



MULTICHANNEL ATOMIC EMISSION SPECTRA (MAES) ANALYZER

"ATOM" software User Manual

VMKO.157UM

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MAES
Multichannel emission spectra analyzer
Measuring Instrument Type Approval Certificate RU.C.31.001.A № 42605



The main goal of this Manual is to provide users with necessary and appropriate information on atomic emission spectral analysis using MAES. MAES analyzer and "ATOM" software allow performing spectral analysis in a more effective and convenient way.

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Software General Information

"ATOM" software package is a flexible tool for atomic emission spectral analysis. It provides MAES operation, performs necessary processing of spectra to calculate element concentrations, has a high performance, optimizes procedures and performs analysis with the maximum efficiency.

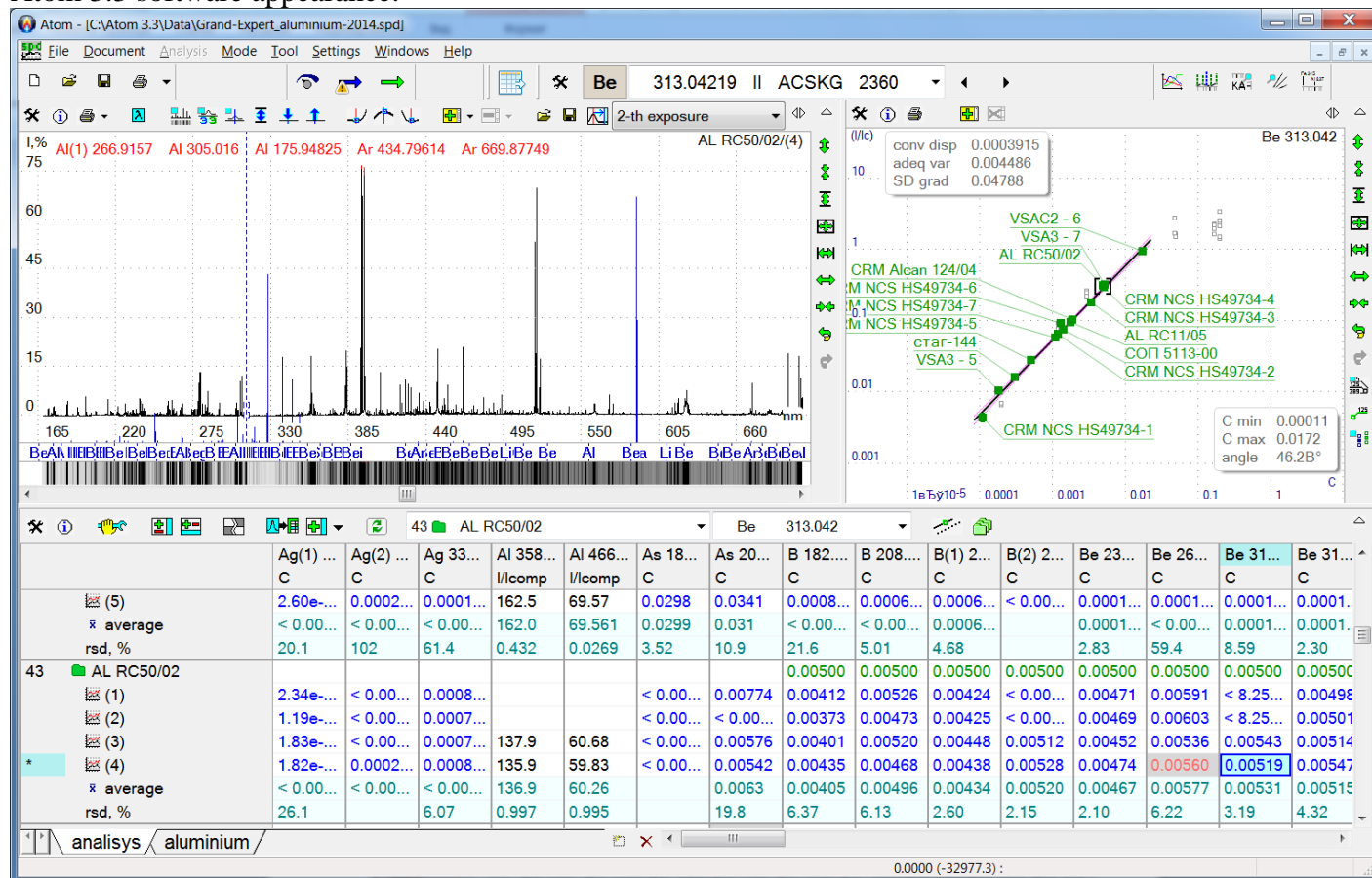
Key Software Features

- Visualization of measured spectra in any scale, displaying the whole spectrum, spectral region, neighbour of a specific spectral line.
- Profiling provides identification of the spectral lines.
- Superposition of images of several spectra for visual comparison. Comparing spectra measured using various types of spectrometers.
- Automatic correction of possible spectrum shift during the analysis.
- Automatic general semiquantitative analysis — search and processing of spectral lines with assessment of element concentrations.
- Automatic calculation of spectral line parameters — searching the line centre and points for background assessment under the line.
- Statistical processing of calibration graphs and analysis results. Discarding gross errors by the specified criteria.
- Calculation of calibration graphs on specified coordinates. Operation in the constant graph mode with re-calibration by reference samples (RS).
- Identification of spectral aliasing and interfering lines.
Fractionation of aliasing lines.
- Storage of spectral information and post-processing with reiterated addition of new lines and change of processing parameters.
- Analysis of line intensity variation over time.
- Differentiation of the beginning and the registration time of various elements depending on conditions of spectral excitation.
- Printing and saving spectra, analysis results and calibration graphs to a file.
- Transferring of analysis results to the database — plant-wide integration into the quality assurance system.

User Interface

Software Interface General Information

Atom 3.3 software appearance:



Software includes MDI-interface (multi-document interface). It means it allows simultaneous processing of several open documents (files). Use "Document" item in the main program menu, or "Document" tab on "Mode" toolbar, or "Ctrl+Tab" standard key combination to switch between documents.

Main user interface elements:

- main window header
- main menu
- toolbars
- status bar
- "Mode" toolbar
- document window (see below)

Document window has three main sections:

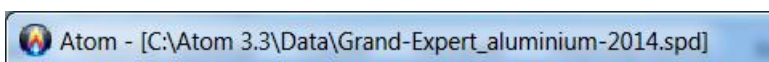
1. spectrum window in the upper left part of the document window
2. calibration graph window (upper right) and
3. analysis table window (below)

Main Window Header

Main window header in "Atom" software:

Header includes the following information:

- icon — "Atom" software logo
- program name



- full path to currently open file (see picture above), if program is in "Analysis" mode
- current mode name (for example, "Profiling", "Alloys", etc.)

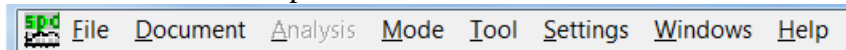


Program header also has standard window control buttons:

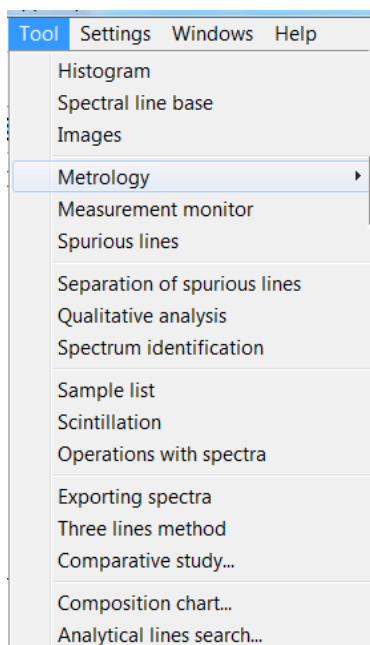
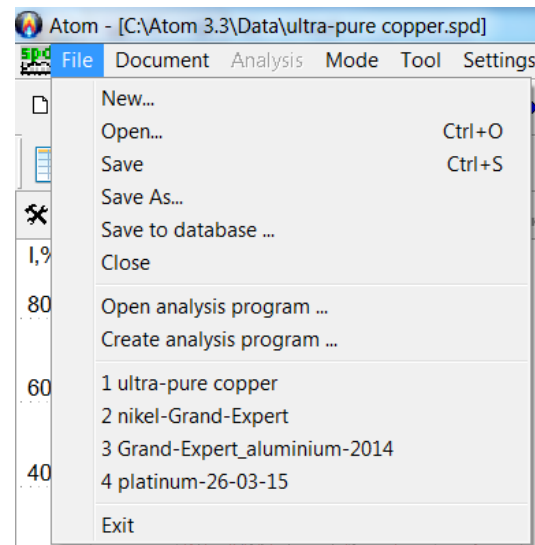
- Far right button (a cross against red background) is used to close the main program window. *Warning! Clicking this button closes "Atom" software.*
- Use left button to minimize main window in the Windows taskbar.
- Central button is used to change main window size: maximize / set necessary size.

Main Menu

main program menu is located under the drop-down bar:



- **File** menu contains such file control commands, as Save/Open File, New File, export current document to the database, create analysis program. List of recently used files is also located there. Use this list (without using "Open" dialog) to open quickly one of the recently used files.
- **"Document"** menu is used for fast switching between open documents (files). Current document is checked with a mark.
- **"Analysis"** menu item allows returning to the current document from any program mode (for example, from "Profiling" or "Alloys" mode). When the current document is active, this menu item is disabled (highlighted with grey colour).
- All available operation modes are located in **"Mode"** menu. When switching to any mode a new window opens, corresponding to the selected mode; current document and other modes become unavailable. Use **"Analysis"** or **"Document"** item (see above) to jump back to the current document. Detailed description of all possible program modes is presented in corresponding chapters of this manual.
- Advanced analysis tools that which do not fall under **"Mode"** item, for which there are no shortcut



Reference Material certification...
Online error control...

keys in any toolbar (since they are used rather infrequently) are located in **"Tool"** menu. Detailed description of all advanced analysis tools is provided in the corresponding chapters of this manual.

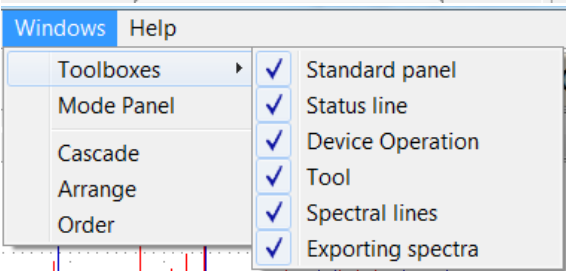
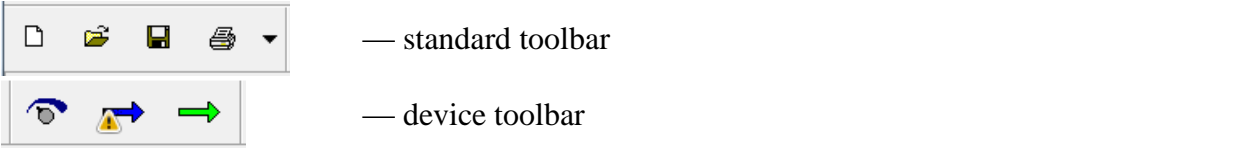
- Main settings of the program are located in **"Settings"** menu. Detailed description of all possible settings is provided in corresponding chapters of this manual.
- **"Windows"** menu item is standard for the majority of programs. Window size and position control commands (such as "Cascade", "Arrange", "Order" are located in this menu. Such commands as "Show"/"Hide" for all main tool-

bars, status bar and "Mode" panel are located in Windows menu as well. All panels currently displayed in the program are checked with a mark.

Toolbars

Toolbars are used to group controls by a feature. Buttons and/or drop-down lists are usually located there. There are three toolbars in "Atom" software:

- floating toolbars are usually located under the main menu; they are used to minimize them ("**Win-**dows" menu) and change their position ("push and drag"). Freeze toolbars through "Settings — Split document windows..." menu.

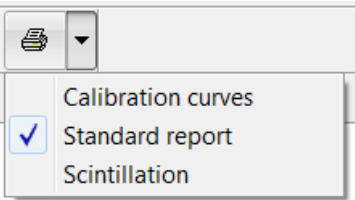
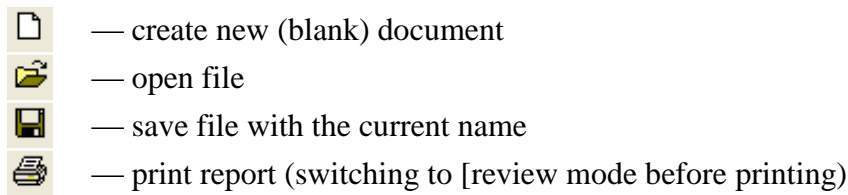


- Frozen" toolbars may not be minimized or dragged. Each toolbar is rigidly attached to its window. For example, spectrum window, calibration graph window toolbars or tables.

- toolbars with window size control buttons:

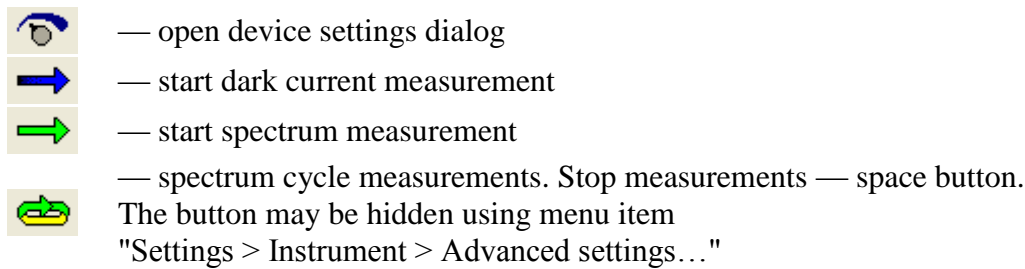


Standard Toolbar

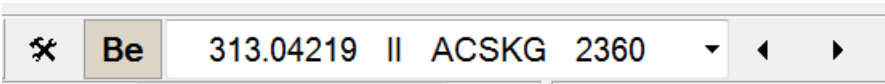


You can print different types of reports:
Standard report with analysis results.
Consolidated report with calibration graph parameters.
Consolidated scintillation report with results.

