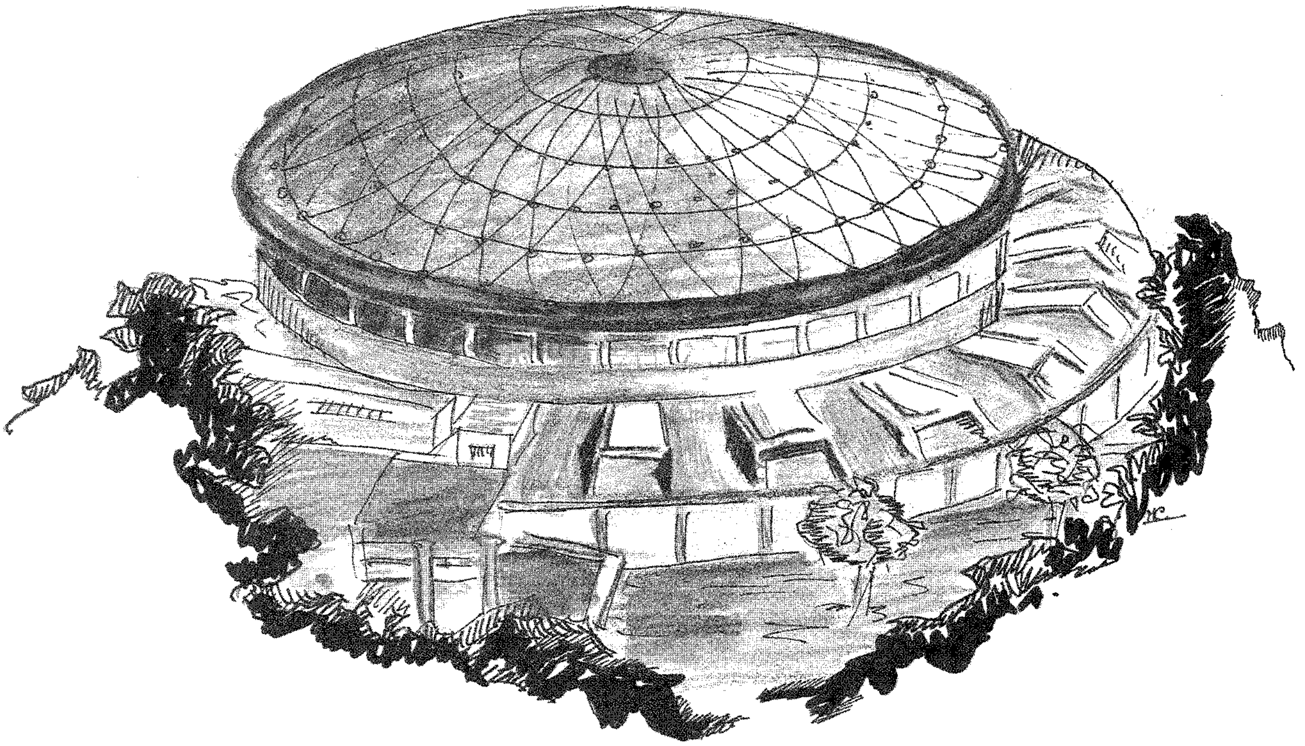
Laboratori Nazionali di Frascati

LNF-89/006R)
13 Febbraio 1989

F. Boscherini, A. Savoia, M. Sanchez del Rio:

RAY TRACING RESULTS FOR A MONOCHROMATOR ON THE SCOW SUPERCONDUCTING WIGGLER BEAMLINE



Servizio Documentazione
dei Laboratori Nazionali di Frascati
P.O. Box, 13 - 00044 Frascati (Italy)

