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The PRSCAL Manual

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The PRSCAL Manual

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Unit conventions:

Energies are given in meV.
Scattering vectors are given in reciprocal lattice units.
Flight times are given in microseconds.
Angles are given in degrees.
Lattice constants and d-spacings are given in Å.

Spaces or commas may be used as separators.

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Contents

1 Introduction

The PRSCAL program is a "simulation" version of the PRISMA operating program. The commands in PRSCAL are, as far as is possible, identical to those in the PRISMA program. Therefore command procedures can be tested out before they are tried out on PRISMA itself. A particular example of this would be with the CD command, where PRSCAL can be used to try out various possible sets of CD values to see which is the best or most appropriate. The PRSCAL program can also provide extra information on the configurations set up with the BR and CD commands which may be useful in planning or interpreting measurements. It also provides routines for calculating the resolution function in different configurations and for plotting the different measuring paths on an appropriate reciprocal space diagram.

On the PRISMA microVax the program can be run in the PRSMGR and PRISMA accounts by typing :

PRSCAL
or
PRSCALU

The situation on the ISIS Vax computers ISISE/ISVS5/etc. is that you can run either of these programs, using just the names given above if you have executed the DCL command file

PRISMA_GENIE_SETUP.COM

This file sets up the various path names and symbols for PRSCAL/PRSCALU, and also for the PRSPLOT6 program and the PRISMA GENIEINIT.COM file. See one of the PRISMA instrument scientists about setting up PRISMA_GENIE_SETUP.COM in your account.

On the PRISMA microVax the program will start by loading the current values of all motor angles and the current parameter list (lattice parameters etc.) of the spectrometer. On ISISE/ISVS5 etc. a default set of parameters will initially be loaded and the user should modify these to their desired values. The PRSCAL program (just as does the PRISMA program) has built-in routines to check for possible analyser or detector clashes when moving. This requires detector and analyser shape parameters to be loaded. On both microVax and ISISE/ISVS5 etc. these files are appropriate for the current detector arms and pyrolitic graphite analyser shapes. It is possible to use other files however (for germanium and mica analysers for example) and if you wish to do this please contact a PRISMA instrument scientist.

The prompt in the PRSCAL program is different from that of the PRISMA control program and is just :

CAL>

The following sections describe the various parameters and the commands that are available. Those that will perhaps be of most use are BR, CD, RE and RC, and these are described in greater detail than the others.

2 PRSCAL or PRSCALU ? — Computer and Library requirements

There are two versions of the PRISMA simulation program, PRSCAL which uses DEC GKS and NAG graphics and PRSCALU which uses UNIRAS graphics. The difference between these two programs on VAX machines only lies in their use of different plotting routines, all other routines being identical. There is a version of PRSCALU which runs on the SUN SparcCenter 2000 (a UNIX system) at Keele University and uses the UNIRAS graphics routines. This program has different routines for calculating the DATE and TIME (printed out by some commands in PRSCAL), the J command, the programs interaction with the terminal status after plotting and also the "logical names" for the spectrometer files. However in all cases the FORTRAN code performing the calculations (of angles, time of flight etc. etc.) is identical. The differences in plotting routines are accounted for by the subroutines PLOTGKS and PLOTUN and the differences in system parameters by the J4JUMP and SYSFIX subroutines, all other subroutines being identical. On the ISIS Vax computers either version can be run, although on the PRISMA microVax the best choice of the which of the two programs to use depends on circumstances. On the Keele Vaxstation (phvax5) only PRSCAL is available and on the SparcCenter 2000 (potter) only PRSCALU is available.

On the PRISMA MicroVax

The choice of PRSCAL or PRSCALU on the PRISMA microVax II depends on whether you want to do any plotting or not. The microVax II is an old machine, plotting UNIRAS graphics is a cpu intensive process for it and Thus if you want to do plots use PRSCAL on the microVax. However if you don't want to plot it is best to use PRSCALU. The reason for this is that GKS interacts with the graphics screen on a Falco/Pericom/Emutek/Teemtalk whether you plot or not. As a consequence it can be a nuisance if you have the dashboard on.

3 Your Terminal and Printer Type

After starting PRSCAL or PRSCALU the user is prompted for the type of terminal and hardcopy (printer) device that they are using. For both programs the choices are basically the same but the names are slightly different.

Option	PRSCAL	PRSCALU
1	Pericom/Falco	Pericom/Falco
2	TEEMTALK/EMUTEK	MT42XX
3	MOTIF	MX11

1) Pericom/Falco

The first terminal option in both programs is a Pericom/Falco choice. This option is a terminal which emulates a DEC VT100 (or higher) for the alpha screen and a Tektronix 4010 series for the graphics screen.