"Device" Toolbar



"Spectral Line" Toolbar

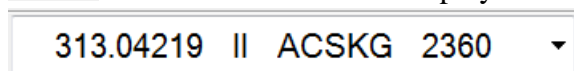




— open spectral line display settings dialog.



— open "Periodic table" dialog to select current chemical element. Name of the currently selected element is displayed.

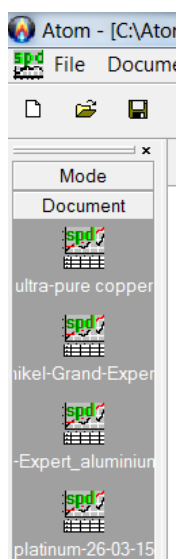
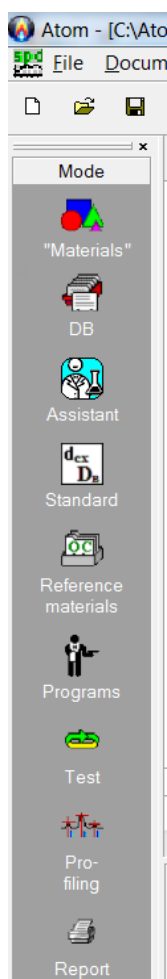


— current spectral line of the current chemical element. Click the triangle button at the right of the current line to display other lines. Select another line in the drop-down list (click it); it will become the current line. Use spectral line display setting dialog to set the list of lines and their position in the list.



— move within the list of lines of the current element (next/previous)

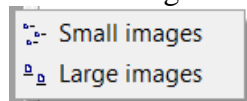
"Mode" Toolbar



"Mode" — "Document" toolbar is located at the left of the document window. Use "Windows"/"Mode" panel menu to show/hide his toolbar. Use "small cross" button located at the upper right side of toolbar to remove toolbar from the screen. Use mouse to change toolbar width by moving the right toolbar border (click-drag&drop). Toolbar is used for fast navigation through open documents ("Document" directory) and to open any program mode ("Mode" directory). Click the required directory name to open it.

The current document in "Document" directory is checked with a mark.

Right-click to open shortcut menu for "Mode" and "Document" menus. It allows resizing toolbar icons.



"Analysis" mode ("Engineer")

Document window

Document window — "Analysis" mode — primary tool for working with the program. Window includes three sections divided with a movable border (splitter).

1. spectrum window is located in the upper left section of the document window
2. calibration graph window (upper right) and
3. analysis table window (below)

Move borders with a mouse (click-drag&drop), which allows changing relative sizes of all three sections of the document. Each section has its unified interface with standard controls:

- Customized "frozen" toolbars. Position and size of these toolbars are fixed, but you can select controls from the list, available for this window section, and the order they are displayed on the toolbars. For further information see "Customize Toolbars".
- , and buttons which are usually located in the left upper corner of each section of the document window.



— open the section settings window



— open the section information window

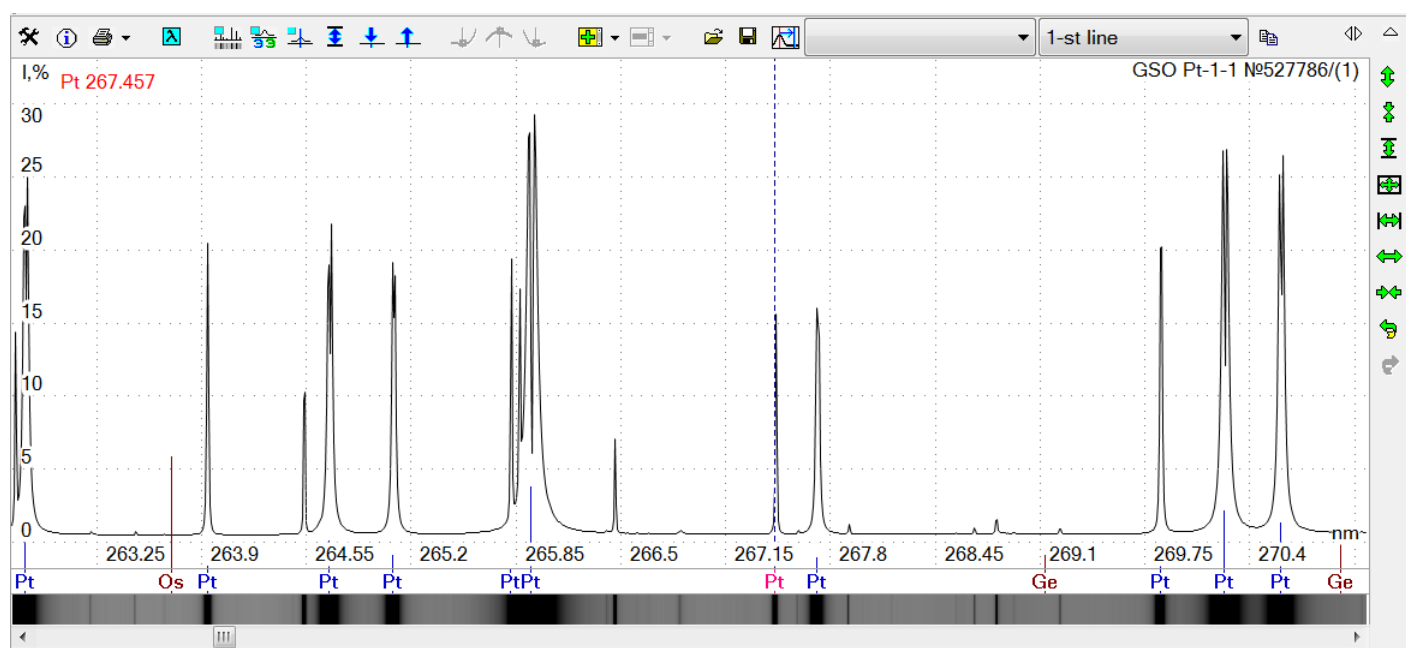


— print of section content (spectrum or calibration graph), switch to preview mode before printing

- Use special toolbars with black triangle buttons in the upper right corner of each document section to control the size of sections such as "maximize"/"minimize". For further information see "Toolbars".
- Use standard Windows controls such as scrolling bar to scroll through the section content (if all information cannot be viewed within the section).

Spectrum Window

Spectrum window is used to display the current spectrum as a graph, measured by MAES or selected in the analysis table.



Use the following tools to control spectrum scale and position:

1. Vertical toolbar at the right of the spectrum (a set of green arrow buttons). See "Main controls in 'Analysis' mode".
2. Right mouse button (see "Zooming with mouse").
3. Standard controls such as "scrolling bar" located at the right and the left of spectrum window. They are used to move the window — the visible part of the spectrum — along the spectrum in any of four directions. For more details, see Windows help.
4. You can also use left mouse button (click-drag&drop with shift key held down) to browse along the spectrum.
5. Double click left mouse button to move the spectrum horizontally so that the click point is in the centre of the window.

Main items of the spectrum window:

- **Spectrum as a Graph** You can view only a part of the spectrum according to the current spectrum scale and position. Horizontal axis (**number of diodes N or wave length (λ)**) is displayed under the spectrum, the vertical axis (**spectrum intensity**), per unit value or in percent (%) of the maximum value of the analogue-digital converter (ADC)) is displayed to the left of the spectrum. **Additional graphs** (8 colours) can be displayed in the window apart from the main current spectrum (highlighted with black colour).




Unit spectrum has the following display features:

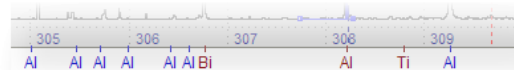
- *red spectrum region*. **ADC overflows** due to high radiation intensity during intensity measurements (off-scale reading). The intensity cannot be measured precisely in this region. Position mouse cursor in this region, "r" symbol will be added to the amplitude value in the status bar. For example, "64.747r".
- *spectrum region is not displayed in two cases*: First, **"faulty" diode** may be present in this spectrum region. Diode is marked as "faulty", if it cannot measure the intensity reliably enough (for more details see "Discarding faulty diodes"). Place mouse cursor in this region, "NODATA" string will be displayed in the status bar as the amplitude. Second, **gap between crystals** may be located in this spectrum region. Spectrum is not measured in gaps and is not displayed in the window.
- *spectrum region is displayed twice*. If spectrum is measured using MAES in a gapless or two-string version, there is an aliasing caused by neighbouring crystals.

- Toolbars are located **above and to the right** of main controls in spectrum window. Detailed description of each button is provided in "Main controls in 'Analysis' mode" section.

Use "Customize toolbars" (click  and choose "Toolbars" tab) to choose, which buttons to display, as well as their order and position).




- Two **"strings"** are located **immediately under** the spectrum image:



- *reference data display line with spectral line peak wavelengths for the selected atoms* (see "Spectral lines" toolbar). In addition to lines of selected atoms, lines of atoms from the analysis table, lines of atoms from the qualitative analysis, reference lines and some other lines may be displayed. Each line has its own colour. Open "Spectral Lines" dialog (click ) and select "Spectral Lines" tab) to control lines and their colours. Use button  or "Strings" dialog (click ) and select "Strings" tab) to show/hide this string. All peak wavelength values of spectral lines displayed in this string, are reference values and are stored in a file with **.mnd extension**.



- *"Photoplate"* displays the current spectrum as a photoplate: darkening value in each image point of a string is directly proportional to the logarithm of intensity in the corresponding spectrum point.



Photoplate is displayed in a scale corresponding to the current spectrum scale. Use button  (options: hide – , show several strings – ) to show this string.



- Red vertical **spectrum cursor** indicates spectrum location, where wavelength are measured, diode number and intensity displayed in the status bar. Click left mouse button in other spectrum region to reposition the cursor. If you set the "Set cursor at the peak" flag in "Peak search" dialog (click ) and select "Peak search" tab), the cursor will be automatically set at the peak nearest to cursor's primary position. Besides, if the flag is not set and the graph is in **N mode** (, see "Main 'Analysis' mode buttons"), then the cursor will be automatically set at the middle of the maximum diode from the histogram, which describes the peak nearest to the cursor's primary position. (step in the graph in **N mode**).
- Blue vertical **cursor** indicates the expected (reference) position on the peak spectrum of the selected spectral line, which was chosen in "Spectral lines" toolbar.

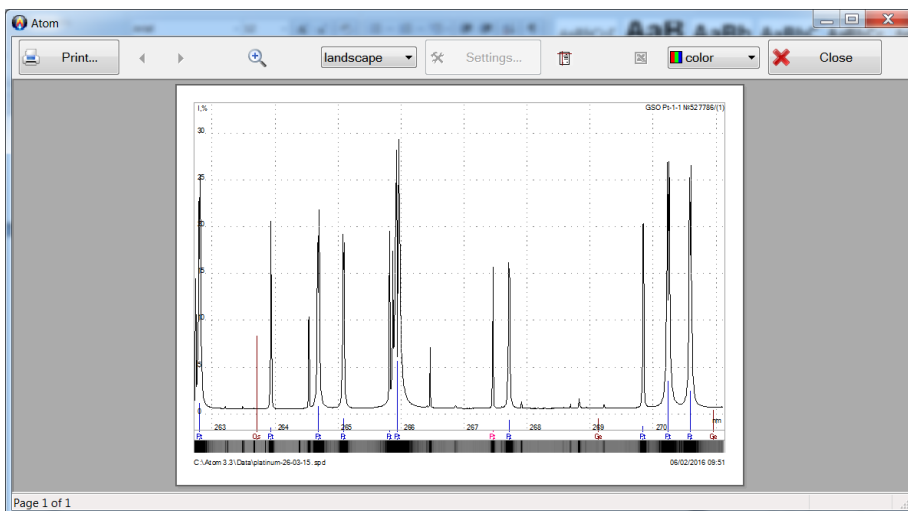
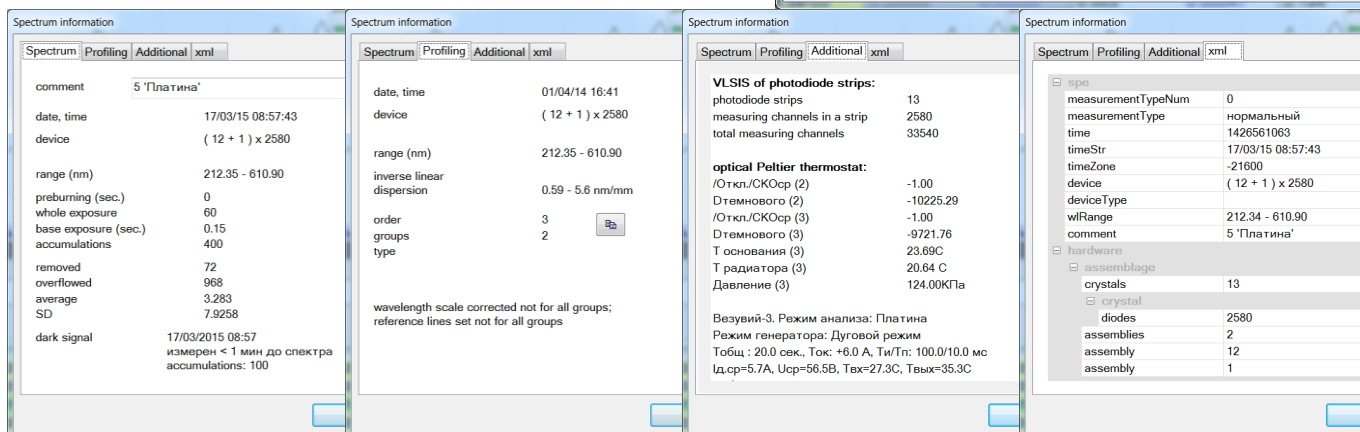
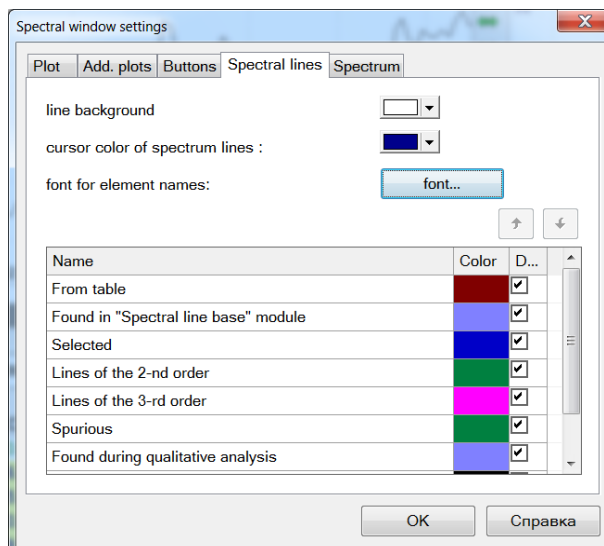
Use this toolbar to select another line or click one of lines displayed in the string displaying *reference data on peak wavelengths of spectral lines*, located under the spectrum. Click directly around this string, do not click spectral region or photoplate.


