

Peakoc

Version 1.0

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1. Introduction and General Information

Peakoc is a profile fitting software written in C++. It has been developed to run on PC's with a 32-bit Microsoft Windows™ operating system (in particular NT, 2000 and XP). It has been designed to perform pattern decomposition of powder diffraction data (X-ray or neutrons) but can be used to perform nonlinear least-squares fitting with other kind of data. It takes advantage of the graphical environment of the Windows OS and provides a friendly and easy to use interface.

It can handle large files with data formats (ASCII format) currently in use in powder diffractometry. Several peak shape functions are proposed like Gaussian, Lorentzian, Pseudo-Voigt, Pearson VII, Voigt, or convoluted functions. Most commands (peak searching, profile fitting) can be performed in manual or automatic mode.

The software uses a version of the Levenberg-Marquardt algorithm for the nonlinear least-squares fitting. Peak shape functions parameters can be refined, fixed or constrained during the refinement. Constraints, which are particularly useful in cases of highly overlapped peaks cluster, can be easily defined using the mouse.

At each step of the refinement, the graphical display (y_o , y_c , $y_c - y_o$), the parameter and χ^2 values are updated in the main window and all the results (refined parameters, sigma values, calculated pattern...) are saved in files.

Disclaimer: Peakoc has no warranty. It is provided “as is”. The author is not responsible for erroneous results obtained with Peakoc. It is the responsibility of the user to check his(her) own data and to validate his(her) results.

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2. Installing Peakoc

- a. Unzip the Peakoc.zip file on your hard disk
- b. You should get the following files:
 - ReadMe.pdf (this file)
 - Peakoc.exe (Peakoc executable file)
 - Test1.txt, Test2.epf and Test3.txt (3 example files)
- c. Just copy the files in your preferred directory (nothing else is needed)

3. The files created by Peakoc

In addition to the output files containing the results of the refinement (see section 4.5), Peakoc creates two files to maintain the current state of the program. These files have the same name as the data file but have different extensions. The .clc file contains the calculated pattern and the .dtb file contains the peak shape function parameters. Thus, to start a refinement from scratch, it is just necessary to delete these two files.

4. Short Tutorial

4.1 Loading data

After starting Peakoc, select the “Open” command from the “File” menu for loading data. The “Open” dialog will be displayed with default file types set to “*.epf; *.txt”. Peakoc uses the file extension name to define the data format. So, even if your data file format is supported by the program you have to rename your file if necessary with the correct extension name.

Data Format: All formats use ASCII characters. All lines starting with the ‘!’ or ‘#’ or ‘;’ characters are ignored by the program. You can use the keyword WAVELENGTH followed by the wavelength value to set the wavelength (e.g. WAVELENGTH 0.48776000, see the test1.txt and test2.epf example files). If no wavelength is specified, the program assumes that $\lambda=1.540598 \text{ \AA}$ (CuK α_1). This value can be changed within the program by selecting the “Pattern information” command of the “View” menu.

EPF files: this file usually contains 3 columns corresponding to x, y and sigma values and the number of lines corresponds to the number of data points. If no sigma values are provided (i.e. 2 columns only) the program assumes that $\sigma(y)=\sqrt{y}$.

TXT files: the first data line should be $2\theta_{\min}$, step, $2\theta_{\max}$. The rest of the file contains the y values given in any, but constant, number of columns (see the test1.txt and test3.txt example files). The program assumes that $\sigma(y)=\sqrt{y}$. The number of used data points is given by the minimum value between $(2\theta_{\max} - 2\theta_{\min})/\text{step} + 1$ and the number of actually read values.

4.2 Inspecting curves

When the data file is loaded, two curves should be drawn in black colour. The uppermost and obvious curve corresponds to the raw data. The lowest curve is the difference between the observed and calculated patterns. By default, the difference is normalised (i.e. $(y_c - y_o)/\sigma$ is plotted). Note that when starting the refinement from scratch, there is no calculated pattern. But when peaks are present (see section 4.3) the calculated pattern is drawn in red colour. You can use the “View” menu or the context menu (by clicking on the right mouse button) to choose between the different viewing options. You can plot your data with a linear, square-root or log scale. You can also zoom in or zoom out, scroll, shrink or expand the view:

Zoom in/out: select a zooming region by pressing the left mouse button and moving the mouse or use the toolbar buttons.

Scroll the view: move the mouse while keeping the ‘Ctrl’ key pressed.

Shrink or extend the view: move the mouse while keeping the ‘Ctrl’ key and the left mouse button pressed.

4.3 Finding Peaks

Before starting the profile fitting, you have to get an initial guess of the peak shape profile parameters (e.g. peak position, peak width, maximum intensity, etc...). This is done by performing a peaks search either in manual or in automatic mode.

Manual peak search: position the cursor at the right location and double-click on the left mouse button. A peak is added at the cursor position. The full width at half maximum of the peak is set to the value given in the "Peak width for manual peak search" dialog box found in the "Peak searching: Options" command from the "Data treatments" menu. This value is given in unit of data points (the default value is 5.0).

Automatic peak search: Select the "Peak Searching: Run" command from the "Data treatments" menu or click on the corresponding  toolbar menu. The peak search is performed on the part of the data displayed in the window. If the full pattern is plotted, peaks are searched in the whole raw data.

