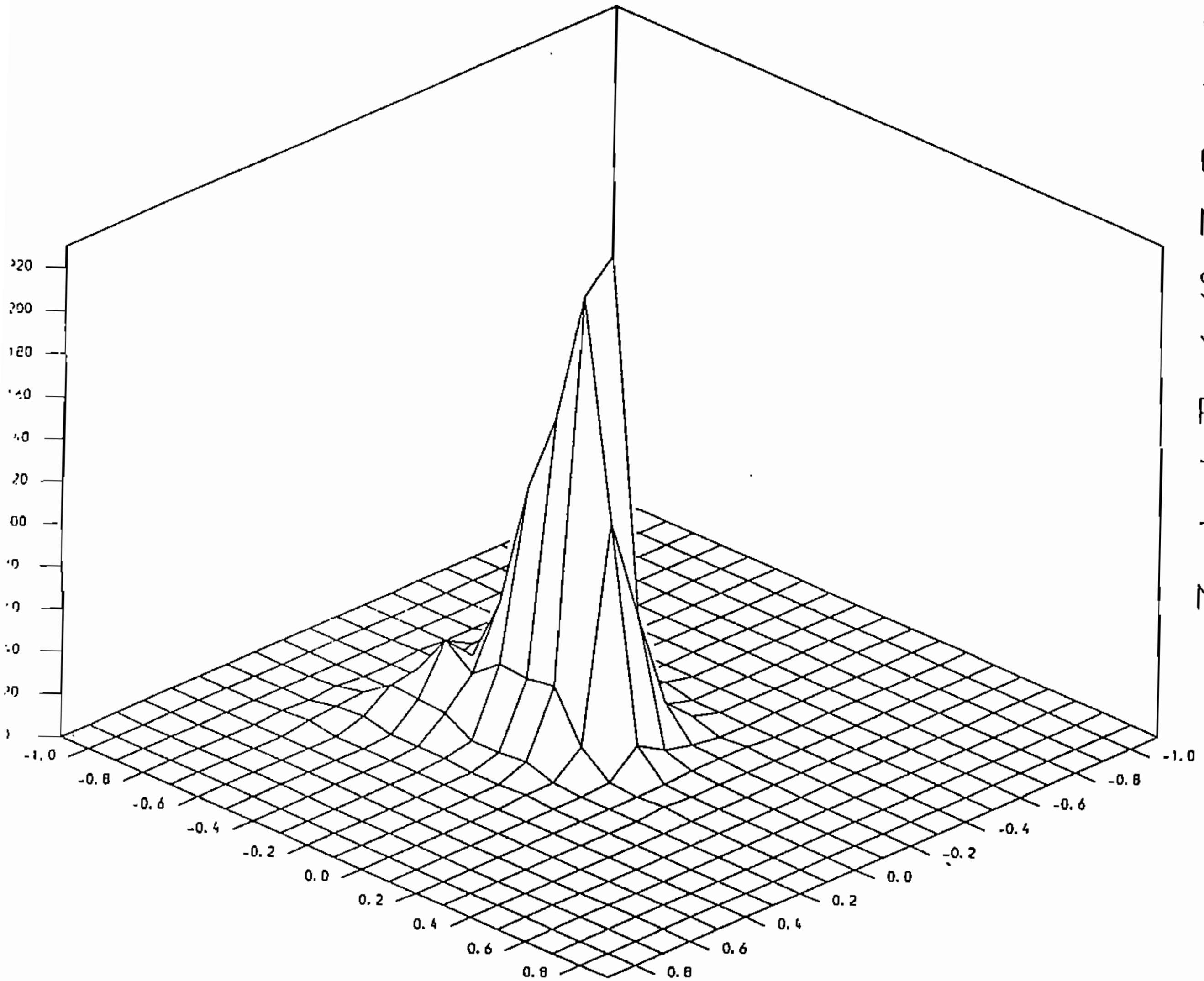
Total plotted rays= 833

[tk.plot]torg27
V. RaJko
15:34:15
7/MAR/90


TOROID RAYTRACE OUTPUT
Fig 5a
T.P. to mirror (m) = 16.500
T.P. to Xtal (m) = 29.500
Graze angle (mrad) = 3.000
Mer. Radius (m) =4847.470
Sag. Radius (mm) = 43.627
Yaw angle (mrad) = 0.000
Roll angle (mrad) = 0.000
Transl. error (mm) = 0.000
Total plotted rays= 1822
sibnorm
V. Rajko
15:45:44
27/APR/90
5
4
3
2
1
0
-1
-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
2
3
4
5

