

EWA (Evaluate in Window Approach)

Version 0.14

A spectrum evaluation program for XPS/UPS

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Contents

I	User's Guide	9
1	Using the program	10
1.1	Starting and exiting the program	10
1.2	Controlling the program	11
1.2.1	Using mouse and cursor	11
1.2.2	Selecting menu items	12
2	Basic terms	14
2.1	Files	14
2.1.1	Spectrum files	14
2.1.2	Batch files	14
2.2	Windows	15
2.2.1	The main window	15
2.2.2	Spectrum windows	15
2.2.2.1	Window for 1-dimensional distributions	16
2.2.2.2	Window for XPS spectra	16
2.2.2.3	Window for 2-dimensional distributions	16
2.2.3	Component windows	17
2.3	Parameters	17
2.3.1	Parameter attributes	17
2.3.2	Linking parameters	17
2.3.3	Adjusting parameters	19
3	Evaluation terms	21
3.1	The principle of the spectrum evaluation	21
3.2	Practice of the spectrum evaluation	22
3.3	Operating modes	23
3.3.1	Normal (or single) mode	23
3.3.2	Cross spectrum mode	23
II	Reference Guide	24
4	Batch	25

4.1	Append	25
4.2	Close	25
4.3	Execute	25
4.4	New	26
4.5	Remark	26
5	Component	28
5.1	Advance	28
5.1.1	Last	28
5.1.2	Next	28
5.1.3	Previous	28
5.1.4	Root	29
5.1.5	Select	29
5.2	Change	29
5.2.1	Adjust	29
5.2.2	Background	29
5.2.3	Delete	29
5.2.4	Label	30
5.2.5	Multiline	30
5.2.6	New	30
5.2.7	Peak	31
5.2.8	Subtract	31
5.3	Display	31
5.3.1	All components	31
5.3.2	Marker	32
5.3.3	Text mode	32
5.4	Link	32
5.4.1	Parameters	32
5.4.2	Multiline	32
6	Component Background	33
6.1	ArcTan	33
6.2	Polynomial	34
6.3	Shirley	35
7	Component Multiline	37
7.1	X-satellites	37
7.2	Vibration	39
7.2.1	Linear	39

8 Component Peak	40
8.1 Drude	41
8.2 Gauss	42
8.3 Lorentz	42
8.4 pVoigt	42
9 File	43
9.1 Execute	43
9.2 Exit	43
9.3 Spectrum	43
9.3.1 Load	43
10 Help	45
10.1 About	45
11 Options	46
11.1 General	46
11.1.1 Batchfile type	46
11.1.2 Confirmation level	46
11.1.3 Datafile type	47
12 Spectrum	48
12.1 Close	48
12.2 Load	48
12.3 Dataset	48
12.3.1 Select	48
12.4 Evaluate	48
12.4.1 Fit	48
12.5 Print	49
12.5.1 Preview	49
12.5.2 Print	50
12.5.3 Setup	50
12.6 Save	50
12.6.1 Components	50
12.6.2 Parameters	50
III Tutorial	51
13 First steps	52
13.1 Installation	52
13.2 Loading a spectrum file	52
13.3 Playing with the mouse	53

14 The simplest evaluation operations	54
14.1 Creating components	54
14.2 Creating background component	54
14.3 Creating peak component	55
14.4 Adjusting component parameters	56
14.5 Finishing model evaluation	56
14.6 Changing the model	56
15 Advanced evaluations	58
15.1 Parameter linking	58
15.2 Non-contributing components	58
IV Appendix	60
16 Bibliography	61
17 Glossary	63
18 Spectrum data file formats	64
18.1 ATOMKI home formats	64
18.1.1 Energy calibrated simple	64
18.1.2 Uncalibrated simple	64
18.1.3 Calibration file	65
18.1.4 ESA-21 format	65
18.2 Nucleus PCA-II	67
18.3 Scienta ESCA-300	67
18.4 Tabular data	67
18.5 VAMAS'88	67

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Foreword

*" To write a good software is hard.
To write a good documentation is impossible."*

For the old users of EWA

The development of EWA was started several years ago and up to now it appeared in several forms. The speed development of both the computing technics as well as the measurement and data evaluation science strongly influenced both its abilities and the user's demands on it. According to this, the 1st time 'native' menus and chained EXEcutable files, compiled with Turbo Pascal 3.0, (version 1.xx) have been followed by a versions (2.xx) which used a single (strongly overlayed) EXE file and were based on a 'revolutionary, high performance graphic system' MetaWINDOW¹. The need to increase the evaluation power and for a modern graphic user interface resulted in versions 2.9x, which were based on the graphic version of the Borland's 'Turbo Vision' package (GVision²). Although this version (with protected mode programming) was already able to break through the 640K barrier characteristic to the MS DOS programming, was completely object oriented also internally, was equipped with a powerful, event-driven windowing shell, in the meantime both the language used in the development (Borland's Turbo Pascal) and the platform (MS DOS) lost their importance. Also, the developer realized his inability to keep pace with the speed development of platforms (computers and operating systems), compilers, always starting the new development from scratch.

The (hopefully good) decision was made to change practically everything, keeping only the ideas from the old development and start the new development in a way which poses no copyright, royalty, etc. problems and supports (practically) all popular platforms and its user community guarantees a long term usage. The multi-platform C++ macro package wxWindows³ was chosen as the development platform for the new version. Because of this change, the whole program (letter by letter) has been rewritten, so it is brand new, with brand new errors.

¹©1986 MetaGRAPHIC software corporation

²Reference to GraVis

³<http://www.wxwindows.org>

About EWA

The EWA program is a high-performance, menu-driven, object-oriented, multi-platform, interactive computer program for evaluation of spectroscopic data. It provides a lot of general tools for the spectroscopists to evaluate their spectra. These tools are more or less common in all spectroscopic fields. Based on the demands of its users, the program has been extended to serve some special spectroscopic needs, mainly in the field of electron- and X-ray spectroscopy as well as electronic and atomic collisions. The special program options, primarily intended to evaluate spectra of such fields of spectroscopy, are extensively cited in the chapters devoted to these special fields. The present document is the manual of the program, available both in printed and electronic form. The manual is continuously updated as the development proceeds. Sometimes it happens that for some reason that the implementation of a particular feature or command stops for a while. In this stage the you might see these (half-implemented) menu commands, but they are not (yet) documented. Please do not 'try' such commands! they might kill the application, together with your valuable work.

How to use this manual

The user is strongly advised to study the *User's Guide* first. Although EWA tries to be user-friendly as much as possible, for using its advanced options, the necessary external information can be feed into the program only through the use of the (quite numerous) options. The different versions of the program might differ in that some new commands and options are added and (less frequently) some old commands are modified. Also, some bugs might be fixed between versions and also sometimes optimization takes place. So -especially after receiving a new version of the program- it is worth to study this guide carefully.

A different source of information is the *Tutorial*: from the simplest to the more complicated you will find examples how to use the different options to evaluate your spectra. Here you can see how to apply the different commands and can learn the tricks of using EWA.

The *Reference Guide* provides the most detailed information about what the arguments of the commands are and what their effect exactly is. Here you find also the default values and the notes about their usage. Most of the (non-trivial) operations, algorithms, as well as some parameter values, are known from scientific publications. These sources are referred to as usual with a [code], and under the correspondingly designated item in *Bibliography* you will find the real source, typically widely available books or well-known journal articles.

The available platforms

Thanks to the used multi-platform package, the program can be (in principle) available on different computers (IBM-PC, a range of UNIX workstations, McIntosh, VAX, etc.) under different operating systems (MS Windows 3.x, '9x, NT, Linux, UNIX, VMS, Mac-OS) and is supported by different graphic packages (like GIMP and Motif). The program on different platforms has a native 'look and feel' and because of this, it behaves a little bit differently. Of course, the basic options must work in any combination, but it would not be wise not to use out the extra possibilities provided only on one of the platforms. These extra possibilities are explicitly marked in the text. The main developer platforms are MS Windows NT, Linux and SGI IRIX. (The availability of the program on other platforms depends on the availability of development capacity for the author on that platforms.) The screen shots are taken from Windows NT and Linux screens.

Typographic notations

When looking at the format of this document, you'll occasionally notice things in different fonts:

- ▷ *Emphasized Style* is used for general emphasis, generic arguments, book titles, names of sections of other manuals, and notes from the author.
- ▷ `Typewriter` is used for program and file names, $\text{\LaTeX}$ code, etc.
- ▷ `NOUN STYLE` is used for command and keyboard button names.

Part I

User's Guide

Chapter 1

Using the program

1.1 Starting and exiting the program

The program can be started in various ways, depending on the platform you use. Please consult the corresponding manuals. Anyhow, the directory which the program is started from, as well as the directory the executable file can be found in, will play a special role. The former ('data') directory will be used when looking for the user's files, like data file, calibration, result files, etc. The latter one will be referred to as the 'program' directory and the program will look for its components relative to this directory.

When everything was OK during the initialization, a window called the 'main window' appears on your screen, similar to that shown on Fig. 1.1. On its top line, in the heading, it contains the program's icon, the name and version of the program as well as the icons for changing the size and closing the program (platform-dependent).

Below the heading, you will find the *menu bar* where some main menu items are displayed. The large area in the middle of the main window contains a text window which receives messages from the program. These messages include the generated menu commands, together with the parameters, the results of the evaluation, error messages, etc. The text cannot be edited, so here you cannot type in command lines, to be executed by the program. This window cannot be closed, it is always open when the program is working. The menu bar corresponds to the text window mentioned above as well as to some general features of the program.

The exit command is in the 'FILE' menu. Select that or the corresponding 'close' icon from the menu bar (or its hotkey 'ALT-X') to finish with EWA. Note that before exiting, the program asks for confirmation on exiting (see *Confirming selection* below) if any evaluation is in progress as well as for closing the open windows.

The spectrum evaluation takes place in so called 'child windows', i.e. for the individual spectra new windows are opened, see below. These windows have separated menus, allowing for the evaluation of the spectrum shown in that window.

At the bottom of the windows you will see the status bar (sometimes split in two parts). This area (or the left half of it) is used to display some status information, as well as some short help message to guide you when selecting menu items, see later. When split, the

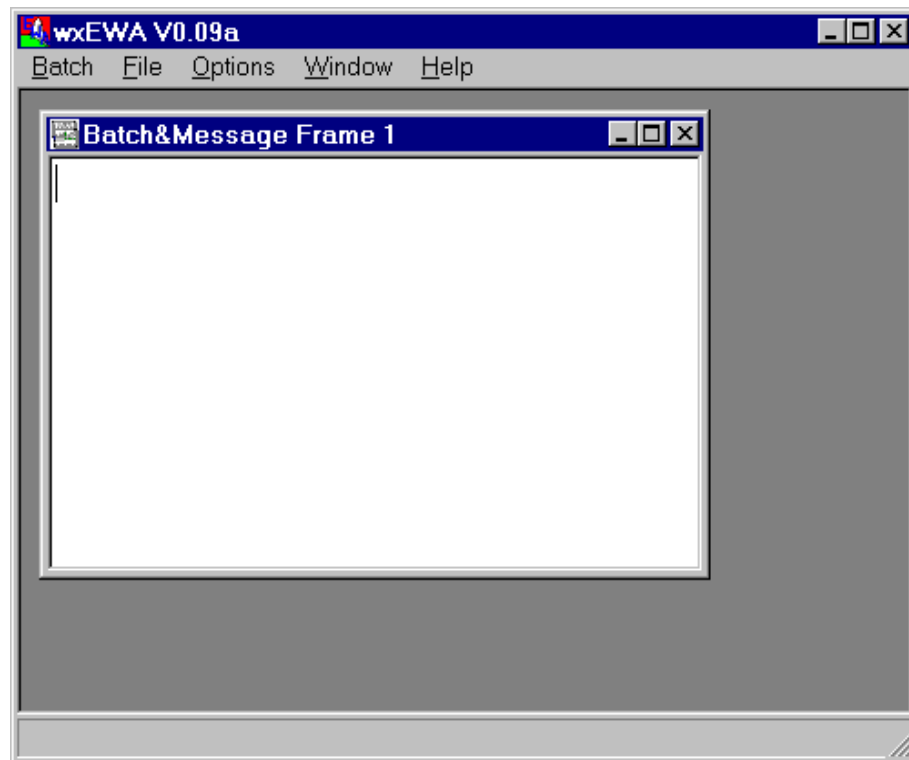


Figure 1.1: The initial desktop screen of EWA

right area is used to display some other information, like the position of the cursor, etc.

