MacDiff Release Notes

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 circumstandes 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 crashs 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 mulit-peak 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 about10% 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!).
- Serveral 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 profile 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. Asymnetric (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 hkls.
- 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.
- 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 multipe 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)

- 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 always 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)

- 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)

- Installation: The Database is a separately file to download. It is no longer bypacked in both of the single 68K and PPC MacDiff versions. 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)

- Adds a "no progress bar" option as preference for fast Macs (as my new 8600) of 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)

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

Version 3.2.6 (May 2, 1997)

- 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)

- Bug fixed: ASCII-"tails" in MacDiff-files coming from Text format import files (Thank you, Harry Gorter!).
- 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)

- 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)

- 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.

Version 3.2.2 (Jan 23, 1997) 68K + PPC

- There is an internal error after opening a peak database as a part of a folder placed on the desktop. In version 3.2.2 you cannot longer open such a database (in older versions a crash No. 11 follows). A database must be launched from a volume. I hope to fix the internal error.
- Closes each DIFF window after printing files launched from the Finder.

Version 3.2.1 68K (Dec 14, 1996)

This is the first release of the 68K version made by VIP-BASIC 2.0R2 and Code-Warrior 10. It works 2 to 6 times faster than older 68K versions of MacDiff. Please test the new release if all works correctly.

Version 3.2.1 PPC (Dec 12, 1996)

- Bug fixed: Wrong icon of mineral database files after first call of "Identify".
- MacDiff now reads files of up to 16768 data points (10000 up to now).
- Failure in saved report files fixed: wrong calibrated FWHM.

Version 3.2 PPC (Nov 26, 1996)

This is the first non-beta of MacDiff 3.2. You do not need no longer any Libs (VIPLib or ANSI_CLib) in your System extension folder to run MacDiff!

- New R2.01 release of VIP-BASIC development tool.
- Recompiled with CodeWarrior 10 (little faster code)
- New: Reads MDI and OUT ASCII File format (Thank you, Henry LaViers).
- Some minor bugs fixed.

Version 3.2b6 PPC (Nov 19, 1996)

- New: Reads Sietronic ASCII File format (Thank you, Peter Talbot).
- A new menu item "Window" comprises the "Diagram Size" of the old "Prepare" menu as well as all the current open Diff windows.
- Bug fixed: Scoll bar.
- Bug fixed: Wrong peak identify list redraw if no intensities available.
- Bug fixed: Cancelled Report file Saving
- Some minor bugs fixed.

Version 3.2b5 PPC (Nov 12, 1996)

- Minor bug fixed: date and time in printouts, report files.
- Crash during writing report files with long names fixed.
- Some faster redraw of a diff.

Version 3.2b4 PPC (Nov 5, 1996)

- Bug fixed: Open Multiple File folder problem on PCI-Macs.

Version 3.2b3 PPC (Nov 4, 1996)

- Some smaller bugs fixed.
- Speed problem after peak database calls removed.
- More speed in the entire graphic recall.

Version 3.2b2 PPC (Oct 31,1996)

- Bug fix.

Version 3.2b1 PPC (Oct 29,1996)

- This is the first version of MacDiff, developed with VIP BASIC 2.0 and auto-translated to ANSI C, compiled with CodeWarrior 8.0. Because I have tested MacDiff only in its main features, there can be remain some failures or bugs. But you have two big improvements:
      - MacDiff is much speedier now (2 - 3 times faster in graphics and **3 to 5 times faster in most calculations!**)
      - MacDiff needs less RAM (the application is more than 700 K smaller).

Important! If you want to start MacDiff 3.2 for the **first** time, you have to install the file "VIPLib" into your system extensions folder! Otherwise your system may crash! MacDiff do not need no longer the file "ANSI_CLib".
The 68K-Version of MacDiff 3.2 is in preparation. I hope to finish it next time.

Because of several bugs in the development environment, there are some old features of MacDiff still disabled (I hope to fix them with the next release):
      - there are no longer working in the background.
      - the window hierarchical menu is unusable.
      - the fast redraw option is always enabled and do no longer appear in Edit menu.

Under some circumstances, mostly after many calls to the peak database, I observed an overall speed loss. If so, you should restart MacDiff. I hope to fix this problem.

Please let me know, if you discover any bug with MacDiff 3.2. Send me an e-mail!

Other changes:

- New: A test of the n strongest peaks of a peak database phase, if available in your diagram (go to "Filter..." in "Identify" list).
- New: The Anode wavelength is editable.
- Cursor handling in the Trace Plot routine is improved.
- The "Info" dialog also works if no diffractogram is present.
- Bug fixed: failure after changing the folder in session- or multiple file dialog.
- The delay times after click on buttons are shorter.