INFN - Laboratori Nazionali di Frascati
Servizio Documentazione

LNF-89/006(R)
13 Febbraio 1989

RAY TRACING RESULTS FOR A MONOCHROMATOR ON THE SCOW SUPERCONDUCTING WIGGLER BEAMLINE

F. Boscherini, and A. Savoia
INFN - Laboratori Nazionali di Frascati, CP 13, I-00044 Frascati, Italy

M. Sanchez del Rio
Dept. de Fisica de la Materia Condensada, Universidad de Zaragoza, E-50009 Zaragoza, Spain

ABSTRACT

We analyze here the combined effect of focussing and diffraction for a double crystal monochromator which is being designed for the Superconducting Wiggler beamline (SCOW) on ADONE. A double separated crystal system has been chosen; we study the possibility of obtaining focalization in two steps, by bending dynamically the crystals in order to obtain both tangential and sagittal focussing. Non-focussing and semi-focussing systems have also been considered. The calculations have been performed with the ray tracing program SHADOW. On the basis of these results we select a 1:3 geometry for the monochromator position and estimate performance for the various focussing geometries. The effect of anticlastic curvature is also considered.

1. - INTRODUCTION

The superconducting wiggler to be installed on ADONE will produce a high photon flux in a rather wide energy range (critical energy 9 KeV). Because of the long distance between the source and the sample, it is convenient to focus the photon beam into the smallest possible spot. A double crystal focussing monochromator is studied to this end. One possibility for focussing is to bend dynamically (i.e. as a function of photon energy) the independent crystals to obtain both tangential and sagittal focalization. This configuration should be compared to other simpler ones, for example only sagittal focalization (semi-focussing system). When focalization is used, the relative position of source, monochromator and sample becomes very important, because of its connection with the magnification factor and diffraction properties. In order to chose the geometry which yields the highest photon flux onto the sample we have performed ray tracing calculations with the SHADOW computer program.

2. - WHAT IS SHADOW?

SHADOW(1) is a software package developed by F. Cerrina at the University of Wisconsin, with the goal of computing the propagation of a photon beam through an optical system. The program is designed to provide an optimal simulation of synchrotron radiation sources. Among its many capabilities it can generate different sources with different optical characteristics, monochromatic or white photon beams, and can also include polarization. The elements of the optical system can be mirrors, gratings, crystals, multilayers, filters, etc. with different surface figures (for example plane, parabolic spherical or toroidal). SHADOW calculates the incidence and reflection angles, the effect of diffraction and absorption of all the rays from the source. A set of satellite programs is designed to visualize the results in plots of intensity, absorption and resolution, and also it is possible to obtain the image on all the optical elements. SHADOW is available to all interested as a utility program on the LNF VAX computer.

3. - CHARACTERISTICS OF THE SOURCE

The source consists of the photon beam emitted from the 6T superconducting wiggler to be installed on ADONE. The characteristics of the electron beam at the wiggler midplane used for the calculation are:

σ_X=2.3mm	$\sigma_{X'}$=0.0549 mrad	ε_X=0.12 π mm mrad
σ_Z=0.16 mm	$\sigma_{Z'}$=0.03 mrad	ε_Z=0.0048 π mm mrad

Critical energy for the photon beam = 9 KeV.
Horizontal divergence accepted by the beamline = 8 mrad.

An image of the source is shown in Fig. 1.

