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### MacDiff Latest Infos

#### Version 4.2.6 (February 19, 2010)

- Works in SheepShaver Emulation (no code changed)
- in Classic Mode of OS X: reads Windows-Files without („TEXT“, „dosa“) Resources.
- Bugs fixed: several glitches in the Print Profile & Data function.
- MDI filter reads files with line feeds (thanks to D. Cardace).

#### Version 4.2.5 (May 17, 2001)

- New option in multifly plots - normalizing the counts of a 2-theta range (proposed by N. W. Hayman, Seattle, thanks!)
- Profile fit dialog option: profile function line thickness changeable (thanks to J.Jung)
- Find Base routine: Exclude (skip, only smooth) first angles of a scan.
- Automatically sorts the file list by names as showing in file session or multiple file dialogs, if a non-HFS volume is called (for example Windows NT) - thanks to J.Forsman!)
- New option: showing d-values of peak search marker (thanks to Louis Evrard!)
- The manual lists two ways to collect a group of single AID files coming from PDFWin software for fast importing into a Peak database file using BBEdit Light or by a Word-VisualBasic Macro Script (thanks to Louis Evrard!)

- Very old bug fixed: no longer forget the source folder of a profile after changing to a new folder using the Open/Save dialog.
- Another old bug fixed: Data loss or crash after calling the undo command, if a Philips APD or any kind of Siemens RAW file was used.
- Bug fix: No longer crash after moving the Comment dialog.
- Bug fix: Session file dialog, "New folder" if no file is selected - no longer finishing the dialog.
- If MacDiff is still not able to find the Preference folder, as observed in rarely cases, the "MacDiff Prefs" file will be located in the system folder.
- To OS X users: Up to now MacDiff only works in the Classic environment of OS X. For the future, a "carbonization" is planned.

#### **Version 4.2.4 (February 20, 2001)**

- Problem fixed: Gradually performance loss after reading more and more profiles if one (or more) of the three data windows are constantly opened (Report, Peak Info, Identify) .
- New option to copy the record list of a peak database into the clipboard: use command-C (thank you, Louis Evrard!).
- New option during import or update of a peak database: removal of duplicates (thanks Louis Evrard too!)
- Optionally print and copy peak data of a phase using 2-theta values instead of d values (as used in the peak database dialog).
- 'Print Profile & Results' routine improved and accelerated.
- Bug fix: "Change Start Angle" dialog glitch (no longer change to zero 2-theta without editing a new angle)
- Bug fix: problem after Peak fit error alert (infinite alert call).
- Bug fix: problem in appending a peak database corrected (thank you, Louis Evrard!)
- Bug fix: MacDiff does no longer overwrite a peak database after creating a new one having the same name.
- Bug fix: Now allows reading data of angles lower than 1 and data > 32768 counts from TEXT files.
- 'Isolated' half height widths lines as a consequence of too small peaks removed.
- Minor bugs of the Peak Info display fixed.

#### **Version 4.2.3 (December 20, 2000)**

- Bug fix: Problems to find the Preferences folder on some non-US and non-German MacOS versions (thank you Faisal A. Butt!)
- Bug fix: Wrong results in calculating Mean Diffs from session files.
- Bug fix: Crash on systems earlier than MacOS 9 after click on one of the comment radio buttons in the Save Report dialog (thank you Michael!)

#### **Version 4.2.2 (December 8, 2000)**

- Some changes of the design of the Peak Identify window. Number of peaks of the current profile as found in the database is documented now.

- New zoom-in and zoom-out function now localized in front of the button bar - Alternatively, use the space bar on keyboard. ALT key for unzooming.
- Changed position of count buttons for zooming/unzooming counts now found in the button bar.
- Bug fix: crashes on systems earlier as 9 after click on some elements of dialog windows for peak correction and for peak comments. Thank you, Michael!
- Fixes a problem in the alpha-2-stripping routine (since 4.2)
- Fixes wrong initial peak parameter used for profile fit (since 4.2)

#### **Version 4.2.1 (October 31, 2000)**

- Peak comments dialog: adds navigation buttons for changing report records.
- Several problems of peak comments dialog solved.
- Missing report data in "Print Profile & Results" routine solved.
- Bug fixed: Disappearance of some buttons in non-modal data windows.
- Bug fixed: Crash under certain circumstances in the "Separate Profile" function, (also problem in window sizing removed)

