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REFLEC

A PROGRAM TO CALCULATE

VUV/X-RAY OPTICAL ELEMENTS

AND

SYNCHROTRON RADIATION BEAMLINES

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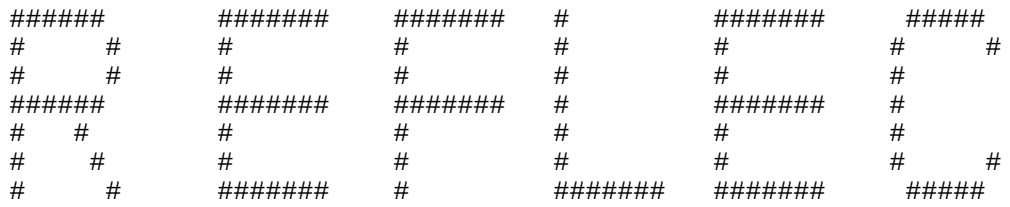
Version from 17.12.02



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WELCOME TO

R E F L E C

a program to calculate
VUV/X-RAY OPTICAL ELEMENTS
and
SYNCHROTRON RADIATION BEAMLINES

Version 21.2 of OCT./29/1996

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NEWS:
- VERSION 1.2 on PRG: -- Rs of Au -- (3. 1.87)
- including Rp and phase difference (21. 4.89)
- logarithmic axes implemented (23. 8.89)
- calculation of beamline with 5 mirrors (6.12.89)
- NEWS-Menue available (27. 7.90)
- Stokes Formalism for polarization (21. 8.90)
- Higher order reflectance (6.11.90)
- Synchrotron dipole-sources calculatio (6. 3.91)
- Multilayer reflectance with roughness (21. 2.92)
- Multilayer transmission (27. 2.92)
- Grating efficiency code of Neviere (30. 4.92)
- automatic BRAGG-Scan for multilayers (29. 6.92)
- calculation of absorbed/reflected Power 27. 4.93)
- implementation of crystal optic 8. 3.94)
- rearranging all (Michael's special) (23.11.94)
- crystal structure factors calculation (2. 2.95)
- MO_nochromator SX700-option (KJS Sahwney) (2.6.95)
- including Cromer tables (5-50 keV) (19. 1.95)
- Absorbed/transm. power also for foils' (19. 1.95)
- REFLEC installed at BESSY-II VAX-PRG (25. 7.94)
- with supermirror option (25. 8.95)
- new Henke-tables installed (30.11.95)
- ALPHA-version of REFLEC available (14. 2.96)
- NEW VERSION 21.1 -- BETA RELEASE -- (3. 7.96)
- including Quartz-crystal calculation (20. 3.96)
- Beamline calculations incl. gratings (5. 6.96)
- ADDITIONAL MULTILAYER FEATURES (25. 9.96)
- PS-Files now on SYS$SCRATCH (28.10.96)

SUMMARY

Based on data-sets for optical constants and/or atomic scattering factors for the UV, VUV and x-ray region, available for all elements and composite molecules, the program package REFLEC has been developed for calculation of the most relevant interaction parameters of radiation with matter:
Starting with the simulation of various synchrotron radiation lightsource characteristics, the reflection, diffraction, absorption, transmission and polarization as well as resolution parameters of the radiation can be calculated for a variety of optical components and graphically displayed.

Special attention was paid to a comfortable handling of the program and to practical applications. It is usefull for a quick survey of the performance of an optical design consisting of different optical components. In addition, it has become an inevitable means for optimization or comparison of individual elements such as (Multilayer-)mirrors, gratings, (ML-)foils, crystals or synchrotron sources or simply for calculation of material properties. Thus, REFLEC is an important tool for the design and optimization of of optical components as well as for complete synchrotron radiation beamlines.