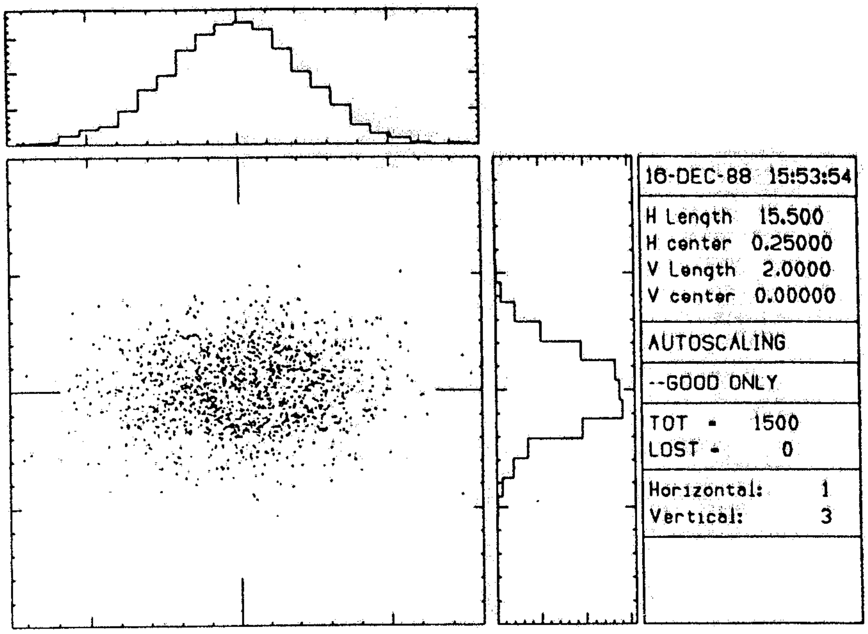


FIG. 1 - Image of the source at the wiggler midplane at 3 KeV. Distances are expressed in mm. Different horizontal and vertical scales have been chosen.

4. - X-RAY FOCUSSING

We study the combined effect of diffraction and focussing of cylindrically bent crystals. Ideally, the photon beam should be focalized in two directions, in the vertical plane (tangential focalization) and in the horizontal plane (sagittal focalization). We study the possibility of obtaining this double focalization by independently bending the two crystals of the monochromator. The radii of curvature are calculated by the focussing formulae:

$$1/s_1 + 1/s_2 = 2 \sin\theta / R_s$$

$$1/s_1 + 1/s_2 = 2 / (\sin\theta \ R_t) \qquad [1]$$

where s_1 and s_2 are the source-monochromator and monochromator-sample distances, R_t and R_s are the tangential and sagittal radii and θ is the Bragg angle. As the Bragg law fixes θ as a function of the energy, keeping s_1 and s_2 fixed, we must change R_s and R_t as a function of the energy in order to maintain the focalization at the sample position. This is illustrated in Fig. 2.

For our calculations we fix $s_1+s_2=32$ m, which is dictated by experimental floor requirements and we try two different geometries:

i) 1:1 geometry, where $s_1=s_2=16$ m and a magnification factor = 1;

ii) 1:3 geometry, where $s_1=24$ m, $s_2=8$ m and gives a magnification = 1/3.

Studying diffraction with bent crystals we have to note that: 1) for tangential focalization the optimal geometry of the system in terms of intensity and resolution should be 1:1 because in this case R_t approximates better the logarithmic spiral, that is the curve that provides no dispersion in θ ; 2) for sagittal focalization at high energies (> 5 KeV) a geometry around 1:3 is claimed to be best in reference 2 because the error in θ across the crystal is predicted to be minimized.

5. - RESULTS

The results of SHADOW calculations are reported in Appendix 1 for a number of Si diffraction planes. The double crystal system is abbreviated by two letters, the first one for the first crystal and the other for the second. F means flat crystal, T (S) means that the crystal has been bent cylindrically, according to [1], to provide tangential (sagittal) focalization. In many cases a horizontal slit has been considered before the first crystal of the monochromator and is abbreviated by "sl" and its extent in the vertical plane is given.

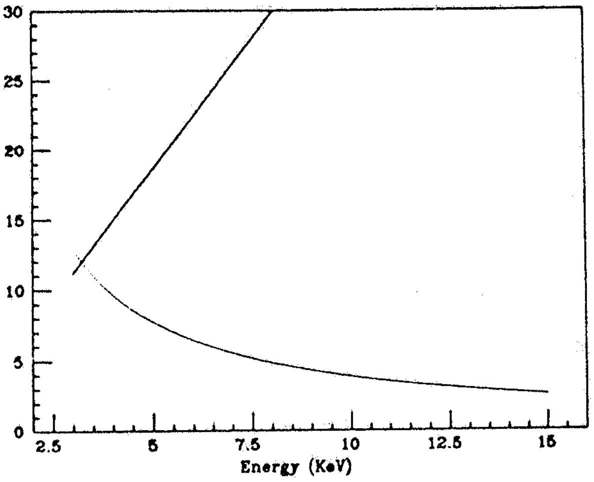


FIG. 2 - Plot of sagittal (dotted line) and tangential (solid line) radii (in meters) vs. energy for focussing with cylindrically bent crystals in a 1:3 configuration for Si (220) crystals.