2) TEEMTALK/EMUTEK

In PRSCAL the second option is the GKS driver for a Tektronix 4200 series terminal which is described as the TEEMTALK/EMUTEK option. In PRSCALU the second option is MT42XX, which is the UNIRAS multi-driver for a Tektronix 4200 series colour terminal, which is the type of terminal emulated by the EMUTEK and TEEMTALK terminal emulators on a PC.

3) MOTIF/MX-11

The third option in PRSCAL is described as MOTIF, and is the GKS X-11 Motif windows driver. This is appropriate for the Vax workstations and the eXcursion emulator on the PC's at ISIS and for

the phvax5 Vaxstation in Keele. In PRSCALU the third option is MX11, this is the multi-driver in UNIRAS for an X-11 windows terminal (or workstation, eg. the Vaxstations at ISIS, the eXcursion emulators on the PC's at ISIS, the phvax5 Vaxstation and the SUN workstations at Keele).

The hardcopy plot files produced by both programs is in the POSTSCRIPT format and is contained in the file called POST.DAT. Text files produced are given a variety of names (the routine in PRSCAL/PRSCALU that produces the output will inform you of the filename) in the VMS "carriagecontrol" format.

4 Spectrometer parameters and angle names

In this section the names used for the various spectrometer and sample parameters in the PRISMA and PRSCAL programs are described. It is divided into two sub-sections, the first describes the names used for the different angles involved in defining the spectrometer configuration and the second describes the parameters used to define (i) the motor zero and limit angles, (ii) the sample, (iii) the analyser crystals and (iv) the time of flight channels.

4.1 Description of Angle Names:

The convention used to represent (name) the angles (motors) on PRISMA is as follows :

A< nn >	-	Analyser angles, < nn >= 1 to 16.
D< nn >	-	Detector angles, < nn >= 1 to 16.
PHI< nn >	-	ϕ angle (scattering angle) for analyser-detector system < nn >. < nn >= 1 to 16
OMEGA or OM	-	The omega angle of the sample.
GX,GY	-	The tilt angle of the two perpendicular arcs.

The angles D1-16,A1-16 and PHI01 are displayed on the P.C. screen under the headings DET1 to DET16, ANA1 to ANA16 and PHI. Please note that there are in fact two angles printed beneath each name on the PC screen, it is only the top of the two numbers that is relevant, ignore the one underneath. These "top" angles should be the same as those printed by the PRint command. The angles OMEGA, GX and GY are displayed on the "dashboard" display under the names PSI, ANG1 and ANG2. There is a difference between the values of OMEGA, GX and GY and those of PSI, ANG1 and ANG2. The latter are the "absolute" angles on the goniometer, while the former are defined with respect to the crystal axes. The omega angle is defined as the angle that the direction PX makes to the direction of the incident beam, ie. omega is 0 when PX is parallel to $\mathbf{k}_i$. These differences between OMEGA and PSI are therefore just the zero angles for the crystal ie. :

$$\text{PSI} = \text{ZOM} + \text{OM} \quad ; \quad \text{ANG1} = \text{ZGX} + \text{GX} \quad ; \quad \text{ANG2} = \text{ZGY} + \text{GY}$$

where ZOM, ZGX and ZGY are the zero angles themselves.

4.2 Description of PRISMA parameters:

There are 4 groups (or families) of parameters in the PRISMA program, the motor zero/limit parameters, the sample parameters, the analyser parameters and the time of flight parameters. Within each of these groups there is a sense of order (this is relevant to the SE command), eg for the sample parameters the order is A,B,C, <AB,<AC,<BC,PX(1),PX(2),PX(3),PY(1),PY(2),PY(3) and the parameters are presented in this order. There is however no sense of order between groups.

4.2.1 Motor parameters:

Z< nn > zero offset of motor nn

L< nn > lower limit of motor nn

U< nn > upper limit of motor nn

4.2.2 Sample parameters:

A,B,C	lattice constants
<AB, <AC, <BC	lattice angles
PX(1), PX(2), PX(3) PY(1), PY(2), PY(3)	Vectors defining the scattering plane

4.2.3 Analyser parameters:

DD	d-spacing of the analyser crystals in Å d=6.71 for pyrolitic graphite d=5.6569 for germanium d=6.71 for mica
AH, AK, AL	Miller indices of analyser scattering plane (0,0,-2) for pyrolitic graphite (1,1,1) or (1,1,3) for germanium (0,0,-1) or (0,0,-2) for mica
DMIN, DMAX	first and last of the array of active analysers
IANAL	default analyser ; some commands require a designated analyser, if not expressly stated otherwise, the program will use this default analyser
MOD	scattering sense of the analysers ; MOD=+1: scattering to the left MOD=-1: scattering to the right (looking in the direction of the neutron beam) MOD=0: corresponds to the straight-through position of the detector(2-axis mode of PRISMA)

4.2.4 Time Of Flight parameters:

MNT — type of monitor counting unit.
MNT=0 is "forever" (ie. until an END command is issued by the supervisor)
MNT=1 is for ISIS frames
MNT=2 is for neutrons in the monitor
MNT=-1 does not perform any counting, the spectrometer is positioned but does not count.