Contents

I. Introduction

For the design of new beamlines at synchrotron radiation facilities or the improvement of existing beamlines, the calculation of the properties of optical components is a very powerful tool. Thus, e.g. the reflectance of different mirror coatings or the influence of different values of the surface roughness can be compared before ordering a new mirror. An even more demanding but very helpful feature is the calculation of the performance of complete beamlines. The program REFLEC developed at BESSY offers the possibility to compare up to 10 different elements or to calculate a complete beamline consisting of up to 10 optical elements. It is thus an essential tool of the BESSY software library for optical computations.

The flow chart in figure 1 shows the structure of the program. The graphical examples illustrate the capabilities of REFLEC for the calculation of individual optical elements and complete beamlines. The connection and interplay between the different programs available at BESSY, which is realized by exchange of ASCII-files is displayed in the flow chart in figure 2.

This report is supposed to be a quick and practical reference and to give examples for the use of the program rather than to give an outline of the underlying physical and optical principles which have partly been summarized e.g. in /1-6/.

II. Possible calculations

For the calculation of a beamline or the comparison of different synchrotron radiation sources, the spectrum of a bending magnet or a wiggler is calculated according to the Schwinger theory /7/. The parameters of several existing synchrotron radiation sources are already stored in the program.

The optical properties of mirrors, multilayers, filters, gratings and crystals are calculated from a recent compilation of atomic scattering factors in the spectral range from 30 eV to 30 keV /8/. Another data set covers the range up to 50 keV /9/. Additional data for lower energies down to 1 eV are also available for some elements and molecules /10/. For compound materials which can be defined by the case sensitive chemical formula (e. g. MgF_2), the contributions of the chemical elements are weighted. A tabulated or, if not available, calculated value for the density is proposed but can be changed. The surface roughness of mirrors or multilayers is taken into account according to the Nevot-Croce formalism /11/. The stored data sets can also be used to simply display the optical constants or absorption properties of the involved materials.

Due to the increasing interest in multilayers, the optical properties of these structures are calculated in transmission and reflection geometry by a recursive application of the Fresnel equations. For periodic multilayers, the layer thickness, density and surface roughness must be specified for each type of interface. For aperiodic structures like supermirrors, the exact structure has to be provided in a file. The energy dependence of e.g. the reflectance of a multilayer is calculated for a fixed

angle of incidence. As multilayers are also treated as dispersive elements, the angle of incidence can also be coupled to the photon energy for maximum reflectance in a given order.

For the calculation of (monolayer covered) gratings, a code developed by Neviere is