- **Current spectrum string** is displayed at the top right side.
 - select spectrum from the analysis table, to display "sample_name / parallel measurement number".
 - "Current spectrum" is displayed, if spectrum is the current spectrum, measured using MAES.
 - if spectrum is loaded from a file, this name is displayed.

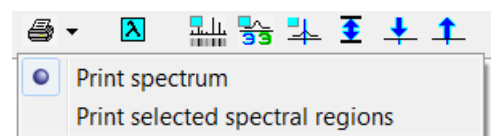
- if additional graphs are displayed, their description is also displayed, whereas text colour matches graph colour.

Use "General graph settings" dialog to turn on/off descriptions.

- Reference line list** is displayed in red colour in the upper left area of spectrum — if it is specified to display the list in the reference line settings; otherwise, just "reference" text is displayed.
- Current peak** is drawn on the spectrum, if you select the cell in the analysis table, which corresponds to the spectral line and the spectrum, and if you select one of the identified lines in the "Qualitative analysis". The following information is displayed when drawing the peak: line centre, left and right background points, resulting background level and peak contour.
- Window resizing toolbar** is located at the upper right part of spectrum window, see "Toolbars".
- Click  button to open the spectrum display settings dialog.
- Click  button to open the current spectrum information window. The window has two or three tabs: "Spectrum", "Profiling", "Advanced" and XML (they are available in all spectra measured using MAES via Ethernet interface or when working with Fireball generator).

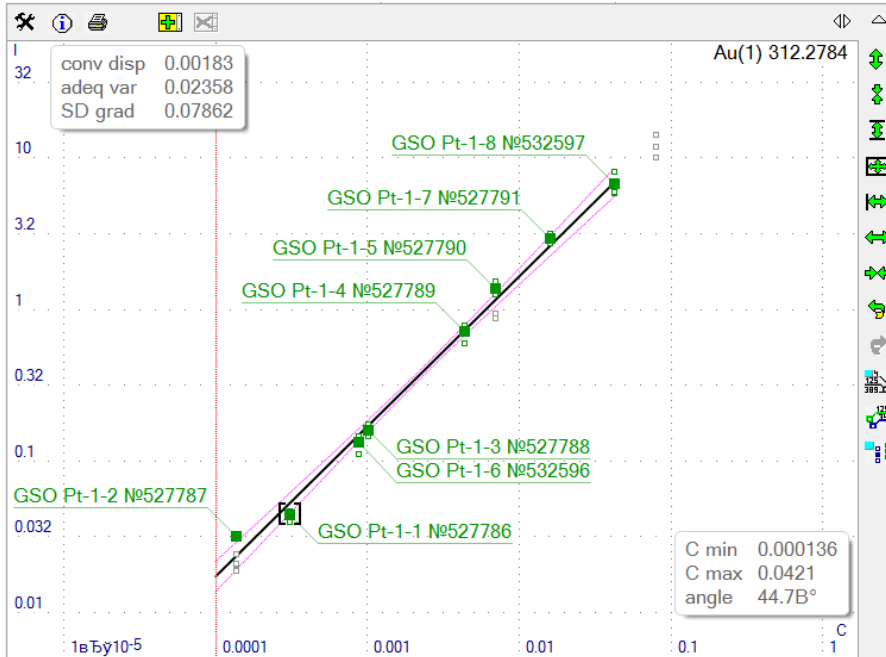


Click  to print the visible spectrum. The program will switch to print preview mode.



You can print the preselected spectrum regions besides the current spectrum. For detailed information, see "Printing several spectral regions" section.

Calibration Graph Window

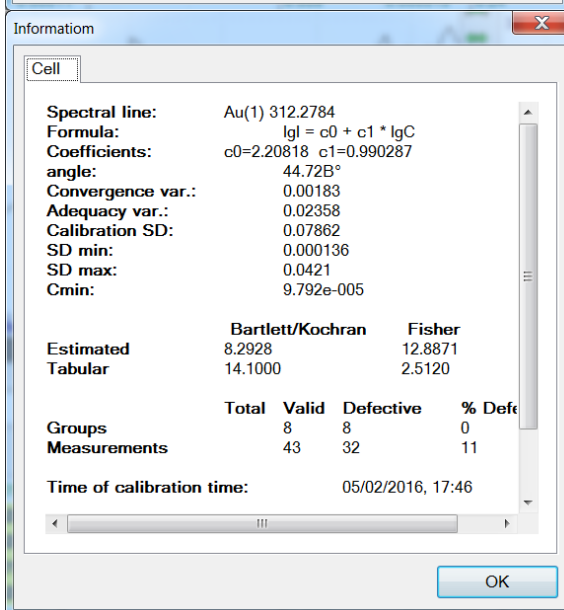
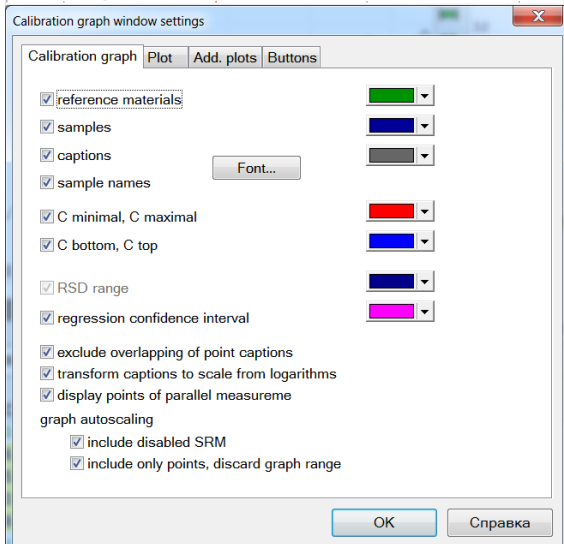



This window is used to display of the current (selected in the analysis table) calibration graph. Main items of the calibration graph window are as follows:

- **Displaying Calibration Graph** as a polynomial of the specified degree. Polynom degree, displayed graph range, as well as coordinates, on which it was built, depend on calibration graph calculation settings. Concentration (X axis) and intensity (Y axis) scales are displayed below and to the left of the graph.





Use the following to control graph scale and position:

1. toolbar located vertically at the right of the graph (a set of green arrow buttons). See "Main controls in 'Analysis' mode".
2. right mouse button (see "Zooming with mouse").
3. standard controls such as "scrolling bar" located at the right and the left of the graph. They are used to move the window — the visible part of the graph — along the graph in any of four directions. For more detailed information, see Windows help.
4. You can also use left mouse button to scroll through the graph (click-drag&drop) with shift key pressed.




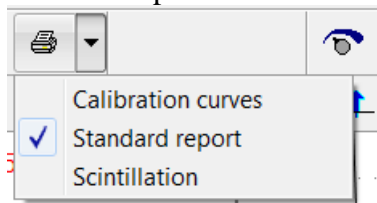
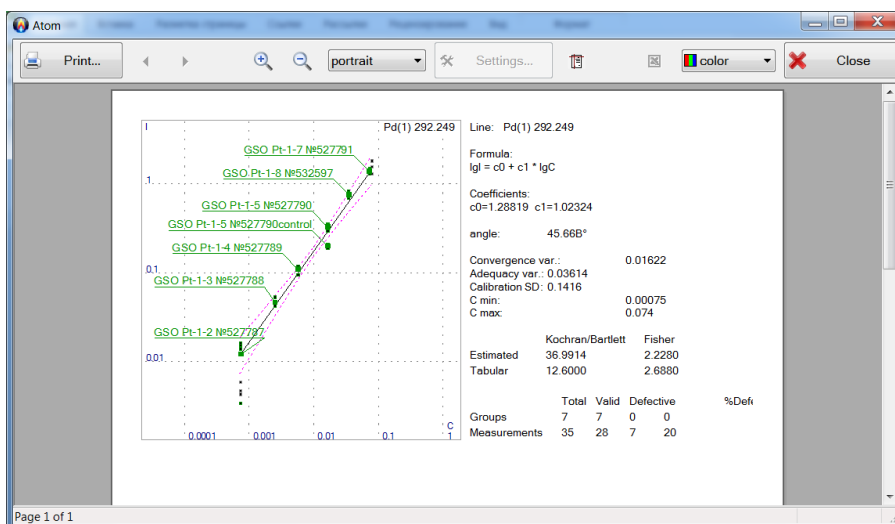
highlighted in red colour. Click red box and click button  in the analysis table to display error information.

Click left mouse button on any box to select a corresponding sample or parallel measurement in the analysis table; selected spectrum and peak will be displayed in the spectrum window (or all spectra of parallel measurements, if you selected the sample). Click by the box, to select the nearest point.

- **Blue vertical dotted lines** indicate positions of C_{lower} and C_{upper} parameters (see "Concentration calculation settings").
- **Red vertical dotted lines** indicate positions of C_{min} and C_{max} parameters (see "Calibration graph calculation settings").
- **Numeric parameters of the calibration graph** are displayed in the upper left part of the graph area: convergence dispersion, adequacy dispersion and calibration SD. To turn on/off the display, use "Calibration graph settings" (click  and select "Calibration graph" tab) using "caption" key.
- Two parameters are displayed in the lower left part of the graph area: **Cmin** and **Angle**. **Cmin** is entered by the user and is equal to the minimum concentration of the reference material among all reference samples, based on which the graph was plotted. To turn on/off display, to use "Calibration graph settings" (click  and select "Calibration graph" tab) using "caption" key. Angle is displayed, only if the graph is linear (linear polynom) and corresponds to the curve slope (in degrees). It is not possible to turn off display of this caption.
- **Spectral line name** is displayed in the upper right part of the graph area, for which the calibration graph was plotted. If additional graphs are displayed, their descriptions are also displayed, with text colour matching the graph colour. Use "General graph settings" (click  and select "Graph" tab) using "Display graph description" key to turn on/off the display.
- Toolbars with the calibration graph window controls are located above and to the right of the graph area. Detailed description of each button is provided in "Main controls in 'Analysis' mode" section. Use "Customize toolbars" dialog (click  and choose "Buttons" tab) to choose the type, order and position of buttons to be displayed.
- **Window resizing toolbar** is located in the upper right part of the calibration graph window, see "Toolbars" section.

Use mouse to select any text in the information window and paste it into Windows clipboard (Ctrl + Ins) to use in other programs (Word, Excel, etc.)

- Click  to print information on the calibration graph. The program will switch to Print preview mode. The program allows generating report for a group of the calibration graphs, including available information on results and the time of calculations, statistics, recalibration, etc. For more information see "Report" item.



Analysis Table Window


Analytical line intensity and concentration calculation results, as well as all contiguous data (such as names of samples and analytical lines, number of parallel measurements, mean calculated values, their absolute and

relative mean-square deviations, difference between parallel measurements, confidence intervals) are displayed in this window.


Main items of the analysis table:

2 GSO Pt-1-2 №527787											
Pd(1) 292.249											
	Pd 340.458		Pd 342.124		Pd	Rh 332.309		Rh 339.685		Rh(1) 343.489	
	I	C	I	C	C total	I	C	I	C	I	C
(2)	12.9	0.0033	5.08	0.0037	0.00293	1.43	0.0018	2.08	0.0017	5.15	0.0019
(3)	10.5	0.0027	4.42	0.0032	0.00264	1.51	0.0019	2.17	0.0018	5.42	0.0020
(4)	12.0	0.0031	4.96	0.0036	0.00306	1.22	0.0018	1.79	0.0017	4.51	0.0020
average	11.8	0.00305	4.81	0.00352	0.00287	1.3	0.00179	1.9	0.00176	4.88	0.00201
median		0.00308		0.00357			0.00178		0.00175		0.00200
repeatability											
4 GSO Pt-1-4 №527789		0.00580		0.00580			0.00468		0.00468		0.00468
(1)	22.0	0.0059	10.4	0.0088	0.00682	3.88	0.0053	5.90	0.0057	14.0	0.0054
(2)	20.3	0.0054	10.5	0.0089	0.00677	3.79	0.0052	5.76	0.0055	13.8	0.0054
(3)	17.2	0.0045	8.32	0.0067	0.00538	3.38	0.0051	5.31	0.0057	12.5	0.0055
(4)	18.6	0.0049	9.68	0.0081	0.00622	4.01	0.0052	6.06	0.0056	14.1	0.0053
average	20	0.0052	9.7	0.0081	0.0063	3.77	0.00520	5.76	0.00565	13.6	0.00538
median		0.0052		0.0084			0.00520		0.00565		0.00540
repeatability											
5 GSO Pt-1-5 №527790		0.0167		0.0167			0.00620		0.00620		0.00620
(1)	36.3	0.010	21.9	0.021	0.0181	4.60	0.0062	6.77	0.0065	16.1	0.0062
(2)	43.0	0.012	25.4	0.025	0.0200	4.21	0.0061	6.39	0.0066	15.6	0.0064
(3)	35.3	0.0098	19.9	0.019	0.0164	3.95	0.0057	5.99	0.0062	14.2	0.0059
(4)	35.9	0.010	21.2	0.020	0.0195	4.65	0.0061	7.04	0.0065	16.7	0.0062
average	37.6	> 0.0064	22	> 0.018	0.0185	4.35	0.00603	6.55	0.00646	15.7	0.00617
median		0.010		0.021			0.00608		0.00651		0.00616
repeatability											

- Table **columns** correspond to analytical and optional spectral lines, which were selected for the analysis.


Use button  in the table window toolbar to add a line to the table. Select the chemical element and its spectral line in the open dialog. Another way is to "click-drag&drop" the selected line from the spectrum window to the table.

To delete a line in the table, click right mouse button on the line to be deleted and select "*Delete column*" in the context menu.

Use "Columns" dialog, which is opened by clicking button  to add/delete columns, especially when it is necessary to delete or transfer several columns to another page.