MNS — size of "monitor" count, either
number of frames (MNT=1) or
number of neutrons in monitor (MNT=2)

BIN — BIN=1: channels are specified in constant time steps
BIN=0: use channels specified in CHANGE program

START — value where the DAE should start taking data, given in microseconds (BIN=1)

STOP — value where DAE should stop taking data, in microseconds (BIN=1)

STEP — Size of time channel (BIN=1) bins in microseconds

5 The Printing, Setting and Positioning Commands

5.1 The PRint command:

This command allows you to print the present value of all the parameters or of a set of parameters. The general form of the command is:

$$\text{PR} < nn >$$

with $< nn >$	=	SAMP	sample parameters
		ZERO	zero offset values
		ANGL	present angle positions
		LIMI	upper and lower limits of angles
		ANAL	analyser parameters
		TOF	time-of-flight parameters
		EF	energy settings of the active analysers
		ALL	everything is printed

or any combination like

PR ANAL SAMP

5.2 The SEt command:

The general form is :

$$\text{SE} < nn >= x$$

All parameter changes which do not involve a positioning of a motor are performed with the set command. More than one parameter can be changed at a time, e.g.:

SE <AB=120,IANAL=10,PX(1)=0

If the order in a parameter string is kept, only the first parameter to be changed has to be named, e.g.:

SE A=6.38 6.38 6.38 90 90 90

will set A=6.38, B=6.38, C=6.38, <AB=90, <AC=90, <BC=90. The parameters which can be set are grouped as sample parameters, analyser parameters, etc. These groups and the order of the parameters within the group were given in section 4.2. Please note that although there is a sense of order between parameters within a group there is not one between groups.

5.3 The DRive command:

The general form is :

$$\text{DR} < nn >= xx$$

This command will drive one or several angles to a new position, e.g.:

DR PHI13=56.66
DR D2-15=23.45
DR D3=60.89 A1=20.5 OM=-13.78

Before a drive command is executed, the program checks if either the upper or lower limits will be exceeded by the new position ; the program also checks that no clashing with neighbouring analyser-detector arms will occur. Please note that the sequence in which the motors will be moved is specified in the sequence of the command ; so in the second example first motor D2, then D3, D4, and last D15 will be moved. Specifying D15-2 instead of D2-15 would move the motors in the reversed order. In the same way also the analyser energies can be changed e.g.:

DR EF1-16=20.0

5.4 The SCan command:

The general form is :

$$\text{SC} < nn >= ct, st, \text{NP} = np$$

This command will perform a scan of one or more angles ; the scan will be centered for every motor around *ct*, the step size will be *st* and the number of points will be *np*. All three input parameters have to be declared, whenever the scan command is used. An example of the use of the scan command is :

SC A6=39.3,0.2,NP=17

This command will make analyser 6 scan from 37.7 degrees to 40.9 degrees in 0.2 degree steps. Several motors can be scanned through the same angles at the same time, only the number of steps has to be the same, for example :

SC A1-10=35.3,0.1,NP=35

Also a desired combination of motors can be scanned, eg. in a theta-2theta scan:

SC A1-6=20.0 0.1 D1-6=40.0 0.2 NP=17

In the same way final energies can be scanned:

SC EF1-16=50,5,NP=19

In an OMEGA scan the scattered neutrons will be counted in the analyser-detector arm that is specified by IANAL. Another detector can be chosen by writing the scan command in the following way:

SC OM16=34.6,-0.23,NP=25
SC OM13-15=-120., 0.5,NP=11

The neutrons will now be counted in detector 16 in the first example and in detectors 13-15 in the second. When scanning the other motors, the neutrons will be counted in the detector(s) associated with the scanned motor(s). In a scan command, like in a drive command the program will check before every new positioning that no limits will be exceeded and that no clashing between neighbouring detector-arms will occur. If a clash situation should arise, the command will be aborted and a message will be printed. Sometimes it may be sufficient just to reverse the sequence of the motors to be moved, e.g D3-1 instead of D1-3. Note that scanning an angle PHIn will automatically change the values of the other 15 PHI angles as there is a fixed relationship between them, ie. $\phi_{n+1} = \phi_n + 2°$.

6 Commands which have little effect in PRSCAL

In so far as is possible the code used in the PRSCAL and PRISMA programs is identical. Obviously those parts of the code which physically do something, eg. position a motor, change a temperature etc. cannot be present in the PRSCAL code. However for consistency the commands which initiate these operations are present. This means that jobfiles can be tested in PRSCAL before being run on PRISMA without running into syntax problems. The following commands can all be entered in PRSCAL but they have little or no effect on the program.