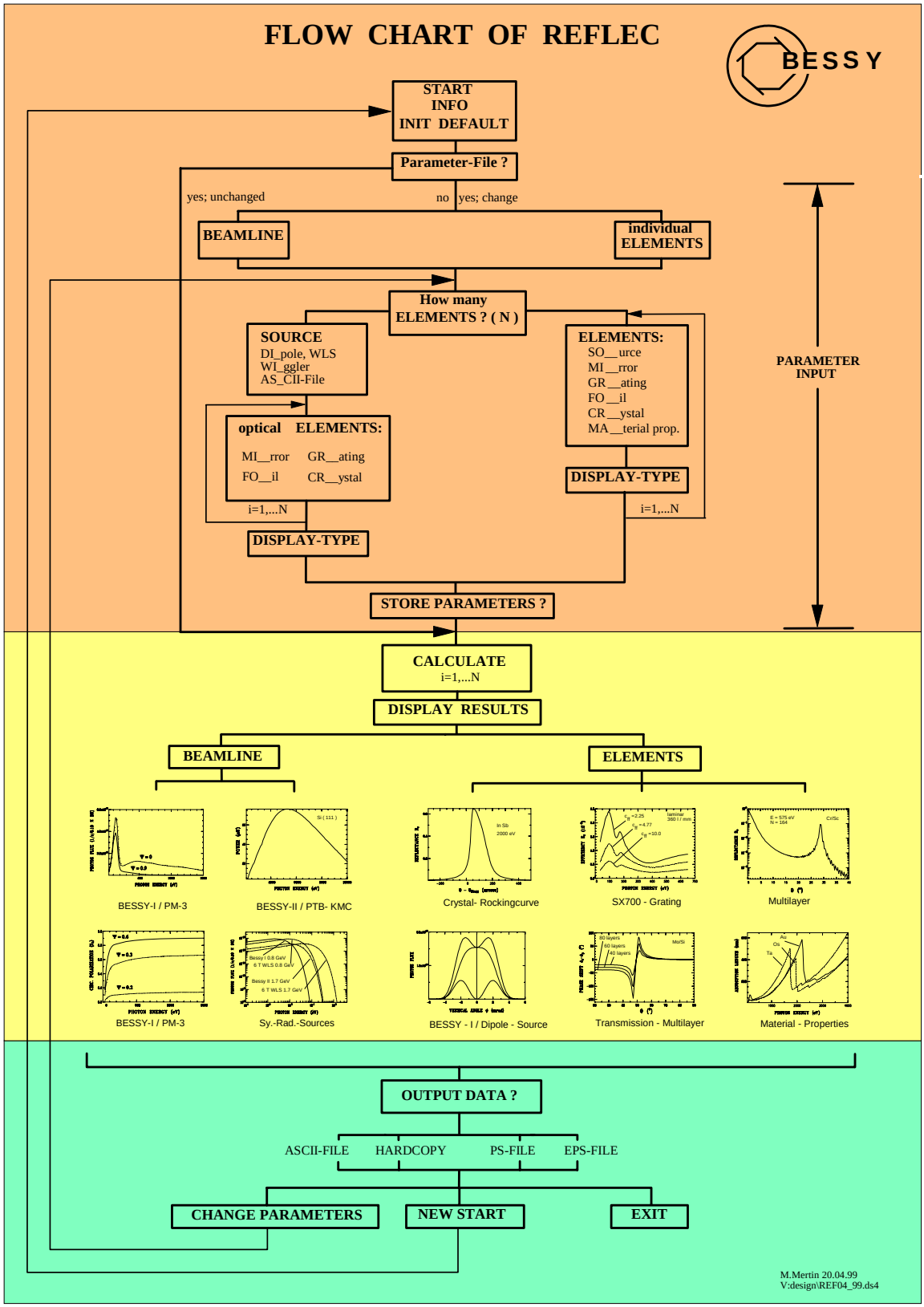

Fig. 1 Flowchart of REFLEC

used /12/, which allows for the calculation for three different grating profiles (sinusoidal, laminar or blazed). In addition to fixed deviation angle mounts, optionally the incidence angle can be coupled to the photon energy in the case of a Petersen monochromator (PM's, SX 700 type) or to any focus curve given as file input.

For crystals the diffraction properties are calculated from the dynamical theory using the Darwin-Prins formalism /13/. For all crystals with zincblende structure like Si, Ge or InSb as well as for quartz and beryl, the crystal structure factors are determined within the program as a function of the photon energy and the corresponding bragg angle. For other crystals, so-called rocking curves can also be evaluated if the structure factors are known from other sources. The calculation is possible for any allowed crystal reflection and asymmetry.

