WinPLOTR,

a graphic tool for powder diffraction

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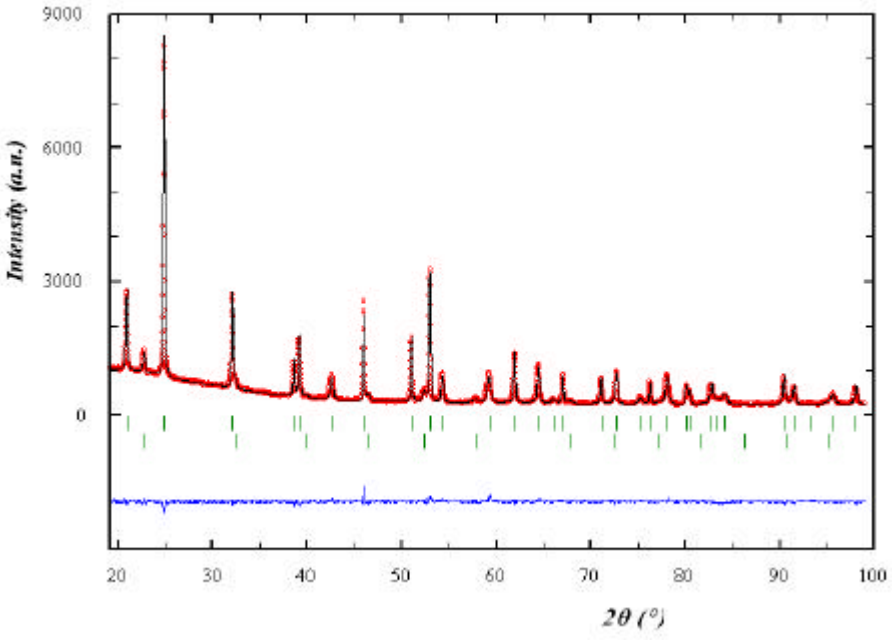

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1. INTRODUCTION

WinPLOTR is a software to plot and analyse powder diffraction patterns. It can be used to plot raw or normalized data files coming from neutron and X-ray diffractometers (conventionnal or synchrotron radiation) as well as Rietveld files created by the several Rietveld type refinement program (FullProf, Jana2000, Rietan2000, Debvin).

WinPLOTR has been also developed to be a preferential graphic interface for the Rietveld type FullProf program: edition of PCR input file, plot Rietveld type plots … can be directed be performed through the WinPLOTR interface.

WinPLOTR can also be used as a Graphical User Interface for programs used frequently in powder diffraction data analysis (ex: DicVol, Treor, ITO ...) or other external programs defined by the user.

WinPLOTR has been developped to run on PC's with a 32-bit Microsoft Windows operating system. WinPLOTR supports Windows 95/98/2000, Windows NT versions 3.51 and up.

This graphic software has been build up with Lahey Fortran 90, using the Windows facilities of RealWin. It has been optimised for a colour screen display with a resolution of 1024 x 768 pixels (or more).

2. WinPLOTR features

- several data file format (neutron, conventional RX, synchrotron, time of flight, dispersive energy)
- data file created by Rietveld type refinement programs FullProf, Jana2000, Rietan2000 and Debvin
- choice of X space:
  - 2theta (deg) / Time of flight (μseconds) / Energy (KeV)
  - $Q(\text{Å}) = 4p.\sin q/l$
  - $d(\text{Å})$
  - $\sin q/l$
- microstructural files for Williamson Hall plots
- graphic options: cursor, zoom …
- plot options:
  - change colours, markers type and size, styles …
  - shifts / offset data
  - hidden part management
- select and save points with the mouse
- automatic peak search and fitting procedures
- automatic background points search procedure
- calculation:
  - summation, difference, smoothing, derivative curves
  - background substraction
  - linear fit
  - profile fitting procedure
  - FWHM calculation (Caglioti formula)
- Rietveld files:
  - (hkl) information
  - (hkl) listing
  - plot the zero difference line
- edit PCR FullProf input file
- Graphical User Interface for external programs (ex: FullProf, Dicvol, Treor, ITO …) and user defined programs

- save patterns plots
- create Bitmap, Postscript and HPGL files
- user's guide on line

3. ARRAYS DIMENSIONS and "WinPLOTR.set" SETTINGS FILE

The arrays dimensions (max. number of patterns, max. number of data points) as well as patterns colour, markers, grid ... can be defined by the user in the "WinPLOTR.set" file. This settings file is stored in the directory defined by the "WINPLOTR" environment variable in the "c:\autoexec.bat" by the following command:

```
example: set WINPLOTR=c:\winplotr
```

or through the "Parameters / Control Panel / System / Environment" command for PC running under Windows NT.

When WinPLOTR is executed, it will look for the "WinPLOTR.set" file in the directory defined by the environment variable. If this settings file doesn't exist, the following dimensions will be used by default:

```
Max_Patterns   =  15     ! number of patterns
Max_Points     =  15000  ! number of points
```

WinPLOTR uses a settings file in order to adapt the capabilities of the program to the different needs and wishes of the user. The following parameters can be defined in this "WinPLOTR.set" file, on the lines following item with "!" as first character:

. ! MAIN WINDOW POSITION AND SIZE:
p1 p2 p3 p4 (real between 0. and 1.)
p1: upper-left x coordinate of the WinPLOTR main Window
p2: upper-left y coordinate of the WinPLOTR main Window
p3: width of the WinPLOTR main window
p4: height of the WinPLOTR main window

. ! LOG FILE:
Y/N => create or not a winplotr.LOG output file with all that has been performed by the user

. ! HELP FILES:
Y/N => display or not in windows user's guide files, depending of the selected option in the WinPLOTR menus options

. ! DIMENSIONS OF ARRAYS:

```
Max_Patterns =              !   max. number of patterns
Max_Points   =              !   max. number of data points
Max_Refl     =              !   max. number of Bragg reflexions
```

. ! SIGMA ARRAYS:
Y/N => create or not arrays for data sigmas

. ! PEAK SEARCH DETECTION THRESHOLDS:
P_T1 P_T2 (reals in free format)
P_T1: sensitivity to find peaks (default value = 0.02)
P_T2: sensitivity to find shoulders (default value = 2.)

. ! BACKGROUND THRESHOLD:
BG_T (default value = 0.05)

. ! RUN PROGRAMS:

```
FULLPROF     =  c:\exe\wfp2k    !  FullProf program       ! Windows version
EDIT         =  c:\exe\notepad  !  my favorite editor     ! Windows version
DICVOL       =  c:\exe\windic   !  DICVOL program         ! Windows version
TREOR        =  c:\exe\wtreor90 !  TREOR90 program        ! Windows version
ITO15        =  c:\exe\wito15   !  ITO1590 program        ! Windows version
SUPERCELL    =  c:\exe\supercel !  SuperCEll program      ! Windows version
MENDEL       =  c:\exe\mendel   !  Neutron periodic table ! Windows version
MYPROG       =  c:\exe\myprogr  !  My favorite MYPROGR program ! Windows version
FullProf_DOS =  c:\exe\fullprof !  FullProf DOS version   ! DOS version (2)
```

Remark:
* First column corresponds to the texts that will appear in the "External Applications" vertical menu
* Second column (between "=" and "!" characters) corresponds to the EXE file that can be executed from WinPLOTR
* Third column (between the "!" characters) corresponds to the help text that will appear in the horizontal status bar in WinPLOTR
* Last item corresponds to the program version (Windows or DOS). In case of DOS programs, the number of arguments acompagnying this program can be specified in parenthesis at the end of the line.