6.1 The DO command:

The general form is :

DO TEST.JOB

This command executes a job file called TEST.JOB. The prompt will be changed to DO>> in order to indicate where the command came from. A job file is a file containing a list of "PRISMA commands", one command per line, which are to be run "in batch". The same sort of idea as a DCL .COM file. Note there is no prompt to be included in the file before a command line and the commands should be left adjusted (no blank spaces at the beginning of the line !!). The filenames for a DO command are limited to 10 characters each and the complete list of files (if more than one) should not exceed one line of 72 characters. Note you cannot DO a file from within a jobfile.

6.2 The TItle command:

The general form is :

TI `title of not more than 72 characters`

This command allows the user to change the run title (as shown on dashboard and stored in the raw file). There should be a single space between TI and the title, apart from that everything else on the line will be interpreted as the title. This command is useful for changing the title between runs contained in a jobfile and run with a DO command.

6.3 The BEgin command:

The general form is :

BE

This command can be used to start the spectrometer counting. The advantage of issuing a begin from the PRISMA program rather than the supervisor terminal is that the angular positions/sample parameters/spectra.dat etc. are stored in the raw file, which they are not if the begin comes from the supervisor. Note the time of flight parameters MNT/START/STOP/STEP used will be those that have been set previously.

6.4 The VX command:

This command can be used to run a Vax system command line from within the PRISMA program. It has two forms :

```
VX  C= Vax command line
VX  F= filename of a file containing Vax command lines
```

An example of the use of VX would be to change the temperature from within the PRISMA program, for example :

VX C=CSET TEMP 100.25

Note there should be no space between the C and the = and and between the = and the command line or file name, although spaces within a command line are allowed. Note: To re-emphasise a point made earlier, this command does not actually do anything in PRSCAL, the command or file of commands is not executed.

6.5 The CSET command:

There is a difficulty with the CAMAC control software on ISIS instruments whereby when moving a motor and logging temperature at the same time it is possible for the motor control command and the log value of the temperature to become interchanged, ie. temperature is sent to angle and angle to temperature ! To avoid this it is necessary to switch off temperature logging while moving a motor. The PRISMA program will do this automatically if (and only if) the temperature logging command was set in the PRISMA program. The general form of the command is :

CSET se_block/log_control

where the possible se_block parameters are TEMP, TEMP1 and LAKES (the Lakeshore controller) and the log_control values are LOG and NOLOG. Note the CSET should be left adjusted, just one space between CSET (all 4 letters) and the se_block name, no spaces between the se_block name, the / and the log_control value. It is intended in the future to extend the CSET command to allow the normal setting of CAMAC values from within the PRISMA program but for the time being this must still be done using the VX command. Note: Again this command does not actually do anything in PRSCAL the temperature is not changed, nor the logging status.

7 The BRagg command

The general form of the command is :

$$\text{BR QH} = \text{h, QK} = \text{k, QL} = \text{l, PHI} = \phi, \text{ DOM} = d\Omega, \text{ NP} = \text{n}$$

although it is usual to issue it without any of the QH = terms as :

$$\text{BR h, k, l, } \phi, \ d\Omega, \text{ n}$$

The Bragg command will position the sample (omega angle) and the phi angle of detector IANAL so as to measure the Bragg peak (h,k,l) and its lower/higher orders in the diffractometer mode. If n > 1 an omega scan through the omega angle corresponding to this point will be performed with n points and an angular step $d\Omega$. If n = 0 the spectrometer will just be positioned and no counting performed.
Examples :

```
BR   1 1 1 -90 0 0
BR   -1 1 0 -80 0.2 21
```

If n=0 is used then apart from "moving the simulated spectrometer" to the relevant angles for the (h,k,l) peak in the diffractometer mode the program will also print out the following extra information :

Omega	-	The omega angle for the (h,k,l) peak (and its lower/higher orders) at a scattering angle ϕ.
Lamda	-	The wavelength corresponding to the (h,k,l) peak at angle ϕ in detector IANAL in Å.
d-spacing	-	The d-spacing of the (h,k,l) planes in Å.
Q_0	-	The magnitude of the wavevector (h,k,l) in $Å^{-1}$.
K_i	-	The incident neutron wavevector in $Å^{-1}$ corresponding to the (h,k,l) peak at angle ϕ in detector IANAL.
E_i	-	The incident neutron energy in meV corresponding to K_i.
T.o.F	-	The time of flight in μs at which the (h,k,l) peak occurs at angle ϕ in detector IANAL.

These parameters can be very useful at alignment time.