1.2 Controlling the program

EWA is an absolutely visual, interactive program, rather than a visual shell to an automatic, command line oriented evaluation program. Although most of the operations can be executed using either the mouse or the keyboard, and it also provides a batch processing facility, it will not work without a graphical screen and a mouse. Note that in this guide, pressing a key on the keyboard is '*typing*', pressing a button of the mouse is '*clicking*', pressing it twice with short time difference is '*double clicking*'. Furthermore, pressing and kept pressed while moving is '*dragging*', while releasing after dragging is '*dropping*'.

1.2.1 Using mouse and cursor

When you move the mouse, the cursor on the screen will follow its motion and it will change its shape. The standard cursor shape (usually an arrow-shaped object) changes when over some special areas of the windows. Namely, it changes to a vertical or horizontal 'RESIZE' cursor when above the vertical or horizontal border of a window. It shows you 'cross hair' over the spectrum canvas (see later). The cursor changes to an 'I-BAR' over the text area of the main window, as well as inside input dialogs, where the user is expected to type characters. The cursor changes to an arrow over the spectrum window 'sensitive

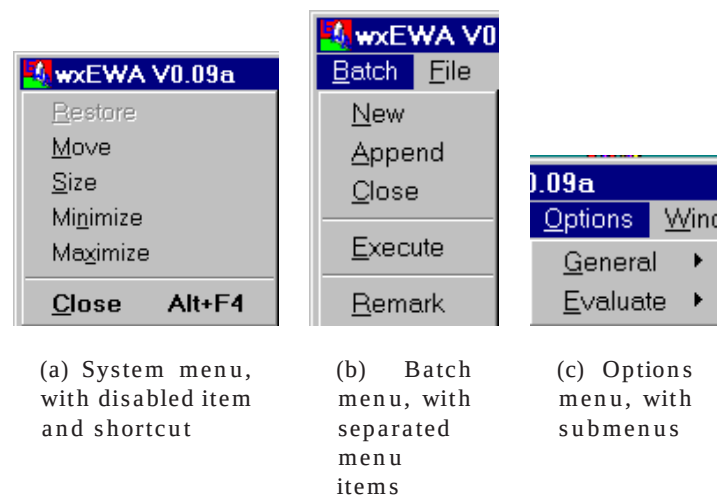


Figure 1.2: Different menu items of EWA

area'. You can display the mouse coordinates in the graph units, measure distances one the screen, drag objects, etc. For details see the *Tutorial*, 'Playing with the mouse'.

1.2.2 Selecting menu items

As it is shown on Fig. 1.2, there are different menu types in EWA. Of course, multiple menu levels are allowed. The upper level menu items are marked with a little triangle on their right, as shown on Fig. 1.2/c, which means that after selecting the item another (deeper level) menu table will appear. Depending on their functionality, the menu items can be divided (using separators) into function groups, like on Fig. 1.2/b.

On the menu screen certain letters are displayed underlined. The given menu item can be activated either pressing 'ALT'+highlighted letter (like 'ALT-F' for 'FILE') or clicking the given item or typing the arrow keys until the selected item reached and typing 'ENTER'. The instruction executed will be the same in all cases, independently of the way as the command was invoked. When you select (any way) one of the items, say 'FILE', a new menu table pops up. Let us select now the 'SPECTRUM' and a new menu will pop up on the top of the previous one. Note a little difference in the menu items: some of the item ends with ellipses (...) which means that after selecting the item a dialog will appear which allows you to provide parameters for the command.

When clicking on the icon in the upper left corner, a special menu (the 'system menu') appears (see Fig. 1.2/a). It handles the general features of a window, like moving and resizing. It is always present with the windows, but most of the functionality it offers, is available also through other methods, see ??.

Some part of the menu items is only legal under definite conditions. When such a condition is permanently absent (like it is no use to select a dataset when evaluating a single-dataset spectrum), the menu item will not be present in the corresponding menu table. When the condition is absent only temporarily (like options using the exciting

energy when the energy of excitation is not known), the corresponding menu item will be present in the menu table, but will be disabled (appears 'dimmed', see Fig. 1.2/a) until the condition fulfilled. The disabled items cannot be activated in such state.

Note that some (frequently used) menu items can be reached via a 'hotkey', i.e. without digging into the menu system. These available accelerator combinations are shown together with the menu items, see for example Fig 1.2/a.

Chapter 2

Basic terms

2.1 Files

The program works with several types of data, stored on mass storage devices, typically hard disks or floppy disks. EWA can use some existing files (like reading spectral data), create new ones (like printing results), or modify them (like appending to the existing log files). For details see the individual commands in the *Reference Guide*.

2.1.1 Spectrum files

The data elaborated with this program are stored in data files, so the term ‘spectrum’ is sometimes used as a synonym for spectrum data files as well as for the spectral data, loaded already in the program’s internal memory. In order to deal with a spectrum, the corresponding spectrum data file should be already loaded in the internal memory, see ‘FILE SPECTRUM LOAD’ in the *Reference Guide*. Following read-in, the program ‘forgets’ about the spectrum file and uses *its own copy* exclusively, i.e. the changes you make to the spectra cannot change the original data file, except if you explicitly replace the original file.

You should not worry about the format of your data: EWA automatically recognizes the file format and chooses the corresponding read-in routine. The program has an internal list of legal formats (see the Appendix) and checks them one-by-one. When a file loaded, a new spectrum window (see below) will pop up to your desktop, showing the data read from the data file. From this point of view the spectrum data and the spectrum window containing them are closely related: to operate the spectrum, you need to select the corresponding spectrum window. Except where explicitly noted, all operations you do, are done with the active spectrum.

2.1.2 Batch files

EWA allows quite complicated string of operations, with using tremendous parameters and options. Their complicated interaction produces your final results. To allow to save and reproduce it, a batch processing subsystem is built into EWA.

The batch files contain evaluation commands, together with arguments and options they use, in ASCII text form. EWA allows to produce such files, and is able to execute them. When producing batch files you can either record, step-by-step, your commands you give EWA in interactive mode, or you can make EWA produce a file which contains commands to reach the current state. When executing batch files, EWA reads the content of the batch file, line-by-line, interprets the content and invokes the corresponding commands, passing the needed arguments. While processing batch files, no interactive processing possibility is provided. The batch files can be nested. For details see the *Reference Guide* and the *Tutorial*.

2.2 Windows

The 'Windows' are some rectangular areas on the computer's screen, around of which some decoration (frame, menu, status bar, etc.) is placed. EWA uses some special kind of windows.

2.2.1 The main window

This is a special text-only window. It pops up when the program is started and will be on the screen until exits.

2.2.2 Spectrum windows

The data files (the spectra) can be browsed and processed in specialized spectrum windows. In the EWA program there are two kinds of spectrum windows: for one-dimensional and for two-dimensional distributions. The higher order dimensions cannot be displayed directly, you should derive one- or two-dimensional distributions from them, via making lower-dimension projections.

Several spectrum windows can be open at a time, but only one of them (the top one) can be active. This window contains the active spectrum, which is the target for the evaluation operations. To make some spectrum data active, just select the corresponding spectrum window. It is common in these window types that the window contains also two scrollbars and an internal part (the 'spectrum canvas'), on which the distribution is drawn. The full spectrum is displayed in the spectrum view and it is drawn on some 'virtual canvas', which can be (and usually is) much larger than the canvas piece shown in the window. Using the scrollbars, you can change the position of the visible canvas on the virtual canvas. When the size of the virtual and visible canvas coincides in some direction, the corresponding scrollbar disappears.

At the top of the window, one line is reserved for the 'window title', below that a one-line 'heading box' is visible. In the middle of the window title, the spectrum file name with full path name is shown in angle brackets. On the left and right side of the file name some other items are displayed, for details see the specialized spectrum windows below.

In the heading box various information is displayed. In its right corner the mouse cursor position is displayed, when the mouse is inside the spectrum view. For details see also the specialized spectrum windows below.

2.2.2.1 Window for 1-dimensional distributions

A typical one-dimensional distribution (measured pulse count in function of energy) is shown on \ref{spwindow1}. Now the spectrum view contains one graph only, namely the measured data. Usually the view contains two more graphs: the corresponding fitted data (the synthetic spectrum envelope) is also shown and the corresponding spectrum component (the ID of which is shown in the window title) is also displayed.

Above the spectrum view one more view, the '*residuals view*' can be seen, if the fitted envelope contains at least one component. It shows the local residuals, see chapter '*Evaluating with EWA*'. The horizontal scale of this residuals view coincides with that in the spectrum view. Since in normal case 99.5% of the local residuals located in the range $[-3\sigma, +3\sigma]$, its vertical scale is fixed to the range $[-4\sigma, +4\sigma]$. The middle line represents the 0 value and the two other lines the -2σ and $+2\sigma$ level, respectively. On the left of this, a separate window shows the distribution of this local residuals, to compare with the theoretical normal distribution.

On the bottom part of the window, a '*status bar*' is shown. Depending on whether the cursor is within the sensitive area, the rightmost two cells are used to show the vertical and the horizontal coordinates of the point over which the cursor stays, or two numbers (the first-order autocorrelation and the χ_n^2 , characterizing the goodness of the fit).

2.2.2.2 Window for XPS spectra

The window for XPS spectra differs from the other one-dimensional spectra only in the form as the energy values are displayed. Namely, the data can be displayed either on binding or kinetic energy scale. In the case of XPS spectra (when the energy of the excitation source is also known), the two energy values can be computed from each other and can be displayed simultaneously. The energy values are appended by the letter 'B' for binding and by 'K' for kinetic energy values, respectively. One of them (the value on the primary scale) is displayed anyhow. The other value (the value on the secondary scale) will only be displayed if this feature is enabled. By default, both energy values are shown.

2.2.2.3 Window for 2-dimensional distributions

(not yet re-implemented) The two-dimensional distributions (measured pulse count in function of the two independent coordinates, like a measurement with a position sensitive detector) is shown on Fig \ref{spwindow2}. The different colors mean different intensity ranges, as shown on the color map at the right side of the canvas.