#### **Version 4.2 (October 25, 2000)**

- New option: save and read peak marker lines into/from DIFF files (edit marker, search marker, and peak database marker, if available).
- Improved Marker lines dialog
- New: File session Info dialog for removing or repeating session files
- New: Peak comments: All the peak data can be explained by a comment, new dialog to handle. The old peak comments are renamed to peak marker.
- New: Print Profile & Results: comprises a smaller profile plot, history, report and comments, as well as peak search lines.
- New: Print Preview window before starting all printing jobs.
- More simplifying printing jobs (no longer changing pageup settings before printing data lists).
- Errors in reading of Rikagu ASCII files removed (Thanks, Brad Johnson!)
- New sort option during update a peak database (sorted to names, JCPDS number, unsorted), thanks Brad Johnson!
- Major revision in the data handling of MacDiff to improve stability.
- Bug fixed: No longer problems on volumes with system folders who are not placed in the root folder (danke, Martin!)
- Bug fixed: Polygon draw of the base line.
- Bug fixed: no longer blocking MacDiff after launching a file from the Finder if a dialog is open.
- Heavy bug fixed: overflow crash after drawing many peak fit functions.
- Fixes the problem to reset the peak limit lines after passing the peakfit prefs dialog.
- Drawing of residuum improved.
- Faster drawing of peak identify list, if test is enabled, but no open profile.
- Fixes a wrong file info for delete records of report data.
- Fixes a problem during changing windows.
- Several minor bugs removed.

### **Version 4.1.2 (June 29, 2000)**

- Peak identify routine: Test of the strongest peak identification in a profile now based on a new peak search routine (2nd derivate method) giving more accurate test conditions.
- Changed: handling the Identify Options dialog.
- New option for printing profiles in correct colors (Preference dialog), thanks J. AbuShama!
- Bug fixed: problem in exporting PICT files of profile graphics.
- Bug fixed: reads Raw1.00 AND Raw1.01 Siemens format (different start angle entries!) - thanks Mr. Michael!

### **Version 4.1.1 (June 1,2000)**

- Changes in the internal data model of the undo operation, may removes crashes during profile preparing (base calculation, smooting, a.o.), as observed on some newer Macs. This increases the memory requirement (1 MB).
- New import file format: Siemens RAW1 (New!) Binary, thanks Stefan!
- New import file format: old Siemens RAW (New!) Binary, thanks Stefan!
- New import file format: Scintag 2000 ACSII, thanks Mr. Schulte!
- New option for marker line text: changeable font size
- Bug removed: Exporting PICT files of profiles and fitting curves, thanks Mr. Jae-Ji!

### **Version 4.1.0 (April 20,2000)**

- New multipeak correction - corrects a profile by a linear regression equation of the deviations of up to eight peak maxima.
- New import: Recognizes film scans (e.g. Debye-Scherrer photo scans).
- Improves choosing peak database record names by typing their first letter key.
- Adds more creator type settings for PICT export (FreeHand 8, 9 and custom creator type).
- Improved Find Base routine.
- Glitch fixed: numbered add-peak-cursor (holding down shift key), if any peak marker is shown.
- Manuals updated. Now they appear as PDF files.

### **Version 4.0.9a (February 2,2000)**

- Bug fixed: Memory overflow (since version 4.0.7).

### **Version 4.0.9 (February 1,2000)**

- Bug fixed: Error during importing several file types (since version 4.0.8)
- Improved background integrity.
- Allows peak maximum marker movements before starting multipeak fit.
- Bug fixed: Copy x5 or Export to PICT \*5 have wrong graph elements, if used together with PeakFit results.

### **Version 4.0.8 (January 17,2000)**

- RAM requirement increases about 500 Kbyte.
- Allows peak ranges down to 0.01 degree 2 theta (no longer 0.05).
- Completely new written peak search routine (second derivation method).
- Reconfigured and improved peak search dialog. Sort by counts/angles and select numbers options added.
- Erroneous text in the Peak Fit Settings dialog: "Lock Peak Limits" changes to "User-defined boundaries!" thank you Dana Giffen!
- Bug fixed: Recognition of files in deep encapsulated folders.
- Bug fixed: Disabled entry of open file name in window menu, if the name contains "(".
- Glitch fixed: too low y scale by using the zoomed window option after mulitpeak fit, if the highest peak is not the first one.
- Some other minor changes.