- The omega value gives the calculated value for use in determining the zero angle from the formula :

$$\text{new\_zero\_angle} = \text{old\_zero\_angle} + \text{omega\_observed} - \text{omega\_calculated.}$$

- The T.o.F value is useful when deciding on the values of START/STOP for the time channel boundaries or alternatively for deciding on the ϕ angle so that the desired Bragg peak is within the time of flight window.

- The d_spacing value is of course useful for identifying Bragg peaks from their experimentally observed d_spacing value.

8 The CD(collect data) command

The general form of this command is:

CD QH = h QK = k QL = l DH = dh DK = dk DL = dl E = en

although it is usually issued without the QH = terms as :

CD h, k, l, dh, dk, dl, en

This command is used to perform an inelastic run along a high symmetry direction. The three components h, k, l determine a point in reciprocal space and dh, dk, dl give a direction in reciprocal space. These six parameters determine the direction in reciprocal space along which the data is taken. The value en determines the value of the energy transfer of the time of flight contour belonging to analyser IANAL at the wavevector (h,k,l). These 7 parameters completely define the energy/wavevector transfer measuring trajectories. The values of omega and for each of the detectors, the ϕ, E_f, k_f, θ_A and $2\theta_A$ angles are printed out. The omega angle of the sample, the analyser and detector angles will be automatically positioned by this command which will also check that the detectors and analysers will not clash in the new configuration and will move them in an order such that they will not clash during the setting up of the configuration.

Assuming that the spectrometer configuration is possible the PRSCAL program will then offer the user a "menu" of the extra information as follows :

0) Save information in a file

1) Plot E vs Q contours

2) Calculate a constant-Q interpolation

3) Calculate a constant-E interpolation

4) Calculate Ki to Ki spurions

5) Calculate Al powder line spurions

6) Return to CAL> level

Apart from number 6 these different options are explained in the following pages.

8.1 Save information in a file

This option writes the angular information etc. printed out on the terminal screen during the CD command to a file called PRSCAL.OUT. Other information is also written to the file, the date and time of the calculation and the sample and analyser parameters. If the file PRSCAL.OUT already exists then the program prompts as to whether the user wishes to overwrite this file or to append to the file.

8.2 Plot the E vs Q contours

This option will make a plot of the energy transfer (in meV) against wavevector transfer (in reciprocal lattice units) paths followed by each of the detectors (from DMIN to DMAX). The scale for the wavevector unit is calculated by Q = Q0 + s.DQ (Q0=(h,k,l), DQ=(dh,dk,dl)) where s is a paramteric variable. Only the first index (ie. h, k or l) which is variable is plotted as the x-axis.

Before plotting these contours the program will prompt to see if "data points" are to be plotted on the contours, ie the positions of peaks in the different detector spectra. The default answer is N, if the answer is Y then the program prompts to ask whether input is from a file or from the terminal. If from a file the then program prompts for the filename (up to 40 characters) and if from the terminal it prompts for the data. In either case the data should be in the format (one per line) :

detector number (integer), energy transfer (real)

and is read by a list-directed (*) format statement. There is no need to include the number of data points, just the data. The program will then prompt to see if the user wants a file of wavevector co-ordinates corresponding to each of the data points (Note this is the same output as for option 5). The default answer is N, if the answer is Y then the program prompts for a filename (up to 40 characters) where the output can be written.

The program will then plot the E vs Q trajectories (and data points if appropriate). It is usually the case that the scales initially chosen by the program are not perticularly sensible. The program will then prompt the user to ask whether the graph is to be replotted. The default answer is N, if the answer is Y, then the program prompts first for XMIN,XMAX and DX and then for YMIN,YMAX and DY. The XMIN/XMAX and YMIN/YMAX define the limits of the graph while DX and DY define the intervals at which "tick marks" are plotted on the scales. The graph is replotted and the user prompted again for replotting.

Following the replotting the program prompts to see if a laser plot of the the graph is required. The default answer is N, at which point the program returns to the menu level. If alternatively the answer is Y then after the program has made the plot file it prompts again to ask whether a further replotting of the graph is required. If the answer is N the program returns to command level, if the answer is Y the replotting/laser plot procedure is repeated.

8.3 Calculate a constant-Q interpolation

This option will list the energy transfer measured in each of the detectors from DMIN to DMAX for a given wavevector along the direction Q = Q0 + s.DQ . The program will prompt for a wavevector. To return to the menu enter the wavevector (0,0,0).

8.4 Calculate a constant-E interpolation

This option will list the wavevector transfers (in reciprocal lattice units) corresponding to a given energy transfer in each of the detectors from DMIN to DMAX. The program will prompt for the energy transfer. To return to the menu enter an energy transfer of -1000.