Version 3.1.5 (Aug 27, 1996)

- The Find Base routine is improved by an option to change the point interval to calculate the background. Thank you, Harrie Gorter!
- Now you can draw more than one records of peak database marker lines into one XRD diagram (up to 256 single lines and 7 phases), a tip from R. Oberhaensli. Thank you!
- And so, a new dialog for handling marker lines with some improvements is added.
- The multiple file dialog is improved. On opening the dialog, the files of the current folder will automatically appear. There is also a new "Clear multiple" button as well as a new option to remove multiple profiles automatically after opening a new window.
- Search of a peak database record now works correctly with capital or small letters.
- Bug since 3.1.4 fixed: the mineral system popup-menu in the peak database dialog works correctly.
- Bug fixed: Disappearance of some tick labels (for example, if start angle is 19.96¡).
- Bug fixed: Memory loss after printing or copying profiles.
- Bug fixed in Report list dialog: Wrong moving up of phase names if an entry of a previous profile is removed.
- Bug fixed: Wrong maximum peak point search, if the maximum count value appears successively several times.

Version 3.1.4 (July 30, 1996)

- New: K-Alpha1 and K-Alpha2 wavelengths implemented.
- New: You can disable/enable the button strip (tip from Thomas)
- More improvement in selecting multiple files from a folder.
- New: Multiple files can be plotted as "stacks" using the new count shift option (thank you, Thomas)

- New: The session files of a folder can be determined individually by selecting or deselecting each file.
- Bug fixed: The window sub-menue works fine again.
- Bug fixed: The scrollbar of some scollable windows works correctly.
- The manuals are updated to version 3.1.4

Version 3.1.3 (June 4, 1996)

- Adds a help display to explain all elements of the diffractogram window.
- Bug fixed: Wrong cursor display if "Invert angles" are enabled.
- Bug fixed: Not completely removed peak lines after several use of the "Search Peak" routine.
- Bug fixed: Accept commas in Preference file!
- Bug fixed: Wrong line colors of multiple diffractograms.

Version 3.1.2 (May 6, 1996)

- A new Diff-File import and export ASCII filter, used for the Mac-Application "XFit4Mac" of Freising (TU Munich, H.Stanjek) is added. If you want to make profile fittings, save your diffs as XFit4Mac-Files (using "File:Export"), and drag it onto the XFit4Mac applications icon.
- The Key code "cdm-m" for the "Manipulate" command is rechanged to "cdm-d" ("m" is used for multiple diffs).
- Bug fixed: Memory overflow error after many zooming or rezooming of the diffractogram.

Version 3.1.1 (April 30, 1996)

- A new Button strip is added, showing 19 buttons of frequently used functions. The old button area is cancelled.
- The FWHM calibration tool is enlarged by two sequences of international FWHM values of illite and chlorite standards, called via "Options" (Thank you, Lawrence).

Version 3.1 (Major Upgrade, April 12, 1996)

- NOTE: Because of the increasing functionality, now you need 3 MB RAM for MacDiff instead of 2.5 MB. On Macs with only 4 MB RAM, you can change the RAM requirements back to 2.5 MB, but you should not work with more than 3 diagrams at one time.

- A JCPDS-card like database interface is implemented, holding crystal name, reference no., formula, crystal system, and up to 255 peaks (_ position, intensity, hkl indices). You can create your own database(s), as required. Each database can hold up to 2048 records by up to 32766 single peak data. An unknown peak of a given diagram is linkable with the database using an index file search. The peak positions of a record are optionally visible as lines within the current diffractogram. MacDiff comes with a standard database holding about 7500 peak data of about two hundred rock-forming minerals. Read the manual for more informations.

NOTE: If you want to build up your own database, make a copy of your files, b e f o r e you want to update the index peak file. I have observed some wrong results (but without any data-loss). It is recommended to restart MacDiff and update the database thenafter.

- The old "Peak Search..." function is strongly improved by 1) linking a peak to the current diagram ("Analyse" button), 2), by linking a peak to the current database ("Identify" button), and 3), better printouts.

- The old "Background" and the "Analyse" menu contents are rearranged as follows. Some menu commands are renamed. Thank you for your suggestions, Thomas!

"Background" is changed to "Base"
"Show Base" without change
"Remove" and "Add Base" is changed to "Subtract Base"
"Base Color", "Base Pattern", "Base Size" and "Base Type" without change
"Find Base" is changed to "Find"
"Find Base Options" is changed to "Find Options"
"Draw Base" (cmd-d) is changed to "Manipulate" (cmd-m)
"Smooth Base" and "Noise reduction" without change.