Each column is an analytical line and consists of several columns:

- **I** — peak intensity;
- **C** — calculated concentration;
- **Iref** — reference line intensity;
- **I/Iref** — relative intensity (i.e. considering the reference line);
- **Csrm** — concentration of the standard reference material, attested (known) concentration, entered by the user. This field value is also displayed in green colour at the intersection of the sample string and the concentration column;
- **Stat. weight** is the statistical weight of reference samples;
- **width** is the spectral line width, measured in diodes.

Type of columns displayed in the table may be specified either by using the context menu (right-click the column header, further see "*Show column*" and "*Hide column*") or using the table window settings dialog (click  and select "Table" tab, then check columns to be displayed).



Optional columns may be displayed in the table apart from analytical lines:

"Concentration by Several Lines", "Sum of Concentrations", "Alloy Identification", "Concentration Factor", "User Defined Column", "Information from Spectrum".


Click small black triangle to the right of button  and select the required type of column in the drop-down menu to add an optional column to the table.


To change width of the column to be displayed, set the cursor on the right border in the table header, the cursor will take the form of horizontal arrows, then use the "click-drag&drop" method. Double click the column border to set automatically its width. Change the column width of the analytical line to change width of the same column for all lines in the table.


- Table strings correspond to the measured spectra, samples and several statistical calculated values (mean value, standard deviation, etc. for the sample).


All spectra added to the table (button ) are grouped by samples and are marked with  symbol. All spectra of one sample are recognized as parallel measurements ("parallels"). Each parallel measurement of a sample has its number, which is displayed in parentheses after the spectrum symbol, for example "(4)".


Each sample has its name which is entered by the user when adding the spectrum to the analysis table, as well as its own symbol indicating the sample type:


 – work sample;

 – reference standard;

 – blank sample (control test);





 – samples that contain burning spectra (for the analysis taking into account the burning of elements);

 – disabled sample – all current and newly added parallel measurements will be disabled.


 – disabled parallel measurement – all current and newly added lines will be disabled.


 – "Blank" parallel measurement, i.e. without a spectrum.


Strings with calculated numeric values are displayed at the end of the group of parallel measurements for each sample:

-  **Mean** value (mean sample concentration, intensity, etc.);
-  **SD** – standard deviation;
-  **RMS deviation** — root mean square deviation, in fractions or as a percentage;
- **Range** is the difference between the maximum and the minimum value = $|X_{\max} - X_{\min}|$;
-  **Confidence interval** of measured concentrations;
- **Median** of measured concentrations;
- **Repeatability** in combination with tabular tolerance from the selected standard;
- **Stability** in combination with tabular tolerance from the selected standard;
- **Result** — calculated according to GOST R ISO 5725-6-2002.

You can specify values in "Table" dialog (button , "Table" tab) to be displayed in the table.

Use button  to add spectra to the analysis table, which displays "Add current spectrum to the table" dialog. Using this command to add the current spectrum to the table and to display it in the spectrum window.

Use "Samples" dialog (button ) to add a sample name to the table without a current spectrum (with the specified number of blank spectra). This method is applied, when the table is filled in advance with sample names, and spectra are recorded only later.

Delete "sample" or "parallel measurements" lines from the table either using the context menu or "Samples" dialog (button .

When "samples" line is deleted, all its parallel measurements are deleted as well.

Use "Samples" dialog to delete only samples, but not specific parallel measurements and spectra. This dialog is especially useful to delete several samples at once.

Right-click the spectrum or sample caption and select "Delete sample or parallel measurement" in the opened menu to delete samples using the context menu. Select several spectra and/or samples to delete them at once. To do so, hold pressed "Ctrl" key and left-click captions of samples and parallel meas-

urements. Selected lines are highlighted with blue colour in the leftmost column (to the left of sample names). After that open context menu by clicking one of the selected lines, and select *"Delete sample or parallel measurement"*. ***It is necessary to right-click one of the selected lines!*** Otherwise, you will be prompted to delete the string you clicked, but not the string that you selected.



Current sample in the table is highlighted with a blue frame. It is displayed by default in "Add current spectrum to table" dialog, as well as in "Samples" dialog. When selecting the spectrum in the analysis table (selection of a cell or sample or parallel measurement header), the current sample name is also changed.


	Ag(1) 338.289	Ag(2) 338.289	Al 257.5094	Al 308.2
	I	C	I	C
* (4)				
x average				
median				
repeatability				
6 GSO Pt-1-6 №5				
(1)				
(2)				
(3)				
(4)				
x average				
median				
repeatability				
7 GSO Pt-1-7 №527791				
(1)				
(2)				
(3)				
(4)				
x average				
median				


Select *"Move sample or parallel measurement"* in the context menu to move all selected samples and parallel measurements to the specified sample. Besides, the selected parallel measurement, one sample or several samples with parallel measurements can be easily moved or copied to any open document.

- Table **cells** contain program calculation results. For example, analytical line intensity in the parallel measurement spectrum is displayed at the intersection of the parallel measurement and "I" column.

Various colours are used to display cells:

- **red colour** means an "error". The cell is mainly highlighted with red colour, if one of statistical criteria is not met (for example, RSD of comparison or Q-criteria), as well as if the analytical line is off-scale (**ADC overflow** takes place in some diode measurements due to high radiation intensity). , Left-click the red cell and press  to obtain information on the error;
- grey background means the cell is disabled. Select a cells to disable/enable it first (information on selection is described below), then press button , or use context menu (right-click) and then use *"Enable"* or *"Disable"* item. Intensity and concentration values of disabled cells do not take part in calculations (mean value, SD, etc.) and do have no effect on the final result. Disabling the cells, therefore, allows discarding some of the calculated values.
- Selected cells are drawn against blue background. Some operations may be performed only with selected cells (for example, enable/disable). Left-click a cell to select it. Click the column header or the parallel measurement header to select all cells corresponding to this column or line. When a sample is selected, all its parallel measurements are selected as well. Hold pressed "Ctrl" key to select several cells.
- Besides, some types of cells are highlighted with their colour. For example, **Coc** is displayed in green, calculated **concentration values** — in blue, sample calculated lines (mean value, SD, etc.) are highlighted with orange colour against yellow background.



Colours mentioned above are default, they can be changed using "Table layout" dialog (button , "Layout" tab).

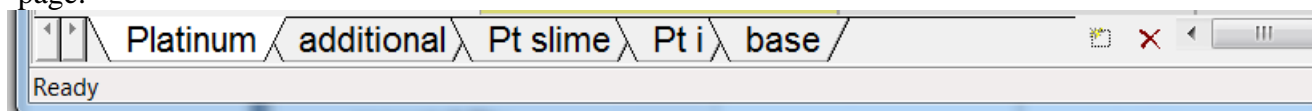
All numeric values displayed in the table are rounded to the specified number of significant digits — see "Table" dialog, "number of significant digits" list (button , "Table" tab).


If the displayed value does not fit in the table cell, only the first several symbols (those that fit) may be displayed + "...". For example, *"1.45..."* If you put the mouse cursor over this cell, a small yellow win-


dow will appear with the full value of the cell. In order to fit values in cells, it is necessary to adjust the respective column width (see "Columns" item above).



Values in some cells may be entered using the keyboard (for example, Coc, stat.weight, concentration factor and other values). To do so, double click the cell, enter the value and press "Enter".


- Use button  in the "Analysis table" toolbar to display **Analysis settings**. In the opened dialog you may change such analysis calculation settings as, for example, calculation method of analysis results or the type of calibration graph.
- Upper left cell of the table** is used to:
 - select the current spectrum registered with MAES;
 - select all table cells. For example, press , to enable or disable all table cells.
- Table page tabs** are located directly under the table and allow splitting one big table into several smaller tables. Different tables have different columns. Samples and parallel measurements are the same for all pages! For example, comparison lines or reference lines can be placed in an individual page.



Use button  to add new page. When the new page appears, you will be prompted to enter its name (input field will appear in the page name area); enter name using the keyboard and press "Enter".


Press  to delete current page. One of the possible actions will be proposed: delete all columns together with the page or move them to another page.



Click page name in the tab area to select one particular page. If you there are too many tabs (or if a tab name is too long), and they do not fit in the screen, use buttons ,  located to the left to browse through these tabs.

All newly added columns are located on the current page. Use "Columns" dialog () to move columns to another page. Or right-click column header, select "Move column" in the opened menu and enter the page you want to move column to.

- Toolbar** is located in the upper section of the analysis table window.

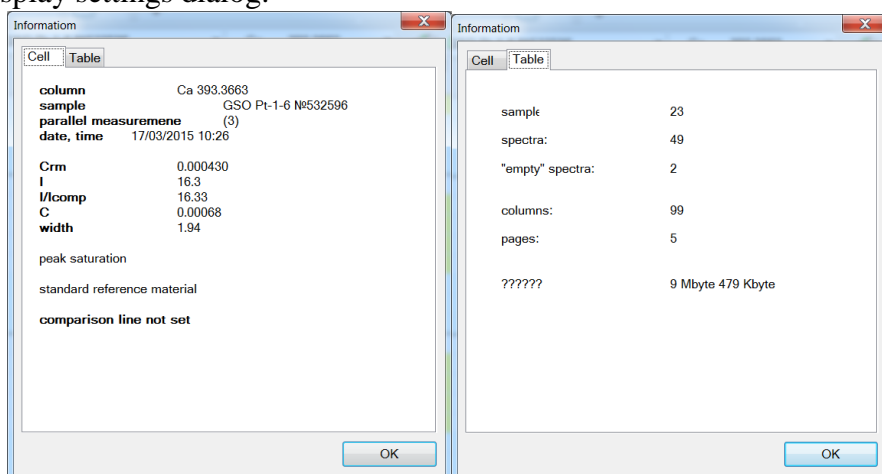
Detailed description of each button is presented in "Main controls in 'Analysis' mode" section.

Using "Customize toolbars" (click  and choose "Toolbars" tab) to choose buttons to be displayed, and their order and position).

- Vertical and horizontal scrolling bars.** Standard controls such as scrolling bar are located at the right and the left of the graph. They are used to move the window — visible part of the table — along the table in any of four directions.
- Click  button to open table display settings dialog.
- Use button  to open information window for the current selected cell ("Cell" tab) and for the entire table ("Table" tab).

Click the header of a respective parallel measurement to display any spectrum from the table in the spectrum window. If you click the sample header, all spectra of the sample parallel measurements will be displayed. Click the header of a respective line in the table to display any calibration graph of analytic lines in the calibration graph window.

Click any table cell to display simultaneously the calibration graph and the spectrum of the parallel measurement. If you click the cell corresponding to the sample header, all spectra of parallel measurements will be displayed.













Main Controls in "Analysis" Mode



Buttons used in main "Analysis" mode and their brief descriptions are presented below. Only buttons located in the frozen toolbars of the main windows in "Analysis" mode (spectrum, calibration graph and table), as well as some dialog buttons, are presented. Description of buttons located in "floating" toolbars under the main program menu is provided in "Toolbars" section.

Standard Window Buttons in "Analysis" Mode



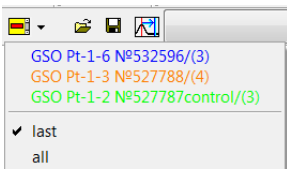
Graph zoom buttons

	— zoom in vertically		— zoom out vertically
	— fit the graph in the window vertically		— fit the graph in the window horizontally
	— fit the whole graph in the window		
	— zoom in horizontally		— zoom out horizontally
	— back to the previous graph scale		— restore initial scale
	— set fixed graph scale (see "Home" dialog)		

Spectrum Display Controls

	— switch graph display mode. In λ mode, graph points are connected using straight lines. In N mode each point is drawn as a step. Each step in the spectrum window corresponds to one diode.
	— enable/disable the spectrum in spectrum window: current (measured by MAES or read from file) or selected spectrum in the analysis table.

Additional Spectra/Graph Controls

	— add current spectrum/graph	
	— delete all additional spectra/graphs	

Save/Restore

Buttons are available in the spectrum window and in histogram window. Save either current spectrum in SPE format or the visible portion of the current spectrum in TXT format as a plain text file in the spectrum window. You can save histograms only in TXT format in the window; histogram is saved entirely, not only the part visible in the window.

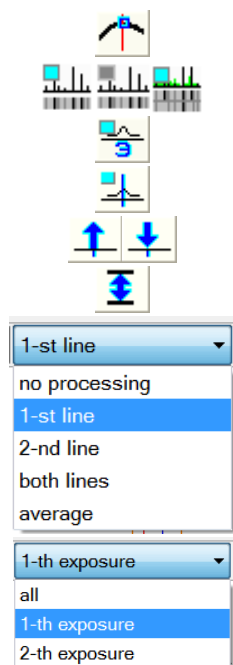
File being opened in the window is moved to additional graphs with the opened file name as a graph description string.

	— save current document to a file		— open document from file
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Spectrum Window



— set left/right point of the peak calculation background to the spectrum cursor position.



- set the peak centre to the spectrum cursor position.
- display or do not display "Photoplate" string/strings under the spectrum.
- display or do not display line of chemical element names under the spectrum.
- display or do not display relative intensity values from the reference book.
- zoom in/out spectral line intensity
- fit all intensity values into window

Set preferences when working with spectra measured by a double line MAES: "no processing" — all information is displayed in succession; "1st (2nd) string" — only the respective string; "both strings" — both strings are displayed simultaneously as per their relative positions; "average" — spectra of certain strings are combined into one average spectrum without gaps and aliasing.

Select the respective view when working with spectra measured in the mode of several exposures.

Calibration Graph Window

- enable/disable sample name view in the calibration graph window:
the program does not allow using the same names for different samples;
- each name is displayed at the upper left of the sample point;
- do not display sample names (only points are drawn).

- control of sample types displayed in the graph:
work samples only; reference samples only; both sample types.

Analysis Table Window



- open analysis settings dialog
- Add analytical line to analysis table dialog is opened by default; click small triangle button to open the optional columns menu.

"Sum of Concentrations" — sums concentration values of the selected chemical elements. It may be used to calculate the main composition.

Spectrum Data — special column with information from the spectrum of each parallel measurement. Any data available in the spectrum (size, time, profiling, generator, reference line parameters, etc.) may be displayed.