TOROID RAYTRACE OUTPUT

Fig 5b



T.P. to mirror (m) = 16.500

T.P. to Xtal (m) = 29.500

Graze angle (mrad) = 3.000

Mer. Radius (m) = 4847.470

Sag. Radius (mm) = 43.627

Yaw angle (mrad) = 0.000

Roll angle (mrad) = 0.000

Transl. error (mm) = 0.000

Total plotted rays = 1822

Maximum z value = 226

sibnorm

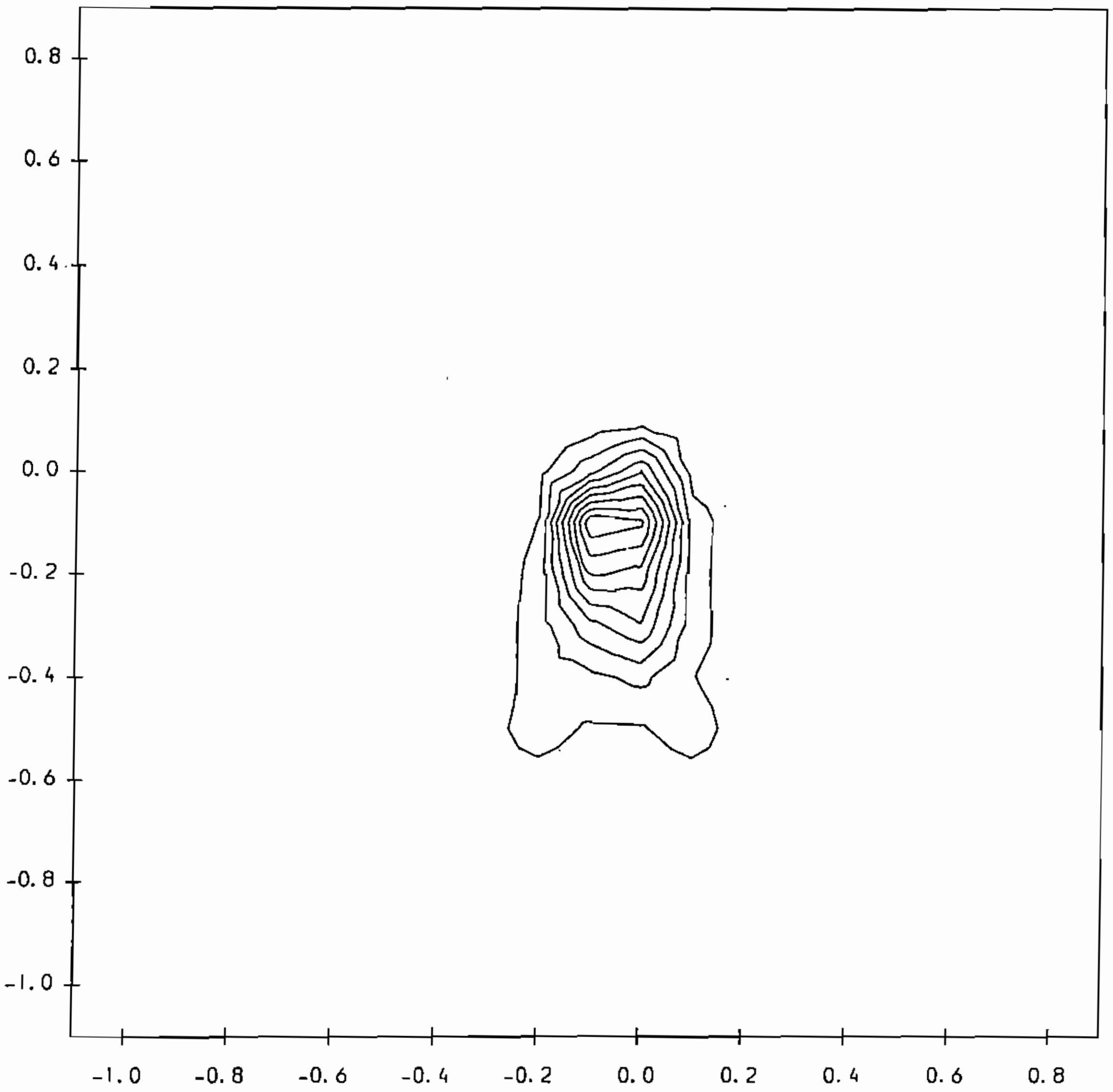
V. Raiko

15:50:15

27/APR/90

TOROID RAYTRACE OUTPUT

Fig 5c



T.P. to mirror (m) = 16.500

T.P. to Xtal (m) = 29.500

Graze angle (mrad) = 3.000