8.5 Calculate k_i to k_i spurions

It is possible to obtain spurious peaks in an inelastic spectrum which result from a Bragg peak in the sample being scattered into the analyser (elastically) and then being scattered by the incoherent cross-section of the analyser into the detector. Because the analysis programs assume that the

neutrons measured had a final wavevector k_f given by the Bragg scattering from the analyser they will analyse these spuriously scattered neutrons as though they were an inelastic scattering process in which the final neutron wavevector is k_f. In reciprocal space this spurious scattering process will correspond to an isosceles triangle with one of the two equal sides along the direction of k_i and the other equal side in the direction of k_f. The third side of the triangle will be the wavevector transfer Q corresponding to the Bragg peak. Since the incident neutron beam is white (all wavevectors k_i) one can think of the situation as scanning along the direction of Q as a function of k_i. A spurious process can then possibly occur if a Bragg peak is close to this path which is traced out in reciprocal space. This is effectively what the program does in its calculation.

Initially the program prompts the user to give the range of detectors and energy transfers in which to investigate if a spurious process is possible. It then prompts for a resolution width A in $Å^{-1}$. It is very unlikely that a Bragg peak will lie precisely on the path traced out, but instead what is relevant is if a Bragg peak lies "close" to the path traced out. The value of A sets a limit, only those Bragg peaks which are within ±A of the path are included. The program then prompts to see if the results should be copied to a file PRSCAL.SPR. If this file already exists then the program will prompt to see whether it should overwrite, or append to, this file. Finally the program prints out on the terminal (and to the file if relevant) the possible spurious processes. The output consists of the detector number, the (h,k,l) of the Bragg peak, the perpendicular distance of the Bragg peak from the path in reciprocal space in $Å^{-1}$ (called SEP for separation) and finally the energy transfer (in meV) at which the spurion would be observed in the detector spectrum after analysis. If the results are written to a file additional information is also written, the date/time, the CD command line and the sample parameters A,B,.....,PY(3). The program then returns to the menu level.

8.6 Calculate Al powder line spurions

In subsection 8.5 the possible spurious scattering process from a Bragg peak in the sample via the incoherent cross section of the analyser into the detector was described. A similar possibility can exist for aluminium powder, which is of course widely used in the construction of cryostats, sample cans etc. This subroutine does the same sort of calculation as in subsection 8.5 but uses the lattice parameters etc. for aluminium and a powder average.

9 The REsolution command/subprograms

If the simulated spectrometer has been set-up for a scattering process using either the DR, BR or CD commands then the command RE can be used to go into the resolution subprogram. This subprogram can be used to calculate resolution widths, lineshapes and contour maps of the resolution function, either in inelastic mode or diffraction mode. This choice is made by setting the value of the MOD parameter (MOD = 0 for diffraction mode and MOD = ± 1 for inelastic mode). The resolution function formalism used is that described in Hagen and Steigenberger, Nucl. Instr. and Meth. B72, 239 (1992). The subprogram has its own set of commands and parameters and prompts with the symbol :

CAL:RES>

The omega and phi angles used in the resolution calculations are those which were set in the main PRSCAL program. The following subsections describe the parameters and various commands available.

9.1 Resolution function parameters

The extra parameters required to define the resolution function are :

In-plane collimation	—	A1 A2 A3 (degrees)
Vertical collimation	—	B1 B2 B3 (degrees)
Sample mosaic spread	—	ES (degrees)
Analyser mosaic spread	—	EA (degrees)
Pulse shape parameters	—	T0 (μs) EC (meV) GE (meV)
Dispersion surface parameters	—	GL GD GMOD (meV/Å^{-1})
Detector and energy transfer	—	DET ENG (meV)

The collimation parameters are the FWHM values of the collimations in the moderator to sample (A1,B1), sample to analyser (A2,B2) and analyser to detector (A3,B3) positions respectively. In diffraction mode the sample to analyser and analyser to detector values are combined into an effective collimation through the formula $(1/A_{eff}) = \sqrt{(1/A1)^2 + (1/A2)^2}$ and similarly for the vertical collimation. The pulse shape parameters describe the slowing down time τ as a function of the incident energy E_i (as described in Hagen and Steigenberger) through the formula $\tau(E_i) = \mathrm{T0}$ for $E_i < \mathrm{EC}$ and $\tau(E_i) = \mathrm{T0}/(1 + (E_i - \mathrm{EC})^2/\mathrm{GE}^2$ for $E_i > \mathrm{EC}$. In both inelastic and diffraction mode the detector parameter DET chooses which detector the calculation is performed for.