#### **Version 4.0.7 (October 18,1999)**

- New in Peak Fitting: Each peak can be fitted by a separated function and by splitted/unsplitted profile function (Thank you, Stefan Taudien!)
- New option in session file batch routine: Calculate a mean profile or a summarized profile of all diff files in a session.
- New: scaleable label font size (Thank you, Mr. Morstein)
- New option in program analysis: "Remove" button to kill the current peak data from report.
- Stores removed report data as zero intensities and areas.
- Bug fixed: Wrong program analysis stop, if cancelled by another routine (e.g. loading new diff, window removal)
- Several minor changes

#### **Version 4.0.6 (July 13,1999)**

- Subtract mode of multiple profiles now works with an optional percentage (1-100). Thank you, Mr. B. Pracejus!
- Plays optional sound on tracing. Some other improvements of the trace routine.
- Bug fixed: Crash after repeated choosing of multiple files.
- Bug fixed: Problem in Multiple or Session dialog after changing to Finder
- Bug fixed: Change Anode/Step Size.. (and Undo): wrong results, if there are more data points than before.
- Bug fixed: Undo after changing anode type was not disabled.
- Serveral minor bugs fixed.

#### **Version 4.0.5 (May 5,1999)**

- Bug fixed (I hope so!): empty or chaotic diffractogram after changing a profile during longer runtime of MacDiff.
- New magnify window to show details of a profile around the cursor (press CTRL key).
- More accurate faster peakfit mode - works 2.5 to 3 times faster as without faster mode, produces about 10% higher residuals.
- Plays optional sound after finishing peak fit.

- Fixes a problem in exporting MacXFit files.
- Fixes an error in switching to subtracting background, if square root axis are shown.

#### **Version 4.0.4 (March 22,1999)**

- New option : Copy the current report window.
- New preference for older Macs or small screens: auto-closing data windows (report, peak info or identify display) after selecting other windows.
- Bug fixed: NBS\*AIDS83 filter problem with files of missing lines (Thank you, Louis Evrard!).
- Sveral minor bugs fixed.

#### **Version 4.0.3 (February 22, 1999)**

- New option in Multiple Diff display: "Get Open Profiles" enables to show all profiles of the currently diffractograms as multiples.
- New option in marker displaying: only hkls and/or only d-values.
- New: disable peak markers by simple clicking the lines of the phase legend list.
- Multiple diffs of other 2-theta as main diffs will be automatically converted.
- Reads NBS\*AIDS83 files of newer versions of PDF retrieval software (Thank you, Louis Evrard!).
- Bug: Memory problem during repeated peak fitting procedures.
- Bug in multiple smoothing: no longer 2-theta drift.
- Minor changes in Undo routine (may remove diagram cluttering bug!)
- Several minor changes.

#### **Version 4.0.2 (December 16, 1998)**

- Draw peakfit interim results: Initial peak profile function displayed. Option to draw the graphics "all in one".
- Bug fixed: "Empty diff" problem after changing/filtering.
- Bug fixed: Crash during auto load session, if "Show each file" option is off.
- Bug fixed: Wrong Multiple Diff diagram, if count shift exceeds 32000 in sum.
- Minor bugs have been fixed.
- Manuals updated.

#### **Version 4.0.1 (December 7, 1998)**

- New options in peak fit - optionally sorting of peaks according to intensities before fitting; graphically display of interim results during fitting.
- New option for peak marker lines, which can be kept as permanent.
- Peak limit lines are changable by mouse before multipeak fitting
- Several bugs fixed, as
  - VMS-Philips files with counts of more than 32768, now readable
  - Wrong order of relative peak results in program analysis.
  - Wrong residuum interim results during peak fitting
  - Window cluttering if a diff was zoomed followed by identify window action.
  - Problems in redraw if a film image or a grid was enabled/disabled and several

diff windows are opened

- Missing increment values of bragg angles by using small angle step sizes (< 0.01)
- MacXFit file export does not work.
- and many minor bugs.
- Manuals updated.

### **Version 4.0.0 (August 31, 1998)**

- About 50% new or changed code.
- New data format: holds 4 byte floating values.
  - works with intensities up to 1.000.000 counts (no longer 32768-count-limit!).
  - holds source file names and formats.
  - holds history info of all modifications to see what's happened with your data.
  - holds comments to each profile as written by the user.
  - holds counting times (also displayed in diagrams).
  - reads and writes the old MacDiff 2/3 data format (write via Export).
  - RAM requirement increases (about 1 MB more: now 3.6/4.4 MB for PowerPC).
- New Undo function - undo of the last change in profile.
- Introducing Peak Fitting - Fit a single peak or a group of (up to seven) peaks - possible profile functions are Gauss, Lorentz (normal, intermed, modified), Pearson VII, and Pseudo Voigt. Least square refinement. Asymmetric (splitted) or symmetric function. Some settings in a new "Peak Fit Settings" dialog.
- ALT-Click-Measurement - Holding ALT only a single click is needed to analyse a peak.
- More exact display of counts (optional) and angle data.
- More exact display in small scaled views.
- Minimum angle interval 0.1° (no longer 0.4°).
- Improved Peak Search accuracy and Peak Limit determination.
- Changed: "Profile" menu instead of "Prepare"
- Changed: "Separate Profile..." moves into the "Profile" menu - some improvements here.
- More Batch options to filter a series of profiles: Separate, Smooth Base, Noise Reduction.
- A new Prefs File! ("MacDiff Prefs 4") The old MacDiff 3 Preferences will be unconsidered.