Mer. Radius (m) =4847.470

Sag. Radius (mm) = 43.627

Yaw angle (mrad) = 0.000

Roll angle (mrad) = 0.000

Transl. error (mm) = 0.000

Total plotted rays= 1822

Maximum z value= 226

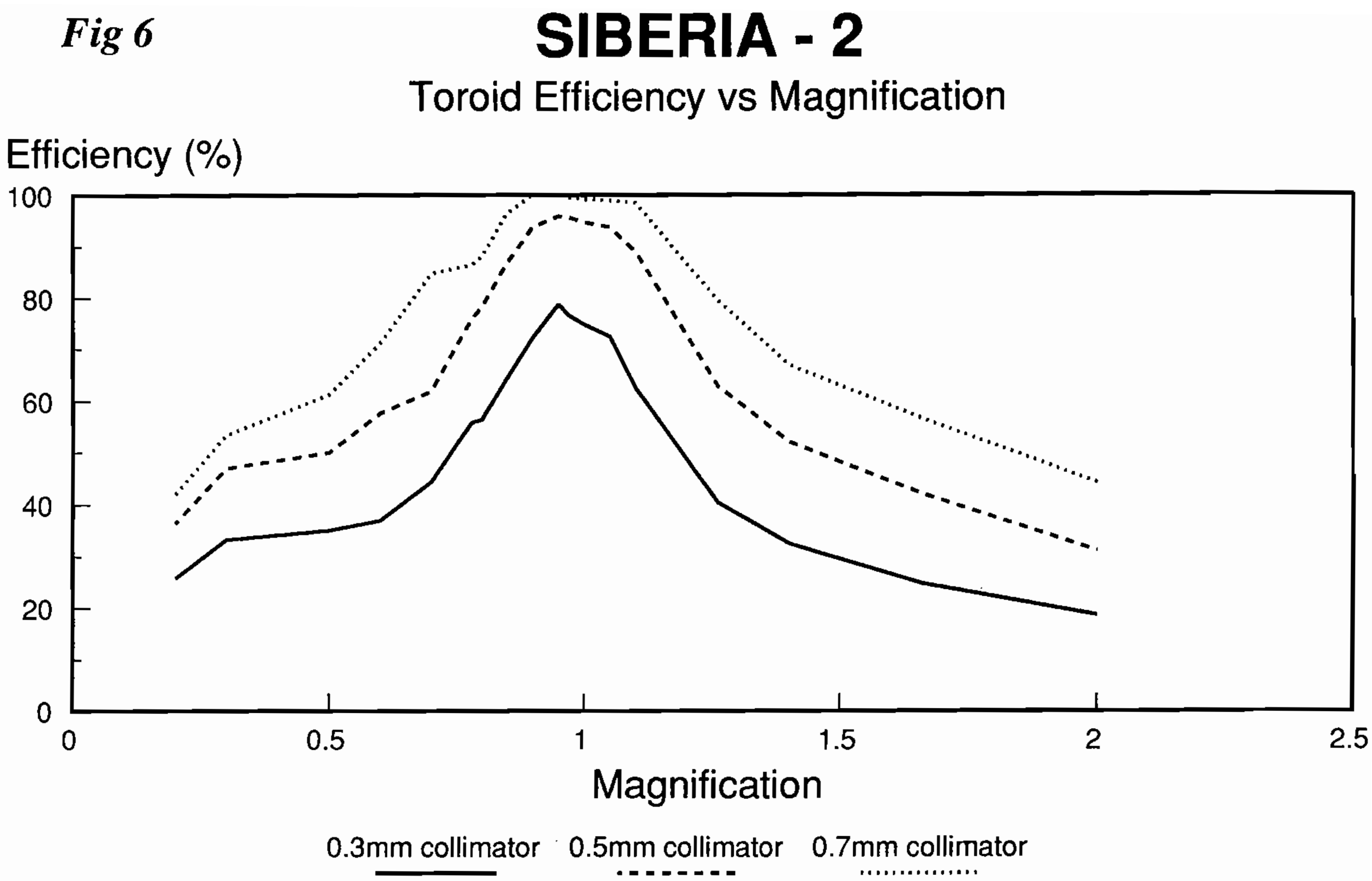
sibnorm

V. Raiko

15:43:09

27/APR/90

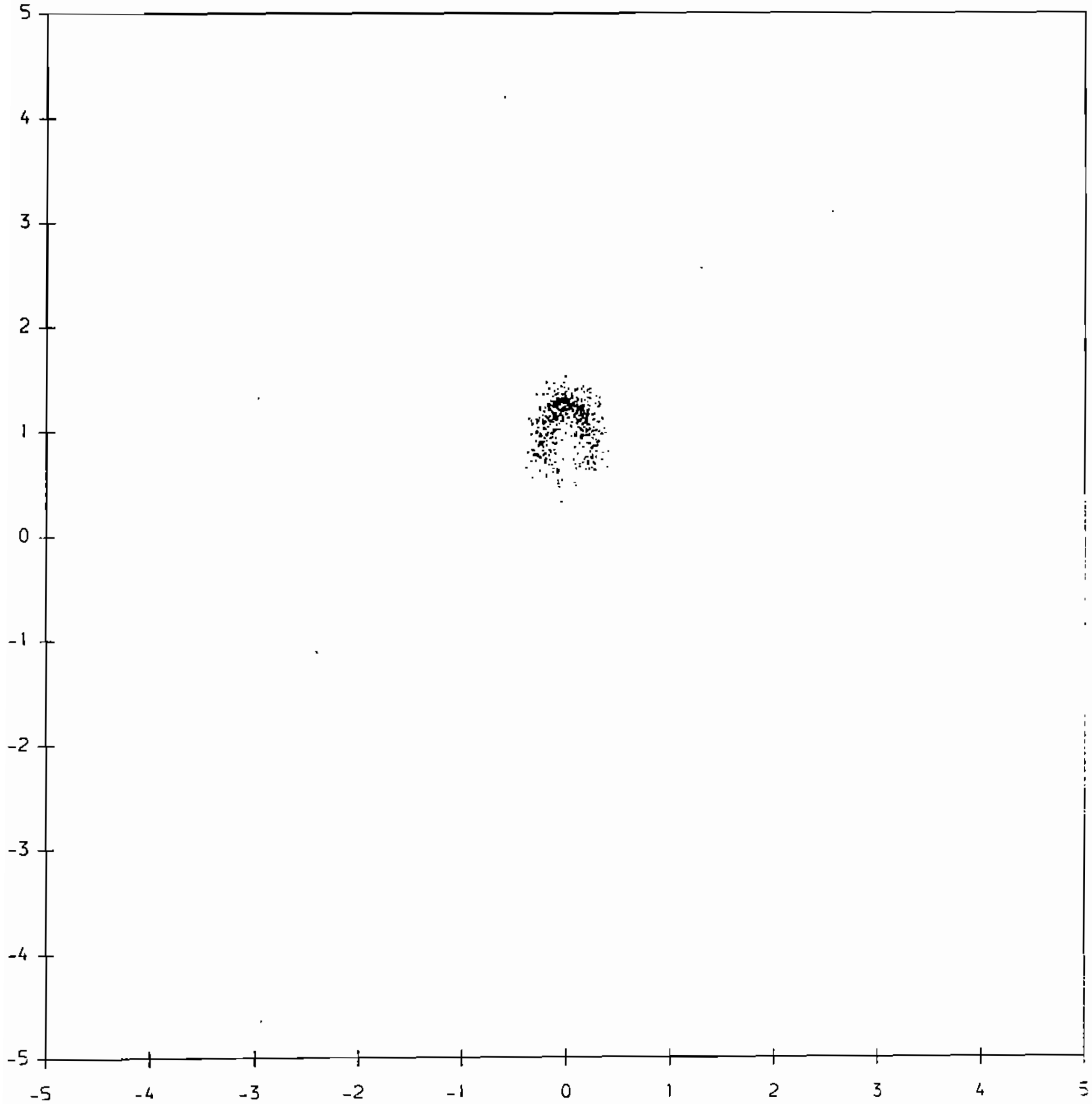
Fig 6



SIBERIA - 2
Toroid Efficiency vs Magnification
Efficiency (%)
100
80
60
40
20
0
0
0.5
1
1.5
2
2.5
Magnification
0.3mm collimator
0.5mm collimator
0.7mm collimator