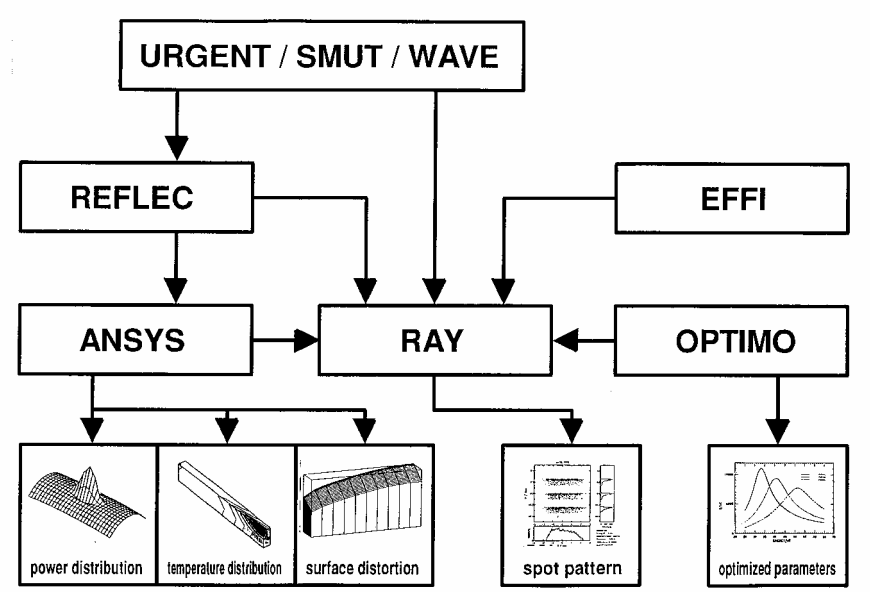

Fig. 2 BESSY soft x-ray computational tools and their interplay (see references 5)

Special attention was paid to polarization effects by application of the Stokes formalism. Thus, not only reflectance, transmittance or efficiency can be calculated for optical elements as a function of photon energy, wavelength or the involved angles, but also the phase change and the phase difference /14/.
If a complete beamline is considered, the photon flux for both polarization components can be calculated, as well as the radiant power or the power absorbed in a specific element. A beamline can consist of up to 10 optical components. Crystal or multilayer monochromators are treated as one element even if the monochromators consists e.g. of four crystals, because the beam divergence is taken into account in a complete integration in the DuMond diagram /15/. For beamlines containing these components the spectral resolution can also be calculated.

III. Computational requirements

The program runs under the operating system VMS on VAX and Alpha computers. The graphics output can be displayed on any X terminal and DEC- or UNIX workstation, send to a printer or saved in a PS or EPS file. It is possible to write the resulting data to ASCII files for input to other programs. The parameters for the calculation can be stored in a parameter file which is a very efficient way if complex calculations have to be repeated later with minor modifications.

BESSY-specific definitions:

At BESSY REFLEC can be started on all VAX or Alpha computers by typing:
RUN PRG:REFLEC.
The preferred printers can be defined as the logicals RAY_PRINTER_1 and _2.
To save disk space during printing, the logical SYS$SCRATCH can be defined as BESSY_SCRATCH.

IV. Summary of the features of REFLEC

- **Data sets (see table 1):**

-- Experimental optical constants n,k for various Materials (VUV-region) /10/
-- Palik-Tables for optical constants n,k for selected elements and molecules /10/
-- Henke-Tables for f_1,f_2 scattering factors for 92 elements (30eV-30 keV) /8/
-- Cromer-Tables for f_1, f_2 scattering factors for 92 elements (5-50 keV) /9/
-- Structure Parameters for crystals with Zincblende-structure (e.g. InSb, Ge, Si) and Beryl, Quartz

Material	**Start-Energy** (eV)	**Stop-Energy** (eV)	**No. of points**
Al	5	40	301
Au	5	9919	301
C	5	30	85
Cr	5	30	102
Cu	5	2017	301
Ir	5	40	301
Ni	1	9919	321
Os	5	2017	301
Pt	2	2017	326
Si	1	2000	242
Al_2O_3	5	100	96
MgF_2	11	83	153
SiC	10	1000	94
SiO_2	1	2000	204
Henke	10 (f_2)	30000	506

(Z=1-92)	30 (f_1)		
Cromer (Z=3-92) (76 elements)	5000	50000	451

Table 1 data sets for optical constants and atomic scattering factors

Material names (chemical symbols) are case sensitive, e.g. MgF_2.
If no experimental datasets are available at the desired energy, a composite material is arithmetically composed from elemental data

-- Source parameters (Ring energy, critical energy) of most Synchrotron Radiation Facilities

• Synchrotron Radiation Sources

-- Bending Magnet radiation
-- Wavelength Shifter radiation (dipole)
-- Wiggler radiation (series of dipoles)
-- Undulator radiation as input file (energy / photon flux / emission angle / bandwidth)

• Optical Elements

-- Mirrors (including multilayers, supermirrors as input file (layer thickness , roughness)
-- Gratings (including monolayer)
-- Foils (including multilayers)
-- Crystals