You should change your settings to an environment of your choice after first start of MacDiff 4 .
- New Alpha-2 Stripping options.
- Import of NBS\*AIDS83 format into MacDiffs peak database, coming from PDF database. Several options to filter PDF data sets.
- Peak database holds 32766 peaks now.
- New main peak database of more than 500 minerals having about 22000 peaks.
- Marker lines of peak data are optionally shown without d-values and hkl's.
- Generates synthetical diffractograms as calculated from records of peak database.
- Improved Session- and Multiple Diff Dialog (long file name display support, scroll by keys, shift-click for choosing multiple file sessions, and several bugs

fixed). Multiple files as earlier determined are no longer automatically removed by opening the multiple plot dialog.

- Redesigned Peak Identify, Report and Info windows. Self updating peak identification, report list and peak Info table, presented on new smaller windows, which can remain constantly opened. The Peak Identify window are resizable now.
- Improved Peak Search routine - Up to 200 lines, redesigned display.
- New Analysis Program features: Profile fitting, peak search method, calculates relative percentages, formula generator.
- New option for count conversion: Free formula calculation.
- Reads NewMod ASCII File format.
- Improved Digitize Plot dialog: Preview tiling of plot, Edit User name.
- Report Save Dialog: new scroll bar
- New Username editing options before tracing diffs.
- Preferences dialog redesigned (splitted into 3 parts). Some new features.
- Noise Reduction of Background: no longer count threshold.
- Manuals can be linked by MacDiff (in Apple Menu), if one of them are placed in the MacDiffs folder.
- More window size menu setting (1600x1200, for big screens).
- Changed position of 2-Theta display in diffractogram printouts.
- Enhanced Mineral database - The database now comes in a "Complete set" of 532 minerals with more than 22.000 peaks. Furthermore, there are sub-databases of Sedimentary rocks, Magmatic rocks, Metamorphic rocks, Ore Minerals, and Clays.
- Manuals updated to 4.0.0 - Thank you for your English translation, Jochen!
- Bug fixed: wrong results in Multiple diff mean, subtraction, or difference, if count shift are used.
- Bug fixed: some wrong release of marker lines.
- Bug fixed: Peak search type was not changeable by holding keys "N", "M", and "P".
- Bug fixed: Screen redraw problem in peak search window.
- Bug fixed: Wrong peak measurement mode if changed during moving of peak position marker.
- Bug fixed: Redraw problem after removing multiple diffs on non-activated windows.
- Bug fixed: No longer removing multiples after closing non-multiple diffs.
- Bug fixed: Wrong data if editing peak positions in database using 2-thetas.
- Many other minor bugs fixed.
- Program and document icons have changed.
- Refreshed Startup Logo.

### **Version 3.3.1 (Nov. 12, 1997) 68K + PPC**

- New file format: H.Lauterjung's ASCII format (Thank you, Christoph!)
- New file format: CIF-Format.
- New option in batched routines (Session file dialog): Export Mode - you can export your data or graphics of file series during coffee break.



- New: Writes Philips UDF, Scintag MDI, Sietronic CPI, H.Lauterjung format files (Export).
- Allowes more Scintag (Rigaku) .MDI format differences.
- Bug fixed in background manipulation. Points-fixed-to-line function works again (key "L").
- Bug fixed - Peak comments remain after closing Diff-windows.
- Minor bug in Export data fixed (Step size allways 0).
- Bug fixed - Error in reading Philips-VMS-Binary files if a count > 32768 did occur (Thank you, Christoph!)