. ! AFTER FULLPROF RUN:

```
item_1 item_2
  . item_1 = plot_prf       => the PRF file is plotted (default value)
             no_plot_prof   => the PRF file is not plotted

  . item_2 = edit_pcr       => the PCR file is edited
             no_edit_pcr    => the PCR file is not edited (default value)
```

. ! EDIT FILES:

```
!    extension          type
     extension(1)        !type(1)
     extension(2)        !type(2)
     extension(3)        !type(3)
     extension(4)        !type(4)
```

Maximum of 4 kinds of files can be defined here by the user. The extension and the corresponding data type has to be separated by the "!" character.

example: *.out;*.sum !FullProf output files

. ! PLOT OPTIONS SETTINGS:

```
!  n   colour   marker   size   style
```

. ! PRF OPTIONS SETTINGS:

```
!  n   colour   marker   size   style
```

. ! XRF OPTIONS SETTINGS:

```
!  n   colour   marker   size   style
```

. ! GRID:

```
g_x g_y  (integers)
  . g_x /= 0  => grid along X axis
  . g_y /= 0  => grid along Y axis
```

. ! GRADUATIONS:

```
X_maj_int Y_maj_int  X_min_int  Y_min_int  (integers in free format)
  . X_maj_int /= 0  => number of major intervals along the X axis
              = 0   => automatic graduations along the X axis
  . Y_maj_int /= 0  => number of major intervals along the Y axis
              = 0   => automatic graduations along the Y axis

  . X_min_int: number of major intervals along the X axis (>1)
  . Y_min_int: number of minor intervals along the Y axis <>1)
```

```
. ! TEXT COLOUR:
    main title:
    X legend:
    Y legend:
    X graduations:
    Y graduations:
    Indices:

  ! LEGENDS POSITIONS AND ROTATION:
     X legend  :  XL_Posx XL_Posy XL_rot
     Y legend  :  YL_Posx YL_Posy YL_rot
     Main title:  MT_Posx MT_Posy MT_rot
```

Remark: A negative value for Posx parameters (X position) will center the text legend

```
. ! FRAME WIDTH [0.2-0.8]:
     f_w (real)

. ! FRAME FEATURES:
     item1 item2 item3 item4 item5 (5 reals: 0. -> 9.)
       item1: frame line thickness  (default = 3.)
       item2: major tics thickness  (default = 3.)
       item3: minor tics thickness  (default = 1.)
       item4: major tics length     (default = 4.)
       item5: minor tics length     (default = 3.)

. ! MY RESOLUTION PARAMETERS (U,V,W): Caglioti's formula parameters
     my_U  my_V  my_W  (reals)

. ! MY X-Rays WAVELENGTHS (A):
     Ka1 Ka2 (reals)

. ! DATA FILES EXTENSIONS:
  !    format_order   extension          type
           1           *.xy           ! X,Y data
           2           *.dat          ! INSTRM = 0
           4           *.dat;*.d1b    ! INSTRM = 3

. ! MY DEFAULT FORMAT [1-16]:
      default_format (enteger)

. ! BACKGROUND SCREEN
    background screen colour:
    background text colour  :
    background plot colour  :
    plot frame colour       :
```

4. Install WinPLOTR on your PC

The WinPLOTR kit consists in a compacted file (WinPLOTR.zip) containing all the files to run install automatically the program WinPLOTR and the Windows version of the Rietveld-type FullProf program, DICVOL91, TREOR90, ITO15 and others programs used in the crystallographic field. The WinPLOTR kit is available free of charge for scientific non-profit institutions. It can be downloaded fr om the Web page http://www-llb.cea.fr/fullweb/winplotr/winplotr.htm.

Installation of WinPLOTR and its tools has to be realized by the different following steps :

1. copy “winplotr.zip” file in a temporary directory of your hard disk

   example: c:\temp\winplotr

2. unzip the “winplotr.zip”

   example: `c:\temp\winplotr> pkunzip winplotr`

   The following files will be expanded in the current directory (c:\temp\winplotr):

   - `install.exe` install procedure
   - winplotr.exe WinPLOTR executable file
   - `winplotr.set` WinPLOTR setting file
   - winplotr.ins user's guide (text mode)
   - winplotr.htm user's guide (HTML language)
   - winplotr.new what's new in WinPLOTR
   - windic.exe DICVOL91 (D. Louër) windows version
   - windic.ins DICVOL91 user's guide
   - wtreor90.exe TREOR90 (P.E. Werner) windows version
   - treor.ins TREOR90 user's guide
   - wito15.exe ITO15 (J. Visser) windows version
   - ito.ins ITO15 user's guide
   - supercel.exe SuperCELL (J. Rodríguez-Carvajal) windows version
   - supercel.ins SuperCELL user's guide
   - FullProf (J. Rodríguez-Carval) program files (EXE, docs, examples …)

3. execute install.exe

   example: `c:\temp\winplotr> install`

4. Reboot your PC if necessary

Remarks:

* The last version of WinPLOTR is available in the ftp area of the Charybde server of the LLB in the “\ftp\pub\divers\winplotr\” directory.
  . ftp address: charybde.saclay.cea.fr
  . IP address: 132.166.20.1
  . login: anonymous
  . password: anonymous
  (please transfer the files in binary and not ascii mode!)

* . WinPLOTR is also accessible via the Web: http://www-llb.cea.fr/fullweb/winplotr/winplotr.htm

5. WinPLOTR functions descriptions

5.1 File menu

5.1.1 Open data file

- choice of the data file format
- access to the Windows directories dialog box to select a data file
- plot on screen the loaded data file

The data file format:

- The INSTRM item corresponds to the same item used by Fullprof in the “PCR” input file

- *npts* is the number of points in a data file. In the case of constant step data, npts is calculated as follows:

$$npts = \frac{(ending\_position - starting\_position)}{step} + 1$$

- For all the following formats, WinPLOTR reads but doesn't take into account the first lines with "#" or "!" as first character. This can help the user to get its own data files compatible with one of the WinPLOTR data file format.

- `X,Y data:`

  ** file with 2 columns (default extension = .xy)*

  Line 1*: text
  Line 1_1: separator (----------)
  Lines l: column 1 = 2θ (deg.) column2 = counting

  Remark:
  . Sigmas are calculated as SQRT(coutings)
  . if a third column exists, the corresponding data are considered as the sigmas of the countings.

  ** INSTRM=10:* X,Y, sigmas with header lines

  Line 1: XYDATA as keyword
  Line 2-6: header lines (comments)
  Lines l: X, Y, sigma values

  Remark:
  . If no sigmas values, the program assumes that sigmas(Y) = SQRT(Y)

  ** RIETAN2000 file*

  - General format:
    Line 1: "GENERAL" keyword
    Line 2: npts
    Lines 3-npts+2: X, Y

  - IGOR format:
    Line 1: "IGOR" keyword
    Line l: "BEGIN" keyword
    Lines l+1 – (l+npts): X, Y
    Line l+npts+1: "END" keyword

  ** Multicolumn file*
    Line 1: X, Y1, Y2, Y3 ... Yn

Remark: if the first X value is greater than 180.00, the data are considered as time of flight data

- `INSTRM=0:` free format file
  (default extension = .dat)
  Line 1: 2θ_min(deg.) step(deg.) 2θ_max(deg.) + optional comments
  Lines l: npts countings

  Remark: sigmas(Y(n)) = SQRT(Y(n))

- INSTRM = 1: data file from multicounters diffractometers
  (default extension = .dat)
  Line 1: 2θ_min(deg.) step(deg.) 2θ_max(deg.) + optional comments
  Lines l: npts pairs (numbers of detectors , countings)

  Remark: sigmas(Y(n)) = SQRT(Y(n)/number of detectors)

- INSTRM = 3: data file from D1B, D20 (ILL) new format
  (default extension = .dat)
  Line 1: nset
  Line 2: data time text
  Line 3: nset1 files numors
  Line 4: par1 par2 2θ_min(deg.) par3 par4 par5 par6 par7 step(deg.)
  Line 5 : npts
  Lines l: npts pairs (numbers of detectors , countings) [format=10(i2,F8.0)]

  Remark: sigmas(Y(n)) = SQRT(Y(n)/number of detectors)

- INSTRM = 4: data file from N.L.S. (Brookhaven) synchrotron radiation
  (default extension = .dat)
  Line 1: 2θ_min(deg.) step(deg.) 2θ_max(deg.)
  Lines l: npts pairs of lines with 10 items like:

```
Y1 Y2 ... Y10   <-- (10F8) intensities
s1 s2 ... s10   <-- (10F8) sigmas
```