• Beamlines

-- Grating monochromators (including SX700, SGM-scan-option, any focal curve by input file (energy / angle))
-- Crystal or ML- monochromators (including 2, 4-crystal option, ML-peak reflectance scan)
-- any optical setup of up to 10 elements (e.g. polarizer)
-- including real source characteristic

• Display Features

-- reflection, diffraction, absorption, transmission, polarizance etc. of optical elements
-- photon flux, power, polarization, resolution etc. of synchrotron sources or beamlines

as a function of the involved angles, energies or wavelengths

-- up to 10 curves simultaneously for comparison of individual elements

OR

-- 1 curve for a series of up to 10 optical elements, including a source

If different beamlines are to be compared, each result should be written to an ASCII-file and then read in for an overall plot

- **Program output**

-- Graphical display of results on VT100, DEC-Term, X-Term Window
-- ASCII-datafiles
-- Hardcopy, PS-Files, EPS-Files
-- Parameter File for all input data

- **Hardware**

-- VAX or ALPHA

at BESSY the REFLEC.EXE Versions are installed on the general accounts PRG:
Program-call from any account at any VAX or ALPHA by

RUN PRG:REFLEC

- **Software installation**

-- BESSY-Graphic-library PLT96
-- Logicals: RAY_OPTCON, SYS$SCRATCH, PLT
-- RAY_SETUP.COM-Commandfile for individual installation of Printerqueues RAY_PRINTER_1 and 2, resp.

- **Directory installations**

VAX, ALPHA at BESSY	**Main directory**	**Subdirectory**	**Subdirectories**
Directory structure	PRG_ROOT =RAY_OPTCON	PRG_ROOT:[RAY]	MOLEC PALIK HENKE CROMER CRYSTAL
Files	REFLEC.EXE	Info-files	Data-files *.f12* *.nk* crystal.txt table.f0

- **Source-Program-Packages**

-- REFLEC.FOR
-- CRYSUB.FOR
-- FUNCTION.FOR
-- RAYLIB.FOR
-- OPTCON.FOR
-- OPTICS.FOR

-- SOURCE.FOR
-- PLT96.LIB

Acknowledgement

Thanks are due to many users of the program, in particular to all collegues at BESSY and PTB. Without their comments, questions, critics, suggestions, problems and patience over the years the program would not exist.

V. References

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VI. Appendix

Internal parameter structure of the program

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I Source parameters (SPAR(10,30):

Parameter \ Source type	NO 1	DI 2	WI 3						
1 = no of source	1	2	3						
2 = name of dipole/wiggler	-	x	x						
3 = start energy (eV)	x	x	x						
4 = stop energy (eV)	x	x	x						
5 =	-	-	-						
6 = S1/S0 (lin. pol.)	x	x	x						
7 = S2/S0 (lin. pol.)	x	x	x						
8 = S3/S0 (circ. pol.)	x	x	x						
9-11 = ...	-	-	-						
13 = ring energy (GeV)(+/-)	-	x	x						
14 = critical energy (keV)	-	x	x						
15 = no of periodes	-	1	x						
16 = beam divergence sig_h'	-	-	x						
17 = beam divergence sig_v'	-	x	x						
18 = diverg. fit Par. A	-	-	x						
19 = diverg. fit Par. B	-	-	x						
20 = beam size (sig-h)	-	x	x						
21 = beam size (sig-v)	-	x	x						
22 = ring current (mA)	-	x	x						
23 = energy resolution (%)	-	x	x						
24 = acceptance hor.(mrad)	-	x	x						
25 = acceptance vert.(mrad)	-	x	x						
26 = start vert. acceptance	-	x	x						
27 = stop vert. acceptance	-	x	x						
28-30 = ...	-	-	-						

II Optical Element Parameters (MPAR(10,60)