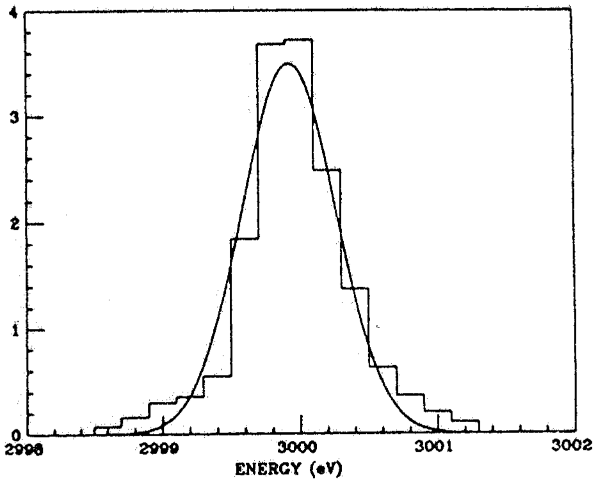


FIG. 3 - Fit with a gaussian of the intensity vs. energy histogram for TS(1:3) Si(111) system at 3 KeV.

I1 and I2 are the intensity after the first crystal and after the whole system, integrated over the image dimension and energy range. They are normalized for an incident intensity of 100 rays in an interval of 1 eV. dE_1 and dE_2 are the resolution, FWHM, after the first element and all the system. These values have been calculated by fitting the intensity vs. energy histograms with a Gaussian (see fig 3). σ_x and σ_z are the horizontal and vertical standard deviation of the ray distribution on the sample. With a Gaussian distribution (usual case) we have FWHM=2.35 σ, and with a box distribution σ corresponds to the total width and is indicated in the table with T.

B is a "brightness" at the sample and it is defined as:

$$B = I2 / dE_2 / W_x / W_z \qquad [2]$$

where W=2.35 σ for a Gaussian distribution and W=0.76 σ for a box distribution. F 5x5 is the total intensity per eV in a 5mm x 5mm spot size; this quantity is of interest because often samples investigated are small and of approximately this size. We note here that the results for Si(331) at 15 KeV have a greater error than the other cases because the total transmission is low and the statistics is not so good.