"Analyse" without change
"Start Analysis" and "Analysis program" without change
"Show Peak Region" is changed to "Zoom Peak Area"
"Peak Info", "Show Report", "Save Report", "Remove Report" and "Peak Search" without change.
"Search Substances" is replaced by "Identify..."
"Peak Database..." is new
"Peak Display Off" is changed to "Remove Marker Lines"
"FWHM calibration" is new.

- All of the dialog boxes now are dragable and can keep in the background (NOTE: Some portions may not completely refreshed on redrawing).

- The settings of the "Show Base" and "Subtract Base" commands can be stored in the "Preferences" dialog.
- The "Optimized Drawing" menu is enlarged to 7 submenus for controlling drawing speed.
- Several improvements in the "Outlier" filter: 1) Option, to remove all outliers, which are higher/lower than the square root of the base line. 2) Fixes a bug, to remove the maximum point of a sharp peak, 3) recognition of outliers within a peak flank.
- FWHM data of your laboratory can be calibrate to standard values using the new "FWHM calibration" dialog (available for up to five different peaks). Such calibrated values are storable in report files. Thank you for your tip, Laurence!
- The "Save Report" dialog is improved by an option, to save 2Theta-angles instead of d-values. Thank your for your tip, Chao R. Li!
- Several other minor fixes and improvements.

Version 3.0.9 (January, 4, 1996):

- Grey scale of the film image can be inverted by mouse click.
- Fixes a bug, that film image orientation are not changeable.

Version 3.0.8 (January, 2, 1996):

- New preference file, the old one will be exchanged by internal prefs!
- New import menu for digitizing diffractogram plots, either by a graphic tablet (you should have at least a 17 inch monitor) or by a greyscaled image of a scanned diagram (Raw-format).
- New feature: An optional film image downside of a diagram, showing a Debye-Scherrer-like greyscaled line graphic. Menu command: "Show Film Image".
- New feature: Scaling the count axis in square roots, adjustable in the "Count Axis..." dialog. That looks better than logarithmical scale.
- New: An alert appears, if memory is low.
- Fixed: Problems to find the MacDiff preference file, if more than one devices are connected.
- Fixed: Only black-and-white printouts, clipboards and export graphics, although colors are used (since version 3.0.7). Some other minor changes during export of diagrams.

Version 3.0.7a (December 8, 1995):

- Fixes a bug, that may yield to wrong logarithmic scale printouts.

- Simplifies the automatic recognition of readable diffraction file formats. During loading time the file format is displayed. Adds a number of error descriptions, if a failure is observed during loading process.
- Changes the "Always" button in the count and angle axis dialog boxes into "Default". A new "Default" button is added to the "Use d-spacings" option. The "Default" buttons are no longer dimmed.

Version 3.0.7 (December 6, 1995):

- Adds the possibility to calculate profiles showing the absolute count difference of two diffractograms (Multiple diagram dialog).
- The print diffractogram and copy to clipboard section is completely rewritten showing more transparency (the printed or copied diagram is no longer invisible; a Page Setup dialog opens, if printout exeeds the A4 or letter format)
- Fixes a bug in using d-spacings for x-axis, if several windows are open.
- Printjobs are of the same name as the window titles.
- Fixes a bug, that cuts parts of entries in edit fields of some dialog boxes.

Version 3.0.6d (November 30, 1995):

- An english manual is ready. Because it is not written in my mothers language, it is still not perfect at this moment. Sorry, that you have to wait so long!
- 68K, PPC version, and the manuals can be installed as separated .sea files.
- Fixes a bug, that parts of profiles have been disappeared after second call of the "Remove Profile" button during peak analysis.
- The "Save As" command now works correctly (the new file name is transferred to the window title, the creation date is not January 1, 1904).
- The "Noise Reduction" filter now works without distortion of peaks.
- Switching the "Show Peak Region" command (or button) during peak analysis do no longer change current peak limit lines.
- Files of the "crlf" file type (as showing by "UDF" files) can be load without changing.
- The window hierarchic menu of the file menu is no longer corrupted, if a slash "/" is used within file names.
- Before "Auto Load" of File sessions now you can decide between overwriting of existing files or (thats new) making new files in a folder "Changed Diffs".
- The Custom Window menu do no longer show reversed axis values.
- Some other minor changes in the "outfit" of MacDiff.

Rainer Petschick

e-mail: Petschick@em.uni-frankfurt.de