- INSTRM = 5: free format file
  (default extension = .dat)
  Lines 1-3: text
  Line 4: npts par1 par2 ivari monitor1 monitor2
  Line 5: 2θ_min(deg.) step(deg.) 2θ_max(deg.)
  Lines l: npts countings

  Remark:

```
If (ivari /=0) then
    Following_lines = npts sigmas
Else
    If (monitor1 > 1. .and. monitor2 > 1.)then
      Cnorm = (monitor1 / monitor2)**2.
    Else
      Cnorm = 1.
    Endif
    sigmas(Y(n)) = SQRY(Y(n) * cnorm)
endif
```

- INSTRM = 6: data file from multicounters diffractometers
  (default extension = .dat)
  Line 1: text
  Line 2: a21 a22 step(deg.) a23 a24 a25
  Line 3: 2θ_min(deg.)
  Line 4: monitor1 monitor2 Tsample
  Lines l: npts pairs (number of detectors, counting)

  Remark:

```
If (monitor2 < 1.) then
    Cnorm = 1.
```

```
    Monitor2 = monitor1
Else
    Cnorm = (monitor1 / monitor2)**2.
Endif
sigmas(Y(n)) = SQRY(Y(n) * cnorm / number of detectors)
```

- INSTRM = 8: data file from DMC diffractometer at Wurenlingen (Paul Scherrer Institut)
  (default extension = .dat)
  Line 1,2: comment
  Line 2: 2θ_min(deg.) step(deg.) 2θ_max(deg.)
  Lines l: npts/10 lines: npts countings
  Lines l': npts/10 lines of npts sigmas(countings)

- INSTRM = 9: X ray data file created by the Socabim software on X rays diffractometers
  (default extension = .uxd)

  Remark: sigmas(Y(n)) = SQRT(Y(n))

- INSTRM = 11: data from variable time X-ray data collection
  (default extension = .uxd)
  Line 1,4: comments
  Line 2: 2θ_min(deg.) step(deg.) 2θ_max(deg.)
  Lines l: time intensity [format 5(F6.0,F10.0)]

- XRF files: output files created by the WinPLOTR profile fitting procedure
  (default extension = .xrf)
  Line 1: titles
  Line 2: `=> Data file name : data file name`
  Line 3: `=> Instrm : data file format`
  Line 4: `=> Lambda(1&2) : lambda1, lambda2`
  Line 5: `=> Number of points: number of points`
  Line 6: `=> Number of peaks : number of peaks`
  Line 7: text
  Lines l: "number of peaks" lines
  X(i), Yobs(i), Ycalc(i), Yobs-Ycalc(i), background(i), Bragg_position(i), integrated_intensity(i), fwhm(i), eta(i)
  Lines l': "number of points" lines
  X(i), Yobs(i), Ycalc(i), Yobs-Ycalc(i), background(i)

  Remark: XRF file is considered as 5 different files (Yobs, Ycalc, Yobs-Ycalc, background, peak positions)

- GSAS data: data files for the GSAS analysis data program
  (default extension = .dat)
  Line 1: legend
  Line 2: item 3 = number of points in the data file (npts)
  Lines l: depending of item 10 and item5
  -item10="STD" item5="CONST"
  . xmin =item6/div
  . step =item7/div
  . read(10(i2,F6.0) iww(i),y(i) i=1,npts

```
      .sigma(i)=sqrt(y(i)/iww(i))     i=1,npts
-item10="ESD" item5="CONST"
      . xmin =item6/div
      . step =item7/div
      . read(10F8.0) y(i),sigma(i) i=1,npts
-item10="ALT" item5="RALF"
      . xmin =item6/32
      . step =item7/32
       read(4(F8.0,F7.4,F5.4) x(i),y(i),sigma(i) i=1,npts
        x(i)=x(i)/32       i=1,npts
        do i=1,npts-1
          div=x(i+1)-x(i)
          y(i)    =1000*    y(i)/div
          sigma(i)=1000*sigma(i)/div
        end do
-item10="ALT" item5="CONST"
      . xmin =item6
      . step =item7
      .  read(4(F8.0,F7.4,F5.4) x(i),y(i),sigma(i) i=1,npts
        x(i)=x(i)/32       i=1,npts
```

Remark: . constant wavelength data: div = 100.
. time of flight data : div = 1.

- `HRMPD files:` data file from the new High Resolution Multicounters Powder Diffractometer (G42/LLB)
  (default extension = .mpd)

  Lines 1-7: comments
  Lines l: npts * 8 lines
  - Line 1: point number
    counting time
    angular positions of each of the 7 counters banks (2θ in deg.)
    setting temperature
    sample temperature
  - line 2: format 10I8: counting of the 10 detectors of bank number 1
  - line 3: format 10I8: counting of the 10 detectors of bank number 2
  - …
  - line 8: format 10I8: counting of the 10 detectors of bank number 7

  Remark: XRF file is considered as 5 different files (Yobs, Ycalc, Yobs-Ycalc, background, peak positions)

- `6T1 file:` data file from the 6T1 diffractometer at LLB

  Remark: sigmas(Y(n)) = SQRT(Y(n))

- G41/G61: raw data file from the G41 (800 cells) or G61 (400 cells) multidetectors neutron diffractometers at LLB

5.1.2 Open Rietveld file

- choice of the Rietveld data file format

- access to the Windows directories dialog box to select a data file
- plot on screen the loaded data file as a Rietveld plot (Y_{obs}, Y_{calc}, Y_{obs}-Y_{calc}, Bragg peaks positions)

The Rietveld data file format:

- `FullProf PRF file:` data file created by the Rietveld type Fullprof program (default extension = .PRF; IPL2=1, -3, +3, 2)
  - powder case: Y_{obs}, Y_{calc}, Y_{obs}-Y_{calc}, hkl, 2θ(hkl)
    remark: PRF file is considered as 4 different files
  - single crystal case: $\sin q/l$, F^2_{obs} , F^2_{calc}
    remark: PRF file is considered as 3 different files ($\sin q/l$ plot) or a single file (F^2_{calc} = f(F^2_{obs}) plot)

- `JANA2000 PRF file:` data file created by the Rietveld type JANA2000 program (default extension = .PRF)
  remark: PRF file is considered as 4 different files
  only available for non modulated structures (for the moment)

- `RIETAN2000 file:` data file created by the Rietveld type RIETAN2000 program (default extension = .PAT)
  remark: PRF file is considered as 4 different files
  only available for non modulated structures (for the moment)

- `Debvin file:` data file created by the Rietveld type Debvin program (default extension = .GRA)
  remark: PRF file is considered as 3 different files (Y_{obs}, Y_{calc}, Y_{obs}-Y_{calc})

5.1.3 Open microstructural file

- access to the Windows directories dialog box to select a data file for a microstructural plot
- plot on screen the loaded data file as a "Williamson Hall plot" (integral breath β* versus $1/d_{hkl}$) or a "average size strain plot" ($\left(b^*/d^*\right)^2$ versus $\left(b^*/d^{*2}\right)$

The microstructural data file format:

- `WHP file:` data file for a Williamson Hall plot (default extension = .whp)
  Multicolumns file:
  . column 1: $1/d_{hkl}$
  . column 2: integral breath β* (in reciprocal unit * 1000)
  . column 3: h index
  . column 4: k index
  . column 5: l index

- `ASS file:` data file from a average size strain plot (default extension = .ass)
  Multicolumns file:

. column 1: $\left(b^{*}/d^{*2}\right)$

. column 2: $\left(b^{*}/d^{*}\right)^{2}$

. column 3: h index
. column 4: k index
. column 5: l index

5.1.4 Open buffer file

- access to the Windows directories dialog box to select a buffer data containing data file names to load simulstaneously
- select the common data file format
- plot all the data files simustaneously on the screen

examples:

6. file1.buf
   file_1.dat (without the directory name)
   file_2.dat
   …
   file_n.dat

