

WinPLOTTR news

June 2025

- New format of Rigaku data file : Profile0.txt file can be read and plot with format=1 (X,Y data + INSTRM=10) or format=15 (Rigaku). In the case of selection of a compressed .RASX file through Format=15, the zipped .RASX is first uncompressed with unzip software defined in the [SYSTEM APPLICATIONS] section of the WinPLOTTR setting file through UNZIP keyword. By default, Profile0.txt file is stored in the \\%TEMP%\Data0 folder if TEMP variable environment is defined and in the current working folder if no TEMP environment variable is defined.

December 2024

- Some shortcuts has been defined to launch some particular tasks :
 - CTRL+F : run FullProf
 - CTRL+E : launch text editor
 - CTRL+C : launch DOS command windows
 - CTRL+R : run previous command (idem REDO button)
 - CTRL+X : Exit WinPLOTTR

October 2023

- Routine of reading .UXD files has been modified to be in total agreement with **FullProf** and **WinPLOTTR-2006** ones : starting point 2Theta_min value of the diffraction pattern is then detected through _2THETA= or _START= items.
In case of .UXD files created by **PowDLL**, it can be generate error in 2Theta_min value if _2THETA and _START= values are different.

June 2023

- New routine of histogram display implemented in april 2023 has been named as "histogram 2" in the "Options / Style" dialog box. Old histogram display is still named as "histogram".
- "Calculation / derivative" has been reactivated : for clearness, data of first derivative curve has been multiplied by Y_max/Yderivative_max.

April 2023

- Histogram display is now compatible with shifts and offsets plot options.

January 2023

- Correction of bug in reading .ipc microstructural file

December 2022

- Correction of bugs :
 - New wavelength input through **X space / Enter wavelength** menu option is now correctly taking into account in the status bar display.
 - Colors changes for data files loaded after plotting a PRF file
- **WinPLOT**R has been compiled with the latest version of CRYSFML, allowing to get informations about trigonal space groups in a rhomboedral description (ex : R -3 C:R)

June 2022

- New `skip_header_lines` item in the [OPTIONS] section of the `winplotr.ini` setting file allows to define the number of header lines to skip when reading a powder diffraction data file.

February 2021

- **File / select files** dialog box is now limited to a maximum of 100 patterns, even if `Max_Patterns` value, defined in the `winplotr.set` setting file, is larger. Routine to create the select file dialog box has been slightly modified to avoid (definitively ?) **WinPLOT**R crash (RealWin bug?).

November 2020

- Minor changes in the reading of .PGF files containing several patterns with the "# DATA: X Y COMMENT" format. This allows to obtain comment for every point of all the patterns when clicking on a particular point.

October 2020

- Lines containing * character as first character in the data file header are considered as comment lines, as well as for ! or # characters. This allows to read and plot .dat or .xy data files coming from Rigaku diffractometers. Please use "1. X,Y data + INSTRM =10" data file format.

June 2020

- **File/Open File/ XY data** menu option can read .csv file containing comma separated values (X,Y) without any header (coming from ICSD for example).

May 2020

- Cosmetic changes in the treatment of excluded regions for Rietveld type files (FullProf, Jana, Rietan, CIF)

April 2020

- **Tools / hkl list generation** is now creating a kind of Debye-Scherrer film with same intensities Bragg peaks. The format of this pattern is a .PGF file with "data_type=3" and "DATA: X COMM" identifiers.
- New PRF_header item in the [OPTIONS] section of the winplotr.ini setting file : allows reading .PRF file created by **CRYSCALC** and containing a file header with profile parameters and structural informations (PRF_header = 1 in the [PATTERN SIMULATION] section of the CRYSCALC.ini setting file).

March 2020

- **WinPLOTTR** web site moved from <http://www.cdifx.univ-rennes1.fr/winplotr> to <https://cdifx.univ-rennes1.fr/winplotr>

December 2019

- **Tools / Molecular weight calculation** can manage real values for stoichiometry (thanks to JGP for the suggestion). Chemical formula can also be input (ie. La1 Mn1 O3).
- New **Plot / Cancel shifts/offsets** menu option : allows to cancel the effects on data of successive shifts and offsets.

April 2019

- **WinPLOTTR** can now read .XRDML files created by new version of DataCollector V6.1 (<intensities unit="counts"> </intensities> tags has been changed to <counts unit="counts"></counts> tags).

November 2018

- **File / save data as / save data as multicolumns file** : If several files has been read, corresponding sigmas can be saved in multicolumns file only if sigma_arrays = Y in the [OPTIONS] section of the setting file.
- RIETAN2000/IGOR format : sigmas are now reading in the file and corresponding extension can be different than .INT.

October 2018

- **File / save data as / save UXD-XRDML as single scans** : if temperature is contained in the raw multiscan file, the created buffer file is directly compatible with the external temperature file used by FullProf in sequential mode.

September 2018

- **File/Open a setting file** routine has been corrected. User can now select particular setting file name with different settings (winplotr.set setting file present in the **WinPLOTTR** folder was always used).

July 2018

- New **Rietveld plot options / plot tics out of X range menu option** : acts as a switch, plotting or not vertical tics (Bragg positions) appearing out of X range. This can be usefull in order to avoid displaying tics of Bragg peaks appearing at angles values higher than the last angular point of the measured pattern but contributing to the counting at this angular point and then present in the reflections list.
- Rietved/profile files (XRFIT, Rietan, CIF ...) can be plotted in different scales (Log, SQRT ...)
- A new routine to calculate difference curve and reflections tics positions has been implemented.

June 2018

- .PRF files created by **JANA2006** can be plotted in log scale.

March 2018

- When **WinPLOT**R is launched in command line and using a buffer file as argument, the data file format can be deduced from the extension of the first file in the buffer. In case of identical extension for different formats (ex : .dat), the associated format can be specified in the MY COMMAND LINE DEFAULT FORMATS section of the winplotr.set setting file.

July 2017

- In case of zoom, normalization procedure is now performed towards the maximum of countings in the zoomed range and not the whole pattern..

February 2017

- The script to be ran by **FullProf** is correctly created in the particular case of sequential mode refinement of multi-patterns (write multi-pattern as "data file code" item in the **FP-CYC/WinPLOT**R dialog box).

September 2016

- **Plot / Offset X,Y / for a particular file** routine has been corrected (offset values were not initialized)

May 2016

- **PRF+/PRF-** buttons were corrupted
- search satellites from .PRF : presence of excluded regions is now considered
- save as .sat file : check if file extension is given for created file
- **Select files** dialog boxes routine has been changed to avoid **WinPLOT**R crash (RealWin bug?). This new routine is applied for number of loaded patterns smaller than 25.
- **Change graduations tex** menu option has been reactivated.

March 2016

- Changes in the routine of reading .dis files created by **FullProf**

October 2015

- Header of output files created by **WinPLOTTR** (.XY, .XYY, INSTRM_0.dat) contain values of used wavelengths.

September 2015

- Cursor position provides 2theta(°) and d(A) values if a single pattern of a PRF **FullProf** file is present on screen and plotted in 2theta space.

August 2015

- Data coming from .UXD (Bruker) and .XRDML (Panalytical) can be plotted in coutings per sec. This can be specified through the data_cps=Y/N keyword in the [OPTIONS] section of the WinPLOTTR.set setting file. If not, a dialog box opens.
- Correction of bug in the reading of .XYY files created by **WinPLOTTR**.

June 2015

- The extension of the **WinPLOTTR** command file can be specified in the setting file trough the command_file_extension= keyword in the [OPTIONS] section :
command_file_extension = .cfe ! winplotr command file extension
Default value for this command file extension is .cmd

March 2015

- A **REDO** button has been added in the toolbar, allowing to execute in the same conditions the previous program launched from **WinPLOTTR**. This can be useful for example to launch **FullProf** with the same arguments as the previous **FullProf** run.
- Default of filenames number to write can be defined in the [OPTIONS] section of the setting file and the following line :
max_write_filenames = 15
- Graphic options (color, marker, style) and X/Y multipliers can now been defined for an individual data file
- New **Text/Display filenames in a window** menu option (not yet fixed)
- Correction in reading new *_dis.SEQ files created by **FullProf**

February 2015

- Number of linked external programs with the "@" character that can be launched from the toolbar has been extended from 3 to 5.
- Minor changes in the code of "exit" procedure.
- **Rietveld plot options** are activated for **RIETAN2000** .PRF file

June 2014

- New parameter in the [OPTIONS] section of the WinPLOTTR.set setting file, allowing to select Y scale for the plot :
Y_scale = LINEAR/LOG/SQRT/YQ2
Default value = LINEAR

April 2014

- Noisy data item has been added in the peak search and background points search procedures dialog boxes

March 2014

- **Points selection / Automatic satellites search** menu option has been implemented. This option is available only after plotting a PRF file and allows to perform peak search on the difference curve. Results can then be saved for **K_search** program to search propagation vector components of a magnetic phase.

February 2014

- After a files summation, difference or average, the resulting file can be saved with corresponding esd's. Of course, sigma_arrays item has to be equal to 1 (or Y) in the winplotr.set setting file.