### Version 3.3.0 (Aug. 7, 1997) 68K + PPC

- Manuals are updated.
- New: External launching of an Analyse program opens the Analyse Program dialog.
- New: A new button in the Database dialog enables a "search in another folder".
- New: Adds an option to draw the same peak lines in diffractogram as filtered in the Peak Identify dialog: "Use Filter in Drawings" - Identify dialog is modified.
- Changed: Choosed objects as shown in several lists appear in hilited color mode now.
- Arrow keys in Peak Search dialog to navigate through the peak list.
- Alpha-2 stripping: Background will be reduced to 2/3.
- New: An asterix "\*" in the hkl field of a peak in peak databases enables to draw an rectangle to the d-value of the following peak, showing variability of d-values.
- Bug fixed: Analyse program was not completely killed if a new analysis program file was launched.
- Bug fixed: Wrong position of main file name in multiple display legend.
- Bug fixed: Wrong names and d-values in header of report output files.
- Bug fixed: Crash in smoothing a profile with more than 10000 points.
- Bug fixed: No more crashes in the case of a profile with more than 8000 points, if the polygon option is enabled (it is automatically disabled above 8000 now).
- Bug fixed: Wrong Enter key behaviour at running program analysis.

### Version 3.2.9 (July 15, 1997) 68K + PPC

- Installation: **The Database must be download and installed separately now.** It is no longer bypacked in both of the 68K and PPC MacDiff versions (but included in the complete package). **If you have already installed the database, you don't need to reinstall, because there is no change.**
- Bug fixed: Database could not be found.
- Bug fixed: Letters of longer file names after "Save As..." were disappear.
- Bug fixed: JCPDS card display has come if a database was called via Identify peak.
- Bug fixed: Wrong Peak correction results (68K version).

- Bug fixed: No File name in printouts.
- Little change in Preferences dialog layout.
- Added: You can disable the "Smart Clicks" in the Preference dialog now. If enabled, and a peak is analysed, a single click within the diffractogram window will finish the peak analysis or will call the next peak in the case of a running analysis program. With disabled smart clicks, you must enter the "OK" button or hit the "Enter" key to finish the peak analysis. **Please, enable the smart click option, if you want to have the same mouse behaviour during peak analysis as ever!**
- Changed: Profile name legend in Multiple display is plotted in the order of their appearance, that means, ordered from bottom to top (former: top to bottom)

### **Version 3.2.8 (July 2, 1997) 68K + PPC**

- Adds a "no progress bar" option as preference usable for fast Macs (as my new 8600) and for little faster working on other machines.
- More flexible filter for MDI-Files - Scintag ASCII compatible (thank you, Mike!),
- Bug in Search Filter Options fixed (Peak Test).

### **Version 3.2.7 (June 23, 1997) 68K + PPC**

- Bug fixed: Mineral database can be changed without problems (Bug in Version 3.2.6)

### **Version 3.2.6 (May 2, 1997) 68K + PPC**

- Manuals are updated (May 2) as stand alone text applications.
- Most dialog windows are improved and redesigned (greyish background, new popup-menus, new scroll bars, no longer loss of objects on update).
- All your peak databases now must be placed into the Preference folder:MacDiff.
- A new Installer for properly installation of MacDiff and the Minerals peak database.
- More stability on corrupted Preference file.
- A new dialog to "Set File format..." to open a profile of a distinct file format.
- Change in reading procedure of MDI-format files.
- Enhanced Info dialog.
- A new "Copy Data" menu command to copy the data (counts) as plotted into the clipboard.
- The clipboard window shows also data (not only graphics)
- A new "Smooth Options..." dialog to set several filter and level for smoothing counts.
- Multiple Diagram: You must select a file to set a folder before choosing multiple files.
- Bug fixed: FWHM Calibrations will appear again.

- Bug fixed: Failure in Multiple File dialog after calling peak database.
- Several smaller bugs fixed.

### **Version 3.2.5 (March 12, 1997) 68K + PPC**

- Bug fixed: ASCII-"tails" in MacDiff-files coming from Text format import files (Thank you, Harry Grooter!).
- Bug fixed: do no longer close Peak database or Peak identify windows after dragging them on screen
- ASCII-Text reader improved (accepts line feeds)

### **Version 3.2.4 (Feb 14, 1997) 68K + PPC**

- New: Rigaku-ASCII-Format-Filter.
- New: Updating XFit4Mac-Filter to XToraya4Mac
- Bug fixed: Undesired removal of single peak comments.
- User handling interface during peak analysis improved.

### **Version 3.2.3 (Feb 7, 1997) 68K + PPC**

- Fixed: Internal error after opening a peak database (no longer error 11 or 1).
- Adds a text editor (menu "Analyse: Comment Peak...") used to give comments to a single peak (tip from Ray Ferrell, Zurich, thank you!)
- Opens a new dialog if intensities higher than 32,768 are observed during loading a Diff. You have an option to divide your intensities by 10 (10%-counts).
- The manuals are updated.

### **MacDiff 3.2.1 for PPC:**

- MacDiff now reads and handles profiles of up to 16768 data points. The maximum in previous versions are 10000 data points.

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