7. file2.buf
   This buffer file can also contain informations about the files (description of the experiment, temperatures)
   file_1.dat T = 5 K
   file_2.dat T = 10 K

   …
   file_n.dat T = 50 K

5.1.5 Open .WPL file

- access to the Windows directories dialog box to select a WinPLOTR (.WPL) file, i.e. a template file
- redisplay patterns with the features contained in the WPL file

5.1.6 Select files

- Select, amoung the loaded files, the patterns to plot on the screen
- *!! This option is not available if more than 80 files have been loaded !!*

5.1.7 Select sections

- Select a single sectio to plot on the screen
- *!! this option is only available for HRMPD file !!*

5.1.8 View files

- access to the Windows directories dialog box to select a file
- Display the text (in ASCII) of the selected file in a window

5.1.9 File infos

- Display in a text window some informations about data file: file name, format, number of points, Xmin, Xmax, Ymin and Ymax

5.1.10 Reset

- Clear all the arrays and reinitialization of all the parameters

5.1.11 Save as .WPL file

- Access to the Windows directories dialog box to select a .WPL template file name
- Save the current plot settings in a .WPL file as follows:

```
. X_space  data_type:  Xspace= 1 (2theta/tof)
                       data  = 0: constant wavelength data
                               1: time of flight data
                               2: energy data
. Main legend:
     . X legend:
     . Y legend:
     . Xmin Xmax: item_1 item_2 item_3 item_4 item_5 item_6
        item_1: Xmin
        item_2: Xmax
        item_3: first_X_graduation
        item_4: last_X_graduation
        item_5: 0/1 => not_auto/auto_first_x_grad
        item_6: 0/1 => not_auto/auto_last_x_grad
.Ymin Ymax:
.X_shift  Y_shift:
.X_offset Y_offset:
.X and Y graduations: X_grab_nb Y_grad_nb X_minor_tics_nb
                      Y_minor_tics_nb
.Write text (X grad., Y grad., Yneg. grad., file_name): 0: no / 1: yes
.Grid (X and Y): 0: no / 1: yes
.Frame features:  item_1 item_2 item_3 item_4 item_5
        item_1: frame line thickness
        item_2: major_tics_thickness
        item_3: minor_tics_thickness
        item_4: major_tics_length
        item_5: minor_tics_length
.Hidden part / 3D lines:    param_1  param_2
        param_1: 0: no / 1:yes
        param_2: 3d_lines_step
.Data directory:
.-------------------------------------------------------------
.file_name  format  colour  marker_type  marker_size  style  pen_width
 title
.-------------------------------------------------------------
.COLOURS:
   . main title              :
   . X legend                :
   . Y legend                :
   . X graduations           :
   . Y graduations           :
   . background screen colour  :
```

```
. background text colour    :
. background plot colour    :
. plot frame colour         :
```

5.1.12 Save as SUP file

- Access to the Windows directories dialog box to select a file name to save data on screen in a multicolumns file
- *!! only available of one pattern on the screen or after running a calculation option (addition, difference, averagen derivative and smooting) !!*

5.1.13 Save as multicolumns file

- Access to the Windows directories dialog box to select a file name to save data on screen in a X,Y file (2 columns)
- Access to a dialog box to select, for all files, X and Y columns to save

5.1.14 Save settings

- Save the current WinPLOTR settings in the "WinPLOTR.set" file (in the WinPLOTR directory defined by the WinPLOTR environment variable):

```
. Main window position and size
 .Log file
. Help file
. Max. number of loaded files
. Max .number of points per file
. Max. number of reflexions
 .Sigma arrays
. Peak search detection thresholds
. Background detection thresholds
. External programs
. Plot options: colours, markers, styles, pen width
. PRF plot options
. XRF plot options
. Grid
. Number of graduations
. Frame width
. User's diffractometer resolution parameters (U, V, W)
. X-ray wavelengths
...
```

5.1.15 Print

- Access to the Windows print dialog box to print the graphic window

5.1.16 Save as PS file

- Access to the Windows directories dialog box to select a file name to save the current plot as a PostScript file
- Access to a dialog box to select "Landscape / Portrait" orientation
- Create a coloured PostScript file (.EPS)

5.1.17 Save as HPGL file

- Access to the Windows directories dialog box to select a file name to save the current plot as a HewLett Packard Graphic Language file

- Access to a dialog box to select “Landscape / Portrait” orientation
- Create a black and white HPGL file (.HPG)

5.1.18 Save as BITMAP file

- Access to the Windows directories dialog box to select a file name to save the current plot as a BITMAP file
- Create a coloured Bitmap file in the Windows-standard “.BMP” format

5.1.19 Exit

- Exit the WinPLOTR program

5.2 Plot menu

5.2.1 Focus

- Access to a dialog box to enter X_{min} and X_{max} for the plot: Y_{min} and Y_{max} will be automatically scaled

5.2.2 Zoom

- Access to a dialog box to enter plot parameters as :
  . X_{min} X_{max}, Y_{min}, Y_{max}
  . Numbers of X and Y major intervals
  . Numbers of X and Y minor intervals
  . First and last X and Y graduations
- Plot the patterns

5.2.3 Shift

- Access to a dialog box to enter X and Y shift values
- The following changes on the x and Y data will be performed
  . first file is unchanged
  . file 2 is shifted by “shift” / first file
  . file n is shifted by “(n-1). shift” / first file
- Plot the patterns

5.2.4 Offset

- Access to a dialog box to enter X and Y offset values
- The following changes on the x and Y data will be performed
  . $X(i,j)=X(i,j)+offset\_X$
  . $Y(i,j)=Y(i,j)+offset\_Y$
- Plot the patterns

5.2.5 Plot 3D+

Plot patterns in a pseudo-3D mode with default parameters:

. X_shift, Y_shift
. color, marker size, pen width
. hidden part
. lines-3d

!! this option is available only after loading a .BUF file !!

5.2.6 Plot 3D-

same as 'Plot 3D+' option with opposite X_shift and Y_shift
!! this option is available only after loading a .BUF file !!

5.2.7 Hidden part

- Plot or not the hidden parts
- *!! Can be useful for pseudo-3D plots !!*

5.2.8 3d lines

- Access to a dialog box to enter a “3D_lines_step” value
- Plot patterns with the following features: draw lines between same indices points (every “3D_lines_step” point)
- 3d lines colour is the common patterns colour or black if no common colour has been previously defined
- *!! Can be useful for pseudo-3D plots !!*

5.2.9 Reverse order

- Reverse the files order to plot the patterns
- *!! Can be useful for pseudo-3D plots !!*
- *!! available if more than 1 file on screen and no PRF and XRF file !!*

5.2.10 Frame width

- Access to dialog box to select a frame width value to control the rectangular shape of the plot
- Plot the patterns with the new frame width value

5.2.11 Errors bars

- Plot or nor the error bars of the countings for the last loaded file
- *!! not available with .PRF and .MPD files !!*

5.2.12 Excluded regions

- Access to a dialog box to enter the number of excluded regions
- Enter lower and upper limits for the excluded regions
- Plot the patterns, considering the previously excluded regions
- *!! not valid for PRF files !!*

5.3 Options menu

5.3.1 Graduations

- Access to a dialog box to enter the following parameters

. number of major X intervals (“O” value leads to automatic graduations)
. number of major Y intervals (“O” value leads to automatic graduations)
. number of minor X intervals
. number of minor Y intervals

- Plot the patterns

5.3.2 Grid

- Access to a dialog box to select to plot or not vertical grid on X and horizontal grid on Y axis

5.3.3 Patterns colours

- Access to a dialog box to select if the same colour is attributed to all the pattern or not
- Access to the Window dialog box that allows the user to select any available colour of his system
- Plot the patterns

5.3.4 Patterns markers

- Access to a dialog box to select if the same marker is attributed to all the pattern or not
- Access to the dialog box to select a particular symbol and the corresponding size
- Plot the patterns