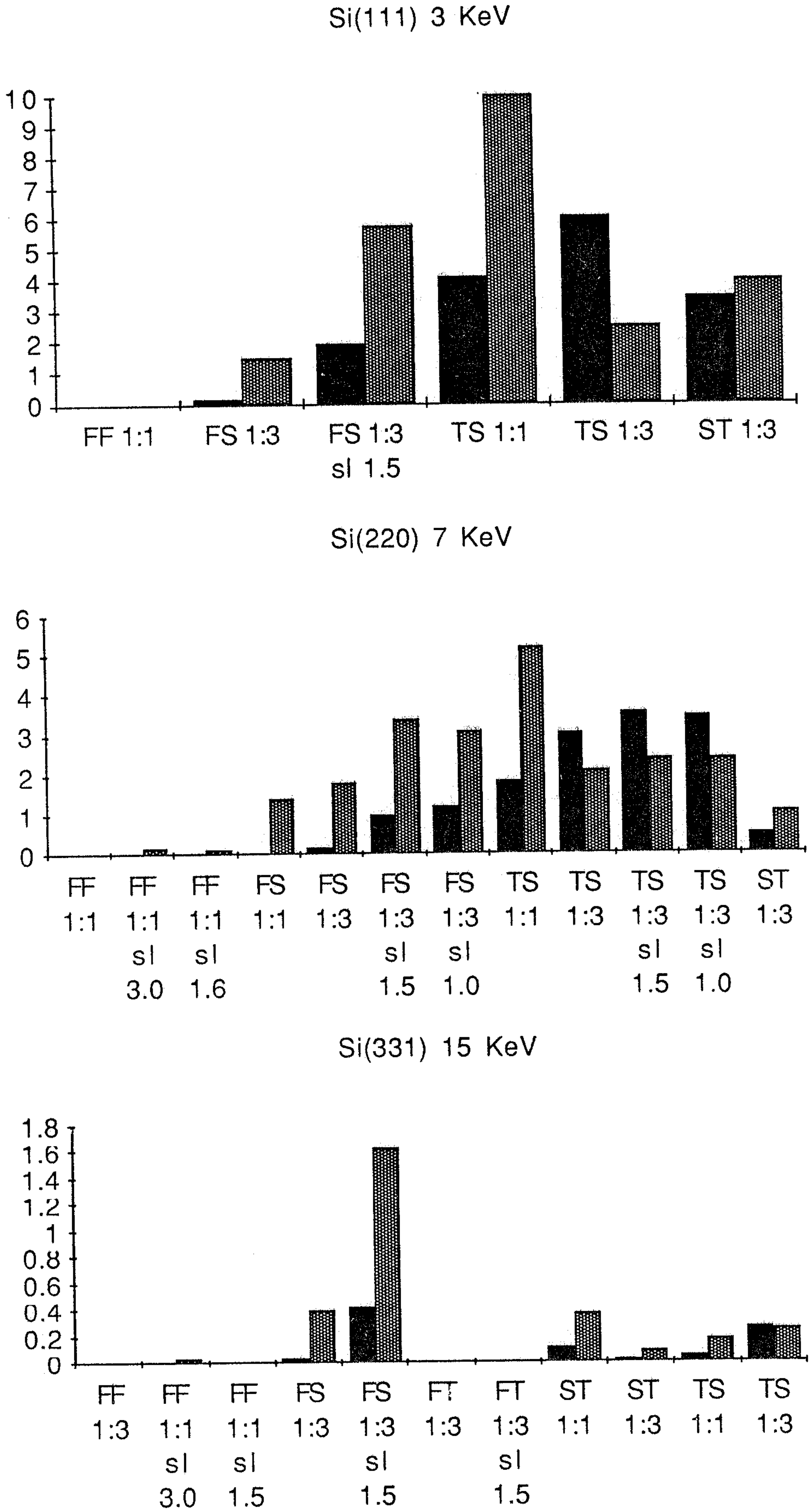
We show in Fig. 4 the histograms of some relevant quantities for different geometries. Some comments are in order:

1) TS versus ST configurations. In a 1:1 geometry these two configurations are equivalent. In the 1:3 geometry, TS is better than ST in both resolution and intensity, because sagittal focalization introduces more aberrations and produces a bigger mixing between horizontal and vertical divergences. These effects appear to worsen overall characteristics more if sagittal focussing is performed before rather than after tangential focussing.

2) Total intensity. The FF configuration yields the highest total intensities because coupling between the two crystals is optimized and intensity loss on double reflection is determined uniquely by the crystal reflectivity. The FS configuration slightly worsens this coupling. All TS configurations exhibit high losses on double reflection.

3) Resolution. A side effect of tangential focalization is to improve resolution, because the spread in Bragg angle is reduced across the crystal. TS(1:1) has a better overall resolution than TS(1:3) at lower energies (3 and 7 KeV), while the situation is inverted at 15 Kev; notice that this is true for the total system resolution, while tangential focussing always has a narrower bandwidth in the 1:1 geometry, as mentioned above. This points to the fact that errors in Bragg angle for sagittal focussing are minimized in a 1:3 geometry at high energy(2).