"Concentration by Several Lines" — calculates the resulting element concentration in a sample as per several analytical lines.

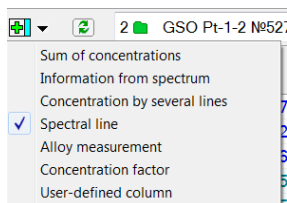
"Spectral Line" — the main column displaying calculated information on elements — intensity and concentration values.

"Alloy Determination" — determines all suitable alloys in "Alloys" mode based on calculated element concentrations.

"Concentration Factor" — factors, which all calculated concentrations are divided or multiplied by.

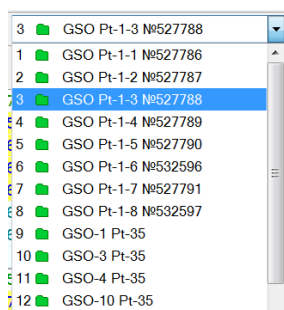
"User-Defined Column" — columns with arbitrary optional numeric or text information.

- add current spectrum to analysis table. Opens Add Spectrum Dialog.
- enable/disable the selected cells in analysis table.





1.
2.



List of current document samples for operative navigation and selection in the analysis table

Ag(1)	338.289
Te	238.578
Zn	213.8573
Zn(1)	334.5015
Zn(1)	334.557
additional	
Co	340.5117
Co	344.9168
Ge	259.2534
Ge	269.1341
Ge	270.9624
Re	221.426
Re	230.03

List of current document columns for operative navigation and selection in the analysis table. The list includes sheet names, spectral lines and additional columns.

List Selection Buttons



— deselect all list items



— invert selected items



— select all list items



— move selected items up/down the list

Status Bar is used to display various context information. It is located at the bottom of the main program window. Status bar may be displayed/hidden using "Windows/Toolbars/Status bar" menu item.

Status bar is split into three sections:

- Text information section. This section usually displays the help string for some menu items/buttons, as well as description text during a long-running operations such as "**calculation ...**" or "**completing the table...**". "**Ready**" means the program is ready for user commands.
- Central section displays spectrum cursor coordinates (red vertical dotted line) or coordinates of any graph (calibration graph, histogram etc.) Displayed information format:

wave_length (diode_number = range_number: range_diode_number): amplitude1, amplitude2, ...
198.8982 (4843.46) : 1.932 1.937 1.961 2.004 2.031 2.225 1.932

Amplitudes of all additional spectra (graphs) are also displayed in the spectrum (graph) window. Amplitude string is sorted in ascending order. Amplitude of the cursor's intersection with the current spectrum without any "additional" spectra is displayed in the last status bar section (see below).

- Last section displays signal amplitude at the cursor position in the current spectrum. This section is also used to indicate the long-running operation progress ("progress indicator").

Description of Modes

"MAES Test" mode

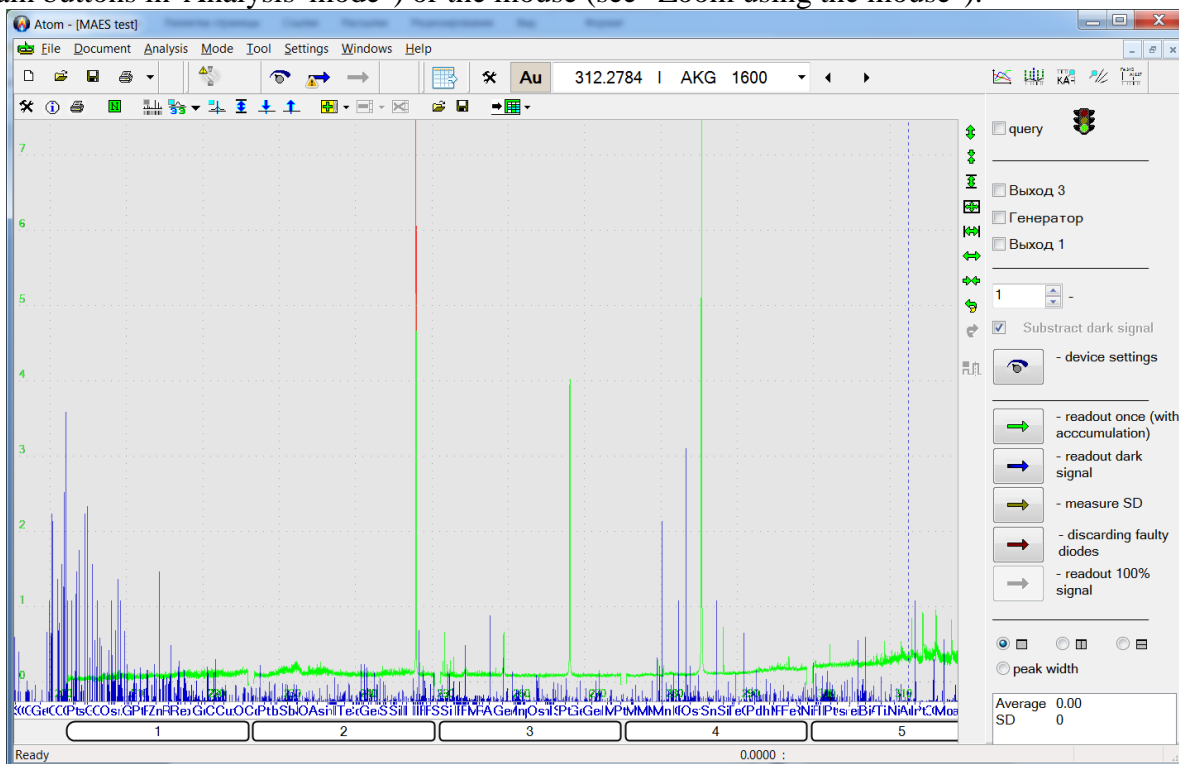
This mode is used to adjust and calibrate MAES and allows performing the following operations:


- measurement parameter setting;
- single measurements or interrogation in MAES cycle with the set amount of accumulations;
- dark signal measurement;
- spectrum SD measurement;
- "faulty" diodes screening;
- measurement of a "100%" signal for correction of diode gain factors;
- status indication and generator, external relay control, etc.;
- display of any part of the signal as a graph;
- splitting the signal window into two sections (vertically or horizontally) to display simultaneously two parts of the signal;

The signal display window corresponds to the spectrum window in "Analysis" mode. The window may be split into two sections, vertically or horizontally. To do so, select the splitting method in the lower right part of the mode window:

☐ — do not split the window; ☐ — split the window vertically into two sections; ☐ — split horizontally; ☐ ширина пиков — histogram with line width for each spectral line in the spectrum is in the lower part of the screen.

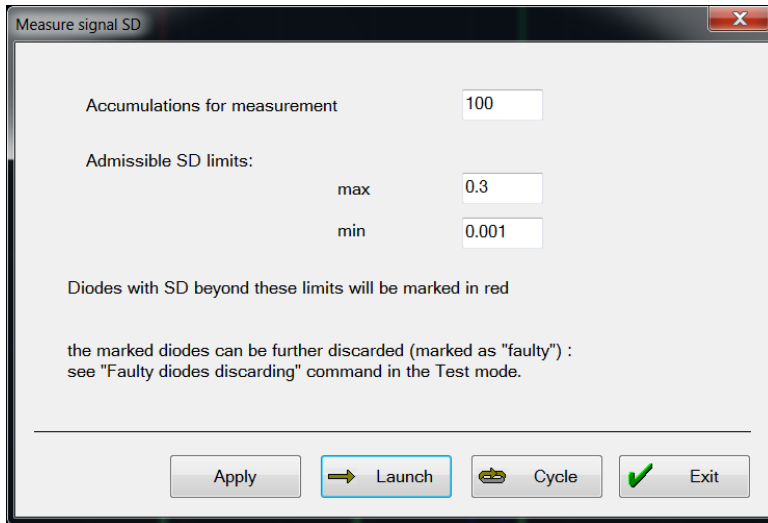
You can display a portion of the signal in each section. To do so, use zoom buttons in the window toolbar (see "Main buttons in 'Analysis' mode") or the mouse (see "Zoom using the mouse").



"Range" string is displayed under the signal image. Each white rectangle in the string corresponds to a specific crystal in MAES range. The digit inside the rectangle is a sequential number of the crystal. Left-click one of the rectangles to zoom the signal in X-axis to display the portion of the signal in the window that corresponds to the selected crystal. Use "Strings" dialog to show/hide this string; this dialog is opened by clicking button  and selecting "Strings" tab.

Traffic light is displayed at the right in the upper part of the window. Red light means "**Attention! Signal measurement...**", green light means "instrument ready for measurement", yellow light means "processing results (drawing, calculation, etc.)".

"Range query" — cyclic signal measurement using MAES. Measured signal is displayed in the window, and the next measurement starts. Uncheck the box to stop measurements. Following that, program will wait until the current measurement is completed and will terminate. Use Space key to start/stop measurements. Press once to start the current measurement, press twice to stop it, press for the third time for the "cold" interruption of the current measurement, if it has not been finished yet. The program switches to standby mode without having to wait for the last measurement to be completed.



Three buttons for device bit control are located below. Click the respective check box to change bit status. Function of bits depends on the instrument configuration. For example, one of the bits may control the start of plasma excitation generator.

"accumulations" — amount of accumulations for signal measurement. Signal is accumulated (summed) and is then divided by the specified number. As a result, we receive some average

signal. One accumulation corresponds to one MAES basic exposure.

"subtract dark signal" — enable/disable subtraction of a pre-registered dark signal from the current signal.

"Advanced" — opens MAES advanced settings dialog, for example, basic exposure settings. *Attention! Only highly qualified user shall change settings in this dialog while configuring the system! Incorrect settings may lead to the impossibility to perform measurements or to incorrect measurements of spectra using MAES!*



"calculate once" — starts single measurement of a signal with the number of accumulations specified in *accumulation* field.



"read dark signal" — starts dark signal measurement. Dark signal is saved, but not displayed in the spectrum window. It may be subsequently subtracted from any measured spectrum.



"measure SD" — opens dialog with SD measurement parameter settings. The signal is registered the specified number of times without accumulations, then signal SD is calculated for each range diode (see SD formula in "Algorithms" section). Calculated SD values are displayed as a graph in the window.

"Accumulations for measurement" — amount of accumulations for signal SD measurement (at least 2, 1000 max).

"SD margin" — specify acceptable range of SD values. If it is not necessary to use one of the range limits, or if the range is not used at all, delete the value from the respective input fields. Diodes, which SD signal exceeds the specified range, are highlighted with red colour and may be later discarded as faulty ones.


"OK" — starts SD measurement.

"Cancel" — terminates SD measurement.




discarding faulty diodes — opens dialog, where you can delete information on faulty diodes or mark all red diodes in the current spectrum as faulty. Measured signals and spectra are not drawn at the positions of faulty diodes. It is recognized that it is not possible to measure the intensity on these diodes with sufficient reliability.

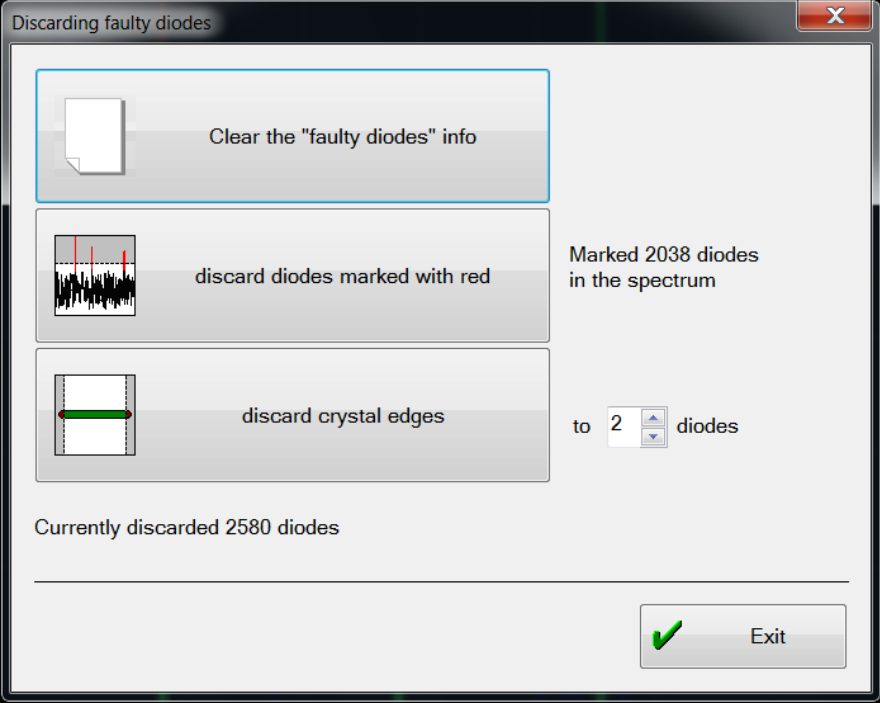
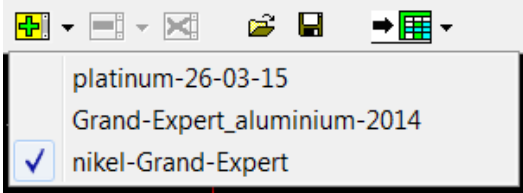
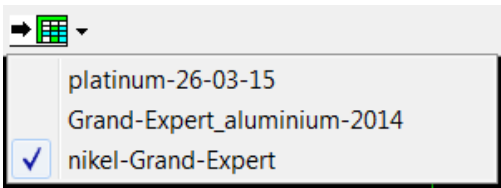
The dialog also allows updating information on faulty diodes when replacing MAES, discarding the specified number (usually, 1 or 2) of diodes, which are extreme for each crystal of photodiodes.

Apart from automatic search and marking with red colour during SD calculations, you can manually mark diodes using button .

read "100%" signal — the signal to be used for correction of diode gain factors (see "Gain factor measurement" in "Working with program" section) is measured and saved.

marked diode — used for manual selecting (highlighting with red colour) or deselecting of diodes. To do so, switch signal display to **N** mode (see "Graph display mode controls" in "Main buttons in 'Analysis' mode" section). Set a red vertical dotted cursor on one of the diodes (left-click it) and check the box to select it (highlighting with red colour), or uncheck this box to deselect it. Marked diodes are used to discard faulty diodes (see above).

