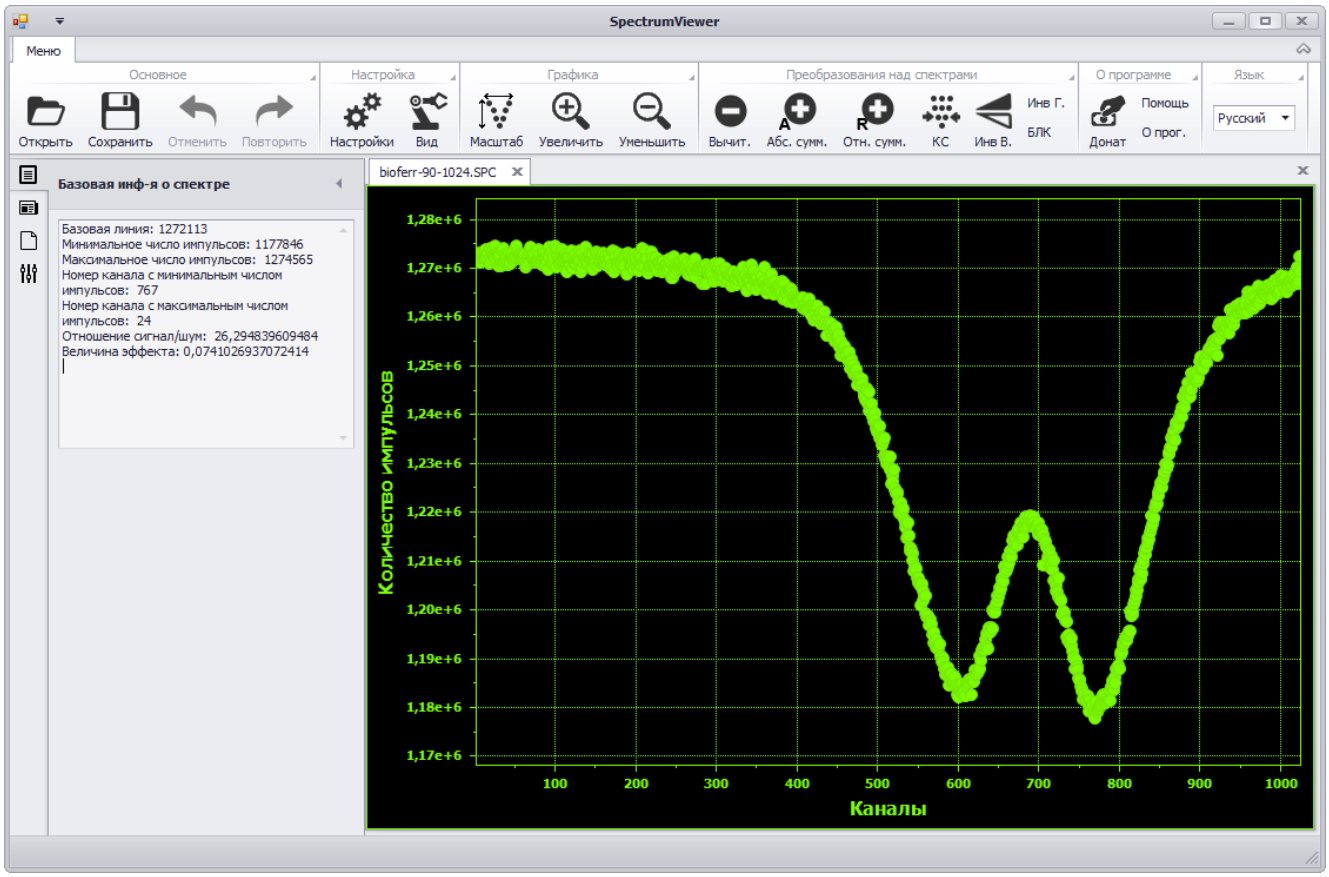
Help SpectrumViewer



Softw are SpectrumView er
Developers: Michael Ushakov, Eduard Lunev.
Ekaterinburg, 2016-2018

Software

SpectrumViewer, version: 2.0

Michael Ushakov, Eduard Lunev

Software application SpectrumViewer is a viewer of Mössbauer spectra. The program also allows to convert spectra to other formats.

Help SpectrumViewer

User manual created: Ноябрь 2018,
Ekaterinburg.

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Software

SpectrumViewer

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SpectrumViewer User manual

1 User Manual SpectrumViewer

User Manual SpectrumViewer

Software
SpectrumViewer

Developers: Michael Ushakov, Eduard Lunev
Ekaterinburg, 2018 г.

1.1 Chapter 1

1.1.1 Introduction

The software application SpectrumViewer is designed for viewing Mossbauer spectra, as well as for simple transformations and converting them to the other formats (binary, plain text, and plain data formats).

The application allows you to work with the spectra of the following formats (extensions): spc, asc, bin, dat, txt:
.spc, .bin - binary format;
.asc, .txt - text format;
.dat - plain data format (It is similar to the text format except that every point of the spectrum is in the separate line (data column)

Current User Manual is for SpectrumViewer v2.0.

1.2 Chapter 2

This chapter describes the basic functionality of SpectrumViewer.

1.2.1 2.1 Basic functionality

This part briefly describes graphical user interface.

1.2.1.1 2.1.1 Toolbar

Toolbar menu is demonstrated in the fig. 1:

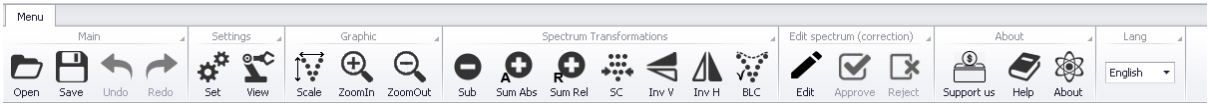

Fig. 1 - SpectrumVievew toolbar.

There is a full access to all instruments and options from the toolbar. It can be hidden/minimized by clicking on the arrow on the top right corner.

Toolbar content:

1. Section **Main**
   - ❖ Open - Dialog to open spectrum.
   - ❖ Save - Dialog to save spectrum.
   - ❖ Undo - Cancel the last action (e.g. transformation), taking back to the previous state.
   - ❖ Redo - Repeat the last action, taking to the further state.

2. Section **Settings**
   - ❖ Set - Application main settings.
   - ❖ View - Spectrum visual settings.

3. Section **Graphic**
   - ❖ Scale
   - ❖ ZoomIn
   - ❖ ZoomOut

4. Section **Spectrum transformations**
   - ❖ Sub. - Spectrum subtraction.
   - ❖ Add Abs - Absolute summing.
   - ❖ Add Rel - Relative summing with weight.
   - ❖ SC - Spectrum compression.
   - ❖ Inv V. - Vertical spectrum inversion.
   - ❖ Inv H. - Horizontal spectrum inversion.
   - ❖ BLC - Base line correction.

5. Section **Edit Spectrum points (correction)**
   - ❖ Edit - Enter edit mode.
   - ❖ Approve - Approve edit changes.
   - ❖ Reject - Reject edit changes.