November 2013

- New sections in the WinPLOTTR.set file :
 - [3D PLOT OPTIONS] (used to customize automatic pseudo-3D plots)
3D_color = RGB(255, 0, 255)
3D_style = 0
3D_marker = 1
3D_size = 2
3D_pen_width = 1
3D_lines_step = 0
 - [SCREEN RESOLUTION] (used for creation of BMP output graphic files)

```
screen_width=1200
screen_height=800
```

- New tool in **Tools** menu : **Remove blank lines in a file** allows to remove all empty lines in a selected file.
- save esd's item has been added in **Save data / save data as XY file** dialog box

October 2013

- A bug in reading .PRF files created by **Jana2006** has been corrected
- External programs can be launched directly from the toolbar (max. = 3) : these programs have to be specified in the [RUN PROGRAMS] section of the winplotr.set setting file through the '@' character before the identifier of the program.
ex: @ MENDEL = mendel ! My period table ! Windows version
- WinPLOTTR can handle .PRF files created by **CALC_PDF** : The observed and calculated PDF are represented as well as the difference curve. Tick marks correspond to atom pairs distances that can be directly inspected.
- New item in the sequential refinement dialog box : temperatures file can be specified see fp2k.inf (25 sept. 2013) for more details

Septembre 2013

- Bugs have been corrected :
 - Different columns for different multicolumns files (WinPLOTTR format #1) can not be mixed.
 - **Calculation / Multiply X-Y** and **Plot / Offset X-Y** menu option procedures are now corrected after **CANCEL** handling
 - Wavelength is correctly read in XRDML Panalytical format files

July 2013

- Implementation (in CRYSFML) of a new treatment for asymmetry parameters due to axial divergency (Finger et al. JAC 27, 892, 1992)
- Buffer file can contain the title of the plot in the first line if begun by COMMENT or TITLE command.
- New loaded data are still plotted in the current Y mode, even if it a non linear mode (log, SQRT ...)
- New RAW data file format : multiscan XRDML (from PANalytical) can now be read (**WinPLOTTR** format = 58). The **Calculation / Multiscan normalisation** can be applied to these data to create a INSTRM10 data file for **FullProf**.

June 2013

- **DOS** button is now opening a DOS window in the working folder

October 2012

- New keyword for **WinPLOT**R command file :
SUBTRACT file_1 file_2 format
 - file_1 : name of first file
 - file_2 : name of second file (Y_2 data will be subtracted from Y_1 data)
 - format : common **WinPLOT**R format for file_1 and file_2

September 2012

- .spc files created by **DIFFAX** can now be read (format = 16). Only the broadened pattern (column #3) is extracted from the data file.

July 2012

- Minor cosmetic changes in PostScript files

June 2012

- Cosmetic parameters have been added for plotting .PRF files (Rietveld plot options menu) :
 - tics positions : 2 parameters (t_1 and t_2) can be specified, relating to the position of the tics for the phase #1 towards the base line, and the interval between tics of different phases respectively. The following formula is used :
$$\text{pos_tics_ph_n} = \text{MIN}(\text{Yobs}, \text{Ycal}) - n * t_2 * (\text{MAX}(\text{Yobs}, \text{Ycal}) - \text{MIN}(\text{Yobs}, \text{Ycal})) / t_1$$
with $t_2=1$ for $n=1$. The default values for t_1 and t_2 are 20. and 1. respectively but they can be defined in the setting file in the [SHIFT AND OFFSET] section with the help of `prf_tics = keyword`
 - Yobs-Ycalc difference curve position :
$$\text{pos_diff} = \text{MIN}(\text{Yobs}, \text{Ycal}) - (\text{MAX}(\text{Yobs}, \text{Ycal}) - \text{MIN}(\text{Yobs}, \text{Ycal})) * K$$
with $K = (1. + t_3 * \text{Nb_phase}) / 5$. t_3 coefficient can now be specified through the **Tics and diff. curve positions** menu option and default value (0.1875) in the setting file in the [SHIFT AND OFFSET] section with the help of `prf_diff_shift = keyword`.
 - colored tics : switch to use or not different colors for tics of different phases. The default value of this `colored_tics` keyword is false but can be defined in the setting file through the `colored_tics= string` in the [PRF PLOT OPTIONS] section.
 - When points are displayed in excluded regions, those of the Yobs-Ycalc curve are not.
- **Zero shifts in 2theta** menu option has been added to input zero shifts value of a powder diffraction pattern (in the case of 2theta display). The whole zero shift is calculated as : $\text{ZERO} = z_1 + z_2 * \cos(\text{Theta}) + z_3 * \sin(\text{Theta})$ and applied as :
$$\text{new_X} = X - \text{ZERO}$$

May 2012

- Single crystal .UXD scans can now be superimposed.

April 2012

- Bugs in Rietveld options (Zero difference, excluded regions) has been corrected.

March 2012

- In the [AFTER FULLPROF RUN] section of the winplotr.set setting file, edpcr keyword can replaced edit_pcr keyword : **edpcr** will then be automatically launched with the current .pcr file.

February 2012

- **DICVOL** and **TREOR** input file created by **WinPLOTTR** after a peak search procedure contains informations about incident wavelength (wave_1, wave_2, wave_ratio). **DICVOL** and **TREOR** have been modified consequently to create .pcr files containing these informations

January 2012

- winplotr.set setting file ([OPTIONS] part) :
 - locked_cursor = Y line (or 1) provides a new type of cursor. This new option, that is activated if only one pattern is displayed, lockes the position of the cursor to the nearest data point.
 - follow_tfp_folder = Y line (or 1) allows **WinPLOTTR** to recover the current working directory of the **FullProf** toolbar if tfp.exe process is activ.

November 2011

- After launching **FullProf** in sequential mode, **WinPLOTTR** is creating .SEQ files (xx_SEQ.dis for distance calculations, xx_SEQ.hkl for profile matching refinement, xx_SEQ.mic for microstructural analysis) for all phases present in the .PCR file.
- Plot microstructural features after a sequential run of **FullProf** is now active.

July 2011

- Some changes in the .PAT files created by **RIETAN**

January 2011

- **WinPLOTTR** command file : PLOT keyword can have 2 optional arguments, delimiting the range to be displayed
- winplotr.set setting file ([OPTIONS] part) :
 - skip_exit_message = Y line (or 1) can be input to skip the dialog box "*Do you really want to quit WinPLOTTR?*"
 - pcr_history = Y line (or 1) can be input to create, when running **FullProf**, a codefile_PCR_history.1 file from the current PCR file

November 2010

- `Exclude_CELL_from_title` item has been added in the [PRF PLOT OPTIONS] of `winplotr.set` setting file. Equal to 1, this item allows to exclude every character after CELL string from the title of a .PRF file.

May 2010

- Profile fitting of the X-ray K_{α} *Fe* doublet has been added
- EDIT_PCR and EDIT_NEW items can be present simultaneously in the setting file
- Save `winplotr.set` was bugged for [PATTERNS PLOT OPTIONS] section

April 2010

- Read PRF files created by **Jana2006** (version April 2010) :
 - **Rietveld plot option** menu is activated
 - if PRF files are associated to **Jana** files in the `winplotr.set` setting file (see [COMMAND LINE DEFAULT FORMATS] section), the **PRF** button can directly load **Jana** PRF files and **PRF+** and **PRF-** buttons are activated.

March 2010

- Correction of bugs
 - Calculation of intrinsic profile components for HG_sample negative values
 - Cration of WHP file
 - Plot of linear fit

February 2010

- **EXPO2009** can now be launched if defined in the setting file
- **Tools / hkl list generation** is creating a txt file that can be read further through the **Text / Open reflexions file** option
- Last point of .XY files was not considered. Now, it is!

September 2009

- **WinPLOTTR** has been compiled with new versions of CFML (4.00)

June 2009

- small bugs have been corrected :
 - read PANALYTICAL format containing end of lines character in the "<intensities unit='counts'>" section

May 2009

- small bugs have been corrected :
 - Export as BMP and Postscript files

April 2009

- small bugs have been corrected :
 - min and max values in the **zoom dialog box** after changing X space
 - character strings length extended to 132 in the profile fitting routine

February 2009

- **Save as DICVOL points** dialog box : add a check box for DICVOL06 option and modify the input file for **DICVOL06**
 - OPTION = 0 : same as DICVOL04 (optimised search, to be used with normal quality data)
 - OPTION = 1 : offers an extended (exhaustive) search (for difficult cases)

Compared to **DICVOL04** (2004), only one additionnal input parameter is added in **DICVOL06**, i.e. DV06_OPTION in card 5

- Read .PLG files created by the Rietveld program **XND** of J.F. Bézar. The **WinPLOT** format is 106. If a filename.HKL exists in the same folder than the .PLG file, hkl indices are displayed. In the other case, background data will be plotted.