2.2.3 Component windows

No additional windows are reserved for the spectrum components. Instead, the spectrum window is used to display all components, one at a time. Immediately before the file name, the window title contains a number which gives the ID of the component which is presently seen in the window. On the right side of the file name, the component type identifier is displayed. The spectrum view contains three graphs: the measurement data, the corresponding synthetic envelope and the current component. Note that for peak components the intensity is shifted so that they appear at the bottom of the view.

In the component windows the merit of goodness is a little bit different. In calculating χ_n^2 the number of the data points m is the number of the points seen in that window and the number of the free parameters p is the total number of the free parameters of that component. Because of this, the value shown can be different for the different components, even without any change in the fitting envelope.

Initially, the program creates a virtual ‘component’, which has no parameters, cannot be deleted or filled with a real component, it serves just to show the spectrum. It is the ‘root window’, which has special meaning when certain commands are invoked. This window also contains the graphs of the measured and synthetic data, as well as it displays the graph of all components when the corresponding flag ‘COMPONENT|DISPLAY|ALL COMPONENTS’) is set.

2.3 Parameters

The parameters are of central importance in EWA, so this separate section deals with their interpretation and handling.

2.3.1 Parameter attributes

The parameter in EWA means not only just a ‘value’ but also some other attributes, including the display format, as shown in Table 2.1 All parameters, all attributes are pre-set for you with some default value. *Please make sure you understand what you are doing when changing them!*

The spectrum components (like peaks, backgrounds, etc.) are described by several parameters which should be handled as a group of interrelated parameters. For example, the peak energy, intensity and width altogether describe the simplest peak line shapes.

2.3.2 Linking parameters

Although by default the parameter values are considered to be completely independent of each other, sometimes you can know certain relation between some of them and you might want to realize this kind of constraints with EWA. Using ‘parameter linking’ (‘COMPONENT LINK PARAMETER’) you can feed this information into the evaluation process, thus enforcing the program to calculate according to the external information. The

Table 2.1: Parameter attributes in EWA

Parameter attribute	Description
Name	the parameters have a unique name
Lower Limit	below this limit the parameter value is illegal
Value	this is the 'parameter' in conventional sense
Upper Limit	above this limit the parameter value is illegal
Uncertainty	expected/estimated uncertainty
Differentiation base	used in calculating numerical derivatives
Digits	the total field width of the format the 'value' is displayed in
Decimals	the number of digits behind the decimal point

parameter linking in EWA means that the value of one of the linked parameters can only be calculated using the value of the other, and is done on a 'master-slave' basis. The value of the 'slave' parameter follows unconditionally the value of the 'master' parameter, but the master parameter will change its value freely and independently. Of course, a slave can only follow one master, but a master can control any number of slaves. Beside the pointer to its master, the slave parameter has also a '*link mode*' information which tells how to calculate its own parameter value from the value of its master. EWA provides three link modes.

Replace mode: the value of the master simple replaces the value of the slave. On linking, the parameter value might (and usually will) change. Of course, changing the (replaced) slave parameter will not change the (replacing) master parameter.

Add mode: the value of the master parameter is added to the value of the slave. On linking, the corresponding difference is calculated for the slave's own value, so linking two parameters will not change the (resulting) value. Changing the slave's value will change the slave's own value (i.e. the difference to its master).

Multiply mode: the value of the master parameter will be multiplied by the value of the slave parameter. On linking, the corresponding ratio is calculated for the slave's value, so linking two parameters will not change the (resulting) value.

Changing the slave's value will change the slave's own value (i.e. the ratio to its master). As you see, after linking the relative value replaces the slave's own value, and there is no

way to calculate the real value without the master's value. Also worth to note that linking affects only the *value* attribute of the parameter, the other attributes can (and should be) set independently. Especially, fixing the value attribute means fixing the relative value. Although possible, both values (master and slave) can be fixed simultaneously or be free simultaneously, but in such case the linking is of no use. This is the reason why EWA fixes the relative value when the linking is established.

2.3.3 Adjusting parameters

When you need to change any of the attributes of any of the parameters, a 'Parameter adjust' dialog comes up, see the Fig \ref{ParAdjust}. At the beginning of the adjust process, the program saves the initial settings of the adjusted object and replaces only in the case if you (before exiting) accept the new settings, i.e. you are effectively adjusting a *copy* of the original parameter set.

The dialog contains two listboxes: the 'PARAMETERS' which contains the name of all parameters in the group while 'ATTRIBUTES' contains the list of attributes mentioned above. One element in both listboxes (initially the first parameter and its 'value' attribute) is always selected. To select another element, just handle the listboxes. The numerical value of the selected attribute of the selected parameter is displayed in an input box above the listboxes, between the corresponding extreme values between which it can be changed.

The value can be set via editing the corresponding text. To do it, just select the input box under the scrollbar. The preset text will contain the current value of the current attribute and you can edit it. You can terminate the editing via typing 'ENTER'. Alternatively, you can use 'ESC' to exit, but in that case the editing you did in the input box will be lost.

There are two checkboxes in the dialog box: the 'FIXED' checkbox displays and allows to set the fixing of the attribute. When this checkbox is checked, you cannot change anyhow the attribute, like on Fig \ref{ParAdjust}. To announce this fact visually, the program disables the input box. Note that *fixing/unfixing a parameter is completely the user's responsibility. Be especially careful when unfixing attributes other than 'value'. Allowing the parameter to take illegal values might crash the program!*

The other checkbox 'Linked' allows to see (only the value attribute and only of the slave parameter) a linked parameter either as unlinked (conventional) parameter value or as linked value, i.e. the relative value to the master parameter value. *This checkbox controls only the display format in this dialog, to link/unlink parameters use 'COMP EVALUATE LINK'.*

The dialog contains also some buttons. The 'OK' button allows to terminate the adjusting normally, i.e. accepting the attributes set during adjusting and continuing command execution. In contrast, button 'CANCEL' restores the saved attributes and aborts processing of the command.

The next two buttons give you again a 'safety net' comfort during adjusting. Sometimes

you go in some wrong direction during adjusting, or just want to try a 'maybe better' case and you fail: in such a case, just press 'RESTORE' and you will be back at the previously 'SAVE'd attributes of the selected parameter. Note that *the 'Save' command overwrites the previously saved value, there is no way to restore the initial value. Even when pressing 'Cancel', the saved (rather than the initial) attribute set will be restored, so handle the command with care.*

Since adjusting is usually invoked from some other command, you might want to see the result with the given settings. In such a case just press 'APPLY'. The adjust dialog will refresh the screen with the current parameter settings and then the adjust dialog re-appears. If the calling command does not want to use this service, the button does not appear.

Chapter 3

Evaluation terms

The present chapter gives some practical advices for the users who are not very well acquainted with EWA and gives some tips even for the profis. For some elementary hints/exercises, see the tutorial part of this guide.

3.1 The principle of the spectrum evaluation

The data called 'spectrum' is a one dimensional distribution (for evaluating two-dimensional data, see a later chapter), sampled as a set of n discrete points, which is given as an n -element vector. The elements of this vector are described by the independent variable (usually energy) where the given sample element was recorded and the measured value (usually counts), that is at the i th point by the coordinates E_i and C_i . Usually an (estimation of the) uncertainty σ_i is also used to describe the point. In practice, the independent variable is a linear function of the sequence number i , so the independent variable can be characterized either by i or E_i .

In practice, these distributions are a superposition of some more elemental distributions (called afterwards components). The task 'to evaluate spectra' is to determine which components are present in the spectrum and what are their quantitative characteristics. In non-routine evaluation the qualitative description can also be problematic, while the routine evaluation requires to determine of the parameters of the components already identified. The EWA program solves the first part of the problem via modelling, i.e. it synthesizes a spectrum which contains the supposed components. A spectrum component is described by a set of parameters

$$C_{j,i} = C_{j,i}(\bar{p})$$

and the spectrum is simply the sum of these components:

$$S_i = \sum_{j=1}^n C_{j,i}$$

where $C_{j,i}$ is the contribution due to the i -th component (out of n) at the i th point. (The parameters can be fixed, moved together, etc., see the previous chapter.) This approach results in an extremely flexible spectrum model.

In the EWA system the quantity

$$r_i = \frac{M_i - S_i}{\sigma_i}$$

(the local normalized residual) describes the similarity of the measured M_i and synthesized S_i data at the i th point (σ_i is the uncertainty of the measured data item). For the series of points analyzed, these values are displayed to show some local trends in the data. This characteristic is a completely differential one. On the other hand, a completely integral characteristic -the normalized (or reduced) chisquare [BPR69]- can be derived :

$$\chi_n^2 = \frac{1}{m - p} \sum_{i=1}^m r_i^2$$

which is practically some kind of average of the local normalized residuals r_i (here m is the number of the spectrum data points considered, p the number of the active parameters). The less is χ_n^2 , the better is the agreement between M and S .

3.2 Practice of the spectrum evaluation

The traditional spectrum evaluation approach can be opposed with the flexible way as EWA approaches to the spectrum evaluation problem can be put in analogy with writing information in a nice bond book, using its rigid structure, margins, with no possibility to tear out sheets or add new sheets, opposed with using a (maybe less nice) cartoon file which allows to add some more sheets, of different shape and origin, to rearrange or remove them, etc. The sheets correspond to the spectrum components and their sum (the synthesized spectrum) to the flexible file.

The spectrum components can be built into the synthetic spectrum one-by-one, for details see 'COMPONENT CHANGE' commands. For setting the initial parameters of such components the program has some 'lazy' algorithms which -in simple cases- provide completely satisfactory results; for details see the corresponding chapters about the different components. The user can, however, change the parameters of the components created by the program manually or can use the built-in optimization routine. To do so, the program provides graphical (the normalized residuals, as well as the measured and synthesized spectrum) and numerical (χ_n^2 , autocorrelation) information, see below, about the similarity of the measured and synthesized spectrum.

In the second step -when the model is correct, i.e. the measured and synthesized spectrum contains the same components- the program determines the 'best' set of parameters describing the synthesized spectrum. In this work (called 'fitting') a built-in mathematical

minimization procedure is used. The user can return at any point to the model improvement until succeeds. From the user's point of view, this is just the automatization of the manual parameter improvement.

3.3 Operating modes

The operating mode changes the programs behavior when doing some operations.

3.3.1 Normal (or single) mode

This is the mode the program uses by default (or when you select 'OPTIONS EVALUATE EVALMODE NORMAL') and most users work in. All other parts of the *User's Guide* refer to this mode. In the description of the other modes it is only given where and how the execution *deviates* from that described in the manuals.

In normal mode all spectra are self-contained, i.e. there is no way to find out in the active spectrum, what is present in some another spectrum. In certain situations, however, a need arises to feed some parameters in the evaluation into the evaluation of some other spectrum. In order to meet these special needs, some other modes **arebe** implemented.

3.3.2 Cross spectrum mode

(not yet re-implemented) A special way of operation can be set using 'OPTIONS EVALUATE EVALMODE CROSSSPECTRUM'. When this mode selected, it makes possible to account some relations between the spectra, beeing simultaneously in the memory. The operation will differ in the following points from that described in the manuals.