6. Section **About**
   - ❖ Donate - Developers support.
   - ❖ Help - Open user manual.
   - ❖ About - Dialog with version, copyrights and contacts

7. Section **Lang**
   - ❖ Localization list - Change application language.

1.2.1.2 2.1.2 Navigation panel

Navigation panel includes four tabs and is located on the left side of the application main view. Panel can be hidden/minimized by clicking on the triangle on the top right corner on any tab.

Tabs:

❖ **Base spectrum information:**

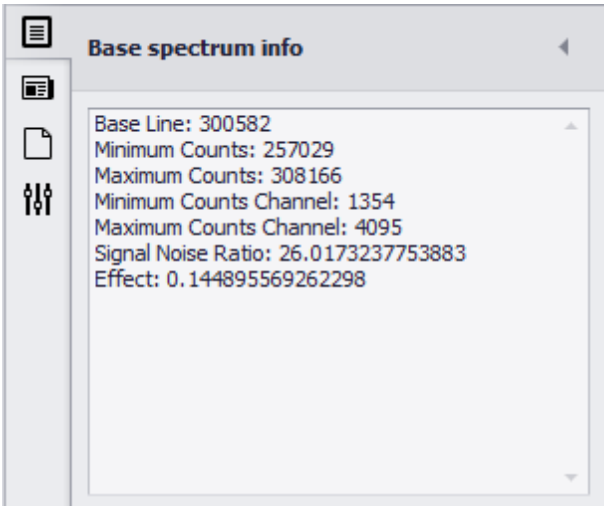

Fig. 2 - Base spectrum info.

This field is populated when the spectrum is opened. (Read only field)

❖ **Extended spectrum information:**

This field is populated when the spectrum is opened. Here is the information about file calibration (in the UnivemMS format).
In this version of SpectrumViewer the field is read only.

❖ **General file information:**

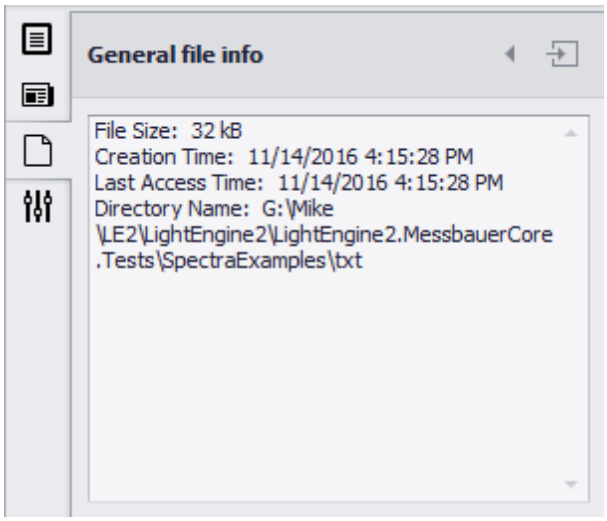

Fig. 3 - Spectrum file info.

Includes the following options:
- File size
- File creation time
- File changing time

- Directory where file is located

❖ **Markers:**

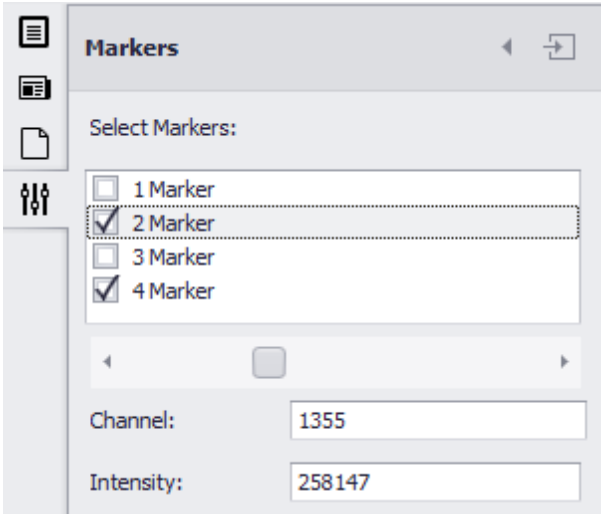

Fig. 4 - Markers display options.

Functionality with markers is described in the part "Markers"

1.2.1.3 2.1.3 Zooming spectrum

There are several ways to zoom spectrum:

❖ By mouse scroll wheel

Rotating the mouse wheel in one direction or another, you can zoom in or out.
If you want to see another part of spectrum, you need to press the left mouse button (don't release it) and drag cursor to the necessary part of the spectrum and (drop) then release the mouse button.

❖ Using hot-key combination and selecting a specific region of the spectrum with the mouse.

1. In order to zoom in the particular area of the spectrum you need to press down Shift-key. The cursor will turn into a magnifying glass with a plus sign. Set the cursor to the particular area and then click the left mouse button, zooming has to be occurred.

Also instead of simple clicking you can select desirable area on the spectrum. For this action it is necessary to press down the left mouse button (shift-key is also has to be pressed) and without releasing the button, move the mouse cursor extending borders of zooming. You will see a rectangle selection area.(pic. 5):

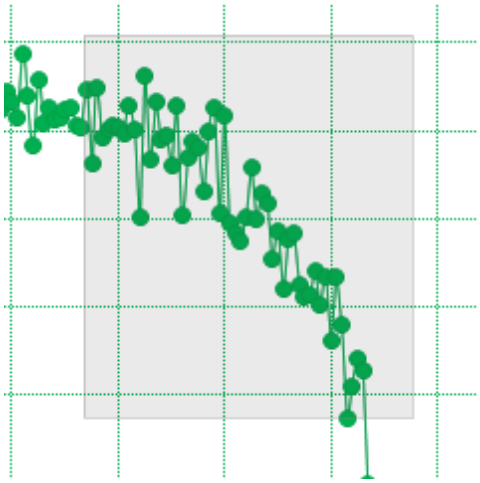

Fig. 5 - Zoom points selection.

In the pic 5 is represented zooming area, selected by mouse with pressing Shift key. This area might be barely perceptible if there is another background color.

2. In order to zoom out press down Alt-key. The cursor will turn into a magnifying glass with a minus sign. Afterwards click the left mouse button, zooming has to be occurred.

❖ In order to return back to the default scale just click the "Scale" button on the toolbar.

This function helps to recover initial state of scale without using mouse wheel or hot-keys in case of zoom changes.

3. Also for spectrum scaling you can use two buttons from the toolbar: Zoom In/Zoom Out.

1.2.2 2.2 Application settings

Here is discovered various settings of the application.

1.2.2.1 2.2.1 General settings

General settings can be called by clicking "Set" button on the toolbar (fig. 6):

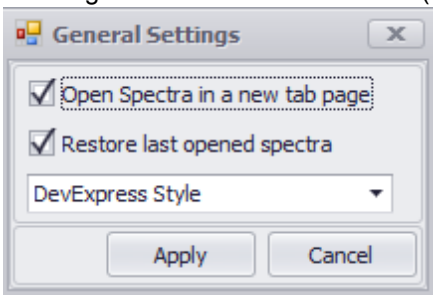

Fig. 6 - General settings form.

Options:

❖ Open Spectra in a new tab page

This option allows you to open a spectrum in a new tab page instead of the current active one in such a way that you can work with several files simultaneously, alternately switching between tabs.(fig. 7).