Button  in the window toolbar is used to send measured signal to spectrum window of the current document. You may also select another open document in the drop-down menu. Current document is checked.



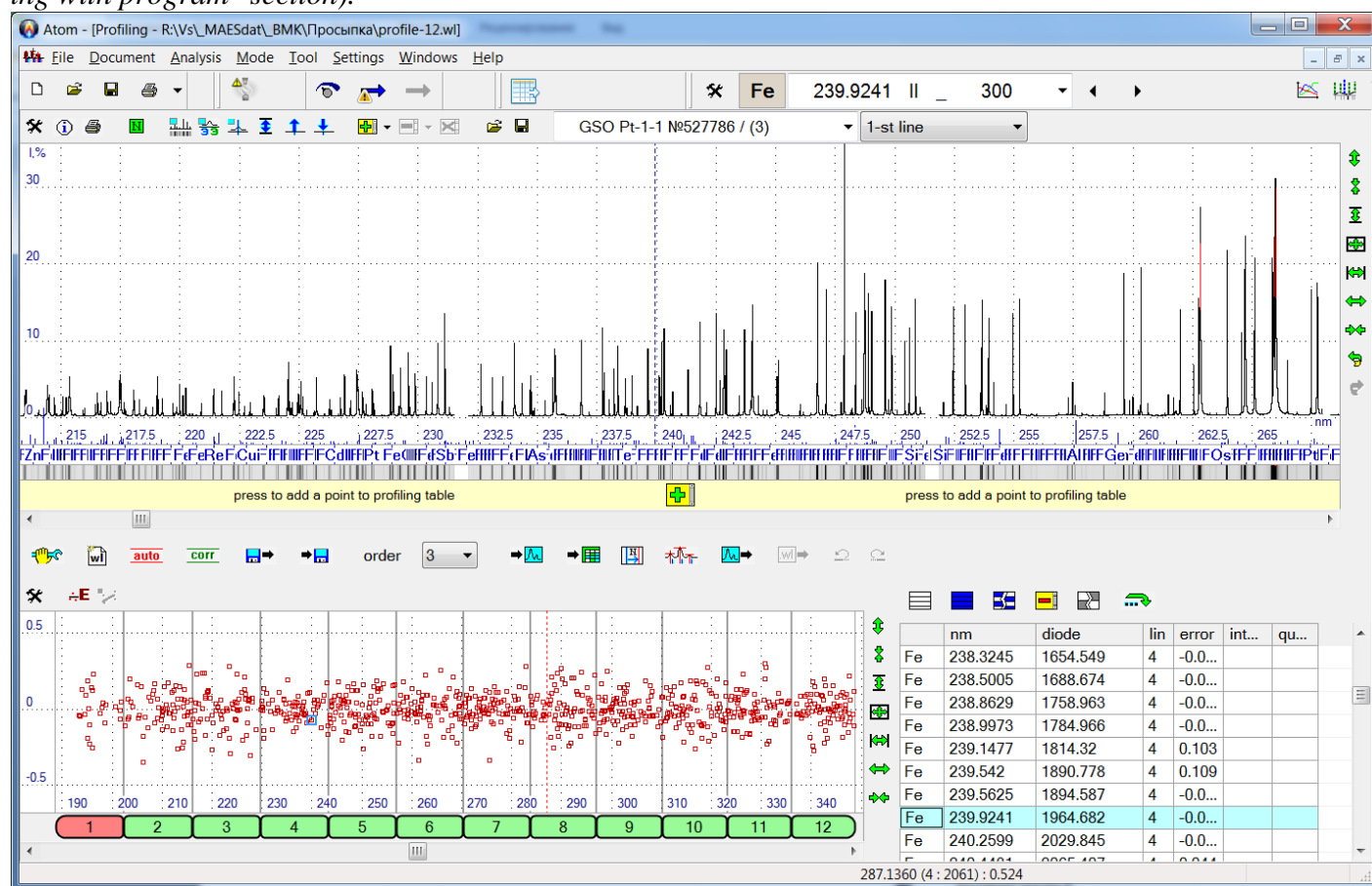
You can also move (copy) the spectrum to another open document as an "additional graph".

"Profiling" Mode

This mode is used to calculate **profiling** — **analytical function** of spectral line wavelength (nm) dependence on the receiver channel number (N), which its peak, as a polynom of the specified degree, corresponds to. Information on profiling is saved in a file with *.wl extension as a **compliance table** λ/N (see below), function polynom factors, gaps between crystals in the receiver and other additional information about the analyzer. Profiling is a process consisting in that the user with his/her knowledge on typical spectral lines of pure elements (carbon, copper, zinc, cadmium, magnesium, silicon, tungsten, etc.) makes up a **compliance table** of the spectral line peak (red cursor), which corresponds to the reference wavelength of the spectral line (blue cursor).

"Profiling" mode is used to find new profiling function or for significant variation of the previous function (for example, in case of intensive shift in MAES analyzer, or when MAES analyzer shall be replaced).

Use reference lines to correct the profiling function during the analysis (see "Reference lines" item in "Working with program" section).









"Profiling" mode window control functions


"Profiling" mode window includes three main sections:




- **spectrum window** in the upper part of the window. Current spectrum of the current document is displayed in the spectrum window. To display the spectrum in "Profiling" mode, select "Documents" in the main program menu, or open a new document and select the required spectrum from the analysis table, register it using MAES or open it from a file. Use the drop-down list to get on-line access to current document spectra.
- **profiling error window** is located at the left bottom. Generally, polynoms, calculated by the program, which describe the profiling function, do not pass exactly through calibration points selected by the user. *Profiling error is a deviation of the polynom from the point expressed in diode numbers.* Profiling errors are displayed for each point as red squares in this window. X-axis designates diode numbers. Display is divided into MAES detector crystals with vertical lines. Left-click the crystal image (white rectangles with sequential numbers inside them) to zoom in/out the error window and the spectrum window along

X-axis, so that the only the selected crystal is displayed. Y-axis designates profiling error in diode numbers. Usually, upon completion of profiling, all errors are within a range of not more than ± 0.5 diodes. It provides reliable detection of peaks corresponding to analytical lines in the analysis table.


- **table of calibration points** is located in the lower right part of the window. All points are located with the wavelength increasing. First column specifies names of chemical elements in the spectral line, "*nm*" column specifies spectral line wavelengths, "*diode*" is the peak centre position in diode numbers, "*lin*" is the crystal number, where the point is located, "*error*" is the profiling error. To add a point, click  (see below); to delete it, select points and click . Selected points may be disabled or re-enabled using button . Double click a point to disable and enable it. Disabled points become highlighted with grey background and with "-" symbol preceding the element name. Standard "Undo" ( button) and "Redo" ( button) operations may be used for all operations with calibration points, such as Add/Delete, Enable/Disable, Profiling shift and Redetermine maximums (more details on these operations are provided below).

To build a new profiling, it is recommended to use button  on the toolbar under the spectrum window. Specify the number of crystals, crystal size (all default values are the same as in MAES), the approximate spectral range (this information is used for the first approximation to the profiling searched for) and comments in open dialogs. Press "Next" or "Back" to navigate through dialogs; press "Ready" to finish; press "Cancel" to cancel. Upon completion the program will clear the table with calibration points and build the first approximation to profiling.

Buttons  under the spectrum are used to add calibration points. First, select the reference spectral line. Blue vertical cursor will appear in the spectral line position. Then specify the line centre in the spectrum, which will correspond to the selected spectral line. It is recommended to specify such spectrum scale, which allows reliable determining that you located the required line in the spectrum, but not one of the neighbour lines.

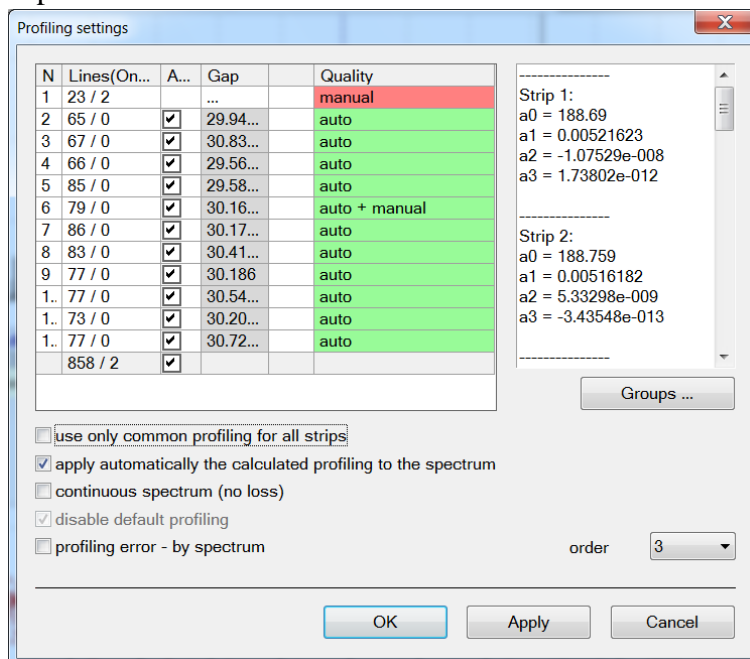
To run correct operation, enable "Set cursor on the line peak" key! (Button  on the spectrum window toolbar in "Profiling" mode, "Line in the spectrum" tab). Red vertical cursor of the spectrum shall move to the specified line peak in the spectrum. Now press  — the specified point will be added to the calibration point table and the program will automatically calculate new profiling. If this point already exists in the table (spectrum line coincides), new point will not be added, information on the line centre in the spectrum will be updated. If "*automatically apply calculated profiling to spectrum*" key is set in profiling calculation settings (see below), new profiling will be applied to the spectrum. If this key is not set, use button  (see below) to manually apply current calculated profiling to the spectrum.

The following operations may be executed with profiling points:)Select, Delete, Enable/Disable, Cancel, Redo (detailed information on these operations is provided above in "*calibration point table*" section), as well as "shift" and "Redetermine peaks" (see below).

Using calibration points, excluding calibration point disabled by the user, the program builds polynoms of the specified degree according to the **profiling settings**, which may be opened by pressing button :

"profiling degree" — specify the minimum required degree of polynoms from 1 to 5. If possible, use the minimal degree to create the final profiling.

MAES range crystal table is displayed In the upper left part of the dialog. First column shows the sequential number of the crystal, the second column displays information on the number of profiling calibration points (lines) in each crystal and how many




points are disabled. "Gap" column specifies the distance between crystal edges (between current and previous) expressed in diodes. "Auto" column allows adjusting the method for gap setting. If the key is set, the program automatically selects the gap value while calculating the profiling (the field is highlighted with grey background, and it is not possible to enter a value using the keyboard); user defined value is applied, if the key is not set (the field is highlighted with the white background and you can enter the value manually). Crystal group number is displayed in "Group" column, if grouping is used. If grouping is not used, "0" is displayed for all crystals. More information on profiling groups is provided below.

Total number of profiling points and total number of disabled points are displayed in the last table line (under the bold line). Besides, check mark in "Auto" column controls all check marks in this column. Enable it to enable check marks for all crystals, and vice versa.


Polynom factors will be displayed for each crystal individually in the upper right part of the dialog.


"use only general profiling for all ranges" — switched on, when one polynom was used for all crystals to create profiling; otherwise, own polynom is calculated for each crystal. Do not use this key to create the final profiling, since one polynom does not allow precise enough description of the consistency of wavelengths and diode numbers.



"automatically apply the calculated profiling to the spectrum" — the program calculates new profiling after adding/deleting, enabling/disabling profiling points, as well as after changing the settings. The key is set so that new profiling can be immediately applied to the spectrum. Use button  to manually apply the profiling to the spectrum.




"Groups ..." — opens Edit dialog for information on Profiling groups. Use this dialog to delete information on groups or to split crystals into groups again. Groups are used to split profiling into several independent areas. No checks (for example, check of monotonicity, profiling function increase) are performed, no gaps are calculated between crystals from different groups. Therefore, one profiling, may be split into several independent profilings. Each crystal belongs entirely to one group only. This splitting may be applied for instruments of "STE-1" type (multiline spectrometers, each line has its profiling), in "Grand", DFS-36 configurations, etc., where assemblages with one or several crystals are located at a considerable distance, or in case when a common spectrum is formed from the spectra of two or more different spectrometers (for example, Grand, SpectroLab).


Use "Next" and "Back" buttons to navigate through the grouping wizard; press "Ready" or "Cancel" to exit. Press "OK" or "Cancel" to exit from "Profiling settings" dialog. "Apply" allows estimating changes in profiling without leaving the dialog.


Use button  under the spectrum window to assign manually a profiling to the current spectrum. If the current spectrum is selected from the analysis table and a new profiling is assigned to this spectrum, while moving to the document, which this spectrum was taken from, the program will report: *"Spectrum profiling from the analysis table was changed. Recalculate analysis table?"* If you answer "Yes", new profiling will be assigned to the spectrum, and the program will recalculate line intensity values for this spectrum; if you answer No, spectrum profiling from the table will remain the same. Profiling is assigned without a confirmation to the currently measured and loaded from file spectrum.


Use button  after the prompt to confirm operation to assign current profiling to all spectra from the current document analysis table. Current document is indicated with a check mark in "Documents" menu of the main program menu.





Buttons  and  are used to copy profiling from one spectrum to another.

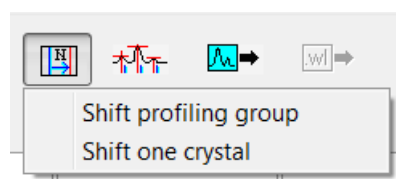
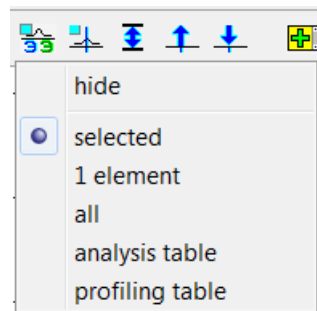
Example: Select spectrum from the analysis table in one of the documents or load it from file and move to "Profiling" mode. Press button ; profiling from the selected spectrum becomes current. Current profiling will be assigned to all spectra to be measured, and is also used to perform operations *"apply current profiling to current spectrum"* (button ) and *"apply current profiling to all spectra in the analysis table"* (button )



In order to apply profiling to another spectrum, move to one of the documents, select the required spectrum, move to "Profiling" mode and press button . When the spectrum profiling is current, several buttons become unavailable in "Profiling" mode, since profiling from the spectra does not contain enough informa-


tion (including **compliance tables**) to perform these commands. In particular, do not add or enable/disable points or change profiling calculation settings; points are not displayed in the table. You can either apply spectrum profiling or save it, you can also load initial profiling from a file and create a new profiling. Press  to load initial profiling from the file.