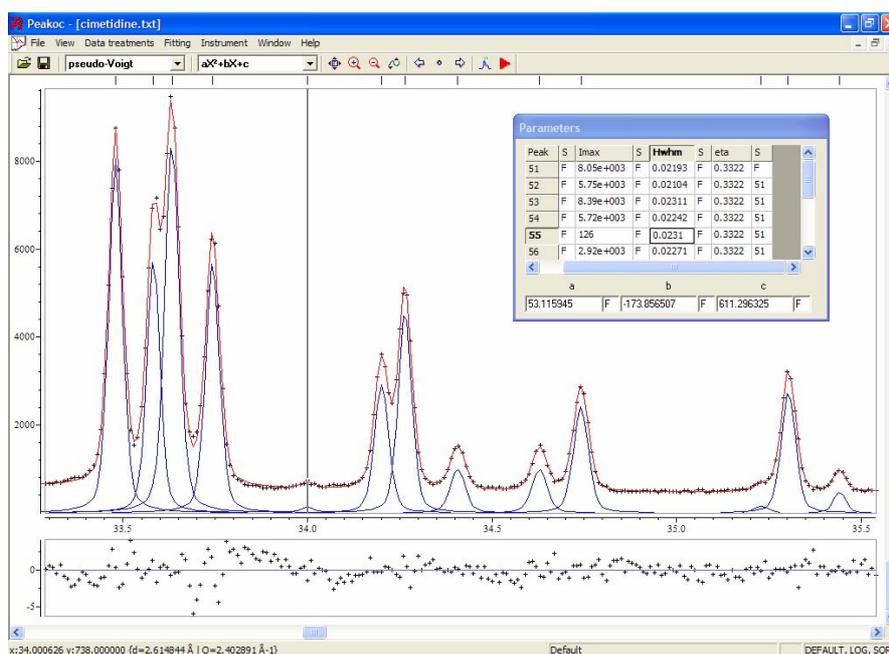
Removing peaks: first select a given peak by moving the mouse while pressing the "shift" key, and then double click on the left mouse button.

Notes: - The peaks are marked with a blue stick in the upper region of the view.
 - When a peak is added or removed, the calculated curve (in red) is updated and the data base is saved in the .clc and .dtb files.

4.4 Fitting Profiles

Now, select a profile shape and a background function with the combo boxes. Also select a region to be fitted (the refinement is always performed on the part of the data displayed in the window). Then select the "Run: Solve" command from the "Fitting" menu or click on the corresponding  toolbar button.

You can examine the fitted parameters by selecting the "Parameters" command from the "View" menu or by pressing the combination <Ctrl+A> on your keyboard. You can also plot the individual peak shape functions, which is useful when the fitted peaks are highly overlapped, by selecting the "Draw individual peaks" command from the "View" or context menus. A typical view is shown on the figure below. You can clearly see the red calculated curve, and the blue individual peak shape functions.



You can use the “Parameters” dialog box to manually change the parameter values. This box is also useful to set some constraints or to fix some parameters. Constraints are used in cases of highly overlapped peaks cluster. By default, the parameters are free to vary during the refinement, but they can also be fixed or constrained. As you can see on the figure below, each line of the dialog box grid contains the values and the states (column “S”) of the peak shape parameters. If the parameter state is "F" (for "free"), the parameter is free to vary. If the parameter state is "H" (for “hold”), then the parameter is kept fixed during the refinement. You can switch between these two states by simply editing the grid or by double clicking with the left mouse button on the appropriate grid cell. You can also constrain a parameter by setting the state equal to the number of the peak to be constrained to. In the example of the figure below, all parameters are free except the “eta” parameter of peak #20, which is fixed, and the Hwhm (half width at half maximum) and eta of peak #24, which are constrained to the Hwhm and eta of peak 23.

The screenshot shows a dialog box titled "Parameters" with a table of parameters for five peaks (20-24). The table has columns for Peak, Location, S, Imax, S, Hwhm, S, eta, and S. Below the table are two input fields labeled 'a' and 'b' with their respective values and states.

Peak	Location	S	Imax	S	Hwhm	S	eta	S
20	49.1891	F	7.82e+003	F	0.1174	F	0.5	H
21	50.0054	F	2.55e+004	F	0.1256	F	0.1927	F
22	51.5728	F	1.54e+004	F	0.1291	F	0.1775	F
23	52.5516	F	1.4e+004	F	0.1413	F	0.09678	F
24	52.876	F	1.84e+004	F	0.1413	23	0.09678	23

a	S	b	S
120.049047	F	1626.820559	F

You can easily change the parameter states of all peaks at the same time by double clicking with the left mouse button on the “S” cell corresponding to that parameter. This will switch the parameter states from “F” to “H” and “constrained”. Also, you can change the parameter values of all peaks at the same time by double clicking the left mouse button on the ‘parameter name’ cell corresponding to that parameter (in this case the parameter states of all peaks need to be “H”).

In some cases, you will need to change some profile fitting options. This can be done by selecting the “Options” command from the “Fitting” menu. In particular, you can change the value of the ‘range of calculated profiles’ (in fwhm units). This fixes the x range used by Peakoc to calculate the peak shape functions during the refinement. The larger the value, the better the line tails are taken into account but at the expense of the calculation time.

Statistics: In addition to a close examination of the differences between the observed and calculated profiles, the quality of the fit can be estimated by the use of a set of agreement factors. Peakoc provides most of the statistics used in Rietveld refinements. To view the statistics, select the “Statistics” command from the “View” or context menus.

When you are happy with your fit, you can change the fitted region by clicking on the   toolbar buttons to move left or right respectively. The options controlling the behaviour of these buttons are found in the “Window options” from the “View” menu.

You can also perform an automatic profile fitting by selecting the “Automatic mode” from the “Fitting” menu. In this case, the program goes from the first to the last peaks and adjusts automatically the fitted region.

4.5 Exporting fitting results

Finally, you can export the results of the refinement by selecting the “Export” command from the “File” menu. Two files can be created:

- the .out file contains all the results,
- the .dif file contains the d-spacing and relative intensity values only.