Jan. 09

- SINGLE_SINGLE_PEAK / FIT_SINGLE_DOUBLE keywords can have two arguments, corresponding to the X range for profile fitting procedure
- **WinPLOT** from a command .CMD file can be launched through the **WinPLOT** GUI (**Tools / Run WinPLOT command file** menu option).
- INSTRM14 (ISIS) data files can now be superimposed.
- **Help/FullProf news/FPS web site** has been added to link to **FullProf Suite** news at the ILL **FullProf Suite** web site.
- New keywords for **WinPLOT** command file :
 - SHIFT_X shift_X_value : shift X values by shift_X_value
 - SHIFT_Y shift_Y_value : shift Y values by shift_Y_value
 - OFFSET_X offset_X_value : offset X values by offset_X_value
 - OFFSET_Y offset_Y_value : offset Y values by offset_Y_value
 - MULTIPLY_X coef_X : multiply X values by coef_X value
 - MULTIPLY_Y coef_Y : multiply Y values by coef_Y value
 - PLOT : plot the open file
 - BITMAP : create a BITMAP file (not compatible with PLOT keyword)

- EPS : create a PostScript file (not compatible with PLOT keyword)
- NORM_UXD : constant time normalization of .UXD multi scans files.
- Read .PGL files created by the Rietveld program **XND** by J.F. Bézar. The **WinPLOT** format is 106.
- The routine to read .IPC files created by **WinPLOT** has been corrected.
- Microstructural analysis : the max_strain value, expressed in %% (1E-04), was not correct but just multiplied by 1000 rather than 10000.

December 2008

- **X_space/Change_X_space_from_X1_to_X2** menu option has been added, allowing X space transformations from every kind of input data.
- new keywords are available for the **WinPLOT** command file, for X space transformations :
 - TRANSF_2THETA_TO_Q, TRANSF_2THETA_TO_D, TRANSF_2THETA_TO_STL, TRANSF_2THETA_TO_S
 - TRANSF_Q_TO_2THETA, TRANSF_Q_TO_D, TRANSF_Q_TO_STL, TRANSF_Q_TO_S
 - TRANSF_D_TO_2THETA, TRANSF_D_TO_Q, TRANSF_D_TO_STL, TRANSF_D_TO_S
 - TRANSF_STL_TO_2THETA, TRANSF_STL_TO_Q, TRANSF_STL_TO_D, TRANSF_STL_TO_S
 - TRANSF_S_TO_2THETA, TRANSF_S_TO_Q, TRANSF_S_TO_D, TRANSF_S_TO_STL
- WAVE keyword for **WinPLOT** command file
- interpolation procedure has been corrected.

November 2008

- **WinPLOT** can read XY multicolumns files with tabulator used as separator

February 2008

- Some tools have been added for launching **FullProf** in a sequential mode :
 - FPCYC dialog box
 - * scripts (.bat file) can be created
 - * Plot interatomic distances
 - **Tools/Run scripts** menu option to execute a script file (.bat)
- **Tools / Create buffer** : access to a dialog box to select a particular extension of data files to be stored in a buffer file.
- **File/Save data as/save data as XXX** menu option has been added. Format is compatible with different software as KaleidaGraph, Origin, SignaPlot or Excel.
- **FPCYC hkl** button : arrays and variables are no more reset, allowing display of evolution of different reflexions.

January 2008

- **SEQ** button : evolution of different parameters coming from different .SEQ files (created by FullProf in cyclic mode) can be simultaneously displayed

October 2007

- .PGF files : comments are automatically displayed for X, Y, TEXT data ("DATA: X Y TEXT" in place of "DATA: X Y COMM" where comment is display only after a mouse click on a particular point).

September 2007

- .PRF files with $K\alpha_1$ and $K\alpha_2$ wavelength :
 - Only plots versus 2θ are correct
 - The calculated d_{hkl} in the 'Reflections positions list' is now correct
 - **Text/Write reflections text** menu option will only display reflections indices corresponding to the $K\alpha_1$ wavelength

July 2007

- Some commands for **WinPLOT**R can be included in a command file called through the command line :
d:\progs> winplotr winplotr.cmd
This command file must have .CMD extension and can contain some keywords and related arguments to order to be performed by **WinPLOT**R . Following keywords have been included :
 - FILE file%name file%format
The file%name file will be read with the file%format **WinPLOT**R format (see user's guide)
 - SAVE_AS_XY
Data of input data file will be saved in a XY 2 columns file
 - SAVE_AS_INSTRM_0
Data of input file will be saved as a INSTRM_0 file for FullProf
 - FIT_SINGLE_PEAK
Data will be fitted with a single peak profile
 - FIT_SINGLE_DOUBLET_CU/FIT_SINGLE_DOUBLET_MO/FIT_SINGLE_DOUBLET_CO
Data will be fitted with a single X-ray doublet profile for Cu, Mo, and Co radiation respectively
- **Calculations / Fit single peak** and **Calculations / Fit single doublet** (for X-ray Cu, Mo and Co $K\alpha$ radiation) has been implemented. This allows automatic profile fitting (without input of parameters through mouse clicking and dialog box).

June 2007

- **Calculations / Polymer crystallinity rate** menu option has been added : access to the cursor to select background points corresponding to the amorphous phase of the compound and calculation of the crystallinity rate of a polymer as follows :
 - integration of the amorphous phase intensities (a)
 - integration of the sample intensity (s)
 - $\text{crystallinity_rate} = 1 - a/s$

March 2007

- **Tools / PCR space group info** menu option has been added and is active if a .PCR file has been edited : informations about the space group in the current .PCR file are then output in a window.
- Links have been created between structural parameters of the current edited .PCR file and input parameters of the **Tools / hkl list generation** and **tools / unit cell volume calculation** dialog boxes.

January 2007

- New facilities in the **Rietveld plot options** menu, activated after loading .PRF files :
 - **Save as .PRF template** : all the plot features of the Rietveld plot (colors, graduations, text legends, fonts ...) are stored in a template file (extension = *.TPL). The format of this type of file is similar to the .PGF files created by **WinPLOT** .
 - **Open .PRF template file** : load all the plot features in a .PRF template file (*.TPL) for a Rietveld plot.

November 2006

- Data file format coming from a Rigaku Rint diffractometer has been add. The **WinPLOT** corresponding format number is #15 and the default extension is *.TXT

October 2006

- **Help / FullProf Suite Web site** links to the **FullProf Suite** at ILL : <http://www.ill.fr/pages/science/IGroups/diff/Soft/fp>
- **Help / FullProf user's guide / FullProf and microstructural effects** menu option links to microstructural_effects.pdf file present in the \doc or \tutorials folder
- **WinDICVOL04** can create .PCR files for **GSAS** diffraction data files

September 2006

- .CIF files created by **GSAS** can be read as profile data files
- **Help / Environment variables** menu option to get informations about environment variables related to **WinPLOT** and **FullProf** .

July 2006

- .CIF files containing experimental and calculated powder diffraction profiles and created by **FullProf** (xx_prof.CIF) can now be read through the **File / Open Rietveld-profile file** menu option. The **WinPLOT** corresponding format is 105.

February 2006

- **MENDEL** : X rays data for Cobalt radiation has been added
- **Tools / hkl list generation** menu option has been added

October 2005

- **FullProf** in cyclic mode :
 - new item in the **Cyclic mode of FullProf** dialog box : the user can select to plot cyclic **FullProf** refined parameters or hkl features (intensity, position) coming from profile matching run of **FullProf** . In this later case, **Save HKL files** has to be activated. A new filename_FPCYC.HKL file is then created by **WinPLOT** from the contains of the filename_1.hkl files created by **FullProf** for the first phase.
 - New button labelled as **CYC hkl** has been add in the toolbar : its function is to allow to select and read a FPCYC.hkl file created by **WinPLOT** when **FullProf** is launch in a cycle mode from the **WinPLOT** interface. The user can then select to plot integrated intensity or Bragg position of a selected hkl towards the external parameter.
hkl- and **hkl+** buttons are then automatically activated to plot previous or next reflexion evolution.
 - Save PCR files of cyclic run of **FullProf** :
 - * before running **FullProf** : initial .PCR file is saved as filename_save.pcr
 - * after running **FullProf** : final .PCR file is saved as filename_final.pcr and filename_save.pcr file is renamed as initial.pcr
- News plot features for .PRF files can be read directly in the setting file (after [PRF plot options] part :
.write_Y_negative_graduations=1/0
.write_PRF_filename=1/0
- **PRF-/PRF+** buttons are now activated after plotting a .PRF file if several .PRF files, are present in the working directory.
- **File/Save UXD file as single scans** menu option has been added : it is active only when multiple scans .UXD files have been plot (load data as RAW data) and allows to split a multiple scans .UXD file to single scan data files (INSTRM10 format)

September 2005

- **WDICVOL04** : .PCR files are now created with a zero shift value compatible with **FullProf** . There was a mismatch in the definition of the zero shift between **WDICVOL04** ($2\theta_{real} = 2\theta_{obs} + zero_shift$) and **FullProf** ($2\theta_{real} = 2\theta_{obs} - zero_shift$)

- **Plot single crystal data PRF files** : a check box has been added in the **Select plot type** dialog box to allow/avoid sorting data by increasing X values. This kind of sort was automatically performed in previous versions of **WinPLOT**R to avoid peculiar plots when continuous line is selected for Y_{obs} .
Skipping this sort can allow to access directly to the reflexion index in the raw file by clicking on a particular reflexion.
- **Help / Links to** menu option has been added to access directly to CCP14 (<http://www.ccp14.ac.uk>) and IUCR powder commission (<http://www.iucr.org/iucr-top/comm/cpd>) web sites. Other internet links can be added by the user by defining web sites name and URL address in the [WEB SITES] part of the winplotr.set file.
Example :
CDIFX = "http://www.cdifx.univ-rennes1.fr" ! cdifx (Rennes)
- **Help / Download WinPLOT**R menu option has been added to access directly to the winplotr.exe file at :
<ftp://ftp.cea.fr/pub/llb/divers/winplotr/winplotr.exe>
A browser has to be defined in the winplotr.set setting file ([SYSTEM APPLICATIONS] part).
- **Help / Download FullProf Suite** menu option has been added to access directly to the **FullProf Suite** package at :
ftp://ftp.cea.fr/pub/llb/divers/fullprof.2k/Windows/setup_FullProf_Suite.exe
A browser has to be defined in the winplotr.set setting file ([SYSTEM APPLICATIONS] part).