The following parameters are relevant to inelastic mode only. The energy transfer parameter ENG chooses at which energy transfer the calculation is performed. The dispersion surface parameters describe the linearised dispersion plane which passes through the chosen detector at the specified energy transfer. The GL refers to the $Q_{\parallel}$ direction and GD to the $Q_{\perp}$ direction. The values of GL and GD define the direction in which the dispersion surface is sloping. The parameter GMOD is the magnitude of the slope of the dispersion surface in meV per Å^{-1}. The sense of slope of the dispersion

surface can be specified in one for two ways either by the sign of GL and GD or the sign of GMOD, but not of course by both simultaneously.

9.2 The LIst command:

This command lists the table of current values for the resolution function parameters. Its form is :

LI

9.3 The SEt command:

As in the main PRSCAL program the SEt command can be used to change resolution function parameter values. Its format is the same as before :

$$\text{SE} < nn >= x$$

where $< nn >$ is one of the parameter names and x is a value. More than one parameter can be changed on a line and if the order of the parameters (as in the table above) is kept then a range of parameters can be changed by specifying the name of the first parameter and a string of values for that parameter and succeeding parameters.

9.4 Inelastic Mode Only Commands

The following 4 commands are specific to the situation where the spectrometer has been set up in an inelastic scattering mode.

9.4.1 The BRagg resolution command:

The BRagg command whose format is simply :

BR

can be used to calculate the width of a Bragg peak in energy transfer in the specified detector DET and at the specified energy transfer ENG (usually zero). In conjuction with the PL command a plot of the Bragg peak lineshape can be obtained.

9.4.2 The PHonon resolution command:

The PHonon command whose format is simply :

PH

can be used to calculate the phonon width and lineshape for the intersection of the time of flight measuring trajectory with the linearised phonon dispersion surface described by (GL,GD) and GMOD. This calculation is performed for the specified detector DET at the specified energy transfer ENG. In conjuction with the PL command a plot of the resulting phonon lineshape can be obtained.

9.4.3 The VAnadium resolution command:

The VAnadium command whose format is simply :

VA

can be used to calculate the width in energy transfer of the scattering from the elastic incoherent line of vanadium. This is done for the detector DET and energy transfer ENG (usually zero) specified. In conjunction with the PL command a plot of the vanadium lineshape can be obtained.

9.4.4 The VT (vertical) resolution command:

The VT command whose format is simply :

VT

can be used to calculate the FWHM of the vertical component of the resolution function for the specified detector and energy transfer. The vertical component of the resolution function is simply a Gaussian lineshape and therefore no plot is available.

9.5 Diffraction Mode Only Commands

At the moment only one diffraction mode command exists, although it performs 3 calculations.

9.5.1 The QR (wavevector resolution) command:

The QR command calculates the FWHM of the resolution function in diffraction mode. The command takes the format :

QR Q_value Q_direction

where Q_value is the magnitude in Å^{-1} of the wavevector Q for which the calculation is performed and Q_direction which must be one of the integer values 1, 2 or 3, indicates the direction in which the width is to be calculated. The 3 direction choices are (1) longitudinal, parallel to Q, in the direction of the time of flight path, (2) transverse, perpendicular to Q in the horizontal scattering plane and (3) vertical, perpendicular to Q out of the scattering plane.

The calculation is performed for the specified detector DET and the values of the widths calculated are given in Å^{-1}. If options (1) or (2) are chosen then in conjunction with the PL command the resulting lineshape can be plotted. For option (3) the vertical resolution component is just a Gaussian and no plotting is available.

9.6 The PLot (lineshape) command:

This command can be used to plot lineshapes calculated with the BR, PH, VA and QR (options 1 and 2 only) commands. The procedure is to execute one of these commands and then to use the PL command to plot the lineshape. The general format of the command is :

PL xmin xmax [ymin] [ymax]

where xmin and xmax are the energy or wavevector x-axis limits for the plot and are obligatory parameters. The ymin and ymax are optional parameters for the y-axis (intensity) limits. After producing the initial plot the program will prompt the user to see if it is desired to replot the lineshape and to see if a hardcopy laser printer plot file is required. After a BR, PH, VA, QR command the PL command can be used as many times as desired to plot the lineshape until another BR, PH, VA or QR command is issued.

9.7 The MA resolution function contour map command:

This command can be used to plot a contour map of the resolution function. The format of the command is simply :

MA

In all cases the plotted contour map has 5 levels measured with respect to the maximum value of the resolution function (ie. effectively max value is 1) of 0.75, 0.50, 0.25, 0.10 and 0.01. A marker is also plotted to show the position of the maximum of the resolution function.