Parameter \ ITEM	SO 1	MI 2	GR 3	FO 4	CR 5	MA 6	WI 7	PO 8		
1 = no of item	-1	1	2	3	4	5	6	7		
2 = type of item	SO	MI	GR	FO	CR	MA	WI	PO		
3-4 = name of substrate	-	x	x	x	x	x	x			
5-6 = name of 1. coating	-	x	x	x	-	x		S1		
7-8 = name of 2. coating	-	x	x	x	-	x		S2		
9-10= name of top coating	-	-	-	-	-	-		S3		
11 = no of layers	-	x	x	x	-	-				
12 = thickness substr(nm)	-	-	-	x	-	-	x			
13 = thickn. odd layers	-	x	x	x	-	-				
14 = thickn. even layers	-	x	-	x	-	-				
15 = thickn. top coating	-	x	-	x	-	-				
16 = density sub.(g/cm^3)	-	x	x	x	-	x	x			
17 = density odd layers	-	x	x	x	-	-				
18 = density even layers	-	x	-	x	-	-				
19 = density top coating	-	x	-	x	-	-				
20 = roughness sub.(nm)	-	x	-	x	-	-				
21 = roughness odd layers	-	x	-	x	-	-				
22 = roughness even lay.	-	x	-	x	-	-				

23 = roughness top coat	-	x	x	x	-	x			
24 = ...	-	x	-	x	-	-			
25 = start BRAGG angle	-	x	x	x	x	-	x	α	
26 = stop BRAGG angle	-	x	x	x	x	-			
27 = start azimuth. angle	-	x	x	x	x	-			
28 = stop azimuth. angle	-	x	x	x	x	-			
29-30 = ...	-	-	-	-	-	-			
31 = F0 IM	-	-	-	-	x	-		δ	
32 = F0 RE	-	-	-	-	x	-		Tp/Ts	
33 = FH RE	-	-	-	-	x	-		Rp/Rs	
34 = FH IM	-	-	-	-	x	-			
35 = FHC RE	-	-	-	-	x	-			
36 = FHC IM	-	-	-	-	x	-			
49 = unit cell volume	-	-	-	-	x	-			
50 = Cff/2.lattice.const.	-	-	x	-	x	-			
51 = ML-num/l-dens/struct	-	x	x	-	x	-			
52 = diffra.order/cr-num.	-	x	x	-	x	-			
53 = gr-type/1.lat.const.	-	-	x	-	x	-			
54 = blaze angl/1. Miller	-	-	x	-	x	-			
55 = apex angle/2. Miller	-	-	x	-	x	-			
56 = groove depth/3. Mill	-	-	x	-	x	-			
57 = groove width/asym.	-	-	x	-	x	-			
58 = limit.vert.beam.div.	-	-	x	-	x	-			
59 = offset angle 2.cryst	-	-	-	-	x	-			
60 = detuning crystal p..	-	-	-	-	x	-			

III Display Parameters

X-Axis parameter-buffer XPAR(10,10,512)

Y-Axis parameter-buffer DPAR(10,100,512)

	Y-AXIS						X-AXIS			
	SO	MI	GR	FO	CR	MA	HV LAM	PSI	ALP BET 2TH	PHI
no of item	-1	1	2	3	4	5	1-2	3	4-7	8
Beamline or individual elements										
1-10 =	-	-	-	-	-	-	-	-	-	-
11 = nat. hor. diverg. WI	x	-	-	-	-	-	x	-	-	-
12 = nat. vert. diverg.	x	-	-	-	-	-	x	-	-	-
13-20=	-	-	-	-	-	-	-	-	-	-
21 = I_par	x	x	x	x	x	-	x	x	x	x
22 = I_perp	x	x	x	x	x	-	x	x	x	x
23 = I_total (N/s)	x	x	x	x	x	-	x	x	x	x
24 = emit./refl. Power	x	x	x	x	x	-	x	x	x	x
25 = abs. Power	-	x	x	x	-	-	x	x	x	x
26 = integr. emitt. Power	x	x	x	x	-	-	x	x	x	x
27 = integr. abs. Power	-	x	x	x	-	-	x	x	x	x
28-30=	-	-	-	-	-	-	-	-	-	-
31 = S1/S0	x	x	x	x	x	-	x	x	x	x
32 = S2/S0	x	x	x	x	x	-	x	x	x	x
33 = S3/S0	x	x	x	x	x	-	x	x	x	x
34 = P_tot	x	x	x	x	x	-	x	x	x	x
35 = total phase phi	x	x	x	x	x	-	x	x	x	x
36 = psi (ellipticity)	x	x	x	x	x	-	x	x	x	x
37 = chi (ellipticity)	x	x	x	x	x	-	x	x	x	x
38 = S3**2 * I	x	x	x	x	x	-	x	x	x	x
39-40=	-	-	-	-	-	-	-	-	-	-
Individual Elements										