July 2005

- **GSAS** file containing the keyword TYPE = FXYE and TYPE = FXY can be read.
GSAS file containing several scans can be read.

June 2005

- **File / Save as / XY file** option is available if only one pattern on screen. The format of this 2 columns is compatible with the **XCH** software of Socabim (no comments, no header)
- raw data file coming from the new 3T2 multidetector with 50 collimators-detectors bank has been integrated. The type of 3T2 file (20 or 50 detectors) is detected automatically.

April 2005

- **The add peaks/background points** and **remove peaks /background points** menu options are now activated after manual peaks/background points selection.
- The constant time normalization procedure for multiscans .UXD files is now adapted to overlapped scans. If several Y values for a single X value are available, only the first Y value is stored in the INSTR_10 file.
- **WinPLOT**R is compiled with the new Crystallographic Fortran Module Library (JRC and JGP).

March 2005

- RGB colors code has been corrected and is now in agreement with Red, Green, Blue color code. The user has now to change the R and B columns in the definition of the different colors used

by **WinPLOT**R in the `winplotr.set` setting file (`RGB(rrr,ggg,bbb)` parts) in order to get the true colors. The RGB color is now defined as :

`color=RED + 256*GREEN + 256*256*BLUE`

Example :

`RGB(255, 0, 0)` corresponds to pure red

February 2005

- Single crystal data coming from the 6T2 neutron diffractometer (LLB, Saclay) is now readable with **WinPLOT**R :
 - multiscan file : Reflections can be plotted ones after others through the **hkl+** or **hkl-** buttons. **Plot / select hkl reflection** menu option has been added to select in the multiscans file a particular reflection to plot.
 - single scan file : **hkl+** or **hkl-** buttons are also activated and allow to change the number of the file to plot file (and then the reflection) in the working folder.
- Fixed bugs : correction of a bug in reading 6T1(LLB) files.
- New buttons to access the programs **GBond_STR** and **GFourier** has been added

November 2004

- Minor changes in **WDICVOL04** and **WTREOR90** : Setting files have been created (`wdicvol04.ini` and `wtreor90.ini` respectively), containing the following optional parameters, united in different sections :
 - [WDICVOL04/WTREOR90 window] : definition of the size and position of the text window, in screen units (0. - 1.0 range). Default values are :
`x_pos = 0.15`
`y_pos = 0.05`
`width = 0.70`
`height = 0.45`
 - [FULLPROF] :
 - * `create_PCR_input_file= item` : creation of PCR input files for **FullProf** (value is y or n)
 - * `IRF_file= item` : definition of IRF file name (`IRESO=1` format) : this kind of file can contained some experimental parameters as wavelength, angular range, diffractometer geometry, profile function, resolution parameters ... (see FullProf user's guide)
 - [CRYSFIRE] :
 - * `create_CRY_input_file= item` : creation of CRY input files for **CRISFIRE** (value is y or n)
 - [EXPO] :
 - * `create_EXPO_input_file= item` : creation of input file for **EXPO** (value is y or n). This corresponds to `HKL=-2` in the .PCR file of **FullProf** .
 - * `space_group, structure` and `cell_content` items : definition of space group, structure name and cell content for **EXPO**

These setting files are installed in the **WinPLOT**R folder but can also be copied in the working directory for another setting.

October 2004

- **WDICVOL04** (new version of the **DIVOL** program : A. Boultif and D. Louer, J . Appl. Cryst. 2004, 37, 724-731) is distributed through the **WinPLOT**R package and the **FullProf Suite** . Please read the `wdicvol04.ins` user guide and the above article to have the features and improvements of **DICVOL**.

September 2004

- Buffer type files can be loaded from the prompt : arguments are the buffer file name and the common **WinPLOT**R format of the data files (1 - 14) :

```
My_prompt> winplotr my_diffraction.buf 2 <cr>
```

- When quitting **WinPLOT**R , name and format of the last selected data file are now saved in the `winplotr.dir` file in the **WinPLOT**R directory. These items are then taken as default in the next **WinPLOT**R run. A `last.PGF` file is also created (in the **WinPLOT**R folder) and can be load rapidly when launch **WinPLOT**R from the prompt by typing the following command :

```
My_prompt> winplotr last <cr>
```

- A new button has been added in the toolbar : click on **Studio** will allow to select a FST file and then launch the **FP_studio** program (see `fp2k.inf` file for details concerning this new crystal/magnetic structure visualisation program that is distributed through the **FullProf Suite**).
The **FP_studio** can also be launch automatically after a **FullProf** run (the relative items in the 'PCR' has to be adapted consequently) by adding as thirs item the `drawfst` string in the `winplotr.set` setting file, in the [AFTER FULLPROF RUN] part.
- A new smoothing procedure has been added, using Fourier filtering

July 2004

- **Calculation / Constant time normalization** : this new procedure can be execute from .UXD data files containing several scans (different angular ranges with different counting time and step) to create `INSTRM10` file with data and sigmas normalized to a constant counting time.
- Profile fitting procedure : if `IRF` is known (and `IRESO/=4`), `U,V,W` resolution parameters are automatically included in the starting parameters dialog box. Consequently, shift values of `FWHM` are fixed to zero.
- *.PIK/*.NEW files for profile fitting : last item of line 1 corresponds to `IRF` and has to be modified by the user. If equal to 1, an .IRF file will be created, containing a list of HG and HL versus 2theta (`IRESO=4`)

June 2004

- Excluded regions and text position can be saved in .PGF files
- display of several 2theta scans contained in .UXD files (**File / raw data file** menu option). Default format associated to .UXD file is 9 (single scan file) but can be modified explicly in

the [MY COMMAND LINE DEFAULT FORMATS] part of the winplotr.set file through the third item (first corresponds to .DAT extension and second to .PRF files respectively). The format number associated to this multiple scans .UXD file is 56.

- fixed bugs :
 - .PCR files created by **DICVOL** were not correctly created (wrong values of resolution parameters, profile function, scale factor ...) for neutron data
 - Protection for XY files containing continuous data with identical X values
 - LOG(Y) option : a protection for zero counting data has been included

May 2004

- Fixed bugs :
 - Profile fitting after reload data and microstructural analysis
 - Plot .SEQ files :
 - * refined parameters are related to the phase
 - * correct Y legend
 - Run **FullProf** in cyclic mode : last number can be lower than first number (inverse cyclic mode)
 - Protections for the case with all data equal to zero

April 2004

- Fixed bugs :
 - **Profile fitting** after automatic peak search procedure
 - plot .XRF file after profile fitting with .PIK input file or after automatic peak search procedure
 - read .PGF files with XMIN XMAX and YMMIN AND YMAX items
 - Ymin graduation in manual mode zoom
 - run user's defined programs

March 2004

- Line width in .UXD files has been extended to 512 characters to allow a correct reading of lines containing 16 data.
- Cosmetic bugs has been corrected (ex : *pen_width* action)
- **Calculation / I.R.F.** menu option : the FWHM of the pseudo-voigt function is calculated from the HG and HL values and the T.C.H. relationship
- access to the **FullProf** manual in HTML format

February 2004

- **Wtregor90** and **WinDIC** are now running with input files stored in directory whose name contains blank character (" ")
- .SEQ file : error bars are automatically display and their values are taken into account in the min and max values calculation in the plot.
- **Open setting file** menu option has been added. The user can then select the setting file useful for his work. The default name of the setting file is winplotr.set but can be more explicit (ex : wpl_neutron.set, wpl_xrays_D8.set ...).
- a link to **FullProf** news and **WinPLOTTR** news (HTML format) has been added (these HTML files are distributed in the last **FullProf Suite** package and copied in the fullprof_suite\docs folder).
- **FP cyc** button has been added : it allows to launch the DOS version of **FullProf** in a cyclic mode (this version is explicitly defined in the winplotr.set file, through the FP_CONSOLE item in the [RUN PROGRAMS] part. The different arguments to launch cyclic **FullProf** are input by the user in a dialog box.
- .SEQ files (output file created by a cyclic run of **FullProf** and RPA=-2) can be displayed (**SEQ** button or automatically after a cyclic run of **FullProf**).
- INSTRM14 data file has been added in the pattern list (corresponding extensions= *.DAT;*.GSS;*.GSA). It corresponds to multi-bank time of flight data (ISIS normalised data)
- .NEW input files can be selected to launch **FullProf**. In that case, it is previously copied to .PCR file (**FullProf** is always running with .PCR input files).