TOROID RAYTRACE OUTPUT

Fig 7a



T.P. to mirror (m) = 16.500

T.P. to Xtal (m) = 29.500

Graze angle (mrad) = 3.050

Mer. Radius (m) =4847.470

Sag. Radius (mm) = 43.727

Yaw angle (mrad) = 0.000

Roll angle (mrad) = 0.000

Transl. error (mm) = 0.000

Total plotted rays= 570

[tk.plot]sibgran4

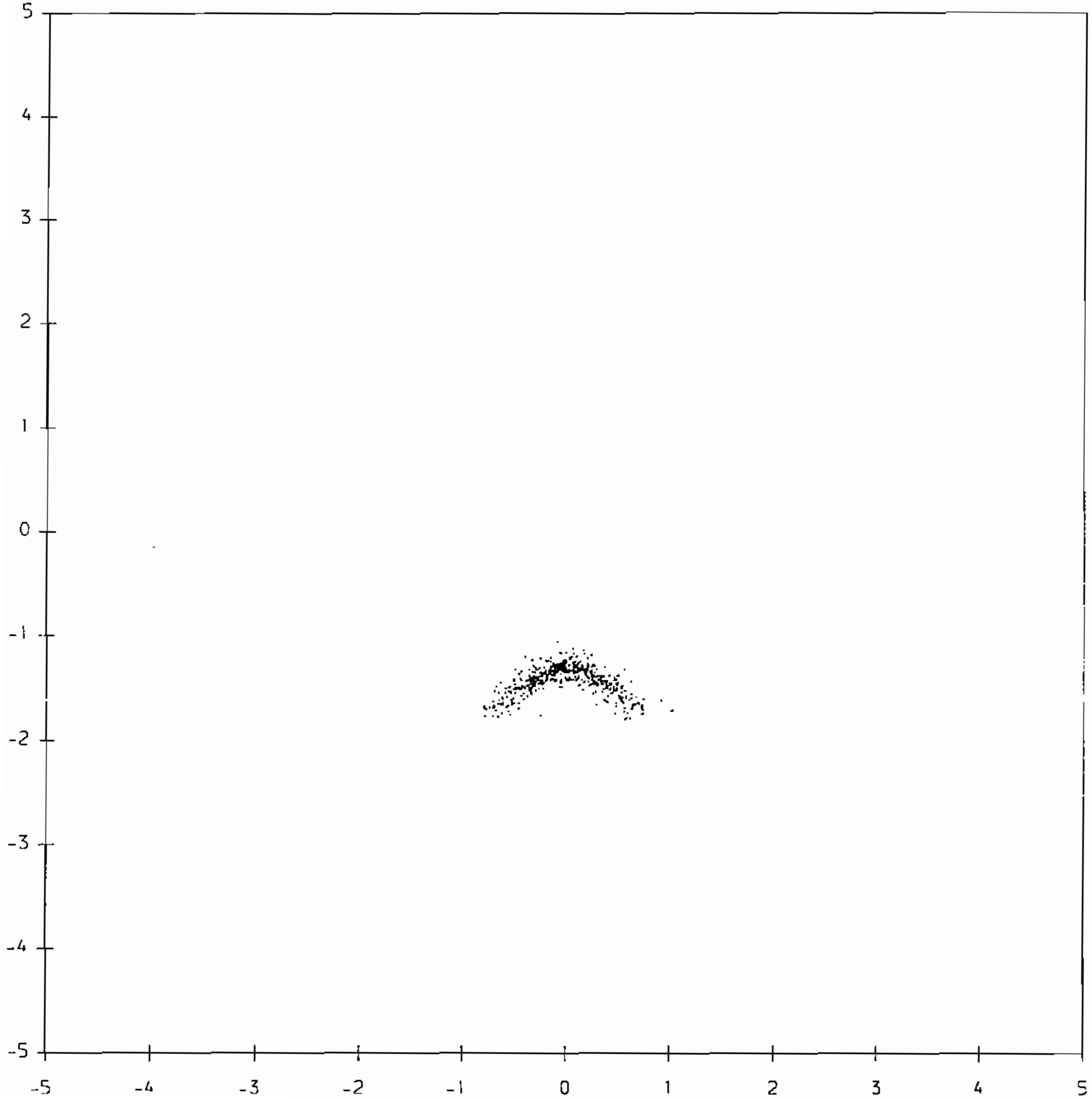
Ron Brammer

17:59:50

27/FEB/90

TOROID RAYTRACE OUTPUT

Fig 7b



T.P. to mirror (m) =	16.500
T.P. to Xtal (m) =	29.500
Graze angle (mrad) =	2.950
Mer. Radius (m) =	4847.470
Sag. Radius (mm) =	43.727
Yaw angle (mrad) =	0.000
Roll angle (mrad) =	0.000
Transl. error (mm) =	0.000