5.3.5 Patterns style

- Access to a dialog box to select if the same plot style is attributed to all the pattern or not
- Access to the dialog box to select a particular style: non-continous line , continuous line, dashed line, dotted line, histogram or filled areas
- Plot the patterns

5.3.6 Patterns pen width

- Access to a dialog box to select if the same pen width is attributed to all the pattern or not
- Access to the dialog box to select a particular pen width value [1-9]
- Plot the patterns

5.3.7 Background colours

- Access to the “Background colours” menu:
  I. Background screen colour
     . access to the Window colour dialog box to select a particular colour for the background screen
     . take into account the previous change

  II. Background text colour.
     . access to the Window colour dialog box to select a particular colour for the background introduction text
     . take into account the previous change

III. Background plot colour
. access to the Window colour dialog box to select a particular colour for the plot screen area
. take into account the previous change

IV. Plot frame colour
. access to the Window colour dialog box to select a particular colour for the plot frame
. take into account the previous change

5.3.8 Frame features

- Access to a dialog box to select the following parameters:
  . line thickness of the frame
  . line thickness of the major and minor tics
  . line length of the major and minor tics
- Plot the patterns considering the previous features

5.4 Options menu

5.4.1 Automatic peak search

- Access to a dialog box to enter the following parameters needed by the peak search procedure: Peak threshold (P_T_1), shoulder threshold (P_T_2), background threshold (BK_T), single/doublets Bragg peaks

- The automatic peak search procedure is performed in three steps:
  - Search of background points (See 4.3)
  - Search of points with zero derivative value:
    . calculation of the maximum amplitude (*delta_max*) of the derivative data when going through a zero value
    . comparison of each amplitude (*delta*) of the derivative data when going through a zero value with *delta_max:*

$$\text{if } (delta/delta\_max > P\_T_1) : \Rightarrow \text{Bragg peak}$$

  - Search of shoulders
    . search of positive minima and negative maxima in the derivative curve
    . calculation of the amplitude (*delta*) of the minima (or maxima)
    . calculation of the maximum background fluctuations (*delta_bf_max*)

$$\text{if } (delta/delta\_bf\_max > P\_T_2) : \Rightarrow \text{shoulder}$$

    remark: for each Bragg peak, points around the Bragg position has to obey to the the following criterium to be taken into account:

$$Intensity(i) = (1 + P\_T_1).background(i)$$

- Search of $K\alpha_1/K\alpha_2$ doublets
  $K\alpha_2$ reflections will be removed from the above reflection list if two successive Bragg reflections obeys suimultaneously to the two following conditions:

1 $\sin(q_2)/\sin(q_1) = l_{Ka_2}/l_{Ka_1}$ (±0.5%)

2 $Intensity(2)/Intensity(1) = 0.5(\pm 0.1)$

- Output files:
  . peaks.APS (X, Y format):
  2θ_Bragg peak_intensity peak_background
  . background.XY (X, Y format)
  2θ background_value

5.4.2 Save peaks

- Access to the Windows directories dialog box to select a file to save the previously automatic founded peaks (.APS extension)

5.4.3 Automatic background

- Access to a dialog box to enter a background threshold value (*BG_T*)
- Calculation of the maximum of fluctuations around a derivative point (*max_delta*)
- Division of the pattern range in several ranges (roughly the square root of *npts*)
- Search the minimum values in all the ranges
- Comparison of the fluctuations around these minima (*delta*) values with *max_delta*

if $(delta/delta\_max > BG\_T)$: => background point

5.4.4 Select background

- Select and plot, by clicking on the left mouse button, background points
- *!! click on the right mouse button to exit from the select background points procedure !!*

5.4.5 Save background

- Access to the Windows directories dialog box to select a file to save the previously background points in a X,Y file (2 columns format with 2θ and background_value)

5.4.6 Select points

- Select and plot, by clicking on the left mouse button, background points
- *!! click on the right mouse button to exit from the select points procedure !!*

5.4.7 Save selected points

- Access to the Windows directories dialog box to select a file to save the previously selected points in a X,Y file (2 columns format with 2θ and corresponding intensity)

5.4.8 Save as DICVOL points

- Access the DICVOL dialog box to create an input file (.DIC) for the Windows version (WinDIC is distributed in the WinPLOTR.zip package) of the DICVOL program (D. Louer & A. Boultif)

- Previously selected points are stored in the .DIC file
- If DICVOL points have been selected by the automatic peak search procedure of WinPLOTR, .DIC input files will contain informations about intensity and background level at the Bragg peak position

5.4.9 Save as TREOR points

- Access to the TREOR dialog box to create an input file (.INP) for the Windows version (WTREOR90 is distributed in the WinPLOTR.zip package) of TREOR program (P.E. Werner, Stockholm Univ., Sweden)
- Previously selected points are stored in the .INP file

5.4.10 Save as ITO points

- Access to the ITO dialog box to create an input file (.ITO) for the Windows version (WITO15 is distributed in the WinPLOTR.zip package) of ITO15 program (J. Visser)
- Previously selected points are stored in the .ITO file

5.4.11 Save as SuperCELL points

- Access to SuperCELL dialog boxes to create an input file (.SAT) for the SuperCELL program (search of commensurate supercell or incommensurate progagation vector)
- Previously selected points are stored in the .SAT file

5.4.12 Add peaks/background points

- Access to the cursor to select (by clicking with the left button) some reflections (position and intensity) / background points to take into account in the reflections / background points list
- Click on the right mouse button to exit from this peak / background points selection
- !! this option is available only after an automatic peak procedure or an automatic background search !!

5.4.13 Remove peaks/background points

- Access to the cursor to select (by clicking with the left button) some reflexions (position and intensity) / background points to remove from the reflexions list / background points list
- click on the right mouse button to exit from this peak / background remove points procedure
- !! this option is available only after an automatic peak procedure or an automatic background search !!

5.4.14 Remove peaks/background points

- After an automatic peak/background search procedure, this option allows to display only the pattern (without the list of peak/background points)

5.5 X space menu

5.5.1 2Theta / T.O.F. / Energy

- Plot the patterns:
  - in the 2θ (deg.) space for constant wavelength data
  - in the time of flight (in µsec.) space for time of flight data
  - in the energy (KeV) space for dispersive energy data
- !! data are considered a priori as constant wavelength data (X_space = 2θ (deg.) !!

5.5.2 Q (Å^{-1})

- Plot the patterns in the Q space:
  - $Q = 4p.\frac{\sin q}{l} = \frac{2p}{d}$ for constant wavelength data
  - $Q = \frac{2p}{tof}.p_1$ for time of flight data
  - $Q = E.\frac{2p}{c_E}$ for dispersive energy data

5.5.3 d (Å)

- Plot the patterns in the d_{hkl} space:
  - $d_{hkl} = \frac{l}{2\sin q}$ for constant wavelength data
  - $d = \frac{tof}{p_1}$ for time of flight data
  - $\cdot\, d = \frac{c_E}{E}$ for dispersive energy data

5.5.4 **sin**q/l (Å^{-1})

- Plot the patterns in the $\sin q/l$ space: $\sin q/l = \frac{Q}{4p}$

5.5.5 s = 1/d (Å^{-1})

- Plot the patterns in the reciprocal space (Å^{-1}): $s = \frac{1}{d}$

5.5.6 Change to W.H. plot

- Plot a Williamson Hall type plot ($b^* = f(d^*)$) from data coming from a ASS file ($\left(b^*/d^*\right)^2 = f\left(b^*/d^{*2}\right)$)
- *!! Of course, this option is only available if a ASS file is plotted !!*

5.5.7 Save data as WHP file

- Save data on screen as a WHP file for a Williamson Hall type plot
- *!! Of course, this option is only available if a Williamson Hall plot is displayed !!*

5.5.8 Change to A.S.S. plot

- Plot a Average Size Strain type plot ($\left(b^*/d^*\right)^2 = f\left(b^*/d^{*2}\right)$) from data coming from a WHP file ($b^* = f(d^*)$)
- *!! Of course, this option is only available if a WHP file is plotted !!*