January 2004

- .IRF file with IRESO=4 can contain WAVE item before the list of HG and HL values
- new item in the **Peak search parameters** dialog box : *Display Bragg peaks positions*
- cosmetic changes in the winplotr.set setting file. Each item is now defined between '[' and ']' characters. This new format is of course compatible with the old one.
- new version of Wtregor90.exe : the *_treor_cell.sum file for **Crysfire** was not correctly created in case of hexagonal solutions
- **Tools / space group infos** : space group extinctions rules are output
- For more clearness, the list of the different kind of powder diffraction data has been splitted in several groups :
 - pattern files (13 formats) corresponding to **FullProf** compatible formats
 - raw data files (5 formats) including multiconounters diffractometers data
 - profile type files (5 formats) : WinPLOTTR/XRFIT, FullProf, Jana2000, Rietan2000 and Debye
 - microstructural files

The corresponding **WinPLOTTR** formats ranges (useful for example when **WinPLOTTR** is launching through a command line) are the following ones :

- pattern files : 1 - 13
- raw files : 51 - 55
- profile files : 100 - 104
- microstructural files : 201 - 204
- 3T2 neutron multiconverters diffractometer (LLB-Saclay) raw data file has been included*
- Fonts are now saved in .wpl files
- a winplotr.set setting file can be present in the working directory. If not, **WinPLOTTR** will use the setting file in the directory associated to the WINPLOTTR environment variable (d:\fullprof_suite for example). The user can then have in each working directory a settings file adapted to the powder diffraction problem he is dealing with.

November 2003

- Instrumental parameters can be read from the .IRF file in the starting parameters dialog box of the profile refinement procedure. This new option is valid for TOF data as well as CWL data.
- The profile fitting procedure for TOF data is now running properly. It uses the `NPROF=9` function defined in **FullProf** (convolution of pseudo- Voigt with a pair of back-to-back exponentials).
- Different kinds of IRF files can be used, depending on the item `IRESO` (as in **FullProf**). It can be defined in the winplotr.set setting file in the MY IRF FILE part : first item corresponds to the `IRESO` value and the second one to the IRF file name.

! MY IRF FILE (IRESO IRF_file_name): 4 d:\fullprof_suite\IRF_files\my_irf.IRF
 For `IRESO/=4`, the .IRF file contains 6 instrumental resolution parameters (*Uins*, *Vins*, *Wins*, *Xins*, *Yins*, *Zins*) which meanings are dependent of `IRESO` value :

`IRESO=-1` pseudo-Voigt profile

$$H^{**2} = UINS \tan(q) + VINS) * \tan(q) + WINS$$

$$ETA = XINS + YINS * q + ZINS * q * q$$

`IRESO=1` Voigt profile (corresponds to `NPROF=7` in **FullProf**)

$$HG^{**2} = UINS \tan^2(q) + VINS * \tan(q) + WINS$$

$$HL = XINS * \tan(q) + YINS / \cos(q) + ZINS$$

`IRESO=2` Voigt profile

$$HG^{**2} = (UINS \tan(q) + VINS) * \tan(q) + WINS$$

$$HL = (XINS * 2q + YINS) * 2q + ZINS$$

`IRESO=3` Voigt profile

$$HG^{**2} = (UINS * 2q + VINS) * 2q + WINS$$

$$HL = XINS * 2q + YINS) * 2q + ZINS$$

This IRF files are the same as used by **FFullProf** and then can contain some informations on the diffractometer setup (see **FullProf** documentation for more details) : WAVE/, GEOM, CTHM ...

For IRESO=4, the .IRF file contains a list of *HG* and *HL* values versus 2theta.

October 2003

- new button **Reset** in the toolbar
- a CIF viewer can be defined by the user in the winplotr.set setting file in the ! SYSTEM APPLICATIONS part. This CIF viewer is associated to .CIF files (created by **FullProf** with RPA=-1) and allows to display crystal structure directly through a single click on the **view** CIF button. The authors strongly recommend the **Mercury** program for visualization of molecular crystal structure (<http://www.ccdc.cam.ac.uk/prods/mercury/index.html>)
- **Calculation / data normalization** menu option has been added

September 2003

- fonts can be defined by the user in the winplotr.set setting file in the ! TEXT FONTS section :

TEXT FONTS	: Typeface	point	italic	underline	strikeout	bold
main title	: Times New Roman	18	F	F	F	F
X legend	: Times New Roman	18	T	F	F	F
Y legend	: Times New Roman	18	T	F	F	F
X graduations	: Courier	14	F	F	F	F
Y graduations	: Courier	10	F	F	F	F
file name	: Courier New	10	F	F	F	F
(hkl) indices	: Times New Roman	10	F	F	F	F
dialog boxes	: Times New Roman	10	F	F	F	F

- Vertical and horizontal lines can be draw (**Plot / draw vertical-horizontal line** menu option)
- HGL viewer can be defined by the user in the winplotr.set setting file
- **LOG(Y)** option : a protection for negative data has been included
- A molecular weight calculation has been included : **Tools/molecular weight calculation** menu option
- Some changes in the peak search algorithm : shoulders positions are determined with better accuracy. The number of iterations for data smoothing procedure can be input by the user

July 2003

- Peaks positions can be saved for **McMaille** program (indexing powder patterns by Monte Carlo method, A. LeBail : <http://www.cristal.org/McMaille/McMaille-v3.html>)

- The **CFML** tools are used in **WinPLOT**R :
 - new profile fitting procedure, available for CWL data and TOF data
 - **Tools menu** is added, leading to new crystallographic tools as **Space group info** and **Unit cell volume calculation**
 -

June 2003

- several TOF GSAS files can be displayed simultaneously

May 2003

- new general graphic file can be created and loaded by **WinPLOT**R . It contents some general features on the graphic plot (legend text, graduations, colors ...) and data in XY format.
- bug in reading .UDF files from Panalytical has been corrected.

April 2003

- New input files for **FullProf** (.new can be automatically edited after a **FullProf** run : change the EDIT_PCR string to EDIT_NEW string in the **WinPLOT**R setting file (! AFTER FULLPROF RUN: section). This can be useful if IPC parameter is equal to 2 in the .PCR file.
- Minor change in the INSTRM_0 data file created by **WinPLOT**R : the step item is now written with a F14.6 format, i.e. with 6 decimal numbers. The previous format (F14.4) was not enough accurate for data coming from continuous scans (step corresponds to an electronic step rather than mechanical step).
- Different Y scales are available : linear, log and SQRT (**Options / Y scale** menu option)

March 2003

- Format #17 (Philips X'Pert) and #18 (Philips X'celerator) have been merged into a single PANalytical format. Different kinds of data file formats can be read and are discriminated from their respective extensions : *.UDF, *.CSV, *.JCP and *.XRDML.
Don't forget to change the data file description in the winplotr.set setting file (DATA FILES EXTENSIONS: section). It has to be as follows :

```

16      *.CPI                                !16 : CPI (Xrays)
17      *.UDF;*.JCP;*.CSV;*.XRDML!17 : PANalytical formats
18      *.DAT                                !18 : ESRF multi analysers

```

- the bug in reading .UXD file with _2THETACOUNTS and _2THETACPSis corrected
- The winplotr.pdf file containing user's guide can be read through the **WinPLOT**R GUI (**Help / User's guide / winplotr.pdf**) if a PDF reader is defined in the winplotr.set setting file
- .XRDML data files from Philips diffractometer has been included. It has been associated to data file format number 18 (Xcelerator)

February 2003

- **Select pen_width option** is now compatible with dashed and dotted lines
- cosmetic changes in automatic 3D plots

January 2003

- small bugs have been fixed :
 - profile fitting with .UXD file and CPS data
 - launching **WinPLOT**R through a command line for data file (Rietveld or Microstructural files were OK)
- Windows explorer can be launch from the **WinPLOT**R GUI through the **External applications / Explorer** menu option or by a button in the toolbar
- output files created by the profile fitting procedure in **WinPLOT**R are now labelled as filename_pf.*.