Total plotted rays= 551

[tk.plot]sibgran5

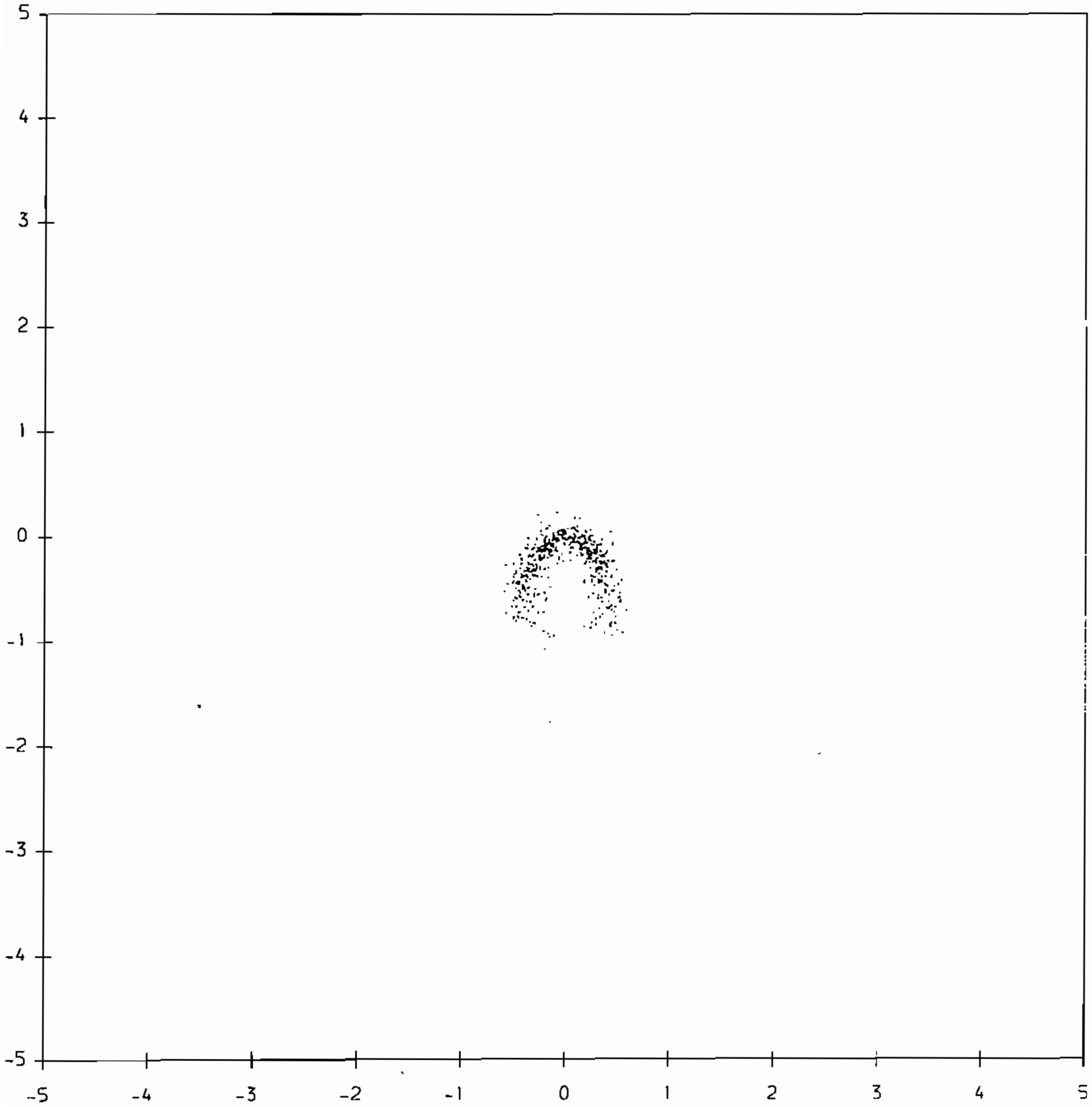
Ron Brammer

18:00:55

27/FEB/90

TOROID RAYTRACE OUTPUT

Fig 8a



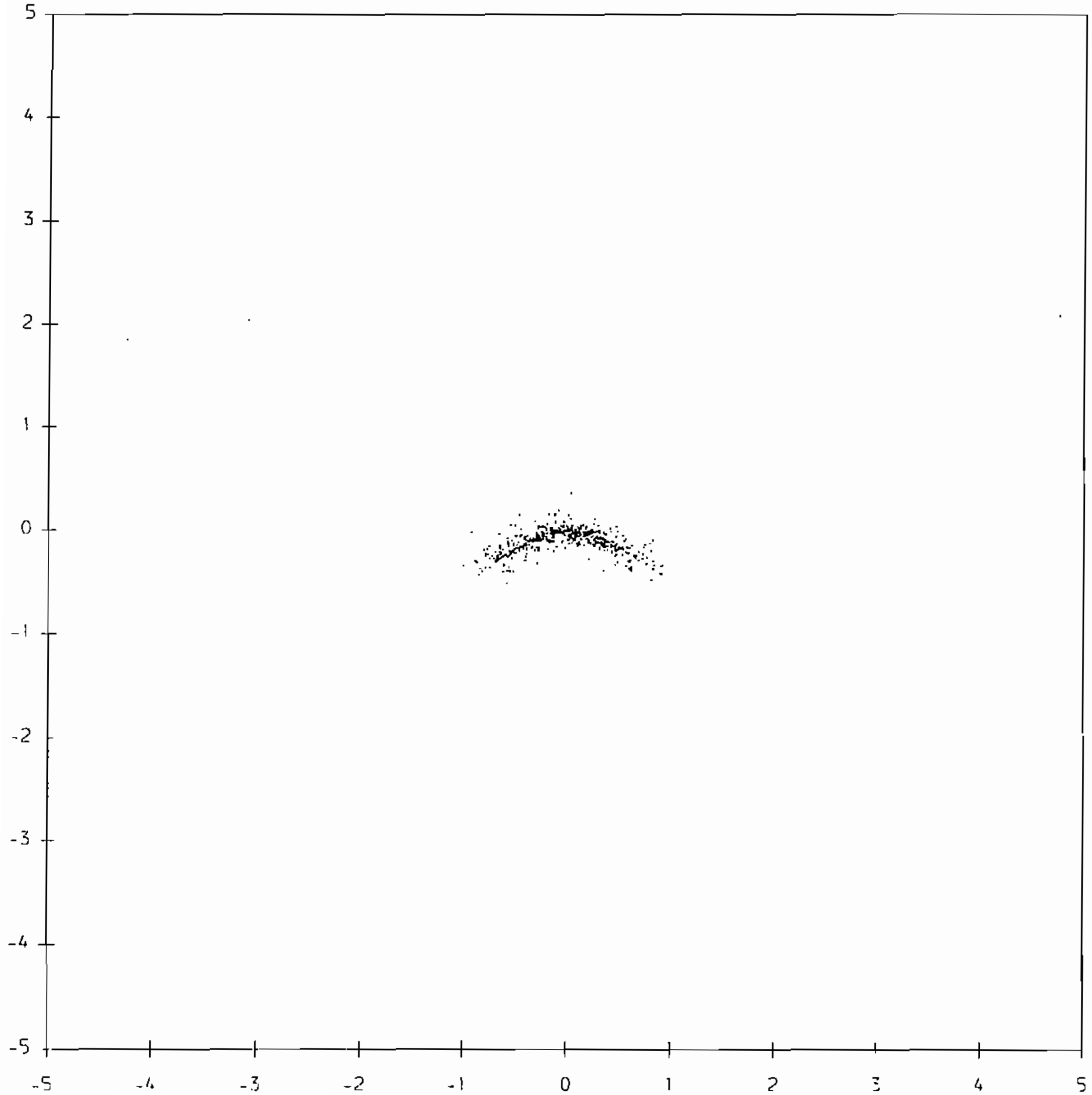
T.P. to mirror (m) = 16.500
T.P. to Xtal (m) = 29.500
Graze angle (mrad) = 3.000
Mer. Radius (m) =4847.470
Sag. Radius (mm) = 42.627
Yaw angle (mrad) = 0.000
Roll angle (mrad) = 0.000
Transl. error (mm) = 0.000