4) Brightness. This value takes into account the spot size, and is the flux density in the focal plane in a 1 mm^2 spot. TS(1:3) is always better than TS(1:1), because the magnification factor 1/3 plays an important role in this quantity. The system FS(1:3) with slit also gives very good results. We note here that although substantial flux is lost from bad coupling between the curved crystals the brightness for the TS(1:3) system is always 2 to 3 orders of magnitude higher than the FF case.



Si(111) 3 KeV

Si(220) 7 KeV

Si(331) 15 KeV

FIG. 4 - Histograms of B (full) and F 5x5 (hatched) for a number of double crystal configurations.

5) Flux in a 5x5 mm^2 spot. At low energy TS(1:1) is better than TS(1:3) and we have FS(1:3) in an intermediate position. At high energy (15 KeV) the most efficient system is FS(1:3) with slit while the comparison between TS(1:3) and TS(1:1) is ambiguous.

6. - ANTICLASTIC EFFECT

When thin crystals are mechanically bent the undesirable effect of transversal curvature is produced (3); this is illustrated in fig. 5. The anticlastic radius R_a is related to the bending radius R by

$$R_a = R/\Sigma \qquad [3]$$

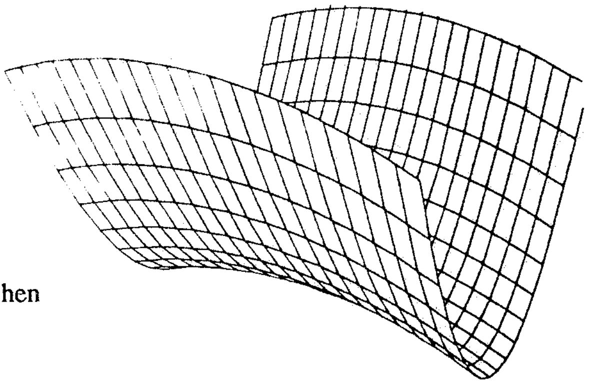


FIG. 5: Effect of anticlastic curvature when bending plates (schematic).

where Σ is the Poisson ratio (about 0.25 for Si). As $R_s < R_t$ (see Fig. 2) the anticlastic effect is much more important for sagittal focalization. In the case of silicon, anticlastic curvature on the sagittally focussing crystal produces a defocussing effect and because $R_a < R_t$ its magnitude is greater than the focussing effect on the first crystal. To avoid this situation one possibility is to cut ribs in the crystal, as shown(3) in Fig. 6. In this case, we have a new anticlastic radius:

$$R_a \simeq [\, 1 + (w/s)\,(h/t)^3\,(1 - \Sigma^2)\,]\, R_s / \Sigma \qquad [4]$$

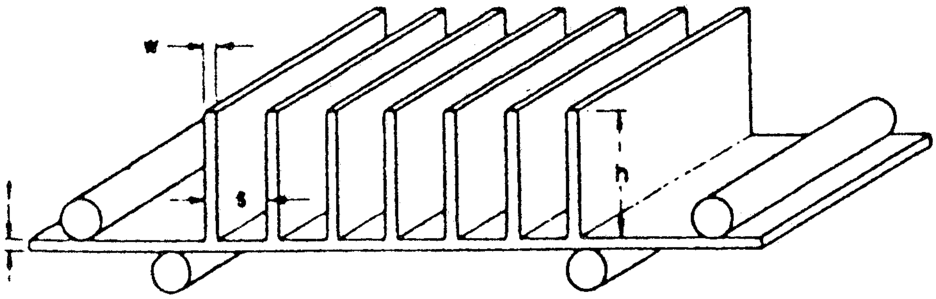


FIG. 6 - Disposition of reinforcing ribs to minimize the anticlastic effect. From reference 3.

where all the symbols are shown in Fig. 6. For our purpose we need to obtain, in TS systems, $R_a << R_t$ in order to maintain tangential focalization. We find that a radius of about R_a=100 R_s is sufficient to obtain good results as it is shown in Table I; this value can be obtained for example with t=w=0.7 mm, s=6 mm and h=4.22 mm. The possibility of changing the curvature of the first crystal to correct for the defocussing effect of the anticlastic curvature (without cutting ribs) has also been considered, but the results are not as good.