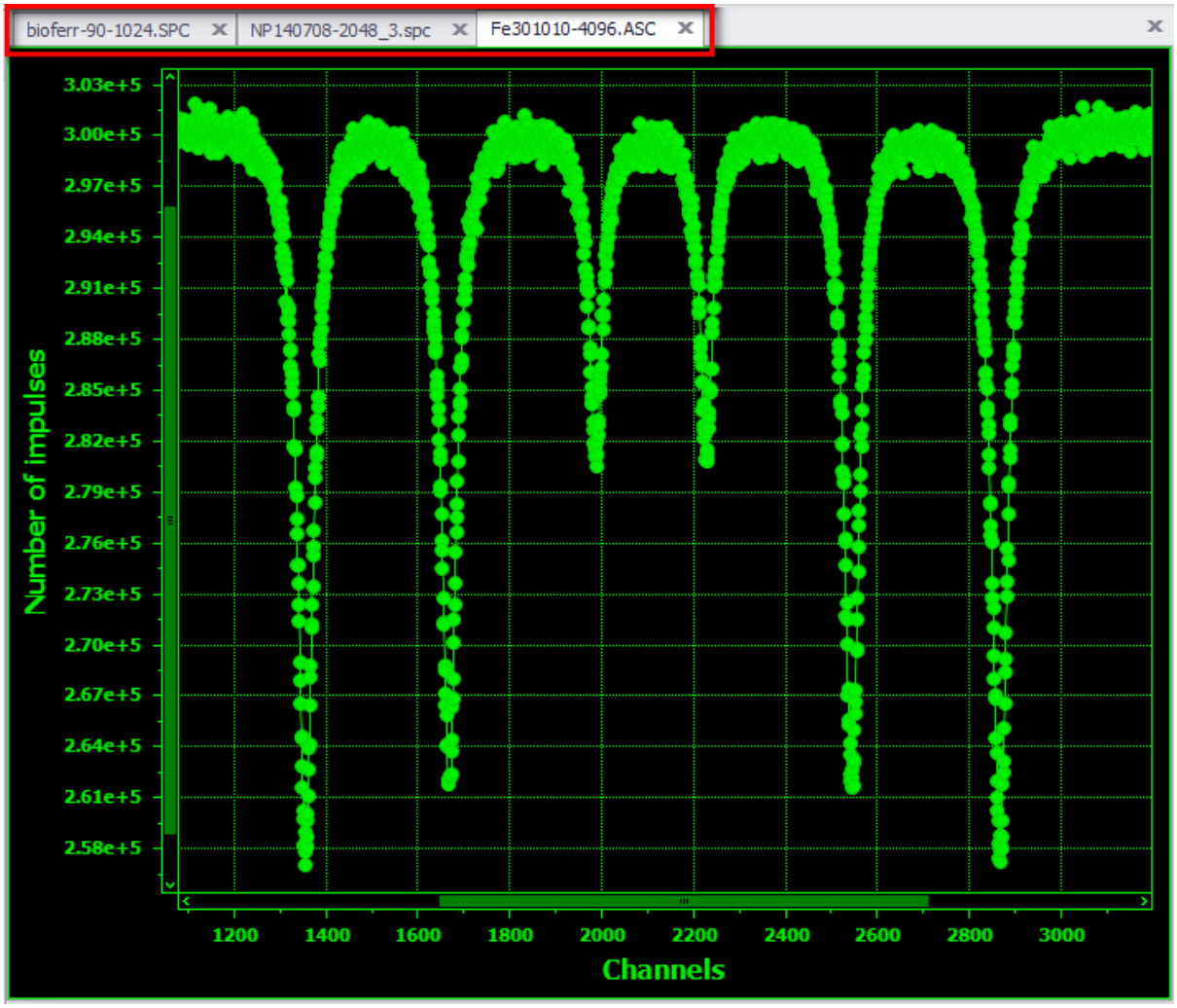

Fig. 7 - Spectra opens in separate tabs.

❖ Restore last opened spectra

It's not necessary to close all the spectra manually when close the program. In the future session you might want to continue working with all these files are opened. This option allows you to open them automatically after application start.
The previous session will be recovered if those files were not removed from the source paths.

❖ List (drop-down box)

This is the list of themes where you can choose a skin to your taste (fig 8).

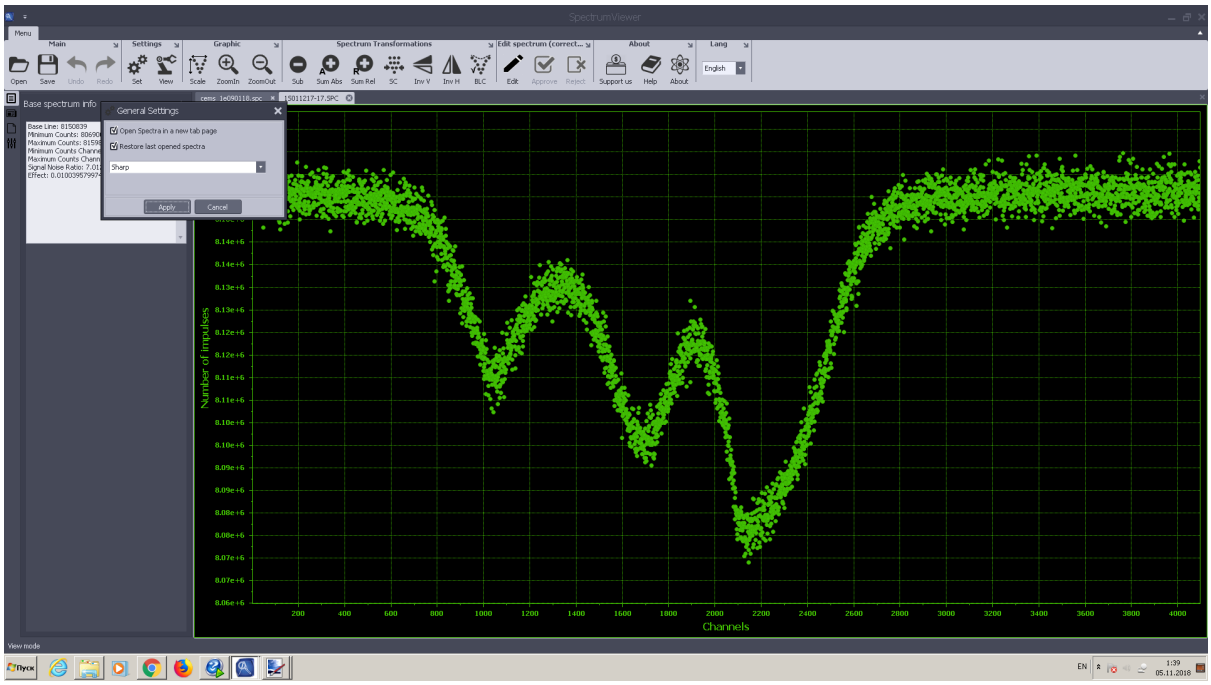

Fig. 8 - Theme selection.