Use Profiling table item from the drop-down menu of control  to display profiling lines in the spectrum window; spectral lines will be highlighted with dark green colour (by default).

Button  is used for profiling shift for all spectra or individual lines. If profiling groups are available, shift is performed for each group individually. Select spectral line (blue spectrum cursor), set red cursor on the corresponding peak in the spectral line and press . The program will displace calibration points of the spectrum profiling (changing diode numbers and, probably, crystal numbers, if the point will move to another line due to shift) and calculate new profiling polynoms. Program will displace polynoms, if there are no calibration points. *Make sure before the operation that spectrum profiling is current (press ).* Upon completion of the operation, if "automatically apply calculated profiling to spectrum" key is not set (see above), press  to see the result of shift. If red and blue cursors were on different crystals, then after shift the reference value of the spectral line may not coincide with its maximum in the spectrum. Repeat the operation in case of a discrepancy.



Measure the final profiling element spectrum (usually, tungsten) and press  — "**Redetermine peak points**" to create final profiling after shift. Program will accurately find positions of line peaks in the place of calibration points and recalculate the profiling. Points with peaks that cannot be found, will be automatically disabled. Both operations may be cancelled later by pressing button .

ATTENTION! Do not forget to press , or specify "automatically apply profiling"!

Use button  to open menu with additional commands for work with points in the table:

"**enable/disable all**" — process all points in the compliance table.

"**enable/disable W**" — process all points for the current element (for example, W) in the compliance table.

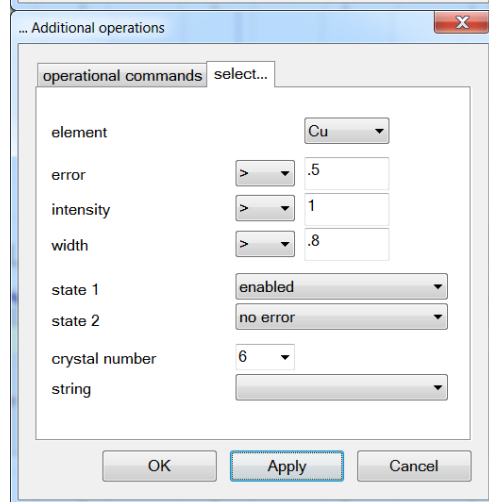
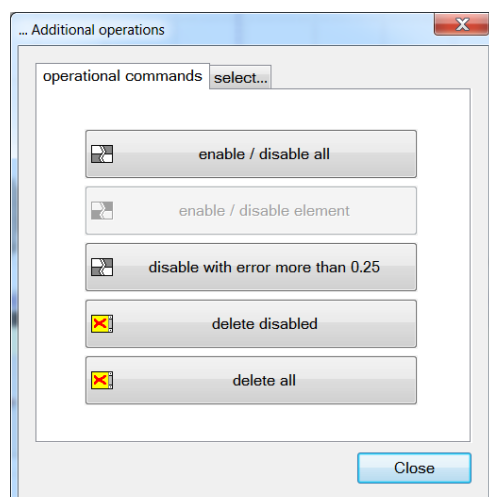
"**Disable with an error above 0.5**" — select all points with error value beyond the range specified in the profiling error window (0,5 in the example). All points with an error value above the specified value will be selected.

"**Delete disabled points**" — delete all disabled points.


"**Delete all**" — delete all calibration points.


"...Advanced parameters" allow selecting more specific conditions for selection of compliance points — for example, a specific crystal or a line in two-line spectrum, a set of points with a specific intensity, etc.


When several criteria are specified, they are combined with "and" symbol, i.e. in order to select a point, this point shall meet all specified criteria.



The following operations shall be performed for manual profiling:

1. Register spectrum of tungsten and several known elements, such as, for example, graphite, copper, silicon etc., and save it in the analysis table. Registration time in arc mode may be set up to 10 s.
2. Select one of the measured spectra. Set red cursor on the peak line in a spectrum, which wavelength is known from the general view of spectrum based on own experience (for example, a group of strong lines with a known ratio of intensity values).
3. Select the reference wavelength of a spectral line of the element (blue cursor), which must correspond to this line in the spectrum.
4. Enter the *spectrum line wavelength and the diode number of the peak line in the spectrum* into the **compliance table** (button  located under the spectrum).
5. Repeat operations 2, 3,4 and add compliance pairs to the table in the amount exceeding the polynom degree, to calculate profiling function. In such case information on spectral lines located uniformly across the spectrum length shall be entered into the table.
6. If the number of spectral lines known to operators in the selected spectrum is insufficient to calculate the profiling function, then the next material spectrum is selected, and the process of filling the compliance table continues. If you can make up a table from two and more pairs, go to item 7 and calculate the initial profiling function. It shall be applied to the next selected spectrum. It will be much easier further to fill the compliance table.
7. Program can create polynoms of the given degree using the least squares method and relying on compliance pairs, which describe the correspondence rule in the form of an analytical function.
8. You can create a very precise profiling using tungsten spectra; however, you can start creating a profiling after you receive the first approximate profiling using more simple spectra.


After the profiling function is created, save it to a file with *.wl extension (usually, "atom.wl") by clicking button . If you forget to do so, the program will ask you to save the modified profiling when exiting. If you want to automatically load the saved file when the program starts, specify this in "Files" dialog, which can be opened using "Settings"/"Files..." item in the main program menu. When starting the program, this profiling becomes current and may applied to all new spectra measured by MAES.


Perform the following operations to run profiling automatically – select tungsten spectrum by clicking button , select spectrometer type in the opened autoprofilng settings window (e.g., STE-1) and press "Profile..." button. As a result, a new set of formulae is calculated for most spectrometers (excluding prism spectrometers).



If the result is satisfactory, "Apply" it, the set of points and formulae will pass to the current profiling, which must be saved to file.

"Report" Mode

"Report" mode is used to set up and preview reports generated by the program before printing them. Open this mode either clicking button  located in the standard toolbar, or using "Mode"/"Report" item in the main program menu.

Program shows in this mode the way the printed report will look like. Press button  in the upper left corner to print the report.

organization
Name
device
analysis
date, time

Gold Plant Laboratory
John Smith
BAIRD
Platinum method № 026-C-2009
18/03/2015 08:33

GSO Pt-1-2 №527787

Elem	%mass	rsd, %	(N)	Elem	%mass	rsd, %	(N)	Elem	%mass	rsd, %	(N)
Ag	0.0010	12.8	4	Fe	! 0.000297	6.83	4	Pd	0.000626	8.97	4
Ag	0.0012	16.4	4	Fe	! 0.00029	12.3	4	Pd	0.00070	11.3	4
Al	0.00059	11.1	4	Fe	! 0.00028	10.1	4	Rh	0.000468	5.37	4
As	0.0012	15.7	4	Ir	! 0.00057	18.9	3	Rh	0.000604	5.19	4
Au	0.000182	2.39	4	Mg	0.00040	26.3	4	Ru	0.00033	10.4	4
Bi	0.00020	11.5	4	Mg	0.00039	25.5	4	Sb	0.00053	19.0	4
Ca	< 0.00041	15.5	4	Mn	0.00045	15.4	4	Si	...	0	
Ca	< 0.00010	39.1	4	Mo	0.0020	23.4	4	Sn	0.000284	9.74	4
Cd	0.0021	33.3	4	Ni	0.00035	13.7	4	Te	0.0018	13.0	4
Cr	0.0014	20.3	4	Pb	0.00029	21.7	4	Zn	0.00031	18.5	4
Cu	< 0.00030	18.2	4	Pd	0.000712	9.46	4				

GSO Pt-1-3 №527788

Elem	%mass	rsd, %	(N)	Elem	%mass	rsd, %	(N)	Elem	%mass	rsd, %	(N)
Ag	0.00126	8.13	4	Fe	...	0		Pd	0.00278	4.93	4
Ag	0.0016	10.5	4	Fe	0.00115	4.30	4	Pd	0.00305	8.90	4
Al	0.0037	19.7	4	Fe	0.00113	4.31	4	Rh	0.00176	2.10	4
As	0.00257	4.60	4	Ir	! 0.0015	11.1	4	Rh	0.00201	2.90	4
Au	0.000915	8.18	4	Mg	0.0020	16.0	4	Ru	0.0012	11.1	4
Bi	0.00149	7.22	4	Mg	0.0021	13.6	4	Sb	0.000999	4.00	4
Ca	0.00132	8.05	4	Mn	0.00133	6.48	4	Si	0.0039	16.7	4

page 1 of 12

C:\Atom 3.3\Data\platinum-26-03-15.snd

06/02/2016 18:23

Print...

landscap

Settings...

color

Close

Page margins, mm

Top

5

mm

Left

5

mm

Right

5

mm

Bottom

6

mm

OK

Cancel

Report template selection

median

report to customer A



statistical report


template


OK

No template


Cancel


Buttons  and  show previous and next pages of report respectively.


Button  prints one page or two pages of the report respectively;

Button  is used to zoom in/out report pages.

"Page Orientation" – "portrait (vertical) or "landscape" (horizontal).


Use button  to open Page settings dialog (space from page edge). Page fields are specified in mm from the edge of print area of the printer. Print area depends on the printer model.

Use button  to copy report to system buffer as a text, which can be pasted into Microsoft Word file or OpenOfficeWriter word processor file.

Use button  to open dialog to export report to Excel program. Select template from the list and press **"OK"**. Or press **"No template"** to export it without a template. Press **"Cancel"** to cancel export.

"Template" — Excel file saved earlier in "Templates" directory of "Atom" software root directory. Use template to create headers, signatures, fonts, etc. according to formats accepted in your organization. If one of cells is called "Start" in the template, program report will display starting from this cell, otherwise, it will be displayed starting from the upper left A1 cell.

Only calculation results and table headers are exported. Report header, title and signature are not exported, because the template already includes them.

Use button  to open report settings dialog with several tabs.

"Format"

"Report form":

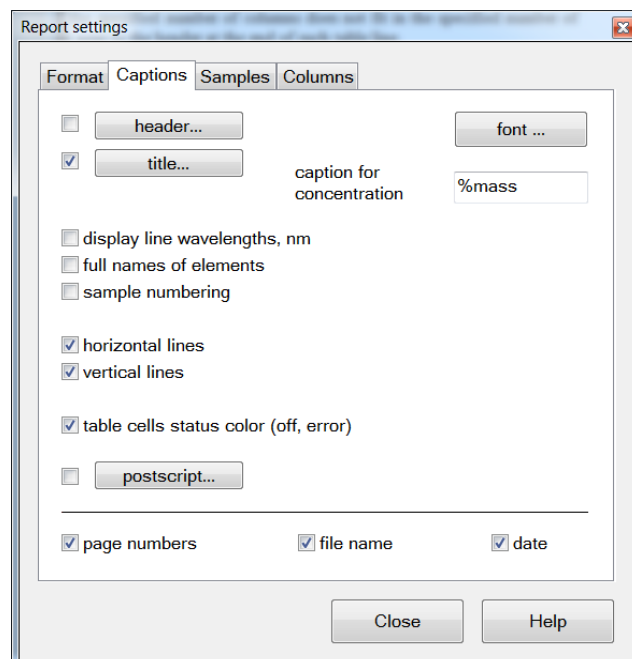
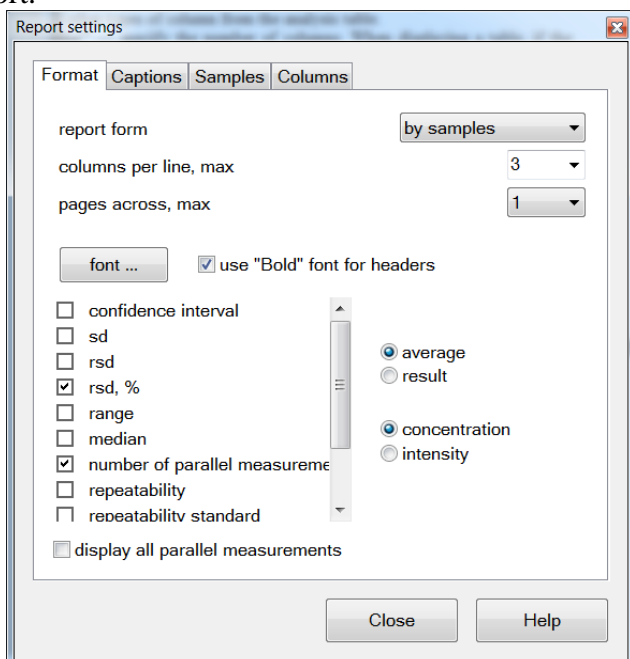
"Sample form" — analysis result table is displayed for each sample individually.

"Element report" — all analysis results are displayed in one table, where strings correspond to samples, columns correspond to analytical lines or other types of column from the analysis table.

"Max number of columns in a string" — specify the number of columns. When displaying a table, if the number of columns is more than the specified value; the remaining part of the table is moved down, allowing thus printing bigger tables on paper of any format.

"Max width of pages" — when displaying a report the program can move data not only down (previous item), but also to the right, if the specified **"Number of columns per string"** (previous item) did not fit in one sheet. Letters corresponding to the number of page widthwise are added to page numbers while moving to right. For example, *"1.a, 1.б, ..."*. If the specified number of columns does not fit in the specified number of pages widthwise, *"..."* symbol appears next to the header at the end of each table line.

"Choose font ..." — opens standard Font dialog, where you can specify the font and its size to output the report.



"Use 'bold' font in headers" – enables output of headers of table lines and columns with bold font.

Besides the calculated analysis results, concentration or intensity values, the program can output calculated statistical numeric parameters:

"RSD", "difference", "confidence limit", "median", "SD", "number of parallel measurements", etc.— various statistical parameters as per the analysis table data. They may be displayed both individually and in groups.