TABLE I - Comparison between TS 1:3 at 7 KeV with and without anticlastic curvature.

Crystal	sigmaX	sigmaZ	dE2	I 2	B	F 5x5	Rtang	Rsag	Ranticl
111	0.75	0.26	1.15	5	4.03	4.3	42.5	3.4	infinity
111	0.65	0.66	1.4	5.4	1.63	3.86	42.5	3.4	335.6
111	0.65	7.6	1.45	5.4	0.137	1.04	42.5	3.4	30.5
111	0.71	20.4	2.1	0.6	0.004	0.15	42.5	3.4	13.6
220	0.78	0.16	0.8	1.7	3.08	2.12	26	5.5	infinity
220	0.73	0.33	0.6	1.8	2.2	2.93	26	5.5	548
220	0.73	3.6	1.1	3.8	0.236	2.2	26	5.5	49.8
220	0.73	9.7	0.8	2.7	0.088	0.75	26	5.5	22.1

7. - CONCLUSIONS

The ray tracing calculations show that it should be possible to obtain relatively high fluxes into small spot sizes by using the TS (1:3) configuration. Alternatively, the FS (1:3) configuration will provide comparable results if a slit is used to improve the first crystal resolution; in any case at least two orders of magnitude in brightness are gained with respect to the double flat configuration. The 1:3 layout of optical elements is compatible with space requirements in the SCOW laboratory, and is the geometry which we have chosen. It will be necessary to cut ribs into the sagittally focussing crystal to reduce anticlastic curvature.

ACKNOWLEDGEMENT

This work has been partially supported by the cooperation agreement between INFN (Italy) and CICYT (Spain).

REFERENCES

[1] B. LAI and F. CERRINA, "SHADOW: A Synchrotron Radiation Ray Tracing Program" Nucl. Instr. and Meth. A246, 337 (1986).

[2] C.J. SPARKS, B.S. BORIE and J.B. HASTINGS "X-Ray Monochromator Geometry for Focussing Synchrotron Radiation Above 10 KeV" Nucl. Instr. and Meth. 172, 237 (1980).

[3] C.J. SPARKS, G.E. ICE J. WONG and B.W. BATTERMAN "Sagittal Focussing of Synchrotron X-Radiation with Curved Crystals" Nucl. Instr. and Meth. 194, 73 (1982).

APPENDIX 1

Results of SHADOW simulations for a number of geometries.