1. When making parameter linking in this mode, is is possible to select the master component from a spectrum, different from the active spectrum, but beeing in the memory at the time of linking.
2. \

Part II

Reference Guide

Chapter 4

Batch

The EWA program provides also advanced features for batch (called also macro) processing. The commands in this group enable the user to document the evaluation, to execute evaluation of series of similar spectra, etc. It is worth to store the repetitive, short processes in short disk files and to instruct the program several times to execute that process. Using the program you can create batch files and also execute them. For details on how to use the batch files, see the user's guide.

Note: Although these files can be edited, be extremely careful when editing. When executing batch files, there is no way to correct mistypes, etc.: all errors are fatal and abort batch file processing. The item names are case sensitive, i.e. the lower case and upper case letters cannot be interchanged.

4.1 Append

Similar to 'BATCH NEW', but the commands are appended to the former content of the file, rather than replacing it. If the selected file does not exist at the time of opening, its effect is identical with 'BATCH NEW'.

4.2 Close

Finishes writing the executed commands into a file. It simply closes the file and the file will be ready for use for evaluation. Note that the file will be saved after exiting, even if you do not 'BATCH CLOSE' it explicitly.

4.3 Execute

Allows the user to select the file which contains the commands to be executed. When invoked, a file dialog box appears and the user is expected to select the name of the file containing the commands to be executed. The default file extension is '.LRN'. There is no need to specially mark the end of a command file; when the end of the command

file reached, the program returns to the place where it was instructed to execute the commands stored in that file. That place can also be somewhere in another command file, i.e. the command files can be nested. Although the program does not limit explicitly the nesting depth, implicitly the resources of the computer (the max. number of files that can be open simultaneously and the available memory) surely do so. Set that parameter properly when setting up your system, taking into consideration the different files which can be opened simultaneously either temporarily or permanently.

4.4 New

Allows to create a new file in which the commands you type will be saved. When invoked, a file dialog appears and the user is expected to type in the name of the batch file to create. If the file does not exist, a new file is created. If the file exists already, the file will be destroyed and its content will be replaced (compare to 'BATCH APPEND').

Of course, in batch mode you cannot append. Once the batch file is open, the program will write a copy of the commands you instruct it to execute into the opened file, until you 'BATCH CLOSE' this action. The commands are written up in textual form, i.e. the command names are taken from the menus and the full menu path used to reach the given command is recorded, separated with a '|'. Sometimes the commands also take parameters. These can be numbers, strings or other structures, depending on the command. For their description see the command in question.

Note: Only the commands invoked through the menu system (as opposed with typing hotkeys and clicking icons) generate writing to the file.

Note: EWA itself also makes batch files, either during fitting ('SPECTRUM EVALUATE FIT') or when explicitly asked ('SPECTRUM SAVE PARAMETERS')

4.5 Remark

The self-documenting feature of the program required this command.

- ▷ When *preparing a batch file*, it asks for a (max. 255 character long) string in an input dialog box. The string will be written in the batch command file, as the argument of the command.
- ▷ When *executing a batch file*, this text will be displayed on the screen. These features can be used in several ways.

Its typical usages:

- ▷ The program itself documents the data changing operations (corrections, smoothing, arithmetic operations, etc.) in this way. Due to this, the data spectrum has its 'history' together with the spectral data.

- ▷ The user can also comment the operations, add remarks, etc., i.e. (s)he can use the program and the batch command file as a notebook. On the other side, when executing batch files, these comments are displayed on the screen, so the state shown in the graphics windows can be commented.
- ▷ Allows to make 'demo' programs for the beginners and to illustrate the advanced features for the advanced users.

Chapter 5

Component

The commands in this group deal with the spectrum components, so it is probable the most important (but surely the most extensive) chapter of the *Reference Guide*. Of course, you can deal only with the component of some spectrum, so these commands appear only on the menubar of a spectrum window.

5.1 Advance

On the screen, only one window is accompanied with each spectrum. In that window you can see only one component (the selected/active one), so to move between the components, you can use this command group. The components are implemented as a list, so in this sense, there exists first(also called *root*) and last component as well as each component has previous and next neighbours.

5.1.1 Last

This command makes the last component (the one at the end of this chained list) the active component.

5.1.2 Next

This command turns the component, standing before the currently active component, into the active component.

Note: Only for this command the component list is circular, i.e. when the current component is the last one, the first one will be selected.

5.1.3 Previous

This command turns the component, standing before the currently active component, into the active component.

Note: *Only for this command the component list is circular, i.e. when the current component is the first one, the last one will be selected.*

5.1.4 Root

This command turns the very first component (the root, ID 0) into the active component.

5.1.5 Select

Allows to select any component in the list . When invoked, a selection box appears with the ID and the label of the available components. The components are ordered as they are inserted into the list of components. The active component will be highlighted. You can choose any of the components shown in the box. The chosen item will be the active one.

Note: *sometimes the order of the components is important. For details see the User's Guide*

5.2 Change

Causes some change in the collection of components, belonging to the currently active spectrum.

5.2.1 Adjust

The command can only be used when the active window is not empty, i.e. it contains some component, which has adjustable parameters. When invoked, a parameter adjust dialog pops up with the parameters of the object in the window, and allows to change any attributes of the corresponding parameters. When the APPLY button pressed, the fitted spectrum is updated with the active component using the current parameters and the display is updated. For more details see section *Adjusting parameters* in the *User's Guide*.

5.2.2 Background

Generates a background in the active window if it contains no component (i.e. it turns an empty component into a background). Because of its special importance and because the available background types are also listed there, Chapter 6 (Component Background) is devoted to this command.

5.2.3 Delete

If you do not need a component (either empty or not), you can delete it with this command. If the window contains some component, the corresponding component will be subtracted

from the fitted data and the component entirely deleted. Of course, the occupied memory will be freed and the measured data will not be changed.

5.2.4 Label

The component also has an identifier string, `itslabel`. Some unique identifying string is given to the components when they are created, but these names are not very descriptive ones. Usually you want to change it to something, which describes the transition, the chemical state, etc. This command allows to do so. Presently, no upper/lower index, greek letters, etc. can be used.

5.2.5 Multiline

Generates a multiline structure in the active window if it contains no component (i.e. it turns an empty component into a multiline). Because of its special importance and because the available multiline types are also listed there, Chapter 7 (Component Multiline) is devoted to this command.

5.2.6 New

Before making anything with a component, you need to create space for it. The only exception is the root component which is created and maintained by the program and the user can just browse but not to manipulate it at all. The command creates space for a new spectrum component to be added later to the current synthetic spectrum. The sequence number (ID) of the newly created component store (window) will be the next available one, while the component itself will be added to the chain of the components *after* the current component. The new (empty) component will be the active one and its settings will be the same as those of the root window.

It is necessary to create 'NEW' place for a component, but it is not necessary to fill the empty component store with a real component. These windows (with no object) can be used for example to browse some part of the spectrum, to compute some 'raw data' parameters, but do not have any effect on the evaluation. The number of the component stores is not limited. The evaluation work usually is not affected by the order of the creation of the components, but there are exceptions. Sometimes the result of the operation will depend on the components already present in the spectrum, see for example presetting the component parameters. In this case the presence of the component(s) has some physical meaning and so needs special attention. In addition, some operations can be carried out more easily if some other components are/aren't present already in the spectrum. Another important exception is when you use efficiency-type component(s). For more details, see the *User's Guide*.

5.2.7 Peak

Generates a peak in the active window if it contains no component (i.e. it turns an empty component into a peak), or, might also turn a peak into another type of peak. Because of its special importance and because the available peak types are also listed there, Chapter 8 (Component Peak) is devoted to this command.

5.2.8 Subtract

This command allows to make 'spectrum stripping', i.e. to remove certain components from the measured data. When invoked, it subtracts the component in the active window from the *measured data* and executes command 'COMPONENT CHANGE DELETE', i.e. subtracts the active component both from the measured and fitted data and removes the component.

5.3 Display

Contains display-related commands, i.e. they have only effect on the appearance of the components, rather than on the evaluation features.

5.3.1 All components

In the root window EWA can display all components, the logical state of which is set properly by this command. The current logical state of the active component is shown in the menu bar: a checkmark is prepended to the command menu name, if it is 'ON', nothing is shown if it is 'OFF'. The state flag has any effect only when the root component is active. The state flag of the root component determines if *any* component is displayed in the root window. The state flag of the non-root components determines *which* components are displayed in the root window if the corresponding flag of the root component is set. All components have such a state information, but it is interpreted differently in the case of the root component and the other components. Component-wide scope.

Root component: enables/disables showing *any of the components* in the root window. Initially it is set to 'ON'.

Non-root components: enables/disables showing *the current component* when the root component is active. Initially, the state of the root component is cloned for the contributing, 'OFF' is set for the non-contributing components.

Note: *The flag has also effect on saving components, see 'SPECTRUM SAVE COMPONENTS'*

5.3.2 Marker

Although you can simple drag the markers to the place you want (see *Using mouse and cursor* in the *User's Guide*), using the present command you can also set the marker values in a dialog box. In the dialog box you can see two (for 1-dimensional spectra) or four (for 2- dimensional spectra) scrollbars and input boxes, and a radio button selects if you want to see (and set) the marker's sequence number or the corresponding energy value.

5.3.3 Text mode

The component windows have two basic appearance forms: the (default) graphic form and the alphanumeric form. In the later one the numeric value of the parameters, describing the component, are shown rather than the corresponding graph. Although it is obvious, the current logical state of the active component is shown in the menu bar: a checkmark is prepended to the command menu name, it if is 'ON', nothing is shown if it is 'OFF'. Initially it is set to 'OFF'. Component-wide scope.

5.4 Link

The commands int this group make the individual components interrelated.

5.4.1 Parameters

Not yet implemented

5.4.2 Multiline

Allows to link a peak type component to a multiline type pseudo-component. When invoked, a select box with the multiline type components, created formerly for the active spectrum, appears. The selected multiline component will be linked to the peak, i.e. this main peak will appear in multiple copies in the spectrum, as described by the selected multiline structure. For details see Chapter 7.

Chapter 6

Component Background

When setting up the initial parameters of the background, EWA uses the position of the component window endpoints and the marker positions as follows, so you can set the *initial values* properly via selecting the positions mentioned accordingly. If you do not, EWA uses the default settings. The generated background (independently of how many points are shown in the active window) is valid for all points of the spectrum.

The region between the left boundary of the active window and the left marker as well as that between the right marker and the right boundary, respectively, are supposed to be 'background-only' regions (the 'net intensity' is used). That means, that the program uses these regions to determine the initial values of the background parameters.

When selecting this command, a background type selection box pops up and you can select the background type you want. When you click 'OK', in a second dialog box you can pinpoint your selection via selecting the needed terms and features, see at the individual background components. After generating the background (presetting the parameters), in the upper information line the component type identifier changes correspondingly. Following that, you can change the pre-set parameters of the background using 'COMPONENT CHANGE ADJUST'

6.1 ArcTan

When the you select the ArcTan-type background, a term selection dialog box pops up, enabling you to select the terms which you wish to include as a parameter. The upper 3 checkboxes are always checked, because they cannot be left out. The lower checkbox, however, is of your choice: the program proposes to use constant background.