Total plotted rays= 572

[tk.plot]sibvnars
Ron Brammer
17:33:37
27/FEB/90

TOROID RAYTRACE OUTPUT

Fig 8b



T.P. to mirror (m) = 16.500

T.P. to Xtal (m) = 29.500

Graze angle (mrad) = 3.000

Mer. Radius (m) =4847.470

Sag. Radius (mm) = 44.627

Yaw angle (mrad) = 0.000

Roll angle (mrad) = 0.000

Transl. error (mm) = 0.000

Total plotted rays= 544

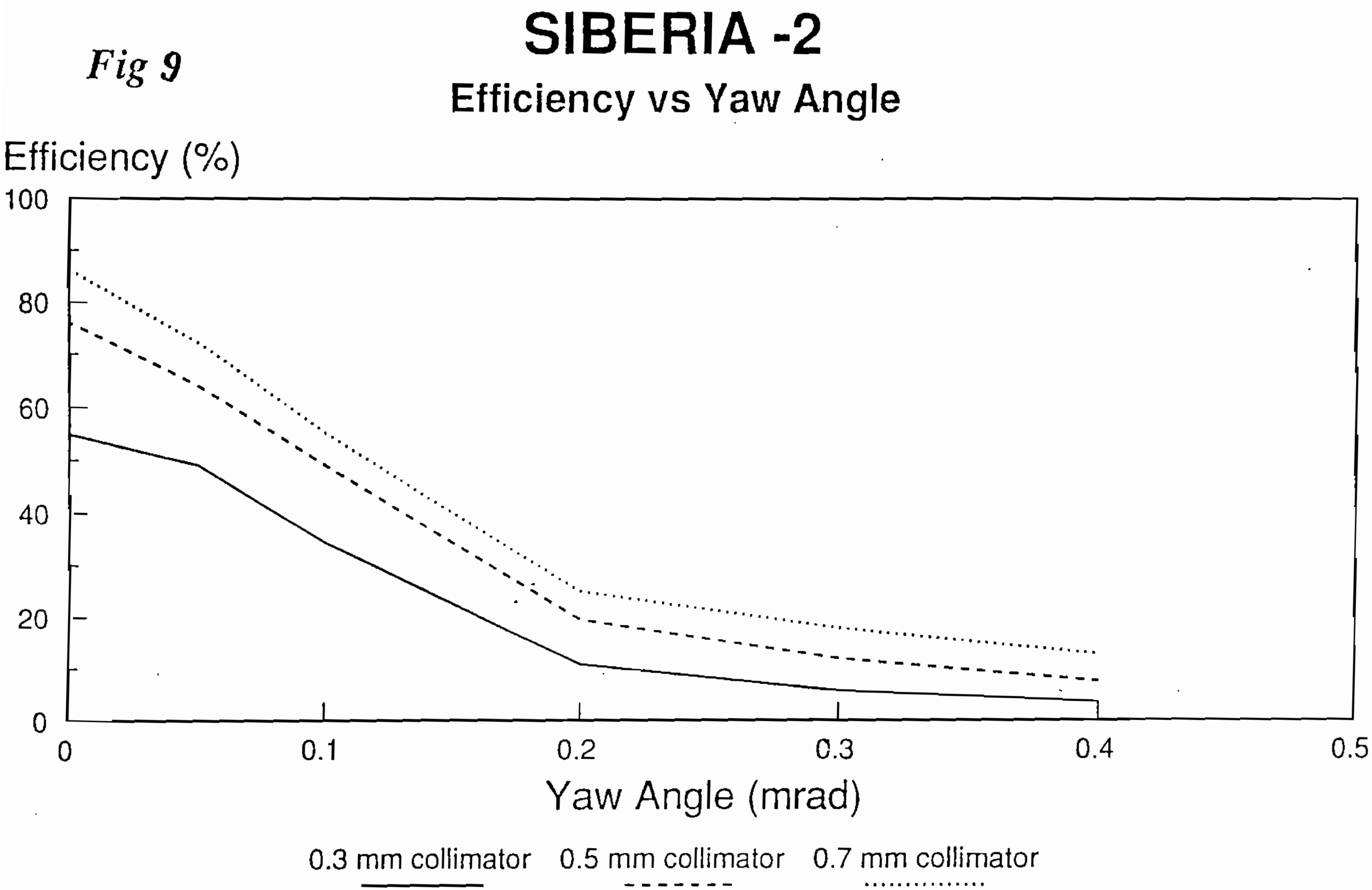
[tk.plot]sibmorsl

Ron Brammer

17:51:52

27/FEB/90

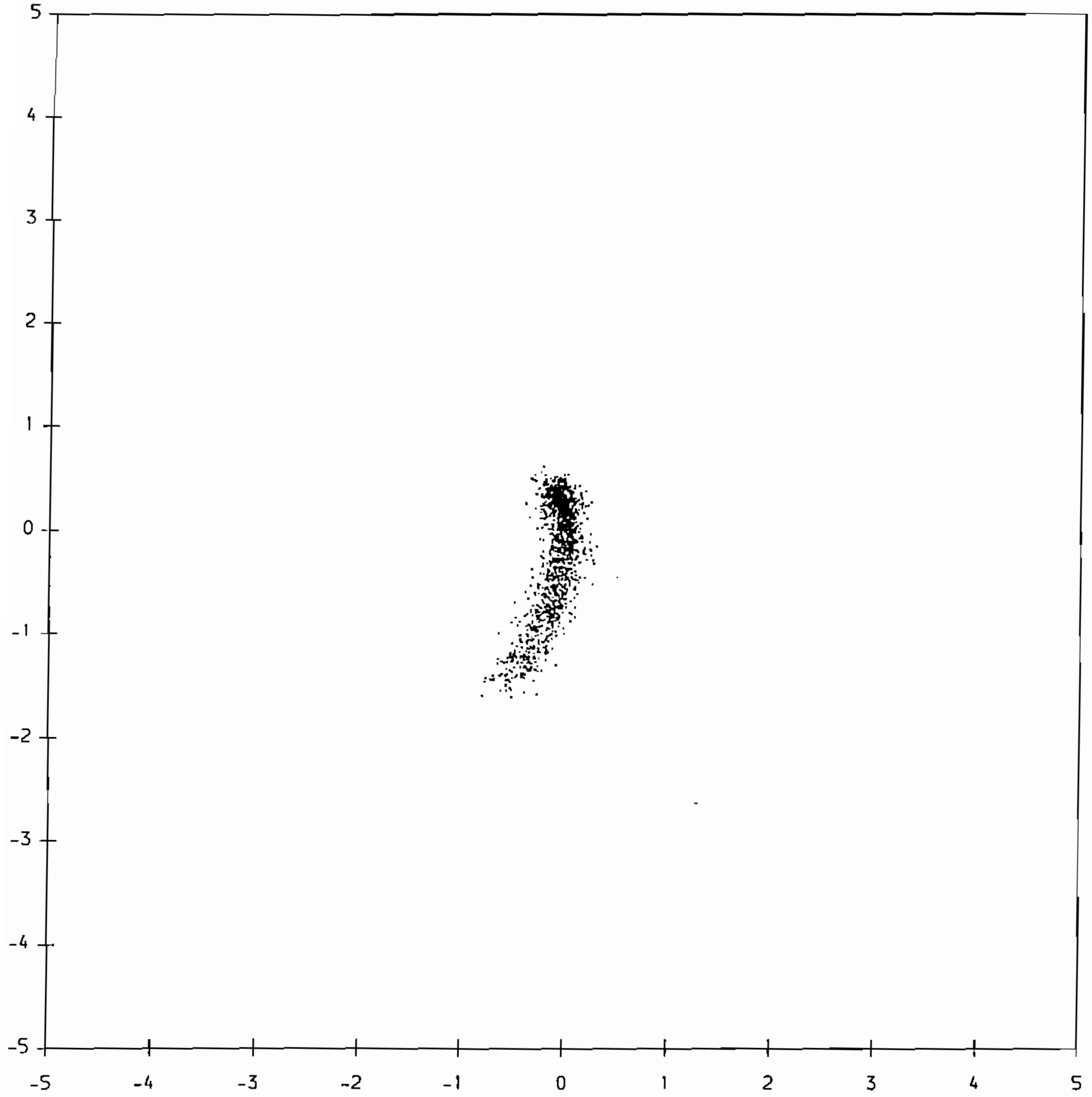
Fig 9



SIBERIA -2
Efficiency vs Yaw Angle
Efficiency (%)
100
80
60
40
20
0
0
0.1
0.2
0.3
0.4
0.5
Yaw Angle (mrad)
0.3 mm collimator
0.5 mm collimator
0.7 mm collimator