1.2.2.2 2.2.2 View spectrum settings

View spectrum settings can be called by clicking "View" button on the toolbar. (fig. 9)
Variation of these options allows you to customize the visual parameters for displaying a spectrum. (The thickness and color of lines, dots and scrolls as well as grid parameters).

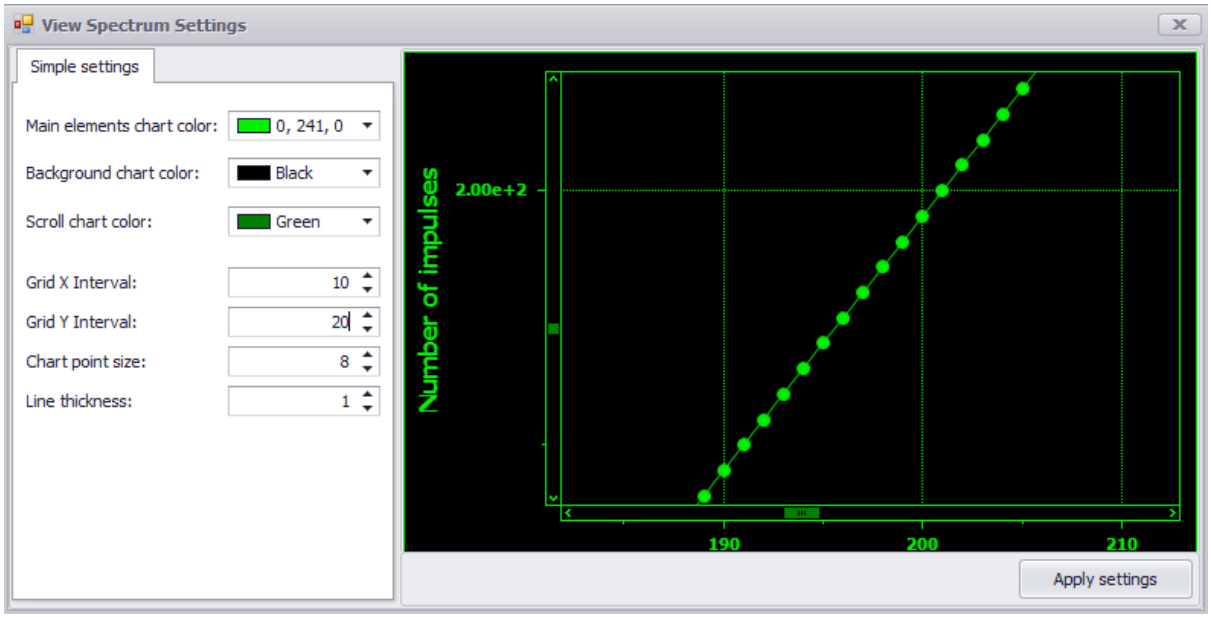

Fig. 9 - Spectrum display style selection.

You need to select the optimal settings for the spectrum display style.
The color of the scrolls can be adjusted separately in the corresponding drop-down box. Scrolls appear when the scale of the spectrum changes.

You can adjust the **color of the spectrum (Main elements chart color)**, as well as the **background chart color**.

You can also specify the grid step parameters and the size of the dots (impulses) and the line thickness that connect dots.

1.2.2.3 2.2.3 Language (localization)

There are two localizations are supported in the current version of the application (Fig. 10):

- English language
- Russian language

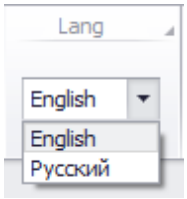

Fig. 10 - Language selection.

To change the language, click on the drop-down list on the toolbar in the Language section and select the appropriate one.
The application will automatically restart after choosing the language. It can take 2-5 seconds.

1.2.3 2.3 Spectrum transformations

Processing algorithms and transforming spectra in this section are considered.

1.2.3.1 2.3.1 Spectra subtraction

Subtraction dialog can be called by clicking on the "Sub" button on the toolbar (Fig. 11):

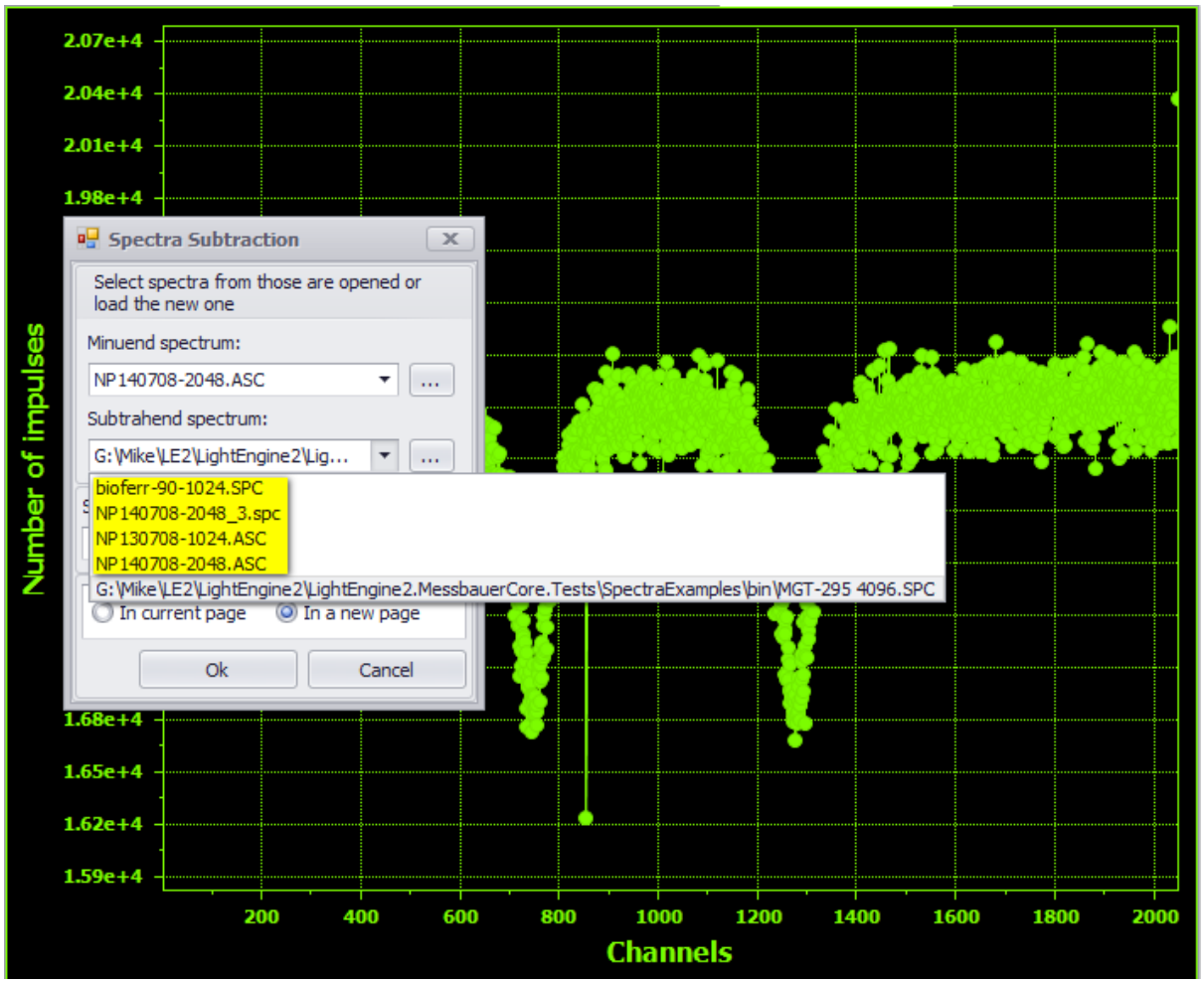

Fig. 11 - Spectra subtraction.