5.5.9 Save data as ASS file

- Save data on screen as a ASS file for a Average Size Strain type plot
- *!! Of course, this option is only available if a Average Size Strain type plot is displayed !!*

5.5.10 Change wavelength

- Access to a dialog box to select a new wavelength
- Simulation of a pattern with the new wavelength in the same $\sin q/l$ range
- Superposition of both diffraction pattern
- *!! Available if only one diffraction pattern on screen !!*

5.6 Calculation menu

5.6.1 Summation

- Summation of the Y values of all the patterns on screen
- Plot the summation result
- *!! only available if more than 1 pattern on screen !!*
- *!! files on screen must have identical X values and same number of data !!*

5.6.2 Difference

- Subtraction of Y values of two patterns on screen
- Plot the difference result
- *!! only available if 2 patterns on screen !!*
- *!! files on screen must have identical X values and same number of data !!*

5.6.3 Average

- calculation of the average of Y values of all the patterns on screen
- Plot the average result
- *!! only available if more than 1 pattern on screen !!*
- *!! files on screen must have identical X values and same number of data !!*

5.6.4 Multiply X and/or Y

- Access to a dialog box to select coefficients to multiply X and Y values for all the pattern on screen
- Plot the result

5.6.5 Derivative data

- Calculation and plot the derivative data (default coefficients = 1.)
- *!! available if only 1 pattern on screen !!*

5.6.6 Smoothing

- Access to a dialog box to enter the number of iterations for the smoothing procedure
- Plot the smoothing result

5.6.7 Centroid

- Determination of the position of the maximum of intensity
- Calculation of the centroid of points, corresponding intensity and estimated FWHM (case of a gaussian profile)
- Results are displayed in a window
- *!! available if only 1 pattern on screen !!*

5.6.8 Integration

- Select with the left mouse button, the lower and upper limits for the integration
- Integration results are display in a window and stored in a file ".INT"
- *!! available if only 1 pattern on screen !!*

5.6.9 Profile fitting

The profile fitting procedure (XRFIT calculation) uses pseudo-Voigt functions (linear combination of a Gaussian profile and Lorentzian profile) with a global FWHM (Full width at half maximum) and a global eta (proportion of Lorentzian), and a linear background. Each Bragg peak is characterized by its position, intensity, FWHM and eta shifts with respect to the global parents. One of the peaks, at least, must have zero shifts to avoid singular matrix error.

The profile fitting procedure is minimizing the c^2 function, defined by:

$$c^2 = \frac{\sum_i w_i.(Y_i^{obs} - Y_i^{calc})^2}{N - P}$$

where:

* $\sum_i$: summation on the N points
* w_i : counting weight ($w_i = 1/sigma(Y_i^{obs})$)
* Y_i^{obs} : observed counting
* Y_i^{calc} : calculated counting
* P : refined parameters number

For each reflection profile characterized by its FWHM and eta component, the H_G and H_L values (FWHM of the Gaussian and Lorentzian profiles of the Voigt function respectively) are calculated from the pseudo Voigt approximation parameters (H=Fwhm, eta) using the following formulation (ref.: Thompson, Cox, Hastings, J. Appl. Cryst. (1987), 20,79-83)

$$H^5 = H_G^5 + 2.69269.H_G^4.H_L + 2.42843.H_G^3.H_L^2 + 4.47163.H_G^2.H_L^3 + 0.07842.H_G.H_L^4 + H_L^5$$

$$eta = 1.36603.\left(\frac{H_L}{H}\right) - 0.47719.\left(\frac{H_L}{H}\right)^2 + 0.11116.\left(\frac{H_L}{H}\right)^3 +$$

Integrals breaths b_G and b_L of the Gaussian and Lorenzian normalised profiles are then calculated as:

$$b_L = \frac{p}{2}.H_L$$

$$b_G = \frac{1}{2}.H_G.\sqrt{\frac{p}{\ln(2.)}}$$

and the integral breath of the Voigt function as:

$$b = p.\frac{H/2}{eta + (1-eta).\sqrt{p.\ln(2.)}}$$

Different output files are created:

* file_name.OUT: detailed output file of the profile fitting procedure (starting parameters and flags, c^2 and $R_{profile}$ values, refined parameters and sigmas, correlations ...)
* file_name.SUM: summarized output file
* file_name.NEW: input file with the refined parameters values
* file_name.REF: multicolumn file with the refined parameters values and sigmas
* file_name.IRF: H_G, H_L values versus 2theta Bragg position value
* file_name.XRF: multicolumn file with Yobs, Ycalc ... (see data files format in 1.1 section)
  This file is automatically loaded and plotted on screen after running the fitting profile procedure. Information about the fitted reflections (position, integrated intensity, fwhm, eta) can be obtained by clicking (with the left mouse button) on the peaks vertical tics.
* peakn.XY: calculated sub-profiles (X-Y type)

This procedure can be performed through three different ways:

1 *after an automatic peak search*

An automatic profile fitting is performed, starting from parameters automatically determined by the peak search procedure (positions, intensities, background levels) and the following parameters:

```
. λ1 / λ2 = 0
. JOBTYP = 2
. asymmetry parameter = 0
. global FWHM = 0
. global ETA  = 0.02
. shift-fwhm  = 0.
. shift-eta   = 0
. icyc = 10
```

Profile refinement is performed with the following codes conditions:

```
. asymmetry parameter = 0
. left background  = 1
. right background = 1
. global FWHM      = 0
. global ETA       = 0
 . positions        = 0
. intensities      = 1
```

```
 . shift-fwhm       = 0
. shift-eta        = 0
```

2 From a .PIK file

Profile refinement is performed with all the conditions defined in the input .PIK (or .NEW) file. This file has the following format:

```
. line 1: title
. line 2: AIN, AFIN, NBACK, NPEAK, NCYC, INTER, INST, JOBT, CONT, IW,
          CORR, CONSTR
          1. AIN  : initial angle (in degrees)
          2. AFIN : ending  angle (in degrees)
          3. NBACK: number of background points
          4. NPEAK: number of reflexions in the angular range
          5. NCYC : number of cycles in the refinement
          6. INTER: 0: shirt listing
                    1: detailed listing
          7. INST : data format (as INSTRM in FullProf)
                      (see data file format in section 1.1)
                    0: Free format
                    1: multicounters diffractometers format
                    3: D1B, D20 format
                    5: general two-axis format
                    6: multicounters diffractometers format
                    8: DMC diffractometer
                    9: X-Y format with a title (INSTRM=10)
          8. JOBT  : 1: fit Ka1/Ka2
                     2: fit single peaks
                     3: simulation of ka1-ka2 doublets
                     4: simulation of single peaks patterns
          9. ICONT : 0: no more angular range
                     1: after the end of this angular range, another set
                         of parameters will be read in the same file
         10. IW    : data weight
                      0: weight(i) = 1/Yobs(i)
                      1: weight(i) = 1/Ycalc(i)
         11. CORR  : ?
         12. CONST : ?
. line 3: lambda1, lambda2
. lines 4: global profile parameters (i: 1 -->9) value(i)    flag(i)
                      i = 1: Ka1 / Ka2 ratio
                          2: asymmetry parameter 1
                          3: asymmetry parameter 2
                          4: U resolution parameter
                          5: V resolution parameter
                          6: W resolution parameter
                          7: Z resolution parameter
                          8: Eta0
                          9: X

    These profile parameters are defined as follows:
         .   pV(x) = Eta*L(x) + (1-Eta)*G(x)
    with:
             pV: pseudo-Voigt function
              L: Lorentzian function
              G: Gaussian function
            Eta: lorentzian component (Eta = Eta0 + X*2Theta)
              x: 2theta - 2theta_Bragg
        . FWHM = SQRT((U*tan(Theta) + V)*tan(Theta) + W) + Z/cos(Theta)

. lines 5: background parameters (NBACK lines)
           2Theta/TOF    background_intensity   Flag
. lines 6: reflections parameters (NPEAK lines)
    2Theta/TOF  intensity  shift-FWHm  shift_Eta  & corresponding Flags


          Remark: flag = 0 => fixed parameter
                         1 => refined parameter
```

3 Handling mode

- select, with the left mouse button: left and right background, intensity, position and FWHM for any peak to fit (max=15).
- exit with the rightmouse button
- access to the dialog box to change starting fitting parameters and select parameters to fit (see XRFIT user's guide)

5.6.10 Reload data file

- reload previous data file on screen
- !! only available after plot of XRF file !