TOROID RAYTRACE OUTPUT

Fig 10



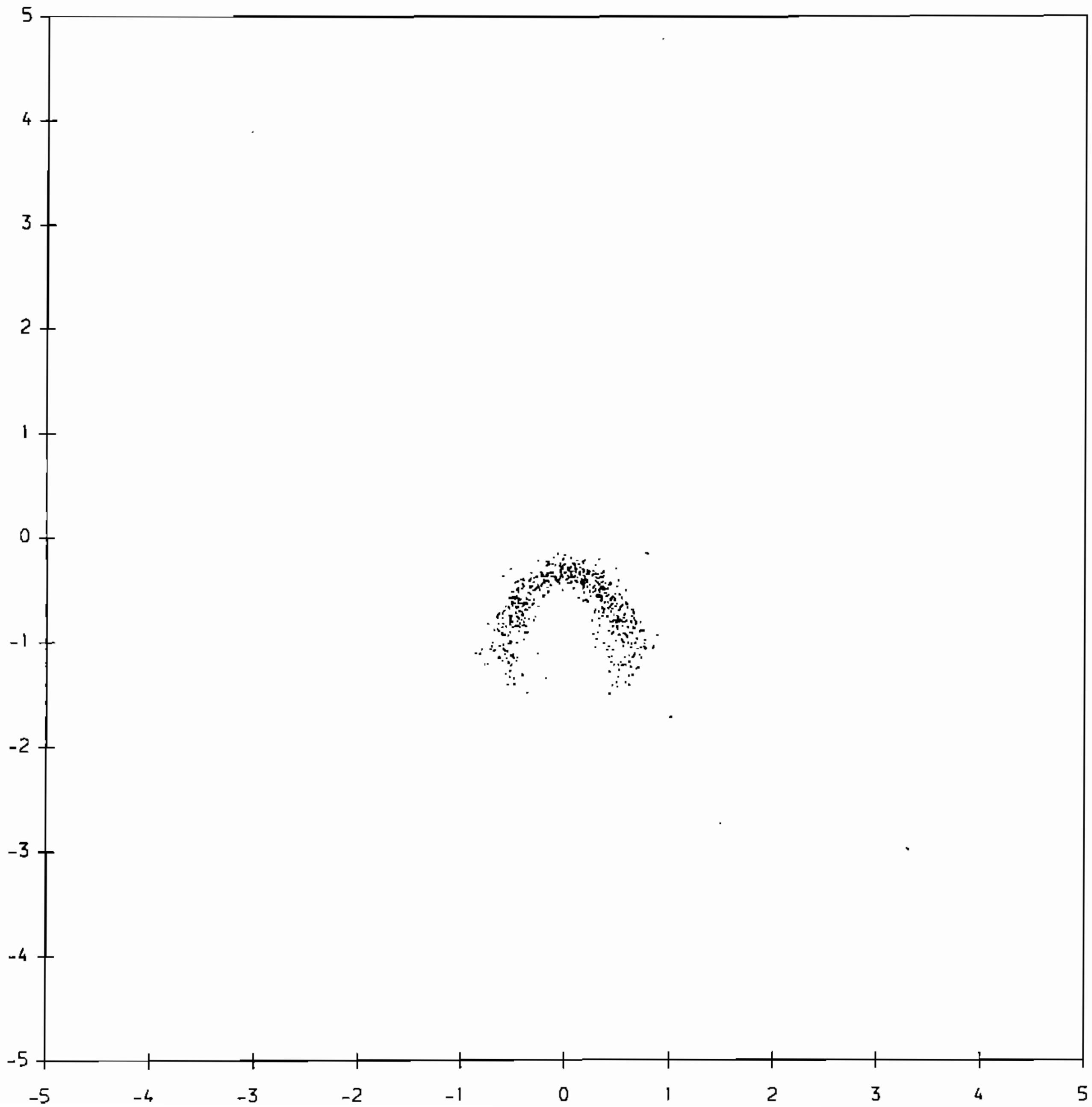
T.P. to mirror (m) = 16.500
T.P. to Xtal (m) = 29.500
Graze angle (mrad) = 3.000
Mer. Radius (m) =4847.470
Sag. Radius (mm) = 43.627
Yaw angle (mrad) = 0.100
Roll angle (mrad) = 0.000
Transl. error (mm) = 0.000