FOCALIZATION	I1	I2	dE1	dE2	I2/dE2	sigmaX	sigmaZ	B	F 5x5
	rays	rays	eV	eV	rays/eV	mm	mm	ry/eV/	ry/eV
								mm.mm	
Si(111) 3KeV									
FF 1:1	34	16	2.5	2.1	7.6	T 277	10.5	0.0015	0.037
FS 1:3	34	16	2.5	2.1	7.4	0.75	10.5	0.17	1.5
FS 1:3 sl 1.5	2.9	1.3	0.4	0.3	5.75	0.75	T 2.2	1.95	5.75
TS 1:1	34	4	0.5	0.4	10	2.2	0.2	4.12	10
TS 1:3	32	2	2.6	0.8	2.5	0.75	0.1	6.04	2.5
ST 1:3	34	2	2.5	0.5	4	0.77	0.27	3.48	4
Si(111) 7KeV									
FF 1:1	107	71	12.7	10.4	6.8	T 279	7.7	0.0018	0.044
FS 1:3	103.4	71.8	12.9	10.4	6.9	0.8	7.7	0.2	1.9
FS 1: 3 sl 1.5	10.3	7.3	1.6	1.2	6	0.8	T 2.8	1.5	6
TS 1:1	115	9	1.2	1.1	8.2	2.25	0.3	2.19	8.2
TS 1:3		5		1.15	4.3	0.75	0.26	4.04	4.3
ST 1:3		2.5		3.6	0.7	0.81	0.78	0.2	0.7
Si(220) 7 KeV									
FF 1:1	49.8	34.6	7.1	5.3	6.5	T 279	7.7	0.0017	0.042
FF 1:1 sl 3.0	16.4	11.8	1.9	1.4	8.4	T 279	T 6.4	0.0081	0.2
FF 1:1 sl 1.6	9.3	6.8	1.2	1	6.8	T 279	T 3.9	0.011	0.16
FS 1:1	49.8	30.1	7.1	5.3	5.7	2.31	7.76	0.058	1.44
FS 1:3	49.8	34.6	7.1	5.3	6.5	0.78	7.76	0.2	1.8
FS 1:3 sl 1.5	4.5	3.1	1	0.9	3.4	0.78	T 2.5	0.99	3.4
FS 1:3 sl 1.0	3.1	2.2	1	0.7	3.1	0.78	1.8	1.22	3.1
TS 1:1	49.7	2.6		0.5	5.2	2.3	0.22	1.86	5.2
TS 1:3		1.7		0.8	2.1	0.78	0.16	3.08	2.1
TS 1:3 sl 1.5	5.14	1.61	0.75	0.66	2.4	0.77	0.16	3.6	2.4
TS 1:3 sl 1.0	3.46	1.52	0.68	0.64	2.4	0.77	0.16	3.5	2.4
ST 1:3		1.4		1.3	1.1	0.79	0.45	0.55	1.1
Si(111)15keV									
TS 1:1	240	11.7	3.5	2.9	4	4.82	0.59	0.26	1.8
TS 1:3		5.5		2	2.75	0.78	0.58	1.1	2.75
ST 1:3		3.1		5.6	0.6	0.86	1.74	0.07	0.6
Si(220)15KeV									
FF 1:3	106	80	31.1	27.5	2.9	T 279	5.9	0.00099	0.025
FS 1:3		74.3	31.1	30.1	2.5	0.8	5.86	0.1	0.9
FS 1:3 sl 1.5		10.3	3.2	3.1	3.34	0.8	1.7	0.45	3.34

FOCALIZATION	I1	I2	dE1	dE2	I2/dE2	sigmaX	sigmaZ	B	F 5x5
	rays	rays	eV	eV	rays/e	mm	mm	ry/eV/ mm.mm	ry/eV
Si (220) 15 KeV		cont'd							
TS 1:1	100	4.6	1.9	1.7	2.7	2.81	0.88	0.2	2
TS 1:3		1.6		0.9	1.8	0.77	0.35	1.2	1.8
ST 1:3		1		4.1	0.24	0.84	1.1	0.05	0.24
Si(331)15KeV									
FF 1:3	25	18.4	15.1	15	1.23	T 279	5.9	0.00042	0.01
FF 1:1 sl 3.0	8.9	6.4	3.8	3.7	1.73	T 279	T 6.6	0.0016	0.041
FF 1:1 sl 1.5	3.5	2.3	2.9	2.8	0.82	T 279	T 3.6	0.0014	0.019
FS 1:3	25	16.7	15.1	15	1.11	0.78	5.85	0.044	0.4
FS 1:3 sl 1.5	3.7	2.6	1.7	1.6	1.63	0.78	T 2.7	0.43	1.63
FT 1:3		0.3		0.8	0.38	T 279	0.05	0.015	0.009
FT 1:3 sl 1.5	3.7	0.3	1.7	0.8	0.38	T 273	0.05	0.015	0.009
ST 1:1		0.41		1	0.41	2.3	0.28	0.12	0.38
ST 1:3		0.13		1.3	0.1	0.8	0.66	0.034	0.1
TS 1:1	26.8	0.21	1	1	0.21	2.3	0.27	0.06	0.19
TS 1:3		0.26		1	0.26	0.77	0.22	0.28	0.26
last rev	12	12	88		fb	msdr			