5.6.11 Fit from .PIK

- access to the Windows directories dialog box to select a .PIK (or NEW) file (input file for a profile fitting procedure) (see the corresponding format in 6.9 section)
- access to the "Windows directories dialog box" to select a data file to run the fitting profile procedure
- execute the profile fitting procedure with these selected two input files (if a .NEW file is selected, this file will be renamed as a .PIK file before executing the profile fitting procedure)

5.6.12 Background subtraction

- Access to the "Background subtraction" menu:
- !! only available if only one pattern on the screen !!

I. Background point

Access to a dialog box to select the background points selection type (automatic - see 4.3- or manual background 'see 4.4-)

II. Data - background

- interpolation of the previous selected background points to determine the background contribution for each point in the pattern (linear or spline interpolation)
- calculate and plot the pattern without the background contribution

5.6.13 FWHM (Caglioti)

- Access to a dialog box to enter U,V,W parameters (Caglioti formula) for a calculation of the angular dependence of the Fwhm, and two others parameters defining the angular 2theta range.

  Caglioti formula (*Caglioti, Paoletti, Ricci, Nuclear Instruments and Methods 3 (1958) 223-228*):

$$Fwhm^2 = U.tg(q)^2 + V.tg(q) + W$$

- Automatic plot of the FWHM=f(2theta) resolution curve
- *! Diffraction data files can not be loaded after a FWHM file. Reset WinPLOTR !*

5.6.14 Linear fit

- Fit the points with a linear function
- Display results in a window
- Plot the linear curve
- *!! only available if one "microstructural" file been plotted (W.H.P. or A.S.S.) !!*

5.7 Rietveld plot menu

5.7.1 (hkl) list

- Open a window and display the list of Bragg positions and indexation of all Bragg reflections on screen
- *!! only available for Rietveld files !!*

5.7.2 Zero difference

- Draw an horizontal line to represent $Y_{obs} - Y_{calc} = 0$
- *!! only available for Rietveld files !!*

5.7.3 Reload Rietveld file

- Load the last plotted Rietveld file and plot it with the same graphic options (plot range, colours...)
- This can be useful if FullProf is running in another window without exit WinPLOTR
- *!! only available for Rietveld files !!*

5.7.4 Excluded regions

- Plot or not data in the excluded regions (use as a switch)
- *!! only available for Rietveld files !!*

5.7.5 Plot equi F^2 line

- Plot or not the $F^2_{calc} = F^2_{obs}$ line (use as a switch)
- *!! only available for single crystal FullProf refinement .PRF files !!*

5.8 Text menu

5.8.1 Write reflections indices (ON/OFF)

- Write on the plot the indices of (hkl) reflections (use as a switch)
- *!! only available for Rietveld files or microstructural files !!*

5.8.2 Filename

- Display or not the filenames on the plot (use as a switch)

5.8.3 Legend text

- Access to a dialog box to enter texts for X and Y legends and main title
- Plot the patterns with the previous legends

5.8.4 Write graduations

- Access to a dialog box to select to write or not X and Y graduations
- Plot the patterns with the previous features
- *!! Can be useful in pseudo-3d plots !!*

5.8.5 Write negative graduations

- Write or not the negative Y graduations
- Plot the patterns with the previous features
- *!! Can be useful for Rietveld plots where the Y_{obs}-Y_{calc} curve has been shifted !!*

5.8.6 Text colours

- Access to the “Text colours menu”

  - *Main legend colour*
    Access to the Windows colour dialog box to select a new colour for the main legend text

  - *X legend colour*
    Access to the Windows colour dialog box to select a new colour for the X legend text

  - *Y legend colour*
    Access to the Windows colour dialog box to select a new colour for the Y legend text

  - *X graduations colour*
    Access to the Windows colour dialog box to select a new colour for the X graduations text

  - *Y graduations colour*
    Access to the Windows colour dialog box to select a new colour for the Y graduations text

  - *Indices colour*
    Access to the Windows colour dialog box to select a new colour for the indices text
    (!! Only available if the “write reflections indices” option has been validated in microstructural plots !!)

5.8.7 Text fonts

- Access to the “Text fonts menu”

  - *Main legend font*

Access to the Windows fonts dialog box to select a new font for the main legend text

- *X legend font*
  Access to the Windows font dialog box to select a new font for the X legend text

- *Y legend font*
  Access to the Windows font dialog box to select a new font for the Y legend text

- *X graduations font*
  Access to the Windows font dialog box to select a new font for the X graduations text

- *Y graduations font*
  Access to the Windows font dialog box to select a new font for the Y graduations text

- *Filename font*
  Access to the Windows font dialog box to select a new font for the filenames text

- *Indices font*
  Access to the Windows font dialog box to select a new font for the indices text
  (!! Only available if the "write reflections indices" option has been validated in microstructural plots !!)

5.8.8 Legends positions

- Access to a dialog box to enter position (in X and Y) and the rotation value to write text of X and Y legends and main legend title
- Plot the patterns with new legends text positions and rotation
- *!! Negative X positions leads to center the text horizontally in the window !!*
- *!! Rotation values are defined towards the horizontal line (horizontal text: rotation = 0.;vertical text: rotation = 90.)*

5.8 External applications

5.8.1 DOS window

- Open a DOS window in the working directory
- !! WinPLOTR window is still active !!

5.8.2 Edit a file

- Access to the "edit a file" menu to select a particular type file and load it into an editor (the text editor can be specified in the "WinPLOTR.set" file, via the " Edit = " keyword in the "! RUN PROGRAMS: " part; if not, the "NOTEPAD" editor will be used)

  - **.* file*
    - ↘ Access to the Windows directories dialog box to select a file to edit

  - **.PCR file*
    - ↘ Access to the Windows directories dialog box to select a .PCR FullProf input file to edit

- **.PIK file*
  - ↘ Access to the Windows directories dialog box to select a .PIK (or .NEW) to edit for the profile fitting procedure

- **.DIC file*
  - ↘ Access to the Windows directories dialog box to select a .DIC WinDICVOL input file to edit

- **.INP file*
  - ↘ Access to the Windows directories dialog box to select a .INP WTREOR90 input file to edit

- **.ITO file*
  - ↘ Access to the Windows directories dialog box to select a .ITO WITO input file to edit

- **.SAT file*
  - ↘ Access to the Windows directories dialog box to select a .SAT (.PIC) SuperCELL input file to edit

- *WinPLOTR.SET file*
  - ↘ Edit the "WinPLOTR.Set" settings file

Remark: Files with particular extensions (maximum = 4) can be defined by the user in the WinPLOTR.set settings file, via the " EDIT FILES:" keyword. In such a case, the corresponding options are automatically added in the "edit a file" menu

5.8.3 Run FullProf

- Access to the Windows directories dialog box to select a .PCR input file for FullProf
- If necessary, access to the Windows directories dialog box to select the data file name for FullProf
- Run the Rietveld-type FullProf program
  Remark: if the version of FullProf to be used is not defined in the "WinPLOTR.Set" file (via the "FULLPROF=" keyword in the "! RUN PROGRAMS:" part, the "wfp2k.exe" Windows version of FullProf will be used)
- Plot the last .PRF file created by the previous run of FullProf, as a Rietveld type plot (Y_{obs}, Y_{calc}, Y_{obs}-Y_{calc}, Bragg_positions)

5.8.4 Run DICVOL

- Access to the Windows directories dialog box to select a .DIC input file for DICVOL
- Run the DICVOL ((D. Louër & A. Boultif) program
  Remark: if the version of DICVOL to be used is not defined in the "WinPLOTR.Set" file (via the "DICVOL=" keyword in the "! RUN PROGRAMS:" part, the "windic.exe" Windows version of DICVOL will be used)