December 2002

- **WinPLOT**R is now distributed via the **FullProf Suite** package (http://www-llb.cea.fr/fullweb/ftp/pub/divers/fullprof_suite/setup_fullprof_suite.exe). This suite contains **FullProf** , **WinPLOT**R , **GFourier**, **EdPCR** ...
- Data file from ESRF multi analysers diffractometers (i.e. : ID31) has been included

November 2002

- IRF file (IRESO=4 format) can be defined in the winplotr.set through the ! MY IRF FILE (IRESO=4) item
- small change in the **profile fitting parameters** dialog box : CREATE .IRF FILE / CREATE .IPC FILE / NO OUTPUT FILE radio button has been added.
- some system applications can be defined in the winplotr.set file, in the ! SYSTEM APPLICATIONS part :

```
Browser      ="C:\Program Files\Netscape\Communicator\Program\netscape.exe"
PostScriptViewer="C:\Program Files\gstools\gsview\gsview32.exe"
PDFReader    ="C:\Program Files\Adobe\Acrobat 4.0\Reader\AcroRd32.exe"
BMPviewer    ="c:\winnt\system32\mspaint.exe"
```

- **Help / WinPLOT**R web site menu option : access to the **WinPLOT**R web site (<http://www-llb.cea.fr/fullweb/winplotr/winplotr.htm>) through the previously defined browser
- **Help / User's guide / FullProf manual** menu option : load the fullprof_manual.pdf file ('fullprof_directory\docs folder) into the previously defined PDF reader

- **External applications / PostScript viewer** menu option : access to the Windows directories dialog box to select a PostScript file and view it with the previously defined PostScript viewer
- **WinPLOT**R web site can be accessed directly in the **Help** menu option, if a browser has been previously defined in the winplotr.set file.
- PostScript files can be viewed through a previously defined PostScript viewer (**External applications / PostScript viewer** menu option).
- some small changes in the procedure to launch **WinPLOT**R from a command line : the two arguments in the command line are not order depending :

```
winplotr 101 fullprof_file.PRF
```

and

```
winplotr fullprof_file.PRF 101
```

are correct.

In the second way, if the second argument (data format) is missing, the format is deduced from the file name extension. In the case of .DAT files or .PRF files, the default corresponding formats can be defined in the winplotr.set file through the ! MY COMMAND LINE DEFAULT FORMAT items. This new option can be helpful to visualize patterns in **WinPLOT**R directly from the Windows Explorer by just clicking on a data file (the corresponding extension has of course to be associated to **WinPLOT**R).

October 2002

- Microstructural analysis
 - new items in the winplotr.set :
 - * ! MY RESOLUTION PARAMETERS: part can contain until 6 parameters values (reals) to define the Instrumental Resolution Function.

Number of
parameters I.R.F.

3	Pseudo-Voigt $H^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W$
4	Pseudo-Voigt $H^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W + Z/\cos(\theta)$
5	Voigt $HG^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W$ $HL = X.\tan(\theta) + Y/\cos(\theta)$
6	Voigt $HG^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W$ $HL = X.\tan(\theta) + Y/\cos(\theta) + Z$

The last *HG* and *HL* angular dependances are corresponding to the the format IRESO=1 of .IRF file in **FullProf**

- * ! DETERMINATION OF INTRINSIC PROFILE COMPONENTS: leads to perform, at the end of a profile fitting procedure, a deconvolution from the instrumental part described just above. Output .IPC file (containing intrinsic profile and microstructural parameters) is created.
- * **Calculation / Read IRF file (IRESO=4)** menu option :
 IRF can be read in a file, containing a list of $2\theta(^{\circ})$, $HG(^{\circ})$, $HL(^{\circ})$ values, as for the IRESO=4 IRF file format in **FullProf** .
 This IRF file is then used after the fitting procedure to perform a microstructural analysis (HG_instr and HL_instr for the refined positions are calculated through a cubic-spline interpolation of HG_instr 's and HL_instr 's contained in the IRF file)
- profile fitted angular ranges are now graphically distinguish : they appear with a particular color after **Calculation / reload data file** menu option. These angular ranges are treated as excluded regions. The default color for these ranges is grey (in not defined in the winplotr.set file through the !EXCLUDED REGION COLOR: item), but it can be changed in the **Plot / excluded regions color** menu option.
 Excluded regions in .PRF files are now plotted by this way. If you don't want to see any points in these regions, you just have to select for the Excluded region color the same color than the Background plot color.
- for more clearness, colors in the winplotr.set can be now defined using a RGB code :
 color=RED*256*256 + GREEN*256 + BLUE
 Example :
 ! BACKGROUND SCREEN:
 background screen color: RGB(228,255,255)
 and ! BACKGROUND SCREEN:
 background screen color: 15007743

 are equivalent
- **Calculation / IRF** : access to dialog box to enter instrumental resolution parameters, calculate the I.R.F. and then plot it on the screen.
- peak positions can be saved as .PRN file (**CHECKCELL** format)
- **Add/remove peak** : the list is updated in the text window after clicking with the right mouse button to exit from the procedure
- profile fitting can be followeg graphically during the fitting procedure (flag in the starting parameters fitting procedure dialog box)
- PRF files with single crystal data containing flipping ratio refinements can be plotted

September 2002

- **WTREOR90** version in the last package was bugged : it has been corrected
- the possibility to read a reflexion list from an external ASCII file has been included (**Text / Open reflexion file** menu option). Then, this file content is written as text over the pattern. The format of this file is the following (lines beginning by '!' or '#' are comments) :

```
!Example of reflexions file
! silicium a=5.4307 Fd-3m
! wave=1.54056 A
! X-ray pattern
```

!2Theta (hkl)				
28.4430	(1	1	1) Si
47.3038	(2	2	0) Si
50.0000				<<< impurity ?
56.1236	(3	1	1) Si
58.8576	(2	2	2) Si
69.1316	(4	0	0) Si
76.3780	(3	3	1) Si
88.0324	(4	2	2) Si
94.9550	(3	3	3) Si
94.9550	(5	1	1) Si
106.7116	(4	4	0) Si
114.0957	(5	3	1) Si
116.6474	(4	4	2) Si

June 2002

- data can now be saved in a INSTRM=0 format (available only if one pattern on screen) : interpolation is performed through a cubic spline procedure. The format is compatible also with Rietveld format (*.dat) in **CHECKCELL**
- new facilities in **WinTREOR90** and **WinDICVOL** (thanks to Alain Lafond for suggestions and discussions) :
 - output files (.SUM and .CRY) for the **CHECKCELL** program (J. Laugier and B. Bochu : <http://inpg.fr/LMGP>)
 - corrections of bugs in **WinTREOR90** in the .PCR creation procedure (wavelength, space group)
- New dialog box in the **Save as TREOR points** option in **WinPLOT** : MONO, CEM, MERIT parameters can be modified by the user
- Profile fitting procedure : sub-profiles (peaks_n.xy) are now correctly calculated
- **EdPCR**, the new GUI for editing and modifying the .PCR input files for **FullProf** , is now distributed in the **WinPLOT** package and can be launched through the **WinPLOT** interface. Thanks to Javier Gonzalez-Platas and Juan Rodriguez-Carvajal for their hudge work to create this interface.

May 2002

- **WinPLOT** can now be launch through a command line following by two arguments :
 - first argument corresponds to the format number (integer) :
 - * format = 1,2 ... 18 : diffraction pattern with format corresponding to the list number in the **format dialog box**
- Example : format=0 for X,Y format
 format=1 for INSTRM=0
 ...

- * format = 101, ..., 104 : Rieveld format for **FullProf** , **Jana2000**, **Rietan2000** and **Debvin** respectively
- * format = 201, ..., 203 : microstructural file (same order than in the **Open microstructural file** section)
- second argument correspond to the data file name

Example : > winplotr 101 fullprof_file.PRF
 > winplotr 7 pbso4.dat

This new opportunity can be interesting to be launch by the own user application that can create data file those format is compatible with **WinPLOT**R .

- a **PRF** button has been added in the toolbat to open and display a .PRF **FullProf** file
- the bug to display multipattern .PRF file with $NPAT > 9$ has been corrected
- the **Text / display reflections list** option has been added : it is valid only for .PRF, .XRF file or after an automatic peak search. It allows to display and store the position list (in 2θ (°), $d(\text{\AA})$, $Q(\text{\AA}^{-1})$, $\sin\theta/\lambda(\text{\AA}^{-1})$)
- the **Text / write reflexions text** menu option is valid after the profile fitting procedure
- the **Text font / (hkl) indices font** option is now valid after writing reflexions indices and/or positions
- $Xmin$, $Xmax$, $Ymin$ and $Ymax$ values in the zoom dialog box are related only to previous values entered by the user in this dialog box : they are not corresponding the extrema values selected by the mouse. This change has been implemented to help to user to keep some $Xmin$... values.

April 2002

- some bugs have been corrected :
 - in the reading *.WPL files procedure
 - display reflection positions
- multi-phases .PRF files created by **Jana2000** are now recognised

March 2002

- last version of Wfp2ks and fp2ks are included (previous one was bugged for .PCR files containing distances and angles constraints)
- wavelengths supplied by the user in the winplotr.set file are correctly interpreted
- the bug in the **Save settings** procedure is corrected
- for more clearness, Exit right button text is replaced by Valid & exit

February 2002

- Microstructural .MIC file (created by **FullProf**) can now be read
- XRFIT.pik file is created after the validation of the **Profile fitting parameters** dialog box. This file is entirely compatible with the **XRFIT** DOS program. This old program is still useful for a cyclic profile fitting procedure, for example.
- Exit tool has been included in the toolbar
- bug in the **save as multicolumns file** menu option has been corrected
- positions of reflexions can be displayed on Rietveld patterns plot : use the **Text / Write reflexions text** menu option

January 2002

- some small bugs have been corrected
- Executable file is now compacted. Thanks to M. Oberhumer and L. Molnar for their **UPX** free compactor (<http://upx.sourceforge.net/>)

October 2001

- M^2 calculation is included in **DICVOL**, according to the definition in **NTREOR** (ref : *Altomare et al., J. Appl. Cryst. 33, 1180 (2000)*)
- data from the **Fit2D** program (extension=.CHI ; ESRF) has been included the X,Y data formats

September 2001

- Problem with **TREOR** and angular 2theta positions lower than 1.0 deg. : remove such kind of data when you are dealing high energy synchrotron data
- data file from X'Pert (Philips) diffractometer has been included
- the PRF file format is removed from the data file list and is now only in the Rietveld file format list (!! change the data file list in your setting file!!).