There are two drop-down lists:

- ❖ Minuend spectrum
- ❖ Subtrahend spectrum

Both lists contain spectra that are already opened in the application (yellow selection in the pic.11).
If there is no suitable spectrum, you can load it from your hard drive, clicking on the button "..." on the right from the list.
Only spectra with equal number of points can be used for subtraction.

For each point of the minuend and subtrahend spectra the relative value of the number of impulses is calculated:
I[k]rel = I[k]abs/Imax, where
I[k]abs - the absolute value of the number of impulses at the point **k**,
Imax - the maximum value of the number of impulses in this spectrum.
As a result of subtraction you get a spectrum with a number of impulses from 0 to 1 at each point.
It is necessary to scale (multiply) it by the value specified in the scaling factor field, in order to continue working with it further.

In the pic. 11, the last line in the drop-down list: this spectrum is not loaded into the main program

window but can be selected to perform the operation.

Below, there is a switches group allows you to choose whether you want to open the result of the operation in a new tab or open it in the current active tab, thereby replacing the data (spectrum) on the current active tab.

1.2.3.2 2.3.2 Spectra summing

There are two categories of spectra summing:

❖ Absolute

Absolute Summing dialog can be called by clicking on the "Sum Abs" button on the toolbar.(fig. 12):

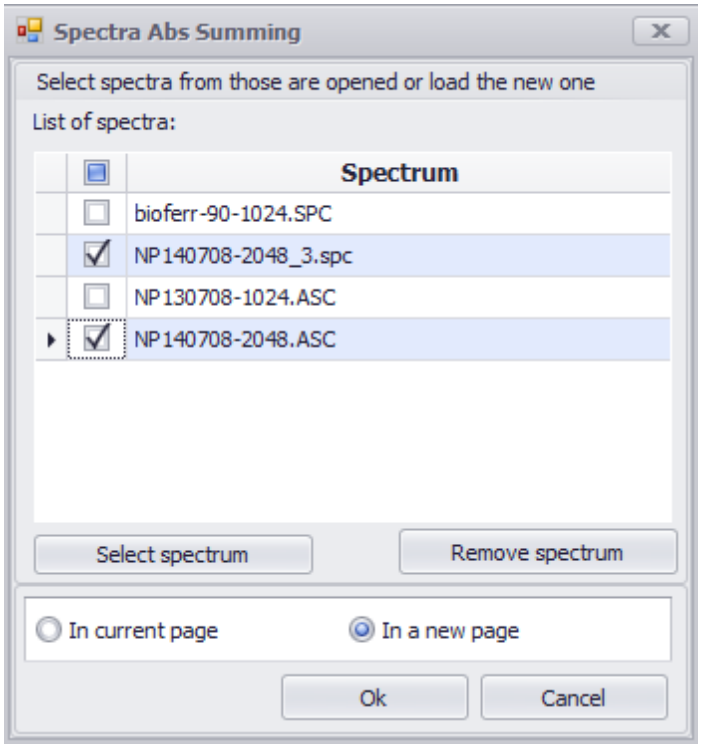

Fig. 12 - Spectra absolute summing.

Only spectra with equal number of points can be used for summing.
For each point of the absolute values will be provided according to the formula:
p[k]=i0[k]+i1[k]+.....iN[k]

❖ Relative

Relative Summing dialog can be called by clicking on the "Sum Rel" button on the toolbar (fig. 13):

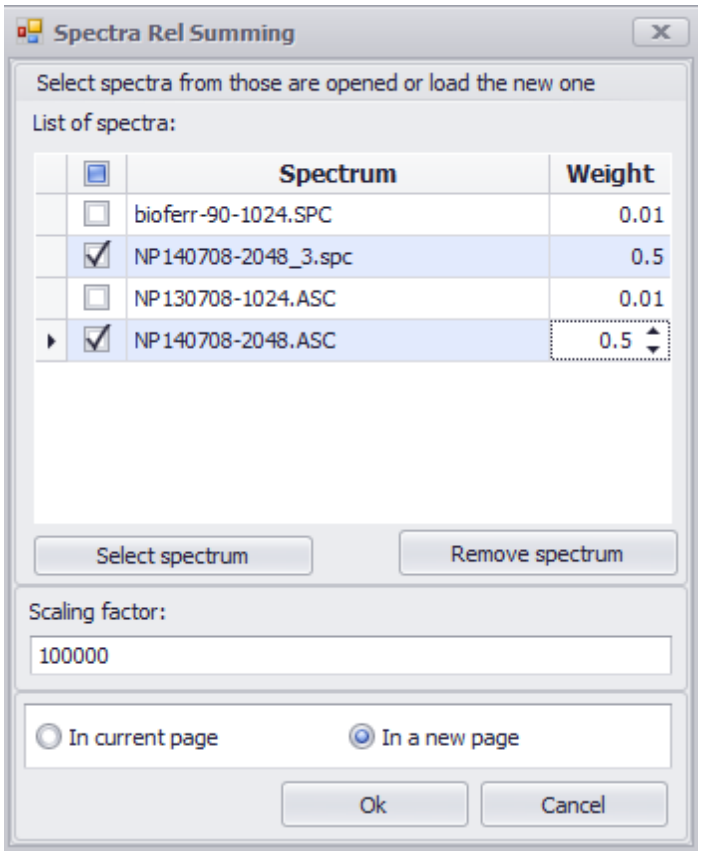

Fig. 13 - Spectra relative summing.

In the grid are represented all the spectra are opened in the application.
If there is no suitable spectrum, you can load it from your hard drive, clicking on the button "Select spectrum".

Each spectrum is normalized to the maximum number of impulses.
For each point of the spectrum the number of impulses is calculated by formula:
i[k]=p0*i0[k]/i0max + p1*i1[k]/i1max + ...pN*iN[k]/iNmax, where
p0,p1,...pN - the weights of the corresponding spectra.
The sum of the weights of all spectra must be equal to 1.

Below, there is a switches group allows you to choose whether you want to open the result of the operation in a new tab or open it in the current active tab, thereby replacing the data (spectrum) on the current active tab.

1.2.3.3 2.3.3 Spectrum compression

Spectrum compression dialog can be called by clicking on the "SC" button on the toolbar (fig.14)

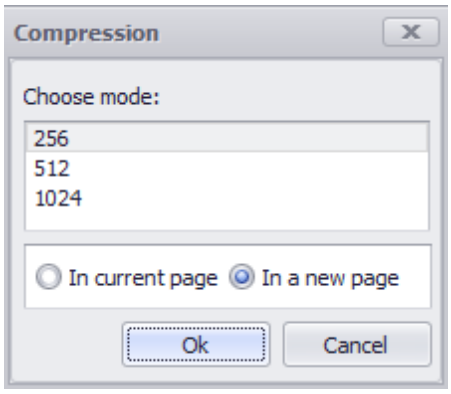

Fig. 14 - Spectrum compression.