When you press 'OK', the program generates an arctan-like background. The exact form of the background at energy E_i is

$$Bg(E_i) = C_0 + Y_0 * \left(\frac{\pi}{2} + \arctan\left(\frac{E_i - E_0}{W_0}\right) \right) * \frac{2}{\pi}$$

where E_0 is some characteristic energy, Y_0 is some characteristic background height, W_0 is some characteristic width, C_0 is some arbitrary constant background level. The

Table 6.1: Default values for the COMPONENT CHANGE BACKGROUND ARCTAN command

Param	Remarks	Low limit	Initial value	High limit	Step size
E_0		E_{left}	$0.5(E_{right} + E_{left})$	E_{right}	$0.05(E_{right} + E_{left})$
Y_0		$Y_0 - 10dY$	$0.5(Y_{high} - Y_{low})$	$Y_0 + 10dY$	$0.05(Y_{high} - Y_{low})$
W_0		$W_0/5$	$0.5(E_{right} - E_{left})$	$W_0 * 5$	$0.05(E_{right} - E_{left})$
C_0	Optional	$C_0 - 10dY$	Y_{low}	$C_0 + 10dY$	$0.01C_0$

inclusion of the (optional) latter term allows this component to represent the background in simple spectra alone, i.e. without using any other background component.

The initial values of these parameters are calculated as follows. The average counts between the left limit and the left marker, as well as between the right marker and the right limit are calculated. The lower of these averages results in C_0 , their (positive) difference in Y_0 . The average of the marker positions sets E_0 and their half distance sets W_0 .

Note: Both arc tan and arc cotg type backgrounds are allowed. The type is selected automatically by the relation of the background heights on the low and high intensity side. For these two background types the sign of the characteristic width is different.

6.2 Polynomial

This command generates a (max) 3rd order polynomial type background in the active window. In the case of polynomial-like backgrounds sometimes it is advantageous to relate the energy to a value E_0 other than to the rather abstract 0 value, as well as to transform either the independent or the dependent variable. The implementation EWA uses allows to do both, independently. Since the individual terms can be calculated independently of each other, you can decide which terms of the background expression to use. Reducing the number of terms you can reduce the computing time, too. To select the needed terms, a dialog box appears. EWA suggests to use the energy transformation as well as the constant and 1st-order term, i.e. a linear background.

The full equation is

$$TrC(Bg(E_i)) = C_{-1} \cdot E_i^{-1} + C_0 + C_1 \cdot E_i^1 + C_2 \cdot E_i^2 + C_3 \cdot E_i^3$$

where $E_i = TrE(E' - E_0)$. E' is the measured energy, E_0 is given as an adjustable/fitable parameter, $TrE()$ represents the transformation of the independent (energy) scale and $TrC()$ represents the transformation of the dependent (counts) scale. When the E_0 paramer is in use, the program 'shifts' the energy scale to the middle of the region analyzed, i.e. $Bg(E_0)$ gives the background height at energy E_0 . The possible transformations are also shown on the term selection dialog.

Table 6.2: Default values for the COMPONENT CHANGE BACKGROUND POLYNOM command

Param	Remarks	Low limit	Initial value	High limit	Step size
E_0	Optional, fixed	E_{left}	$0.5(E_{right} + E_{left})$	E_{right}	$0.05(E_{right} + E_{left})$
C_{-1}	Optional	$-100s_1$	0	$+100s_1$	s_1
C_0	Optional	$-100s_1$	C_0	$+100s_1$	s_1
C_1	Optional	$-100s_1$	0	$+100s_1$	s_1
C_2	Optional	$-100s_1$	0	$+100s_1$	s_1
C_3	Optional	$-100s_1$	0	$+100s_1$	s_1

In the case of polynomial-like backgrounds in order to estimate the initial values of the polynomial coefficients C_0 and C_1 and their uncertainties s_0 and s_1 , the program makes a non-iterative fit to the points between the leftmost point and the left marker, as well as to those between the right marker and the rightmost point. (Due to the noise in the measured data, the higher order coefficients C_2 and C_3 cannot be estimated safely.)

Note: This procedure estimates the uncertainty of these parameters, too. In the case of too few points (the markers have not been moved from their extreme position, so the 'fit' has been done on two points only), the estimated uncertainty would be 0. In such a case the program uses 0.01 times the corresponding parameter value instead.

6.3 Shirley

When the you select the Shirley-type background, EWA generates a background due to the inelastically scattered electrons in the spectrum via method of Shirley [SD-72] as proposed by Proctor and Sherwood ([PS-82]; [BS-83], Appendix 1). Although the method in its original form is a two-parameter method for background *removal*, EWA implements it as multi-parameter *fitable* background component. (To use the original Shirley background removal, just create this Shirley background component, with the default initial values, then use 'COMPONENT SUBTRACT'.)

When invoking the command, a term selection dialog box pops up, enabling you to select the terms which you wish to include as a parameter. The upper 3 checkboxes are always checked, because they cannot be left out. The lower 3 checkboxes, however, are of your choice: the program proposes to use constant background, no iteration and no energy gap. The additional parameters give you more flexibility as follows.

The first two parameters are the originally proposed ones: E_L ('Low limit') and E_H ('High limit') represent the energy values between which the background is calculated according to Shirley. Below and above these limits, respectively, the background is considered to be constant, namely C and $C + D$, on the high and low kinetic energy side, respectively. Note that although formally the two limits are 'parameters' and so their value can be adjusted, it is quite unusual to fit them (better to keep fixed).

Table 6.3: Default values for the COMPONENT CHANGE BACKGROUND SHIRLEY command

Param	Remarks	Low limit	Initial value	High limit	Step size
E_L	Fixed	E_{low}	E_{left}	E_{high}	$E_{stepsize}$
E_R	Fixed	E_{low}	E_{right}	E_{right}	$E_{stepsize}$
D		0	D_0	$10D_0$	$0.01D_0$
C	Optional	$C_0 - 10D_0$	C_0	$C_0 + 10D_0$	$0.01D_0$
I	Optional, integer, fix	1	1	5	1
G	Optional	0	1	10	0.1

The D ('Difference') is the increase in the background level due to inelastic scattering. Originally, this value was calculated as the difference of the background levels, averaged for the points outside the limits E_L and E_H , respectively. In EWA, the initial value D_0 is calculated in this way, too.

Since usually the measured data rather than the background-subtracted data are evaluated, it is very useful to add the parameter C ('Const Bg'), which represents a constant background level, caused by effects other than the inelastic scattering in question. The inclusion of this term allows this component to represent the background in simple spectra alone, i.e. without using any other background component. Its initial value C_0 is calculated as the average level for points above E_H . The C_0 parameter is optional.

The algorithm can even be iterated if the level difference due to scattering is significant. This possibility is provided through the parameter I ('IterCount'). The iteration is finished if either this iteration count is exceeded or the background converged. The I parameter is optional.

Also an important extension is the G ('Energy Gap') parameter, which accounts for the fact that under some minimal energy loss (rather than zero) no inelastic scattering is possible. The parameter is implemented as it was proposed by Bishop [BH-81]. The actual value of the gap (which is interpreted in [eV]) will be rounded to the nearest multiple of the energy step size. The parameter G is optional.

Note: Since the electrons can only be scattered towards lower (kinetic) energies, the lower-energy background level must be of higher intensity than that at the high-energy level. If this condition is not fulfilled, the initial value of D_0 will be set to 0.

Note: The spectrum data might be either on kinetic or binding energy scale, EWA handles the inelastically scattered background correctly.

Chapter 7

Component Multiline

This command group allows to reduce the complexity of the spectrum model and/or the number of parameters in fit via introducing well established relationship between some peaks in your spectrum. When selecting this command, a multiline type selection box pops up and you can select the multiline type you want.

When setting up the initial parameters of the multiline structure, sometimes EWA uses the position of the markers, as described at the individual multiline types. When you click 'OK', in a second dialog box you might pinpoint your selection via selecting the needed terms and features, see at the individual multiline components. After generating the multiline template (presetting the parameters), in the upper information line the component type identifier changes correspondingly. Following that, you can change the pre-set parameters of the background using 'COMPONENT CHANGE ADJUST'.

Note: Multilines are non-contributing (pseudo) components, i.e have no direct effect on the evaluation, until you use them in a 'COMPONENT LINK MULTILINE' command.

Note: The intensity and position of the multilines are only slightly related to the intensity and energy scale on which they are shown within a component window; only some symbolic lines are displayed.

7.1 X-satellites

In a significant part of the XPS spectrometers, the X-ray source is *not* monochromatised. As a consequence, all characteristic energies belonging to the source material will excite separated peaks in the resulting XPS spectrum.

The X-ray satellites listed are built in with characteristic like line position (for the main line the absolute, the others the relative position), intensity and width. The selectable X-ray excitation source structures are listed in tables 7.1-7.3. This kind of multilines are implemented as $3N$ parameter objects, where N is the number of the satellite lines, as shown in the corresponding table. All these parameters are fixed by default.

Table 7.1: The built-in Al K_α [KC-93] and [SDM94] structure

Designation	Energy [eV]	Intensity, rel	Width [eV]
α_1	0	1	0.58
α_2	-0.413	0.5	0.58
α'	+5.452	0.01928	1.3366
α_3	+9.526	0.07774	0.6922
α_3'	+9.958	0.02373	0.6623
α_4	+11.71	0.06139	1.1557

Table 7.2: The built-in Mg K_α [KC-93] and [SDM94] structure

Designation	Energy [eV]	Intensity, rel	Width [eV]
α_1	0	1	0.541
α_2	-0.251	0.5	0.541
α'	+4.74	0.02099	1.1056
α_3	+8.210	0.07868	0.6264
α_3'	+8.487	0.04712	0.7349
α_4	+10.095	0.09071	1.0007

Table 7.3: The built-in He I structure [DKS80]

Designation	Energy [eV]	Intensity, rel	Width [eV]
A	0	1	0.1
B	+1.869	0.02	0.1
C	+2.524	0.002	0.1

Table 7.4: Default values for the COMPONENT CHANGE MULTILINE VIBRATION/LINEAR command

Param	Remarks	Low limit	Initial value	High limit	Step size
dE_0		$dE/2$	$E_{Right} - E_{Left}$	$dE * 2$	$dE/20$
S		0.05	C_{Right}/C_{Left}	0.95	$Y_0/50$
N	integer	2	$N, ?4?$	$2 * N$	1

7.2 Vibration

This type of components allows to handle structures where both the distance and the energy of the multiplet lines vary in a regular way, described by a few parameters.

7.2.1 Linear

This kind of vibration is described by 3 parameters. The number of the lines (multiplicity) N , the damping factor S and the energy distance dE . The lines are equidistant, so the energy (relative to the main peak) of the i th line is given as

$$E_i = i * dE$$

The intensity of the i th line is

$$Y_i = \frac{S^i}{i!}$$

Of course, $i = 0, 1, \dots, N - 1$.

Chapter 8

Component Peak

The command either generates a peak in the active window (if it contains no component) or changes the type of the peak (if the current component is a peak). The generated peak (independently of the size of the active window, i.e. how many points can be seen in the spectrum) will be calculated only at the energies where its contribution is significant, i.e. higher than one tenth of the lowest difference in consecutive channels. After generating the peak (presetting the parameters), its parameters are saved, in the upper information line the component type identifier changes correspondingly. Following that, you can change the pre-set parameters of the peak using 'COMPONENT CHANGE ADJUST'.

When selecting this command, a peak type selection box pops up and you can select the peak type you want. When you click 'OK', in a second dialog box you can pinpoint your selection via selecting the needed terms and features, see at the individual peak components. Since the program allows to select from several peak types and these peak types are more or less independent of the program (they are supplied as elements of some list), they are described in the separated chapter 'COMPONENT PEAK'.