July 2001

- data file from X'celerator (Philips) diffractometer has been included
- a bug in the Wito/WinPLOTTR interface has been corrected

June 2001

- (hkl) reflexions can be displayed on Rietveld patterns plot : **Write reflexions indices (ON/OFF)** in the **Text** menu option
- 3D plots can be realized rapidly (default parameters) : **Plot 3D+/3D-** in the **Plot** menu option

May 2001

- The bug in the **Reload data file** menu option is now fixed
- Position of the files names can be specified by the user (**Text / Legends positions**)

April 2001

- The following bug has been fixed : . text has microscopic size in the **File / Print** procedure
- Linear fit of microstructural data can be performed

March 2001

- Rietveld profiles file created by **Jana2000** (.PRF) has been included
- Bitmap files can be created

February 2001

- Plots for a microstructural analysis can be performed :
 - Williamson Hall : integral breath b^* versus $1/d$
 - Average size-strain : $(b^*/d^*)^2$ versus b^*/d^2
- A Windows version of the **ITO15** program (J. Visser) is distributed within the WinPLOTTR.zip package
- The **DOS command** option has been replaced by the **Open a DOS window** option
- Data file .CPI created by **POUDRIX** (J. Laugier and B. Bochu) has been implemented
- Default version of **FullProf** is wfp2k.exe

January 2001

- some changed in the profile fitting procedure of doublets have been performed : X-Rays Kalpha1 and Kalpha2 wavelengths can be defined by the user in the winplotr.set file by defining two new items :

```
! MY X-Rays WAVALENTHS (A):  
Kalpha1_wavelength Kalpha2_wavelength
```

- Text fonts for legends can be changed by the user in the **Text / text fonts** menu options
- Copy text to the clipboard can be realized in text windows
- the Windows calculator can be spawn through **WinPLOTTR**

December 2000

- Rietveld files created by **Rietan2000** (.PAT) and **Debvin** (.GRA) Rietveld programs have been included
- IPL2=2 .PRF Rietveld file created by **FullProf** has been included (**IGOR** format)
- Data file (.INT) for **Rietan2000** has been included
- Positions and rotation of the legends texts can be defined by the user (**Text / Legends positions** menu option) and stored in the winplotr.set settings file
- Offset X and Y values can be defined for each pattern independently

November 2000

- Xray attenuation coefficient and total interaction cross sections have been included in the **MENDEL** program
- .CPI data file format has been included
- **WinDICVOL** and **WinTREOR90** : .CRY files as input files for **CELREF**, **CHEKCELL** are creating

October 2000

- Profile fitting procedure : the *HG* and *HL* parameters (*FWHM* of the Gaussian and Lorentzian part respectively, of the Voigt function are calculated from the pseudo Voigt approximation parameters (*Fwhm*, *eta*) using the Thompson-Cox-Hastings formulation : A FILENAME.IRF file is created, containaing *HG* and *HL* versus 2θ .
- Powder diffraction pattern can be transformed to another wavelength pattern

September 2000

- Correction of a bug in reading time of flight data coming from Argonne

July 2000

- After plotting a .PRF file, a .SUB file (created by **FullProf**) is automatically shifted according to the shifts parameters of the .PRF file.
- The calculation of the *FWHM* from the Caglioti formula has been implemented (**Calculation/FWHM(Caglioti)** menu option)
- The number of user's defined editable files has been extended from 2 to 4

June 2000

- the bug in **WinDIC** in the triclinic case (display unit cell parameters on the screen and in the .UCP file) has been corrected
- a bug has been corrected in the manual fit dialog box (selected peaks)

May 2000

- a bag version of the **INSTALL** program has been installed in the LLB ftp area : it has been corrected

April 00

- some changes in the **Save as TREOR input file** subroutine have been performed in order to interface the last **TREOR** Windows version :
 - first two lines are beginning with the '!' character
 - reflection intensity and background are stored
- new TREOR windows version :
 - after successfull run, automatic generation of PCR input file
 - for **FullProf** (profile matching mode)
- **WinDICVOL** window size and position can be defined in the `windic.ini` settings file (stored in the directory associated to **WinPLOT**R through the `winplotr` environment variable)

March 2000

- new procedure to plot red selected reflexions and selected background points (it would be more rapid with very large of points in the data files - synchrotron data for example-)
- **Help / WinPLOT**R **help file** menu option has been changed
- **Select files** dialog box has been modified (bug with large number of data files)
- ! **EDIT FILES:** item in the `winplotr.set` file : definition of files (type + extension) that can be edited in the **External applications / Edit a file** menu option
- Peak search and background points search are running correctly with *d* spacing data
- **PFE** editor has been removed from the **WinPLOT**R package
- some bugs in the PostScript and HPGL files have been corrected
- frame features can be modified by the user : line thickness, major and minor tics thickness and length
- bugs have been corrected in the creating/reading *.WPL files procedures
- **SELECT** option in the **External applications** menu : select an .EXE file to run from **WinPLOT**R

February 2000

- Fitting procedure from a .PIK file can be performed with `INSTRM=10` (with sigmas as third column) data files

January 2000

- a background subtraction procedure has been implemented in the **Calculation** menu
- small bugs have been corrected in the following menu options
 - **save as TREOR points** : inversion of the VOLmax and BETAmx item values
 - **PRF+** / **PRF-** tools : problem with the '_' character in the directory name
- the **PFE** editor is now distributed with the winplotr.zip package and is considered as the default editor
- the winplotr.set file can be edited from **WinPLOTTR** through the **External applications / Edit a file / Winplot.set file** menu option

October 1999

- the .PRF file can be automatically plotted and .PCR file can be automatically loaded after a **FullProf** run, by defining two new items in the winplotr.set file :

```
! 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_prf      => the PCR file is edited
           no_edit_prof  => the PCR file is not edited (default value)
```

September 1999

- bugs have been corrected in the **Calculation/Integration** and **Calculation/Profile fitting** menu option of the previous **WinPLOTTR** .

July 1999

- a new zoom and graduations routine has been implemented.
- a winplotr.hlp HELP file has been created. It can be loaded through the **Help / WinPLOTTR help file** menu option.
- The utility launched by **WinPLOTTR** to read the winplotr.hlp file is winhlp32.exe by default. However, it can be defined in the winplotr.set file in the `/! HELP FILES:` part, as the following :

```
. ! HELP FILES:
.   N  winhelp
```

- some bugs in the peak search routine has been corrected

June 1999

- bug in reading the INSTRM=4 data files (Brookhaven format) has been corrected

May 1999

- .PRF files (single crystal data) can be displayed as a $F2_{calc} = f(F2_{obs})$ plot
- sorry for the last bad version of the INSTALL.exe program : it has been corrected now
- winplotr.set / !run programs : program name that will be launched by **WinPLOTTR** can be .LNK files as well as .EXE files
- The number of user's defined programs is extended to 10
- **File / file Infos** menu option : displays in a text window some informations about data file
- **! MY DEFAULT FORMAT**: keyword in the winplotr.set file allows to define the default format in the select format dialog box. If no default format has been defined, first format (X, Y format) will be taken as the default one.

April 1999

- buffer file can contain some optionnal informations, as for example temperature, experimental conditions ...
- **plot / reverse order** option
- user's DOS program definition in the winplotr.set file : the number of arguments accompanying the relative DOS program can be specified in parenthesis at the end of the definition line.
ex : Fullprof_dos = FULLPROF !FullProf dos version !DOS version (2)
In this case, **WinPLOTTR** will open two dialog boxes to select the two arguments files for the FullProf program. The following command line is then executed :
FULLPROF selected_file1.PCR selected_file2.DAT
If the program comment starts with fullprof 'in capital or lower case letters), **WinPLOTTR** will automatically display the last .PRF file created by **FullProf** .
- Windows version of **TREOR** (WTREOR90.exe and the user's guide) are now included in the winplotr.zip file and automatically installed with the INSTALL.exe program.
- user's diffractometer resolution parameters can be defined in the winplotr.set file, via the **! RESOLUTION PARAMETERS (U,V,W)**: keyword in the winplotr.set
- **save as multicolumns file** option : select X and Y columns to save for each file

March 1999

- **Add / remove peaks** options are now available after an automatic background points search
- Windows version of **FullProf** (WFP98.exe and related files) is now included in the WinPLOTTR.zip file. Automatic installations of **WinPLOTTR** and **FullProf** are realized by launching the INSTALL.exe program contained in the WinPLOTTR.zip file.
- **WinPLOTTR** is compatible with dispersive energy data