Total plotted rays= 1822

slbyaw
V. Rajko
15:46:54
27/APR/90

TOROID RAYTRACE OUTPUT

Fig 11



T.P. to mirror (m) = 16.500

T.P. to Xtal (m) = 29.500

Graze angle (mrad) = 3.000

Mer. Radius (m) =4847.470

Sag. Radius (mm) = 43.627

Yaw angle (mrad) = 0.000

Roll angle (mrad) = 0.000

Transl. error (mm) = 1.500

Total plotted rays= 605

[tk.plot]sotrn03

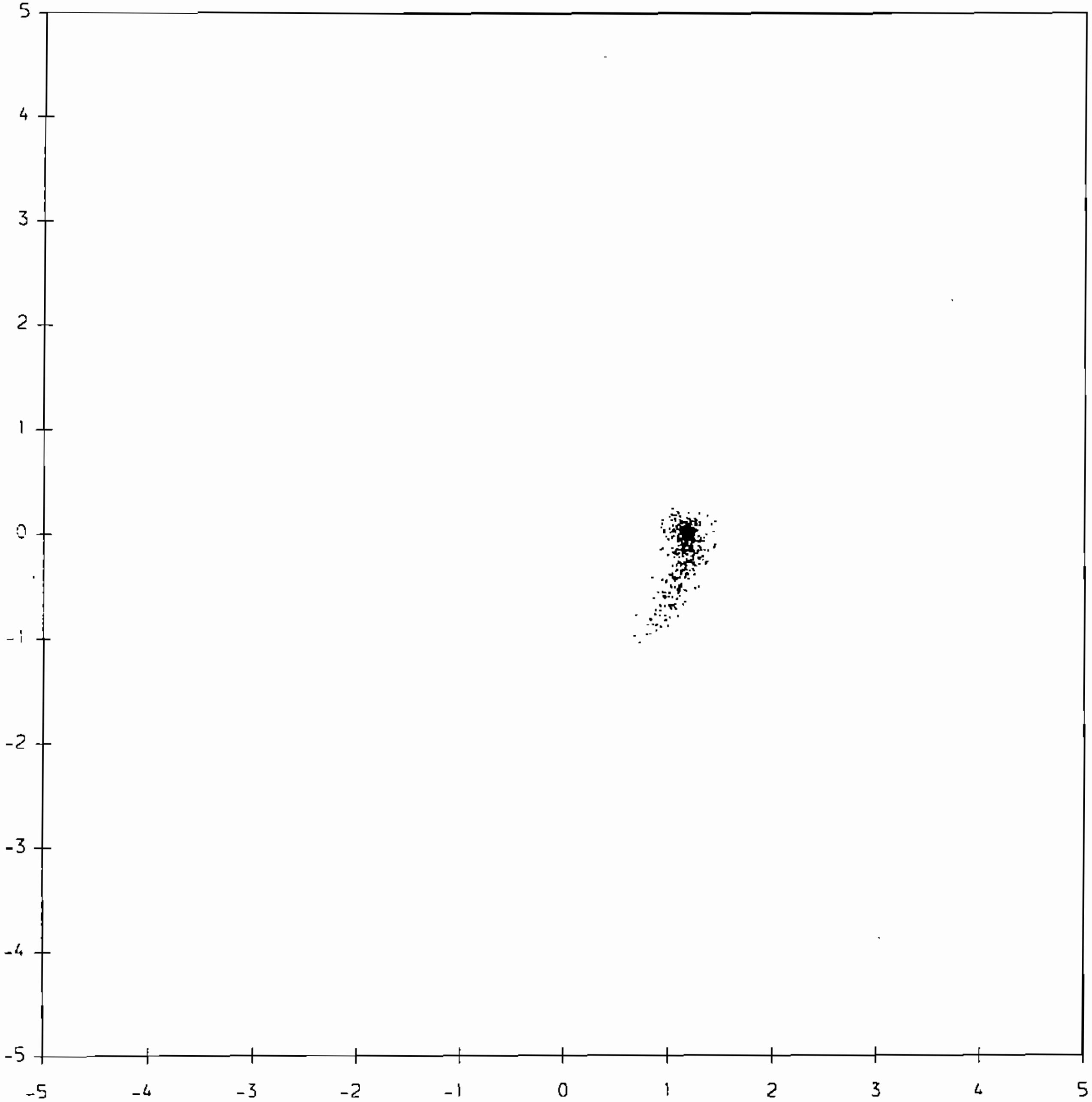
V. Rajko

17:03:51

6/MAR/90

TOROID RAYTRACE OUTPUT

Fig 12

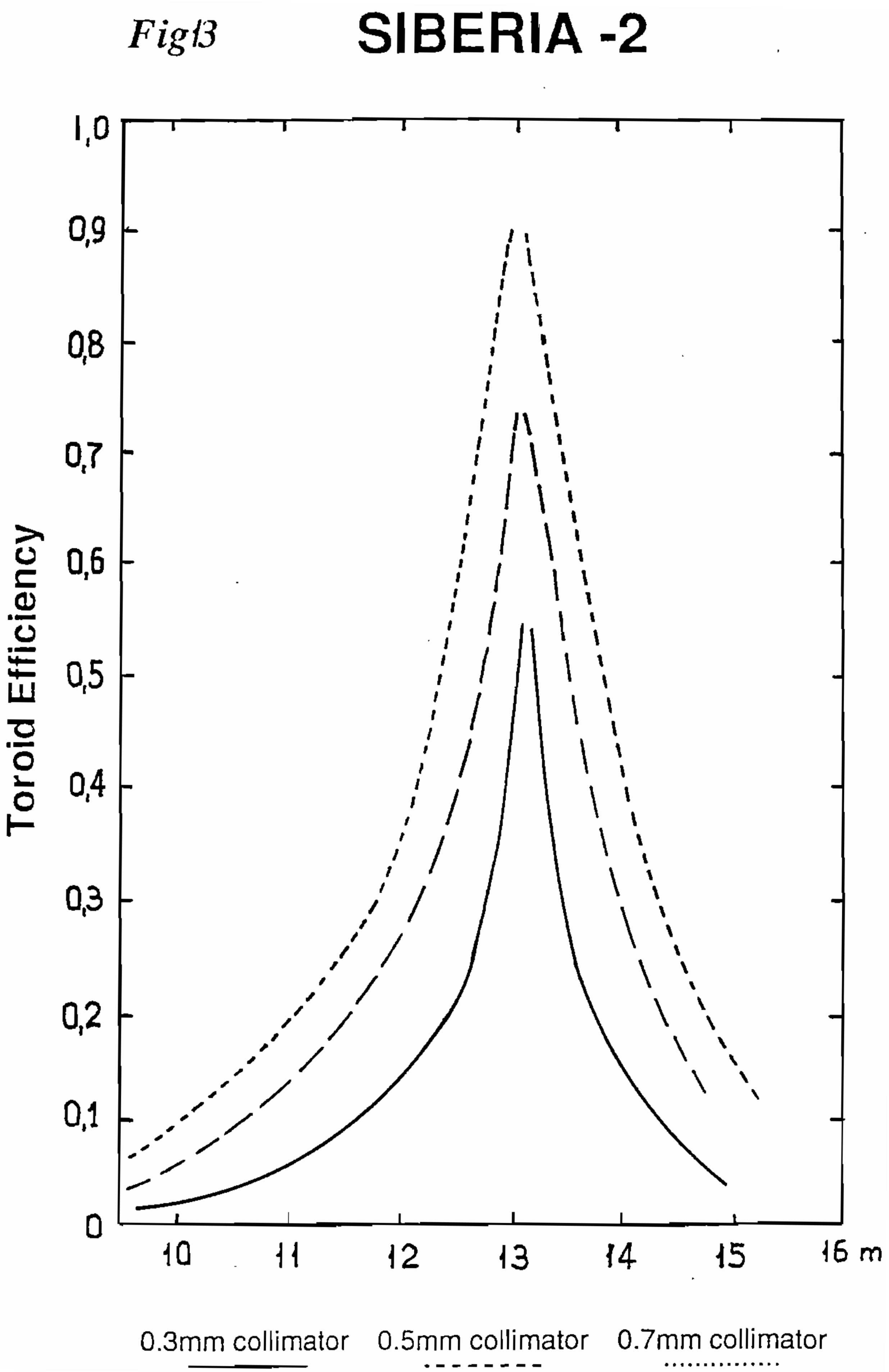


T.P. to mirror (m) = 16.500
T.P. to Xtal (m) = 29.500
Graze angle (mrad) = 3.000
Mer. Radius (m) =4847.470
Sag. Radius (mm) = 43.627
Yaw angle (mrad) = 0.000
Roll angle (mrad) = 15.000
Transl. error (mm) = 0.000

Total plotted rays= 531

[tk.plot]sibrol03
V. Rajko
16:56:53
6/MAR/90

Fig13


SIBERIA -2
Toroid Efficiency
1,0
0,9
0,8
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
10
11
12
13
14
15
16 m
0.3mm collimator
0.5mm collimator
0.7mm collimator