The peak-like components have at least three parameters. Their common meaning (as well as the initial value given to them) is the same for all peak shapes and will be described in the followings. Some peaks have further parameters; their values and interpretation will be given there. In order to generate initial values for the first three peak parameters, the program uses the settings in the active window and uses the net intensity data. The program assumes that the markers have been set previously to the points where the peak half-width is expected (see also the note below).

The 1st parameter gives the *position* (usually energy) of the peak. The program estimates the peak position using various methods for the points between the markers.

The second parameter is its intensity. The program uses the *peak height* or the *peak area* as a primary parameter. Usually the peak area is preferred (it is a more adequate measure of the intensity), but sometimes the peak height is preferred since it can be compared directly to the measured counts. You can decide at generating the peak which representation to use. The peak creation dialog provides a radio box to chose. Some peaks have a height-only representation: in such a case the radiobox cannot be changed to area representation. The initial value of the peak height will be the 'net' maximum

Table 8.1: Default values for the COMPONENT CHANGE PEAK command

Param	Remarks	Low limit	Initial value	High limit	Step size
E_0		$E_0 - W_0$	Calculated position	$E_0 + W$	$W_0/10$
Y_0		$Y_0/5$	Estimated height/area	$Y_0 * 5$	$Y_0/50$
W_0		$W_0/2$	Estimated width	$W_0 * 2$	$W_0/10$
A_0	Optional	-0.99	0	+0.99	0.01

intensity between the markers. Whenever possible, the area is calculated analytically, but in some cases (see the individual peak shapes) the area is calculated via numerical integration, carried out only between the limits of the spectrum root window which *can lead to inadequate results if the peak is truncated due to the (improper) spectrum limits*.

The third parameter is the width. Its initial value will be the difference between the horizontal coordinates of the marked points.

In the case of single or slightly overlapping peaks, the following 'lazy' algorithm can be used. If the markers are in their extreme position (this is the base state after 'COMPONENT CHANGE NEW') the program looks for the maximum net intensity then moves the markers to the points where the net intensity decreases to the half of its maximum, then sets up the initial value of the parameters as described above.

When calculating the initial values of the peak parameters, the program uses the 'net intensity', i.e. it subtracts virtually the already created components.

The symmetric peak shapes can be asymmetrized easily with introducing the function

$$W(E) = W_0 \cdot \begin{cases} (1 - A) & \text{if } E > E_0 \\ (1 + A) & \text{if } E < E_0 \end{cases}$$

which will not change the width and the area, but can be more dynamically used.

8.1 Drude

Generates a peak of form [ACR79]

$$Y_i^{Drude} = Y_0 \frac{W_0 E_i}{(E_0^2 - E_i^2) + (W_0 E_i)^2}$$

(Drude-type function) in the current window.

Table 8.2: Default values for the COMPONENT CHANGE PEAK pVOIGT command

Param	Remarks	Low limit	Initial value	High limit	Step size
η		0	0.5	1	0.05

8.2 Gauss

Generates a peak of form

$$Y_i^{Gauss} = Y_0 \cdot \exp \left(- \left(\frac{E_i - E_0}{W_0 \cdot 0.6005} \right)^2 \right)$$

(Gaussian) in the current window. W_0 can be asymmetric, as given at 'COMP CHANGE PEAK'.

8.3 Lorentz

The command generates a peak of form

$$Y_i^{Lorentz} = Y_0 \cdot \left(1 + \left(\frac{E_i - E_0}{W_0 \cdot 0.5} \right)^2 \right)^{-1}$$

(Lorentzian) in the current window. W_0 can be asymmetric, as given at 'COMP CHANGE PEAK'.

8.4 pVoigt

The command generates a peak of form

$$Y_i^{pVoigt} = (1 - \eta) Y_i^{Lorentz} + \eta Y_i^{Gauss}$$

(pseudo-Voigt) [WBW74] in the current window.

Chapter 9

File

The majority of the commands in this group deals with data files. Some commands, however, do not have much relation to the spectrum files, but they are placed by convention in the FILE group.

9.1 Execute

Using this command you can run commands of the operating system, i.e. the spectrum evaluation program can execute some commands of the operating system. The main difference from the usual shell commands (like 'File Shell') is that the program invokes the operating system for the execution of a single command only and returns immediately. Since the command can be executed from a batch file too, you can program the shell through excuting EWA batch files.

9.2 Exit

The command finishes the work with EWA, saves the necessary information, closes files, etc., i.e. terminate 'orderly' the work and returns to the operating system.

9.3 Spectrum

The commands in this group deal with spectrum files, i.e. with spectral data stored on external devices or their copy stored internally by the program.

9.3.1 Load

The spectral data are stored on some external storage unit in some specific (either ASCII, BCD or binary, etc.) format or some proper mixture of them. The first step of dealing with any of them, is to read them in the program's internal memory. To do so, select this command and then a file dialog appears. You will see all files with the default extension (see OPTIONS GENERAL DATAFILE TYPE). You can walk in the directories, can

change the directories, wildcards, extensions, filenames, drives, and finally you end in selecting one particular file. Pressing 'OPEN', the program tries to find out the format of the file you selected. The program tries one-by-one its known formats, stored in an internal list. When found, it reads in the file in its internal store; otherwise an error message is received.

The directory of the file will be remembered as the user's working directory (i.e. next time you will start file searching from that directory) and

Chapter 10

Help

This command group contains real Help commands, as well as commands placed by convention in the Help menu.

10.1 About

Shows the program's 'business card'.

Chapter 11

Options

EWA sets up all the parameters to some usual, convenient value, for the typical application. Of course, you might need different settings. This command group provides the possibility to change the options of EWA according to your needs. Some of the options affect the active spectrum or component only (they can be found under 'Options' in the individual spectrum windows), some others have effect on all spectra and components or the general program features (they can be found under 'Options' in the main window), the scope of the command is explicitly shown in the description. Depending of the current data, options, etc., some of them can even remain hidden.

11.1 General

This command group contains various, miscellaneous option settings.

11.1.1 Batchfile type

The batch command files usually have some distinct ending, the batch file type ('extension', under DOS). When using the for opening a file, only the data files with some default type are shown in the box. Initially EWA sets it to 'LRN'. This command gives you the way to set it to the type you like. Application-wide scope.

11.1.2 Confirmation level

The one-touch handling provides some chance to mis-press a key, so EWA asks for confirmation sometimes before carrying out the operation. A 3-level selection is available to select when to ask for confirmation:

Level name	When to ask for confirmation
Beginner	Always
Medium	In critical situations
Expert	Never

Using this command you can switch the proper level you like. At the beginning, MEDIUM level is selected. Normally, the beginners level slows down working with the program but sometimes (especially when new to EWA or received a new version of it) it is still necessary. On the other side, using expert level can be dangerous: one mispress can ruin all your work. Anyhow, it is up to you! Application-wide scope.

11.1.3 Datafile type

The data files usually have some distinct ending, the datafile type ('extension' under DOS). When using the file selection dialog for opening a file, only the data files with some default type are shown in the box. Initially EWA sets it to 'DAT'. This command gives you the way to set it to the type you like. Application-wide scope.

Chapter 12

Spectrum

The spectrum-related operations.

12.1 Close

Closes the active spectrum window. All components will be lost!

12.2 Load

Same as 'File Spectrum Load'.

12.3 Dataset

Some spectra contain more than one set of data (i.e. more than one count value is measured at the same energy). These commands allow to manipulate these datasets.

12.3.1 Select

Allows to activate some other dataset. When invoked, a listbox with the available datasets appears. The selected dataset becomes active immediately. After loading a spectrum, the very first available dataset is active.

12.4 Evaluate

Contains comands relating the spectrum evaluation.

12.4.1 Fit

When you created the model spectrum you need (i.e. set the needed options and created all necessary components, adjusted, fixed and linked their parameters, etc.) you can instruct the program to fit the model spectrum to the experimental data. This is done

via optimizing the parameter values of the corresponding components. For the details of the mathematical procedures, see the *User's Guide*. When the fitting starts, a 'Fit dialog' pops up, showing some important parameters of the fitting procedure.

The title bar of this dialog shows the current state of the fitting: either minimizing or estimating the errors of the parameters. The listbox at the top of the dialog shows the current messages: some state information as well as the detected errors are displayed here. Also, some information is displayed at the bottom part of the dialog, like the current value of the χ_n^2 , the parameter and iteration under processing, so you can follow how the minimization proceeds. When you press the 'CANCEL' button, a confirmation dialog pops up if you really wish to abort the fitting (or, when pressed it during error estimation, if you wish to skip the error estimation part).

Apart from the manual aborting, the minimization can also be automatically terminated. Several terminating conditions can be set up at the same time, the first one encountered will terminate the fitting process. You can determine the required relative precision of the parameters ('OPTIONS EVALUATE FITPRECISION', default value is 10^{-4} .) and the maximum number of the iterations ('OPTIONS EVALUATE FITMAXITER'), default value 30). These values -as usual- are pre-set to some proper initial value, but you are free to change them.

The display update also requires time, so EWA tries to minimize it via reducing the number of the screen redraws. The display is only refreshed when the actual iteration number is the exact multiple of the value set by 'OPTIONS EVALUATE FITDISPFREQ', , its default value is 5. With the same frequency are saved the current fitting parameters in the file 'EWAFIT.TMP', in the format described at 'SPECTRUM SAVE PARAMETERS'. The file is ment to store the best values only temporarily, so only the latest parameter values will be stored. It can be used for crash protection or you might simple forget to save the final/intermediate results. If you wish to keep it, just rename them, any time.

The program checks for events (like keypresses or clicks) only when processing of a parameter finishes, so be a bit patient. Note that these events might be also used to ask for services like using menu items, etc. Since the program is not working in multitasking (multithread) mode (it simple interrupts the fitting processing to give the control to some other processing), until you finish the other task, the fitting will not continue.

12.5 Print

This command group contains the printing-related commands

12.5.1 Preview

In a separate frame, you will see how the current spectrum will be put out to the printer.

12.5.2 Print

Makes actually the printing, according to the settings of the operating system.

12.5.3 Setup

Invokes the system's printing setup facility.

12.6 Save

These commands save different evaluation objects in disk files.

12.6.1 Components

Allows to save in a file the fitted envelope as well as the individual components. The individual data are saved only when the corresponding 'Display All components' flag is set, see 'COMPONENT | DISPLAY | ALL COMPONENTS'. The root's flag enables/disables saving the fitted envelope.

12.6.2 Parameters

Allows to save the parameters of the components which the fitted envelope consists of. The format of the file is such that 'BATCH EXECUTE' can execute it. The basic difference is that 'Batch New' records the commands you type (i.e. the *actual path on which the current state was reached*), while the present command creates a batch file which generates *the current state on some optimum path*.

Part III

Tutorial

Chapter 13

First steps

Well, lets make the very first steps together. Here it is only assumed that you have already used some applications on your platform and want to check the evaluation possibilities.

13.1 Installation

Usually, the installation is very much platform-dependent and -typically- simple.

Under Windows, just create a directory where you start the EWA executable from and uncompress the executable file here. Under Unix/Linux, the procedure is essentially similar, but the access limitation can complicate the things. Later, install program/script will help you.