41 = Resol. E/dE (s-pol)	-	x	-	-	x	-	x	-	-	-
42 = Resol. E/dE (p-pol)	-	x	-	-	x	-	x	-	-	-
43 = Resol. dE (s-pol)	-	x	-	-	x	-	x	-	-	-
44 = Resol. dE (p-pol)	-	x	-	-	x	-	x	-	-	-
45 = Bragg Angle	-	x	-	-	x	-	x	-	-	-
46 = FWHM (s-pol)	-	x	-	-	x	-	x	-	-	-
47 = FWHM (p-pol)	-	x	-	-	x	-	x	-	-	-
48 = Integ.refl.power (s)	-	x	-	-	x	-	x	-	-	-
49 = Integ.refl.power (p)	-	x	-	-	x	-	x	-	-	-
50 =	-	-	-	-	-	-	-	-	-	-
51 = R_s, T_s, E_s	-	x	x	x	x	-	x	-	x	x
52 = R_p, T_p, E_p	-	x	x	x	x	-	x	-	x	x
53 = R, T, E_unpol	-	x	x	x	x	-	x	-	x	x
54 = Polarizance s/p	-	x	x	x	x	-	x	-	x	x
55 = Delta_s	-	x	x	x	x	-	x	-	x	x
56 = Delta_p	-	x	x	x	x	-	x	-	x	x
57 = Delta_s-p	-	x	x	x	x	-	x	-	x	x
58 = Complex rs RE	-	x	x	x	-	-	x	-	x	x
59 = Complex rs IM	-	x	x	x	-	-	x	-	x	x
60 =	-	-	-	-	-	-	-	-	-	-
61 = mass abs. coeff.	-	-	-	-	-	x	x	-	-	-
62 = linear abs. coeff.	-	-	-	-	-	x	x	-	-	-
63 = abs. length	-	-	-	-	-	x	x	-	-	-
64-70=	-	-	-	-	-	-	-	-	-	-
71 = n / (RE(F0))	-	-	-	-	x	x	x	-	-	-
72 = 1-n / (RE(F0))	-	-	-	-	x	x	x	-	-	-
73 = k / (IM(F0))	-	-	-	-	x	x	x	-	-	-
74 = f1 / (RE(FH))	-	-	-	-	x	x	x	-	-	-
75 = f2 / (IM(FH))	-	-	-	-	x	x	x	-	-	-
76 = eps1 / (RE(FHC))	-	-	-	-	x	x	x	-	-	-
77 = eps2 / (IM(FHC))	-	-	-	-	-	x	x	-	-	-
78-100=	-	-	-	-	-	-	-	-	-	-

IV General parameter-buffer IPAR(100)

```
 1-10  = no of y-axis display parameter for 10 OEs
 11-20 = x-axis data points for 10 OEs (max=512)
 21 = beamline or individual elements (1 or 2)
 22 = how many items (beamline elements or OE)
 23 = start-value not equals stop value (flag f. x-axis display)
 24 = display y-axis survey
 25 = display as function of hv,lam,psi... (x-axis)
 27 = crystal/ML-mono flag (=0,1)
 30 = parameter file (IPF)
 31 = no of turns (ITURN)
 41 = Terminal type (ITERM)
 42 = Hardcopy device (IHCP)
 51 = No of lines to plot (NOLNS)
```