In diffraction mode the resolution function depends on 3 wavevector components, the longitudinal (radial) component in the scattering plane, the transverse (perpendicular to Q in the scattering plane) component and the vertical (out of plane) component. The out of plane component is a decoupled Gaussian function and is not plotted by MA. The in-plane components are plotted as a function of ΔQ_{lon} and ΔQ_{tran} which are in Å^{-1}. If the resolution function subprogram is set up in diffraction mode then after entering MA the program will prompt for the magnitude of the wavevector Q in Å^{-1} at which the contour map is to be drawn. The detector for which the calculation is done is that set by the DET parameter. The program then prompts for the maximum and minimum limits of the plot in ΔQ_{lon} and ΔQ_{tran}. With this information the contour map is plotted.

In inelastic mode the detector and energy transfer for which the contour map is calculated are as given by the parameters DET and ENG. The program therefore first prompts the user for the maximum and minimum limits in ΔQ and ΔE over which the contour map should be plotted. The inelastic mode resolution function is a function of 4 variables, $\Delta Q_{\parallel}$, $\Delta Q_{\perp}$, ΔQ_v and ΔE. The vertical component (in ΔQ_v) is a Gaussian which decouples from the rest of the function and is not plotted by MA. This leaves a coupled 3 dimensional function and therefore the program next prompts for a choice of one of the 3 possible planes in which it should plot a contour map. The 3 choices are (1) E vs $Q_{\parallel}$, (2) E vs $Q_{\perp}$ or (3) $Q_{\parallel}$ vs $Q_{\perp}$. Finally the program prompts to find out if the desired contour map should be (1) the intersection of the resolution function with the desired plane or (2) the projection of the resolution function onto the desired plane. Once these 3 pieces of information have been input the program then plots the desired contour map.

In both cases once the plot is complete the program will prompt to see if it is desired to replot the contour map and then to see if a hardcopy laser printer plot file of the contour map is required.

9.8 The EXit command:

In order to leave the resolution function subprogram the EXit command can be used. Its format is just

EX

and it returns the program control back to the main PRSCAL program. However if the resolution function parameters have been changed these changed values will be preserved and if after moving the "simulated" spectrometer in the main program the resolution function subprogram is re-entered these values will still be available.

10 The RC (reciprocal space plot) command

This command just takes the form :

RC

It can be used to make a plot of reciprocal space and possibily to include the paths followed by inelastic or diffraction measurements on the plot. It assumes that the reciprocal lattice points in the scattering plane can be generated from the vectors PX and PY used in the PRSCAL program, ie. G = M*PX + N*PY where G is the reciprocal lattice vector and M and N are integers. Note: (a) PX and PY do not have to be at 90 degrees to each other and (b) the plot created by the program (in a plot file) is as close as possible to scale in $Å^{-1}$.

After typing RC the program prompts to see if the user wishes to include a structure factor for missing Bragg peaks. This structure factor must be of the form :

a1*H + a2*K + a3*L = a4*n + a5

where a1,a2,a3,a4 and a5 are co-efficients entered by the user and n is an integer (0,1,2,3,....). Note: it isn't currently possible to enter structure factors of the form, all odd, all even, mixed odd/even etc. After this the program prompts for the X and Y limits of the plot, ie. the maximum and minimum values of M and N above to be used in creating the plot. The axis scales of the plot will be adjusted so that the plot is as close as possible to scale (in $Å^{-1}$). Note: The program can only plot about 50 Bragg peak/reciprocal lattice points in total.

The program will then prompt to see if any measuring paths are to be included in the plot. There are 3 possibilities, (1) a CD path, (2) a CF path and (3) a SC path. The first two are inelastic measurements and the third a diffraction measurement. The CD path is specified by the QH, QK, QL and DH, DK, DL parameters as explained in section 8. The CF command is the situation where the analyser-detector systems have been driven to a value of E_f and the omega and phi angles driven to a particular setting but which does not correspond to the high symmetry CD scan. In the case of the SC measurement, the omega and phi angles must be entered for a diffraction measurement along with the Q range of interest in $Å^{-1}$. The program prompts for the various parameters for each type of scan. Note that more than one type of scan can be plotted on the same reciprocal lattice plot.

When all of the desired scans have been entered the user enters an extra <return> and the program creates the plot. After the plot is completed an extra <return> may be necessary to get back to the alpha screen. The user is then prompted to see if a plot file containing the reciprocal space plot is required or not. The default answer is N (no). Control then returns back to the CAL> level.

11 The J and J/P (jump) commands

It is possible to use the J command either to run a system command from within PRSCAL or to create a subprocess from which system commands can be run without stopping PRSCAL. The first usage takes the form

J "command line"

where the command line to be run is enclosed in the quotation marks. The second usage takes the form J/P on the Vaxes. This creates a subprocess and runs the users login.com. To get back into PRSCAL one just logs out of the subprocess by typing LOG. On the UNIX systems J/P doesn't work, instead one must use control-z which suspends PRSCALU. To get back into PRSCALU one then types fg.

12 The EXit command:

The general form of this command is:

EX

This command terminates the PRSCAL program.