On all platforms, the directory where the executable/binary file can be found (the program directory), as well as where the spectrum data are (the data directory), play a special role. So do also some subdirectories of the mentioned directories.

13.2 Loading a spectrum file

The very first step is to load the spectrum data file, which contains your spectral data. EWA recognizes and uses several data formats, without your interaction. Check the appendix for the file formats to find out if you have (or can prepare) data files in format which EWA knows. If not, it is also no problem: EWA knows also some standard formats, used in international spectral data bases and also you can download some sample data files from its WEB site (http://esca.atomki.hu/~vegh_j/EWA/).

Start EWA (usually just type 'EWA') and the main window appears. (For details see the User's Guide.) Select command group 'FILE' on the menu bar, then 'SPECTRUM' on the pop-up menu, then the subcommand 'LOAD...'. As '...' in the command name signalizes, a dialog, namely the file selection dialog pops up, where you can select the file you want to load into EWA. In the dialog box you will see the available files, subdirectories, etc. Depending on the file extension (please consider the *file filter*) and the position of the data file, you will find the data file in the directory structure. Double click on its name, or

single click + 'OK', and you will have one more window on the screen, showing the chart corresponding to the data file you selected.

Say, you downloaded the tabular format standard spectra from the NIST site, unzipped file 'FILE001.DAT' to some subdirectory, and now load its content into the memory. Your new window will be like Fig X. (The chart is shown according to the defaults of EWA, later you will learn how to change them.)

13.3 Playing with the mouse

Using EWA, you can do a lot of evaluation, via just playing with the mouse. If you do *not* keep pressed the mouse buttons and you move the mouse, as the cursor gets into the frame (the 'sensitive area', between the axes frame), in the rightmost two cells of the statusbar you will see the coordinates of the cursor in the actual horizontal and vertical scale coordinates, usually energy and intensity. Note that these fields are used to display different values when the cursor is outside the sensitive area, see below.

A different action is taken if you *drag* the mouse. If you keep the *right* mouse button pressed while moving the mouse, an 'L' shape will be drawn between the initial position of the cursor and the current one. At the same time, the coordinate display fields will change: they will contain the *difference* of the coordinates of the two endpoints. The simplest way to determine peak distances, half widths, intensity, etc.

Dragging the *left* button has another meaning. There are some draggable things on the screen and you can change their position. For example, now on the screen you have two 'bulbs' at the rightmost and leftmost position of your spectrum: they are the 'markers', some tools used to mark certain points in the spectrum. Change their position: move the cursor over them, grasp them (press the left button and keep pressed while moving) and move the cursor to some other place; release the button to finish. While dragging, a line section will be drawn between the initial and the current position; however, in this case the bulb will remain all the time on the graph, you are allowed only to change its horizontal coordinate.

Chapter 14

The simplest evaluation operations

14.1 Creating components

In order to evaluate the spectrum, you need to create components (backgrounds and peaks), one by one. The components are summed up, their common envelope will be the fitted spectrum. The more similar the fitted spectrum and the measured spectrum is, the better you know the composition of your sample.

The components are created in two steps: the first one just creates an empty component store, which in a second step can be turned to something useful. Between the two steps you have the possibility to prepare the components, allowing this way much better initial values. Usually, the mouse (i.e. dragging the spectrum markers) are used to reach this goal.

14.2 Creating background component

Usually, one starts with the background component. In the spectrum there are regions where peaks appear superimposed on background, also there are -usually at least at the leftmost and rightmost points of the spectrum- background-only regions, but hardly if ever happen peak-only regions. So, you can easily show the leftmost few points and the rightmost few points as background-only regions, which allow to derive easily very good initial parameters for the background. To do so, create first an empty component ('COMPONENT CHANGE NEW'). Now, the displayed picture changes: a new horizontal line (representing the 'fitted' spectrum, which initially is an all-zero line) appears. Also notice that the numbers shown in the rightmost cells of the status bar change.

Now you *can* prepare the background parameters: drag the two markers to the position where the 'background-only' region ends: now the region between the leftmost point and the left marker, furthermore the region between the right marker and the rightmost point contain no significant contribution due to the peaks. Moving the markers in this position is helpful in general; however in some cases it is absolutely necessary. For example, in the case of the Shirley type background we will use here, the algorithm only

works between the markers; outside that simply constant average levels are taken, so it is absolutely necessary to move the markers to the correct position.

Having moved the markers to the correct positions, you can turn this empty component to a background: select 'COMPONENT CHANGE BACKGROUND'. Now a list selection box pops up, showing the available background types. Select 'SHIRLEY' here. Following this, you can pinpoint the selection via correcting the number of the terms in this background. Until you know precisely what you are doing, do not change the default values the program suggests. Having finished this second selection, too, your component (with the initial parameters calculated from the marker positions and the two background-only regions) is ready to use.

Note: Not only the initial values, but also their uncertainties are determined from these settings. If you do not move the markers previously, the two regions degenerate to two points and the uncertainty might reduce to 0. Although EWA tries to correct for this, please check/correct the uncertainty of the parameters in such cases.

Finishing the second step of the component creation causes a drastic change in the picture you see in the spectrum window: the height of the graph frame is decreased, a new graph corresponding to the generated component appears and the 'fitted' spectrum envelope changes. On the top of the main area some new frame with a new graph (the local normalized residuals, characterizing the similarity of the measured and fitted spectra) appears; and even on the left side of this frame again another frame with a graph (showing the expected and the realized distribution of the local normalized residuals) appears. Their role is discussed in the User's Guide. Also, the two numbers displayed on the statusbar are smaller.

14.3 Creating peak component

Creating peak components is quite similar to creating background components. The important difference is in setting up the initial values. As described at 'COMPONENT PEAK', the two markers should be moved to the positions where you guess the FWHM position. Now you use the 'lazy' algorithm: just create a new component, do not move the markers, then use 'COMPONENT CHANGE PEAK', and select 'GAUSS'.

Now the change on the displayed graph is much less: still, the fitted component envelope changes and the new (peak) component appears. However, it is obviously bad: there is a doublet in the spectrum, but the 'lazy' algorithm is prepared for a single peak. So, obviously the parameter value initial estimates should be corrected.

14.4 Adjusting component parameters

Select now 'COMPONENT CHANGE ADJUST' while the peak component is selected. A specialized dialog box pops up, the 'adjust parameter dialog'. Both the attributes of the parameters, and the parameters names are shown in a special listbox, a combo box. To handle them, just click on the arrow on their right side. Then, on the open listbox select some other item. The actual value of the selected attribute of the selected parameter is shown immediately under the combo boxes, in the middle field. The left and the right side fields show the lower and the higher limit for the middle value, respectively. On the slider bar in the next row, the same information is duplicated, now in graphical form. The sidebar shows the position of the current value relative to the corresponding limits. Dragging the sidebar thumb, you can change the value also in this graphical way.

The peak height is more or less O.K., but you should correct both the energy and the half width. Initially, the 'parameter value' is selected in the left-side combo box and the first parameter, the peak energy in the right-side combo box. Increase the peak energy with 0.5 eV, either editing the value shown in the middle field or via dragging the thumb on the sidebar. Apparently, nothing will change.

Now select the half width (the 3rd parameter) in the right-side combo box and set it to 1 eV. Now select O.K. and leave the dialog. Now you make the new parameters effective: the display refreshes with the component having the new parameters. Yes, now the initial estimates are much better: the left-side peak component is nearly O.K.

14.5 Finishing model evaluation

Still the right-side peak is missing. Just create one more component and turn it into a Gaussian peak. In this case there is no need to move the markers: because EWA uses the net intensity (i.e. measured data minus the already synthesized fitted envelope), the 'lazy' algorithm places the second peak correctly.

Of course, not all parameters have the 'possible best' value. You might try to adjust the parameters of any of the created components (use 'COMPONENT ADVANCE SELECT', then adjust it), until it gets better. Or, just you might use the built-in optimization routine: 'COMPONENT EVALUATE FIT'. Following a couple of iterations, the optimization stops and you will see the components with the best possible combination of parameters. And, you are ready.

14.6 Changing the model

Well, till now we used only the defaults and the simplest settings. At this point you might ask questions of type 'What if ...'. Say, you might know that the two half widths have the same value, or you might know the distance of the two peaks, etc. or, you are just curious about the model if some other background or peak type is used. It is easy to do.

- ▷ Known half width: select the peak, then adjust it. In the parameter adjust dialog, select the half width, set it to the value you know, and check the 'FIXED' box. Now (until you unfix it again) the adjusting/optimizing will not change the parameter, so just restart parameter optimization and you will find out how the fitted spectrum looks like with this (fixed) half width value

Chapter 15

Advanced evaluations

15.1 Parameter linking

Not (yet) re-implemented

15.2 Non-contributing components

The components you used till now, have a direct effect on the spectrum envelope: the backgrounds and peaks are contributing components. There are other components the use of which is more sophisticated. As an example, use the X-ray satellites.

Load now the 'IZOTOP.DAT' spectrum file from the ATOMKI1.zip file. It contains an Ag 3/2 5/2 spectrum, excited by a non-monochromatized Al K_α X-ray source. Because of this, apparently several peaks are present. One way is to create an independent peak for each single line. However, they obviously reflect the structure of the multi-line X-ray source. How can we use this fact to reduce the number of the parameters and simplify the evaluation?

Create a Shirley-type background as we did in the previous chapter. Then create one more component and turn it into 'COMPONENT MULTILINE'. Select 'Al_K_1234', since the spectrum was excited by Al K_α radiation. Some strange triangle-like structures appear on the screen, representing the 6 lines of the X-ray source. You can adjust the parameters: they are initialized with parameters proposed in [SDM94]; all parameters are fixed.

Now you attached this non-contributing component to the spectrum. Create one peak (either use the default initial values or select previously one of the two $K_{\alpha 1,2}$ lines). It will correspond to the main peak (which is unfortunately a doublet). At this point, having this peak component active, you can make use of the multiline structure you created in the previous step.

Select 'COMPONENT LINK MULTILINE' now (this menu command is not enabled until a multiline structure is created for this spectrum). The pop-up window will show all multilines, belonging to this spectrum: this time you can select only the one you created. Select this, and the single peak in the window turns into a 6-line multiplet. Rather than

using 6*3 parameters, you can exactly fit all the 6 peaks with 3 parameters only! And no problems with the too close lying peaks, very low relative intensity satellites, etc.

Create one more peak now, for the another $K_{\alpha 1,2}$ line, then use 'COMPONENT LINK MULTILINE' again, for this peak. In the popup window the same (and only) multiline structure will be shown, select it and you will have one 6-line multiplet again. Now practically all main spectrum components are created for your fitted spectrum, just adjust/fit as you like.

Note: Adjusting/fitting the multiline component, also the peak components, which this multiline component is linked to, will be re-calculated.

Note: You can unfix some of the multiline parameters, too, if you want to determine their value from your spectrum.

Note: You can create more than one multiline structure for a spectrum. For example, 'ghost peaks'.

Note: Although you can link more than one multiline to a peak, it is counteradvised. Rather, create one more peak and link the second multiline to that one.