This transformation reduces the number of channels.

When compression is executing the N-first points are summed (N = number of points of the original spectrum / number of points of the scalable spectrum).

Below, there is a switches group allows you to choose whether you want to open the result of the operation in a new tab or open it in the current active tab, thereby replacing the data (spectrum) on the current active tab.

1.2.3.4 2.3.4 Spectrum inversion

Vertical and horizontal inversions can be executed by clicking on the "Inv V" or "Inv H" buttons on the toolbar.

Be careful: Inversion operation is always occur in the active current page tab. Thereby the old spectrum data is replaced by new inversed one. This data store in RAM until the spectrum is saved to a file.

1.2.3.5 2.3.5 Base line correction

The base line correction is not implemented in the current version of the application (probably this feature will be implemented in 2.1 version).

1.2.3.6 2.3.6 General information about spectrum processing

The asterisk symbol (*) appears in the name of a page tab after any spectrum transformations (pic. 15) what means that this spectrum is not stored in a file yet but in the RAM only.
If you try to quit, the program will ask you whether you really want to close the application or not, because there is unsaved data.

If you close the application, this spectrum will not be stored and opened the next time you enter the program.
After saving the spectrum to a file, the asterisk disappears.
In the fig.15 vertical inversion of the spectrum is performed:

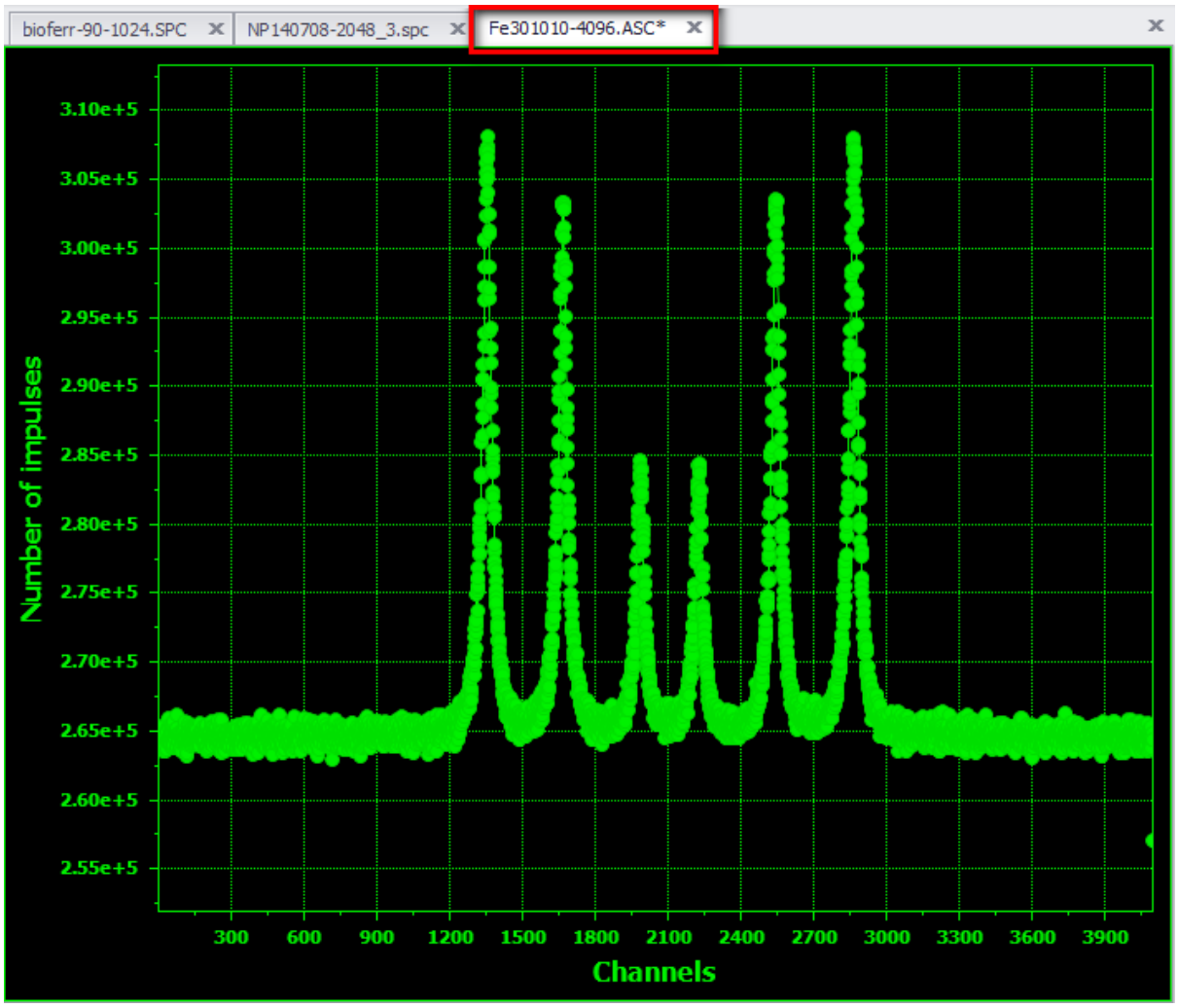

Fig. 15 - Spectrum transformation result is represented at the same tab.

If the conversion is carried out into a new tab, the counter is added to the file name on the page tab (pic. 16):