February 1999

- **WinPLOT**R is a GUI for the **TREOR** program (Windows version) :
 - save selected points as TREOR points to create an input file for **TREOR**
 - edit **TREOR** input file
 - run **TREOR**
- new tools in the toolbar after plot of .PRF or .XRF files : **hkl-** / **hkl+** buttons lead to display in a text window the features of the previous / next Bragg reflexion
- new tools in the toolbar after running the multipatterns version of **FullProf** : **PRF-** / **PRF+** buttons lead to plot previous / next .PRF file.
- **WinPLOT**R is now compatible with the **FullProf** multi-patterns version (**Wmfp99.exe**) : just change the appropriate item in the **WinPLOT**R.set file

January 1999

- **Peak search** dialog box : choice between search single peaks and search Cu Ka1/Ka2 doublets
- **Plot / 3d lines** menu option
- some changes in the menu presentation :
 - **Options / Background colors** menu option leads to the 'background colors menu'
 - **Text / Text colors** menu option leads to the 'text colors menu'
 - **External Applications / Edit a file** leads to the 'edit a file menu'
 - **External Applications / Run user's programs** leads to the 'run user's programs menu'
- **External Applications / Edit a file** new menu option
- **ISNTRM= 1** data file format (data from variable time X-ray data collection) has been included (raw or normalised data)
- **WinPLOT**R can be used as a GUI for **SuperCELL** program (search of commensurate supercell or incommensurate propagation vector) :
 - **Points selection / save as SuperCELL points** option
 - **External applications / edit .SAT file** option
 - **External applications / Run SuperCELL** option
 - **Supercell** program name is stored in the **winplotr.set** file in the ! RUN PROGRAMS: section
- **Help menu** : 'Help Files' option as a switch to display or not help files in windows
- the **INSTRM=9** data files are now correctly read
- **! HELP FILES**: keyword in the **WinPLOT**R.set file : display or not user's guide files in a window
- a new initialization routine has been implemented : I hope the slowness in the **Reset** and **Run Fullprof** options are now disappeared

December 1998

- Colored PostScript files
 - **FullProf** default version is Wfp98 (Windows version)
 - **Dicvol** default version is Windic (Windows version)
 - the ' $s=1/d \ (A-1)$ ' X space is available
 - multiply X values option
 - INSTRM=4 data file format has been included (data from Brookhaven synchrotron)
- position and size of the WinPLOTTR main window can be defined in the winplottr.set file, via the ! MAIN WINDOW POSITION AND SIZE: keyword. The parameters in the following line are related to the upper-left corner coordinates (x and y) and the width and height of the window, respectively. These values have to be between 0. and 1.

November 1998

- fitting profile procedure will create an XRF output file, containing $X(i)$, $Yobs(i)$, $Ycalc(i)$, $Yobs-Ycalc(i)$ and $background(i)$ values and position, intensity, full width at half maximum and eta value for each fitted reflexion.
This XRF can then be loaded by **WinPLOTTR** and is considered as 5 files. Click with the mouse on reflexions tics will displayed in a window the corresponding position, intensity, fwhm and eta
- some changes in the profile fitting procedure :
 - introduction of U,V,W resolution parameters
 - introduction of an angular dependence of the eta parameter (lorentzian part in the pseudo-Voigt function) :

$$pV(2\Theta) = \text{Eta} * L(2\Theta) + (1 - \text{Eta}) * G(2\Theta)$$
$$\text{Eta} = \text{Eta0} + X * 2\Theta$$

- **Selected points / Add peaks** and **Selected points / Remove peaks** option : lead to the capability to add (or remove) reflexions to (or from) a list of Bragg peaks determined by the automatic peak search procedure : an automatic profile fitting procedure can then be executed, taking into account this new reflexions list
- the user can select and save screen background color, introduction text color and plot background color

October 1998

- **File/save as multicolumns file** option : create a multicolumns file with all the data on the screen, with the following format :

X_1 Y_1 X_2 Y_2 X_n Y_n

- some modifications have been done in the **Win_DICVOL91** program (Windows version of **DICVOL91**) in order to create .PCR files for **FullProf** to test rapidly unit cell solutions proposed by progWin_DICVOL91

- Automatically find peaks can then be stored in a .DIC file for a further automatic search of the unit cell
- an automatic background search procedure has been implemented (**Points selection / automatic peak search** option). The results of this automatic procedure are related to background threshold value, that can be stored in the winplotr.set via the ! BACKGROUND THRESHOLD: keyword. Default value is 0.05.
- an automatic peaks search procedure has been implemented (**Points selection / automatic background** option). The results of this automatic procedure are related to background threshold values, that can be stored in the winplotr.set via the ! PEAK SEARCH DETECTION THRESHOLDS: keyword. These values can be changed by the user, and are defined as follows :
T1 : sensitivity to find 'real peaks'
T2 : sensitivity to find 'shoulder peaks'
Default values are the following : T1 = 0.02 and T2 = 2.
- An automatic profile fitting can be performed after the automatic peak search procedure
- an automatic procedure for installing **WinPLOT**R has been realized : all the **WinPLOT**R and install files are zipped into a winplot.zip file. To install **WinPLOT**R on your PC, unzip this file and execute install.exe
- **File / save sup file** option :
 - save data created by the calculation options : Summation, Difference, Average, Derivative and Smoothing procedures
 - format = 2 columns X, Y
- a log file can be created to have a trace of that has been done during **WinPLOT**R using. This file creating is related to the ! LOG FILE: keyword in the winplotr.set, and a winplotr.LOG file is created in the directory defined by the WINPLOT
- order in the format list has been changed : please reload the last WinPLOT
- INSTRM=8 (data from DMC (PSI) diffractometer) has been implemented
- options **Plot/Excluded regions** and **PRF options/excluded regions** have been implemented

September 1998

- problem in **save WinPLOT**R settings option has been corrected in the previous version
- user's programs can be executed from the **External applications** menu : the program name, version and comment are defined by the user in the winplotr.set file, in the lines following the ! RUN PROGRAMS: keyword.
.example : PLOT

As for FullProf, Edit or Dicvol, first item on the line is related to the vertical **External applications** menu item, second (after the '=' character) to the program that will be run, and third (after the '!' character) to the text that will appear in the status bar of **WinPLOT**R
Remark : a maximum of 5 user's programs can then be defined

- data file extensions can be defined by the user in the winplotr.set, via the ! DATA FILES EXTENSIONS: keyword

```

example :      1  *.xy                ! X,Y data
                2  *.dat              ! INSTRM = 0
                4  *.dat;*.d1b        ! INSTRM = 3

```

- multicolumns data files are now accepted in X,Y data format
- **File/print Setup** option has been removed (unused)
- INSTRM=10 data file format has been included (with XYDATA as keyword in the first line)
- Fit procedure bugs have been corrected
- X,Y file (with '!' or '# as first character of the lines) are now correctly read
- Link to **DICVOL** program (D. Louer & A. Boultif) :
 - select some points
 - save as **DICVOL** points : fill a **DICVOL** dialog box to create a **DICVOL** file (.DIC)
 - run the Windows version of **DICVOL** (External links)
- **Calculation option** :
 - derivative data
 - smoothing

July 1998

- **fit procedure** dialog box :
 - global Fwhm and Eta are displayed as refined parameters values
 - add or remove peaks
 - a file.XRF is created (column format) with refined parameters and standard deviations values
- new tools in the toolbar : shrink or expand the plot frame width

June 1998

- a bug in the **difference calculation** option, after selection of files to plot (**Files/Select files**), is corrected
- selected points values are displayed in text windows

May 1998

- G41 and G61 (LLB) files format has been included
- new tools in the toolbar :
 - arrows : move through the patterns
 - **FP** : run FullProf program
 - **Pcr** : edit .Pcr file

- **Fit** : access to the profile fitting procedure
- clicks on frame lines have been replaced by clicks on icons in the toolbar (if the zoom or focus option has been previously activated)
- buffer files with empty lines are read without error
- correction of bugs in :
 - **profile fitting** after **select files** among several files
 - **difference calculation** option
- If a WINPLOTR environnement has been defined, the last current directory is stored in the winplotr.dir file. This file will be read after each **WinPLOTR** executing to open files in the directory previously visited by **WinPLOTR** .
- left mouse click on frame lines :
 - right frame line : move the pattern to the right
 - left frame line : move the pattern to the left
 - down frame line : move the pattern to the down
 - up frame line : move the pattern to the up

April 1998

- After running **FullProf** (Wfp98 Windows version), **WinPLOTR** will plot the last data file used by **FullProf** , if a FULLPROF environment variable has been defined.
- link to an editor to edit a PCR.file : the editor name can be specified in the winplotr.set file. If not, the **notepad** editor will be used. Unfortunately, you have to exit from the editor to run **FullProf** (**WinPLOTR** have to stop a 'call(system) command'.
- The existence of a sigma data array can be specified by the ! SIGMA ARRAYS: item in the winplotr.set file. Sigmas are then associated to all the data files to plot errors bars.
- Plot error bars
- Save pattern plots as file.WPL
- Open templated file.WPL
- Choice of the pen width
- Write or not the negative Y graduations
- Change the frame width of the pattern plot
- Profile fitting procedure

March 1998

- Birthday of the beta version of **WinPLOTR**