Part IV

Appendix

Chapter 16

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Chapter 17

Glossary

- ▷ ACCELERATOR see hotkey
- ▷ CLICKING pressing a button of the mouse
- ▷ COMPONENT ID The components are queued to form an ordered list, which in some respects is circular. Beside their position in the list they have a unique identifier, their ID, too.
- ▷ CONTRIBUTING COMPONENT The kind of components which result in a direct contribution to the spectral data values
- ▷ DOUBLE CLICKING pressing a button of the mouse twice with short time difference
- ▷ DRAGGING pressing and kept pressed a button of the mouse while moving
- ▷ DROPPING releasing a button of the mouse after dragging
- ▷ FILE FILTER in the file selection dialog only the files matching the condition set by the file filter appear
- ▷ HOTKEY a key combination used to access a menu item
- ▷ NET INTENSITY the measured intensity, minus the already ‘fitted’ spectrum
- ▷ NON-CONTRIBUTING COMPONENT The kind of components which do not result in a direct contribution, but might affect the data points in an indirect way
- ▷ TYPING pressing a key on the keyboard

Chapter 18

Spectrum data file formats

The file formats, recognized by EWA, are shortly described here. Note that EWA takes care of things like the different 'end-of-line' formats in different platforms.

18.1 ATOMKI home formats

18.1.1 Energy calibrated simple

These file formats are also able to store the energy calibration data, set during data acquisition. Internal code name is 'Izotop'.

the heading is one value per line

(#1) EnergyStart, the first energy value

(#2) EnergyStep, the energy step size

(#3) EnergyEnd, the last energy value

(#4) TimePerChannel, Collection time, per channel and per cycle in units 0.1sec, one less

(#5) Cycles, the counts are the sum of measuring Cycles times

(#6) NoOfPoints The number of the measurement data points

(#7) ECalibrIntercept The energy calibration parameters

(#8) ECalibrSlope

(#9) reserved, dummy values

(#10) usually 0

from line #11 the 'NoOfPoints' measure counts, one count per line

18.1.2 Uncalibrated simple

These simple formats are used to record data from the spectrometers ESA-11 and ESA-13. Contains no energy calibration, but able to record multiple channel data.

These file forms have a 10-byte heading; contain equidistant data, in one region only (Code name: ESA-11 and ESA-13)

Line #1: (#1) SpectrumNO, spectrum identifier number, 0-65535 (#2) SPMI-IDent spectrometer ID, 0-65535

Line #2: (#3) DependenceNo, typically unused, contains angle at ESA13, sometimes (#4) EnergyStart, the first energy value (#5) EnergyStep, the energy step size (#6) EnergyEnd, the last energy value (#7) TimePerChannel, Collection time, per channel and per cycle in units 0.1sec (#8) Cycles, the counts are the sum of measuring Cycles times (#9) NoOfChannels, ≥ 0 The number of data sets, one less (#10) NoOfPoints The number of the measurement data points per channel

Line #3:... measured counts, 10 value per line, 1st channel measured counts, 10 value per line, 2nd channel

18.1.3 Calibration file

The uncalibrated file formats do not store information about the energy calibration, so a special method is used to calibrate them. The spectra have some internally stored ID number (which is usually also present in the file name) and a calibration measurement is done immediately *after* recording a series of spectra. This calibration is considered to be valid for spectra recorded since the previous calibration. When reading uncalibrated spectra, EWA checks for the presence of the file 'EWA.CAL' in the working directory, and if found, calibrates the spectrum according to the data found here.

This file contains one-line entries, stored as ASCII text. One entry contains the following items (separated by space(s)): a positive integer number *below* which the given calibration data are valid, and the intercept and slope of the calibration. The data are recorded at some DAC (Digital-to-Analog-Converter) addresses (see below) and the corresponding energy is: $E = \text{DAC} * \text{Slope} + \text{Intercept}$.

The entries should be in ascending ID order. EWA looks for a number which is higher than the ID number of the given spectrum. If found, takes the calibration data from that entry, else (if the file does not exist or does not contain such an entry) it remains uncalibrated.

18.1.4 ESA-21 format

This format is in use at the ESA-21 electron spectrometer. The file contains ASCII text only. In the first part the heading describes the data structure.

Heading:

Line #1: characters 1..4 are the format identifier (and checksum): Char(1) is the main type (can be 'R', 'N' or 'X' presently Char(2) is the subtype (presently

can be 'A', 'B', 'C', 'D') Chars(3) and (4) are the checksum to identify the format Chars(5)..(11) is the description of the projectile (Name, mass, charge) Chars(12)..(18) is the description of the target Chars(19)..(23) is the spectrum internal identifier Chars(24)..(29) is the energy of the projectile, in keV Chars(30)..(43) is the date of the data recording Chars(44)..(57) is the date of the last processing

Line#2: (items separated by ',') No of data points, length of data record (Not no of channels!) Energy calibration intercept slope Dummy???? flag if live time data are present in the record (1 if yes, 0 if not) No of comment lines present

Line#3: No of timing counts range of current integrator (No of data cycles total) * 256 * current cycle mask word for multichannel summing no of regions present

Line#4..line#(3+No of regions present) DAC1 start value DAC1 step value DAC1 final value DAC2 value (always 0?)

Line#(4+NoOfRegionsPresent) Slit settings, 2 values, in mm vacuum settings, 2 values, in mbar

Line#(5+NoOfRegionsPresent) ADC parameters, 3 values ADC energy calibration, 2 values Optionally one more parameter can be present : calibration factor

Line#(6+NoOfRegionsPresent) Digital Voltmeter range (=0: not present) scattering flag : =1 present, =0 absent Vacuummeter range (=0: not present) scattering flag : =1 present, =0 absent Average current (calculated from time and charge)

Line#(7+NoOfRegionsPresent)..Line#(7+NoOfRegionsPresent+NoOfComments) Comment lines after this

the data record follow, till the end of the spectrum. ('length of data record' values are read, not some definite number of lines) Their content is different according to the information given above

Format 'R' : (raw data) first the contents of the counters, (the number is calculated from the length of record and the flags, given above) then the DAC1 value, if live time value is present, then its value if DVM values present, then the average DVM value if DVM values are present and its scattering is present, then the scattering value if Vacuum values present, then the average Vacuum value if Vacuum values are present and its scattering is present, then the scattering value The uncertainty of the counts is not stored, the Poisson distribution is assumed.

Format 'N': The calculated channel number (see format 'R') is divided by 2 (here the uncertainty is also stored. The heading as at 'R', the data records: data are stored as value and its uncertainty,(no. of channels times) then the energy value (calculated from the DAC address and cal. constants) and the other data depending on the flags as at 'R'

18.2 Nucleus PCA-II

The format is produced by the Series II Personal Computer Analyzer, as described in the 'Operation and instruction manual' by The Nucleus Inc.

18.3 Scienta ESCA-300

This particular format is described in the corresponding manuals of the data system. When working with such format data, some special conditions need to be fulfilled. The information needed to read in spectra are distributed in the user's subdirectories '\Specific', '\Regions' and '\Results'. In all these directories a file with the same name should exist. You can select any of them to read the file into the memory.

18.4 Tabular data

This format can contain tabular data, with an optional, max. 10 lines heading. The heading lines MUST NOT be interpreted as numbers, they should provide something 'foreign' for the number reading routine. (i.e. they can contain numbers, but also some letters or other characters) The data lines should contain the same number of data items (1, 2 or 3 items are legal, more items can be present, but are neglected). 1 data item: counts only. 2 data items: energy and counts. 3 data items: energy, counts and the corresponding uncertainty. The items can be separated by comma as well as any number of spaces or horizontal tabs. *Be sure not to add extra lines at the end.*

18.5 VAMAS'88

This file format is described in detail in [DHS88]. The VAMAS format uses 'blocks' as atomic units, while in EWA terms like 'spectrum', 'region' and 'channel' are interpreted. The natural choice is to handle one 'block' as one 'spectrum'. The present reading routine checks some relations between the energy range and block ID of the individual blocks and might arrange the blocks differently. When data in the different blocks seem to be measured over the same energy range and have the same ID, they are considered as different scans of the same spectrum and formally will be read in a multi-dataset spectrum, where the individual datasets correspond to the individual blocks in the data spectrum file. Beside this, if the energy range in two blocks seems to be the continuation of each other (i.e. the last point of the first and the first point of the second is within one step size) and the number of the scans is the same, then these regions are grouped into a multi-region (and maybe multi-dataset) spectrum.

Although non-standard, the reading routine allows empty leading/trailing lines.

Index

χ_n^2 , 22

accelerator, 63

active

 spectrum, 15

 window, 15

adjust component, 29

adjust parameter dialog, 56

asymmetry

 peak, 41

attributes

 parameter, 17

autocorrelation of residuals, 22

Batch Append, 25

canvas

 spectrum, 15

Ccomponent Display All components, 17

chi square, 22

clicking, 11, 63

clicking, double, 63

combo box, 56

component

 adjust, 29

 background, 33

 contributing, 63

 creating, 30

 deleting, 30

 ID, 63

 label, 30

 marker, 32

 multiline, 37

 non-contributing, 63

 peak, 40

 root, 28

 save, 50

 subtract, 31

 window, 17

Component Change Adjust, 33, 37

constraints

 parameter, 17

creating components, 30

cursor shapes, 11

data directory, 10

dialog

 adjust parameter, 56

 file select, 43

 file selection, 52

 parameter adjust, 29

directory

 program, 10

double clicking, 11, 63

dragging, 11, 63

dragging the mouse, 53

dropping, 11, 63

evaluation mode

 cross spectrum, 23

 normal, 23

EWAFIT.TMP, 49

exiting EWA, 10

extension

 batch file, 46

 data file, 47

file filter, 52

file select dialog, 43, 46

file selection dialog, 52

File Spectrum Load, 14

fitted spectrum

- save, 50
- fitting
 - LSQ, 49
- goodness of fit, 23
- help message, 10
- hotkey, 63
- initial parameters
 - background, 33
 - peak, 41
- linking
 - parameters, 18
- linking modes
 - parameter, 18
- loading
 - spectrum, 14, 43, 53
- local residual, 22, 55
- marker, 53
- master parameter, 18
- menu
 - program, 12
- menu bar
 - main, 10
- menu items
 - selecting, 12
- minimization
 - LSQ, 49
- mouse
 - dragging, 53, 63
 - dropping, 63
- multiline component, 37
- net intensity, 33, 63
- Options
 - General, 46
 - Options Evaluate FitDispFreq, 49
 - Options Evaluate FitMaxIter, 49
 - Options Evaluate FitPrecision, 49
- parameter
 - adjust dialog, 29
 - adjusting, 19
 - attributes, 17
 - constraints, 17
 - fixing, 19
 - linking, 18
 - linking modes, 18
 - master- and slave, 18
- peak
 - asymmetry, 41
 - initial parameters, 41
- peak component, 40
- program
 - directory, 10
 - menu, 12
- quality of the fit, 22
- residual
 - local, 16, 22
- role, 10
- root component, 28
- root window, 17
- save
 - component, 50
 - current evaluation state, 50
 - fitted envelope, 50
- slave parameter, 18
- spectrum
 - active, 15
 - canvas, 15
 - component, 21
 - file formats, 14
 - interpretation, 21
 - loading, 14, 43, 53
 - window types, 15
- Spectrum Save Parameters, 49
- spectrum window, 15
- starting EWA, 10
- subtract component, 31
- typing, 11, 63

window

- active, 15

- root, 17

- XPS specific, 16