5.8.5 Run TREOR

- Access to the Windows directories dialog box to select a .INP input file for TREOR
- Run the TREOR (P.E. Werner) program (automatic indexing of powder diffraction patterns)

Remark: if the version of TREOR to be used is not defined in the "WinPLOTR.Set" file (via the "TREOR=" keyword in the "! RUN PROGRAMS:" part, the "wtreor90.exe" Windows version of TREOR will be used)

5.8.6 Run ITO

- Access to the Windows directories dialog box to select a .ITO input file for ITO
- Run the ITO (J. VISSER) program

  Remark: if the version of ITO to be used is not defined in the "WinPLOTR.Set" file (via the "ITO=" keyword in the "! RUN PROGRAMS:" part, the "wito.exe" Windows version of ITO will be used)

5.8.7 Run SuperCELL

- Access to the Windows directories dialog box to select a .SAT input file for SuperCELL
- Run the SUPERCELL (J. RODRIGUEZ-CARVAJAL) program

  Remark: if the version of SuperCELL to be used is not defined in the "WinPLOTR.Set" file (via the "SUPERCELL=" keyword in the "! RUN PROGRAMS:" part, the "supercell.exe" Windows version of SuperCELL will be used)

5.8.8 Run user's defined programs

- Access to the "run user's programs" menu to select programs defined by the user in the "WinPLOTR.set" file.
- If the number of arguments relative to the selected program has been previously defined, access to the Windows directories dialog box to select arguments files
- In case of FULLPROF programs, the last PRF file created by FullProf is automatically displayed as a Rietveld type plot

5.8.9 Select EXE file

- Access to the Windows directory dialog box to select an EXE file to be launch from WinPLOTR

5.8.10 Run the Windows calculator

- Launch the "calc.exe" program (Windows calculator)

5.9 Help menu

5.9.1 User's guide

- Access to the user's guide menu to select a user's guide file to edit (WinPLOTR.ins, FullProf.ins, WinDIC.ins, TREOR.ins, ITO.ins or SuperCEL.ins file)

5.9.2 WinPLOTR news

- Display this "WinPLOTR.new" file in a text window

5.9.3 FullProf news

- Display this “fp2k.inf” file in a text window

5.9.4 Settings

- Display this “winplotr.set” file in a text window or the main parameters and associated values used by WinPLOTR if the WinPLOTR environment variable has not been correctly defined

5.9.5 Help files (ON/OFF)

- Display or not help files in windows (use as a switch)

5.9.6 WinPLOTR help files

- Launch the Windows help system with the “winplotr.hlp” file

5.9.7 About WinPLOTR

- Open a message box with authors coordinates and WinPLOTR Email and URL addresses

6. Use of the mouse in WinPLOTR

Many mouse handling capabilities has been implemented in WinPLOTR:

- Select menu options in menu bar and drop-down menus
- Use tools in the toolbar
- Answer dialog boxes
- Resize and move windows
- Select text in text windows (with the “CTRL-C” command)
- Scroll text windows …

Moreover, when a pattern plot is displayed in the graphic window, zoom of the pattern plot can be performed with the left mouse button via the drag operation (pressing, move and release). Click with the right mouse button will redisplay the complete patterns in the pattern window. In any case (zoom or not) moving the mouse inside the graphic windows will give information (in the status bar) about the X and Y position of the mouse cursor, in physical units.

Different kinds of operations can also be realised using the mouse capabilities and some tools in the toolbar, depending on menu selections:

- **Zoom / Focus**
  - left button click on arrows tools in the toolbar leads to move the plot in the corresponding direction, by step of 1/10 of the axis range:

	$X_{min} = X_{mini}$ $X_{max} = X_{min} + 0.1 \, . \, X_{delta}$		$Y_{min} = Y_{min} + 0.1 * Y_{delta}$ $Y_{max} = Y_{max} + 0.1 * Y_{delta}$
	$X_{min} = X_{min} - 0.1 * X_{delta}$		$Y_{min} = Y_{min} - 0.1 * Y_{delta}$

	$X_{max} = X_{max} - 0.1 * X_{delta}$		$Y_{max} = Y_{max} + 0.1 * Y_{delta}$
	$X_{min} = X_{min} - 0.1 * X_{delta}$ $X_{max} = X_{max} + 0.1 * X_{delta}$		$Y_{min} = Y_{min} + 0.1 * Y_{delta}$ $Y_{max} = Y_{max} - 0.1 * Y_{delta}$
	$X_{min} = X_{min} + 0.1 * X_{delta}$ $X_{max} = X_{max} - 0.1 * X_{delta}$		$Y_{min} = Y_{mini}$ $Y_{max} = Y_{maxi}$
	$X_{min} = X_{mini}$ $X_{max} = X_{maxi}$		$Y_{min} = Y_{min} - 0.1 * Y_{delta}$ $Y_{max} = Y_{max} - 0.1 * Y_{delta}$
	$X_{min} = X_{mini} + 0.1 * X_{delta}$ $X_{max} = X_{maxi} + 0.1 * X_{delta}$		
	$X_{min} = X_{maxi} - 0.1 * X_{delta}$ $X_{max} = X_{maxi}$		

Remark: Z_{mini} and Z_{maxi} (Z=X,Y) are related to the lowest and largest X,Y values of the loaded files

- right button click: exit from the Zoom/Focus option can display the complete patterns ($Z_{min}=Z_{mini}$ and $Z_{max}=Z_{maxi}$ Z=X,Y)

- **Select background**
  - left button click: select the current position of the mouse as a background point. This point is then displayed in the pattern window.
  - right button click: exit from the background mouse handling procedure

- **Select points**
  - left button click: select the current position of the mouse as a selected point. This point is then displayed in the pattern window as a vertical bar.
  - right button click: exit from the select point mouse handling procedure

- **Integration**
  - First left button click: select the current position of the mouse as the left background point. This point is then displayed in the pattern window.
  - Second left button click: select the current position of the mouse as the right background point. This point is then displayed in the pattern window.
  - right button click: exit from the select point mouse handling procedure

- **Profile fitting**
  - First left button click: select the current position of the mouse as the left background point. This point is then displayed in the pattern window.
  - Second left button click: select the current position of the mouse as the right background point. This point is then displayed in the pattern window.
  - Following two left button clicks: for each of the Bragg peak, select the current position of the mouse as intensity (for the first click) and the Full Width at High Maximum (for the second click).
  - Right button click: exit from the select point mouse handling procedure

- **Plot of PRF file**
  - left button click on a Bragg reflection positions (vertical tics) will display in a text window the corresponding information about the selected reflection: indexation:(hkl) indices, Bragg position, phase number, wave propagation vector.
  - right button click on a Bragg reflection positions (vertical tics): no particular action

- **Plot of XRF file**
  - left button click on a Bragg reflection positions (vertical tics) will display in a text window the corresponding information about the selected reflection: Bragg position, integrated intensity, Fwhm, Lorentzian eta component, H_g and H_L (see profile fitting procedure).
  - right button click on a Bragg reflection positions (vertical tics): no particular action

- **"Add peaks" option**
  - left button click: select a Bragg peak intensity and position (or a background) point to add it in the reflections / background points list
  - right button click: exit from this mouse handling procedure

- **"Remove peaks" option**
  - left button click: on a vertical Bragg tic / background point will select a reflexion / background point to remove from the reflections / background points list
  - right button click: exit from this mouse handling procedure

7. References

Please use one of the following references for WinPLOTR:

T. Roisnel and J. Rodríguez-Carvajal
WinPLOTR: a Windows tool for powder diffraction patterns analysis
Materials Science Forum, Proceedings of the European Powder Diffraction Conference (EPDIC7), in press

Juan Rodríguez-Carvajal and Thierry Roisnel
FullProf.98 and WinPLOTR: New Windows 95/NT Applications for Diffraction
Commission for Powder Diffraction, International Union of Crystallography, Newsletter N°20 (May-August) Summer 1998