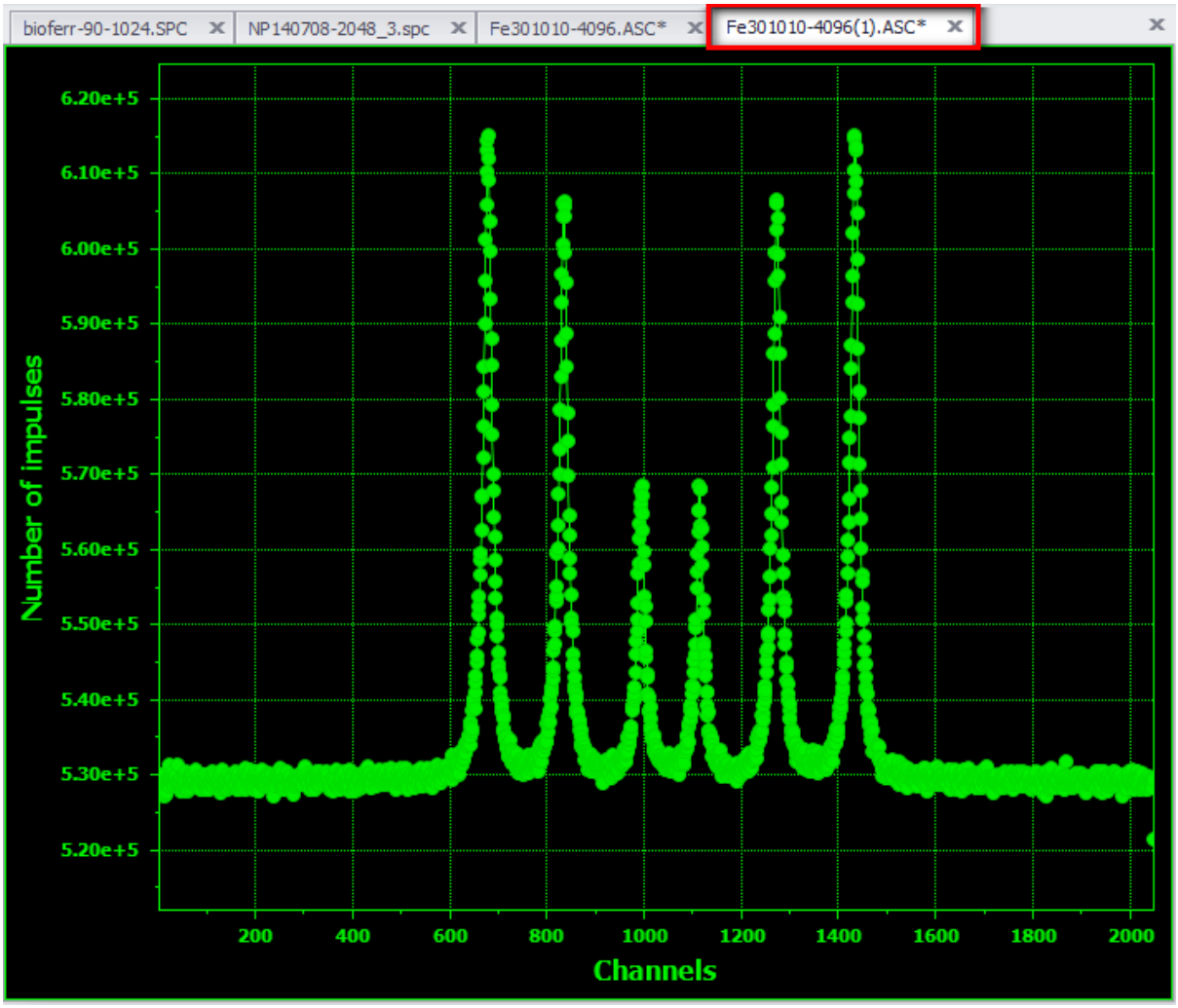

Fig. 16 - Spectrum transformation result is represented in new tab.

Thus you can estimate how many transformations have been made over the original spectrum.

1.2.4 2.4 Markers

In this part of manual you will learn how to work with markers

1.2.4.1 2.4.1 Markers

You can use four makrers in the current version of the application.
Markers allow you to select a channel and estimate the intensity. (fig. 17)

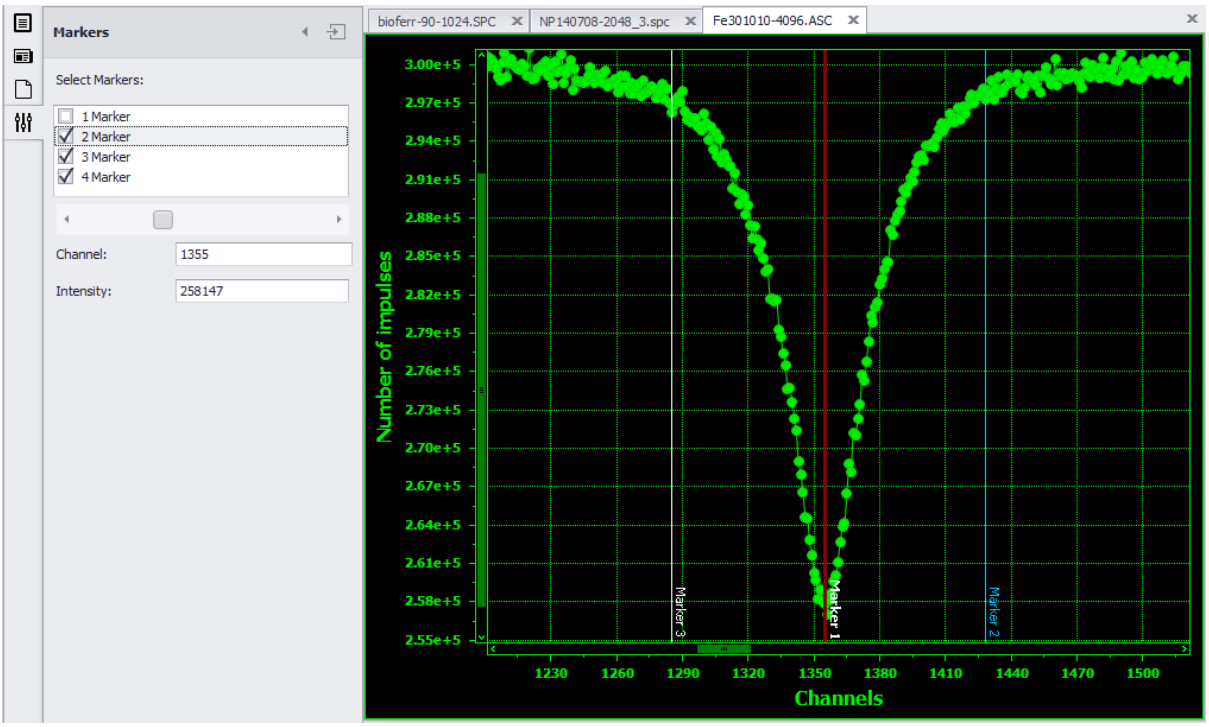

Fig. 17 - Markers management.

To set a marker on the spectrum, you must select any of the items in the list (1-4 Markers) and check the box.
After the checkbox is checked the marker appears as a color line in the spectrum.

To change the marker position you must move the scroll (slider) which is located below the marker list. The selected marker on the spectrum will be highlighted with a thicker line.

The intensity of a channel can be viewed also by the mouse cursor. When you hover the cursor on the points of the spectrum, you can see a hint with intensity and the channel number. (fig. 18):

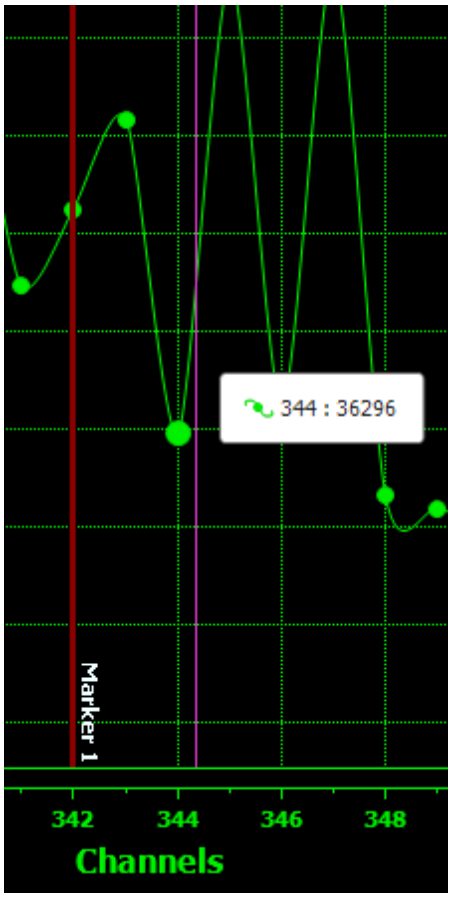

Fig. 18 - Enlarged area and markers usage.

1.2.5 2.5 Spectrum Edit

Enter topic text here.

1.2.5.1 2.5.1 Spectrum edit procedure

There are two modes of working with Mossbauer spectra: view and edit.
To enter edit mode click Edit button on Edit spectrum points toolset on toolbar (see Fig. 19).

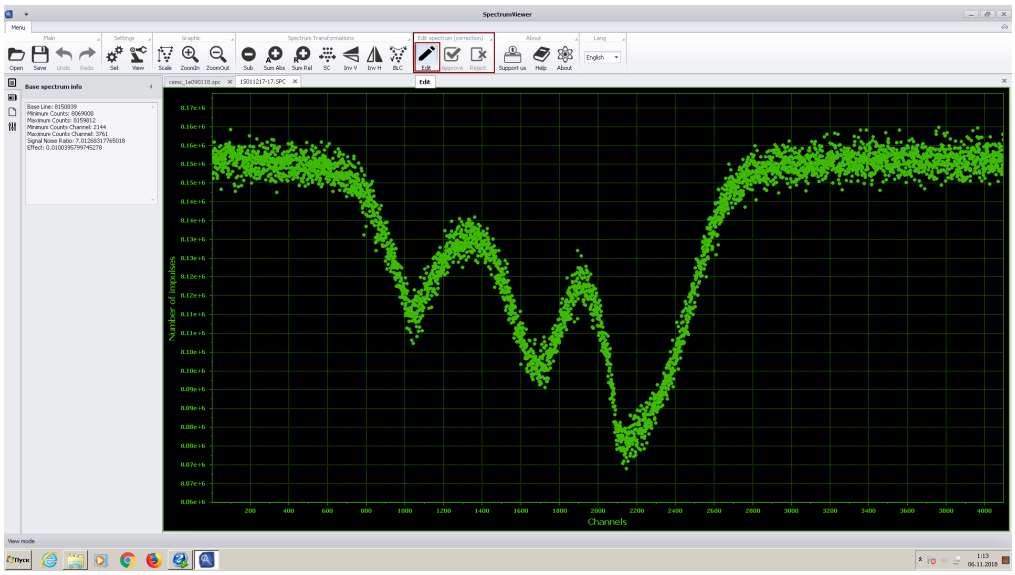

Fig. 19 - Enter points edit mode.

After click on this button text on status bar is changes from View mode to Edit mode.
Points could be selected via:
- mouse click on point (if points is clicked with pressed Ctrl clicked point is added to previously selected)
- via region (mouse button down on begin position pull mouse cursor and button up at the end position, see Fig. 20)

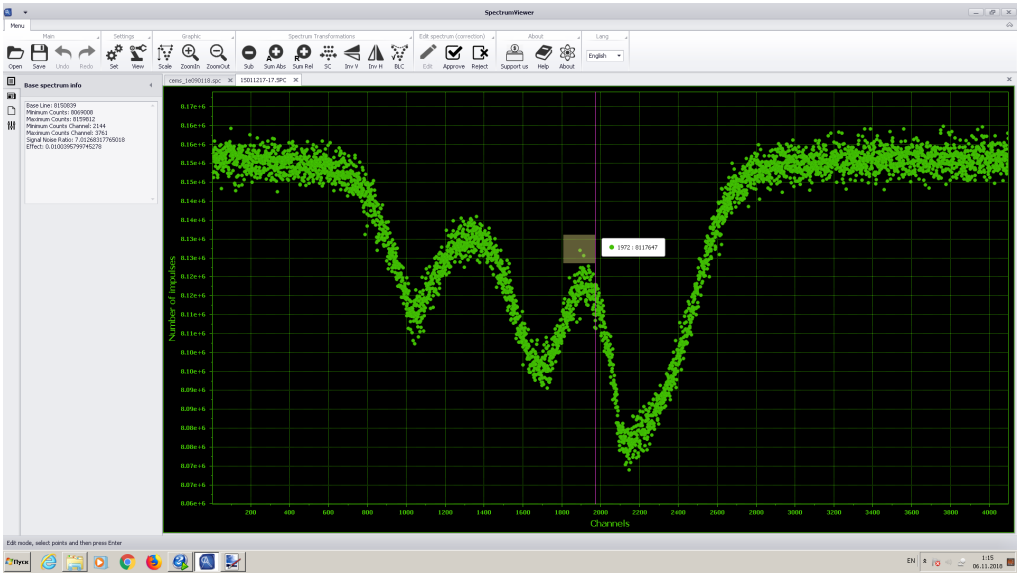

Fig. 20 - Selection of points for edit via region.

When all points have been selected press Enter key for running window for entering points corrected values (see Fig. 21).

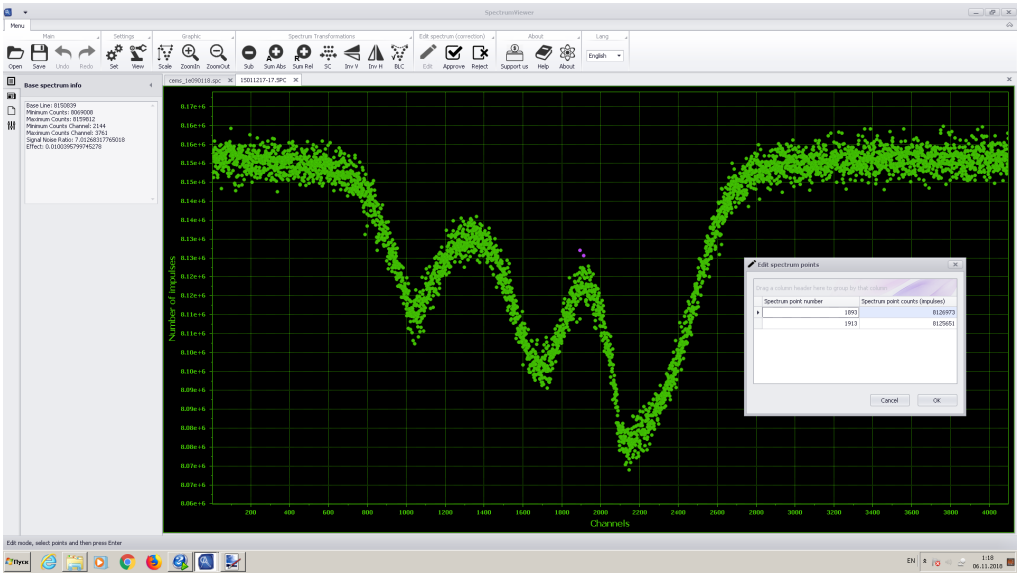

Fig. 21 - Enter points corrected values.

After all correction were entered press OK button and close points edit window. For save applied correction in tab (in RAM) press Approve button otherwise press Reject in this case all corrections will be discarded.

The end

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