"Captions"

"title" — display title at the beginning of the report (company, operator name, date, time, analysis, instrument and comments). This information shall be entered in "Title" dialog ("Settings-Title..." menu). Operator will be asked in "Assistant" mode to enter the title prior to starting the analysis.

"header" — display header at the beginning of the report.

"Header text ..." — opens dialog to enter report header text.

"display line wavelengths, nm" — display wavelengths of analytical lines in the report.

"full name of elements" — display "Iron" instead of "Fe", etc..

"horizontal/vertical lines" — display horizontal/vertical gridlines between table columns/lines.

"cell status" — highlight disabled cells in the report in colour (grey background + strikethrough text, otherwise only strikethrough text is displayed) and cells with error status (red colour text).

"concentration caption" — column header, where concentration values are displayed; used in sample reports only.

"display in table: concentration or intensity" — display calculated concentration or relative intensity values (I/Ic) as analysis results.

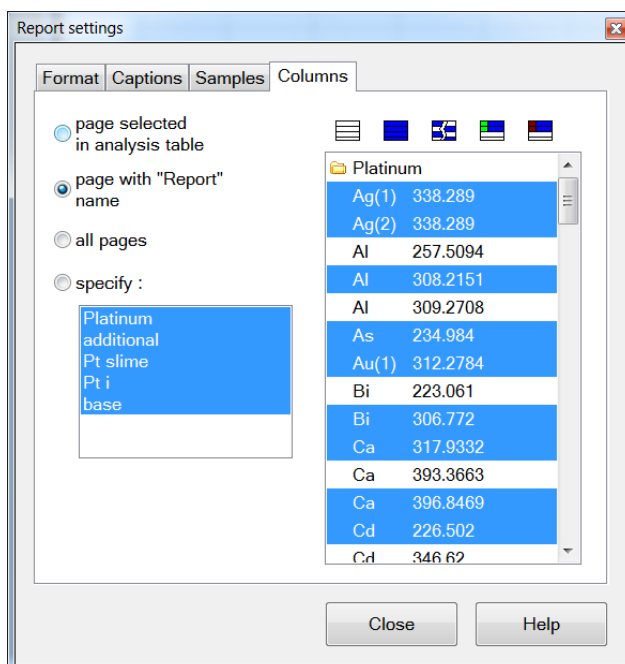
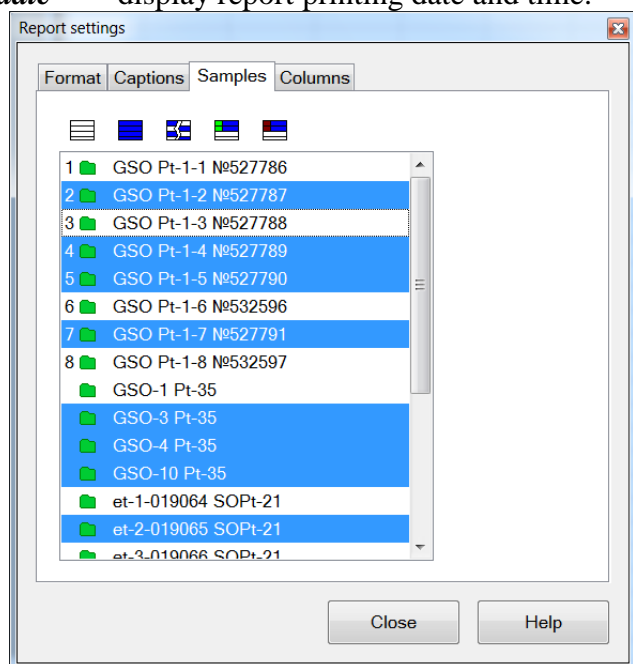
"postscript" — switch on/off postscript text at the end of the report.

"Postscript text ..." — open dialog to enter postscript text.

"page numbers" — display page numbers. "page 1 of N" format.

"file name" — display full file name.

"date" — display report printing date and time.



"Samples"

Select samples from the list. Only the selected samples will be printed in the report. Left-click a sample to select it or to deselect a sample selected earlier. You may also use selection buttons (see Main buttons in "Analysis" mode) to select samples.

"display all parallel measurements" — values for all parallel measurements of samples will be included in the report. Otherwise, only for values samples (mean values) will be included.

	C	Mn	P	S	Cr	Si	P
	193.0906	293.3055	177.4949	180.7311	267.717	212.4123	178.2829
590	2.7	0.27	1.0	0.24	0.087	3.6	1.1
698	3.2	0.11	1.2	0.44	0.088	2.9	1.2
794	3.2	0.13	0.67	0.30	0.17	2.6	0.77
895	3.2	0.073	0.47	0.22	0.23	2.4	0.54
ЧГ10в	2.7	0.84	0.10	0.0076	0.25	2.8	0.11
ЧГ11г	2.4	0.28	0.22	0.035	0.22	1.8	0.22
ЧГ1г	3.6	1.1	0.16	0.032	0.091	1.1	0.16

Проба : 28_4.1-5

Элем	нм	%Масс	Разн	Элем	нм	%Масс	Разн
Mg	II	280.2705	$3.4 \cdot 10^{-5}$	Ni	305.0816	$3.5 \cdot 10^{-5}$	$2.0 \cdot 10^{-5}$
Mn		280.1081	$4.1 \cdot 10^{-5}$	Pb	I	283.3053	$3.8 \cdot 10^{-5}$
Ni	I	300.2485	$3.5 \cdot 10^{-5}$	Sb	I	217.581	...

Проба : 28_1.2-4

Элем	нм	%Масс	Разн	Элем	нм	%Масс	Разн
Mg	II	280.2705	$1.3 \cdot 10^{-4}$	Ni	305.0816	$1.2 \cdot 10^{-4}$	$4.7 \cdot 10^{-5}$
Mn		280.1081	$1.4 \cdot 10^{-4}$	Pb	I	283.3053	$1.6 \cdot 10^{-4}$
Ni	I	300.2485	$1.2 \cdot 10^{-4}$	Sb	I	217.581	$1.3 \cdot 10^{-4}$

printed.

"All" — print the all analysis table pages.

"select" — print pages selected in the list.

Press "Close" button or Esc key to exit Preview mode.

Apart from the Standard report with analysis results, the program can generate report by Calibration graphs, including all information on calculated calibration graphs, statistics, calculation time and re-calibration.

"Columns"

Select analytical lines and other types of columns from the list to be included in the report. Only lines and columns of the selected pages will be included in the report. Left-click lines and columns to select or deselect them. You may also use selection buttons (see Main buttons in "Analysis" mode).

Use the following options to print a report:

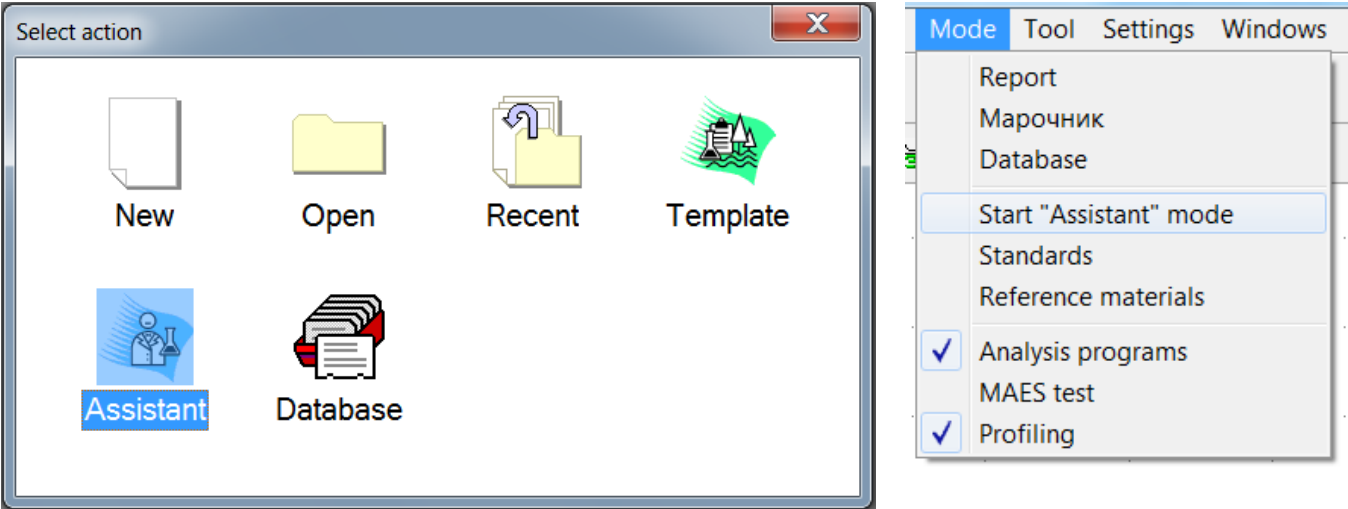
"current" — print the current page displayed on the screen.

"page with 'Report' name" — print only the page with 'Report' name, if it is available in the analysis table. Otherwise the current page will be

The screenshot displays the Atom software interface. The main window shows a table of analytical data with columns: analytical line, angle, SD min, SD max, calibration SD, Cmin, and detection limit. The table lists various elements and their corresponding analytical lines and detection limits. A 'Report settings' dialog box is open, showing options for report generation, including 'title...', 'header...', 'Bartlett/Kochran tabular', 'Fisher', 'Fisher tabular', 'constructed', 'recalibration', 'recalibration factor', 'working range SD min / SD max', 'statistical properties Conv/Adeq/SD', 'Fisher exp/tabular', 'Bartlett/Kochran exp/tabular', 'Cmin', and 'detection limit'. The 'detection limit' option is checked. The 'Report settings' dialog also includes a 'Select font...' button and a 'bold for headers' checkbox. The main window has a 'Print...' button and a 'Settings...' button. The status bar at the bottom indicates 'Page 1 of 2' and the file path 'C:\Atom 3.3\Data\platinum-26-03-15.spd'.

"Assistant" Mode

Enter "Assistant" mode using "Mode" > "Start 'Assistant'" menu in the main program menu, use "Mode" toolbar ("Assistant" item) or "Assistant" shortcut on Windows desktop. As compared to "Engineer" mode, this mode has a significantly simpler interface. Analysis is performed based on analysis programs preinstalled by the engineer. For more details see "Developing analysis programs" item in "Working with programs" section.

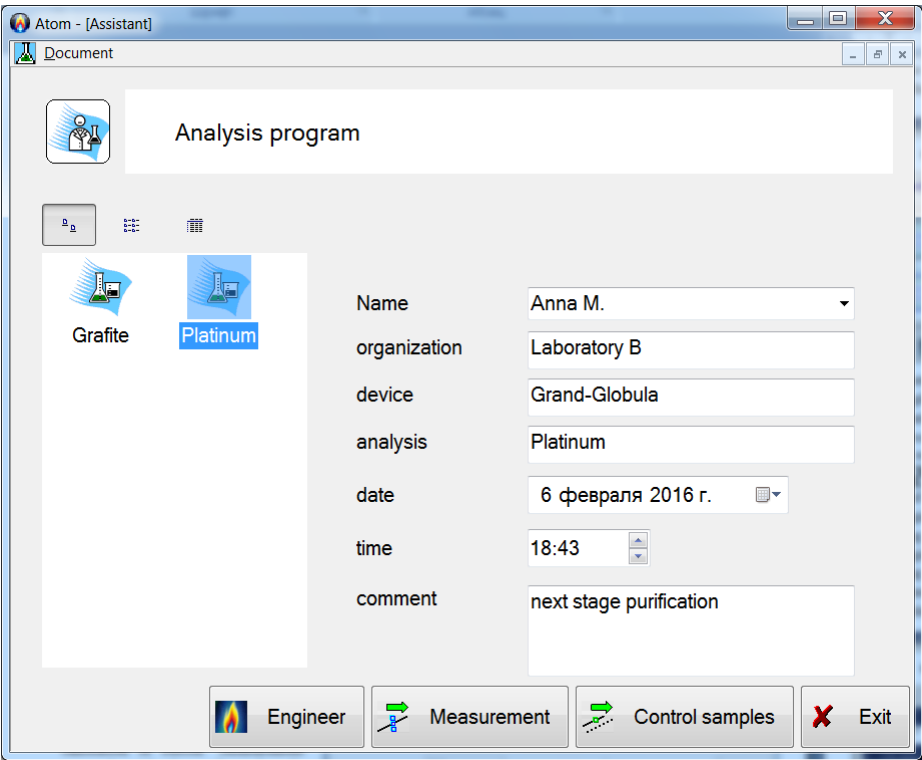


This mode includes several windows; each window is used to perform a specific operation, such as "Choosing analysis program", "Measurement", "Re-calibration", "Title", "Report". Press the corresponding button to enter the required mode. Press Exit to exit "Assistant" mode.

Use shortcut on Windows desktop to launch several copies of "Assistant" mode, it will allow running several analysis program simultaneously and switch between them as different samples are received. Use Windows taskbar to switch between analyses. Each launched "Assistant" mode is displayed as an individual program. When you enter the program, the specified spectrum measurement settings are automatically set (burning, exposure, generator mode, etc.) PC controlled generator modes such as "Fireball" and "Vezuviy-2" are also changed according to the analysis program. Set up of other generators shall be performed according to their operation manuals.

Selecting Analysis Program

Work in "Assistant" mode starts from selection of the analysis program from the list prepared by the engineer. Analysis program settings are as follows: spectrum measurement mode, analytical lines, analysis settings, program types, which the program/assistant interaction scenario depends on, whether the assistant will be prompted to run re-calibration, if the assistant can specify sample names etc. (For more details, see "Analysis programs" section). Click program icon to select it, then click button "Reference samples" to run re-calibration or button "Measurement" to work with the performed earlier calibration/re-




calibration. Double-click the name to enter "Measurement" mode. When the cursor is over the program name, program description (name and type) and comments are displayed. You may select one of three types of analysis program icons in the list: large icons, small icons and the table (see buttons above the list).

Important step: enter user name. Press button with a black triangle to the right of input field to select name from the list. You can edit the list using "User list" dialog (in "Engineer" mode). The program remembers the last entry and proposes it by default. Each new name is automatically saved in the user list. Use Title window (see below) to change name during analysis. You must also enter the following fields: company, instrument, analysis, date, time and comments. This data will be stored together with analysis results and can be printed subsequently in the report or used for search in "Database" mode.

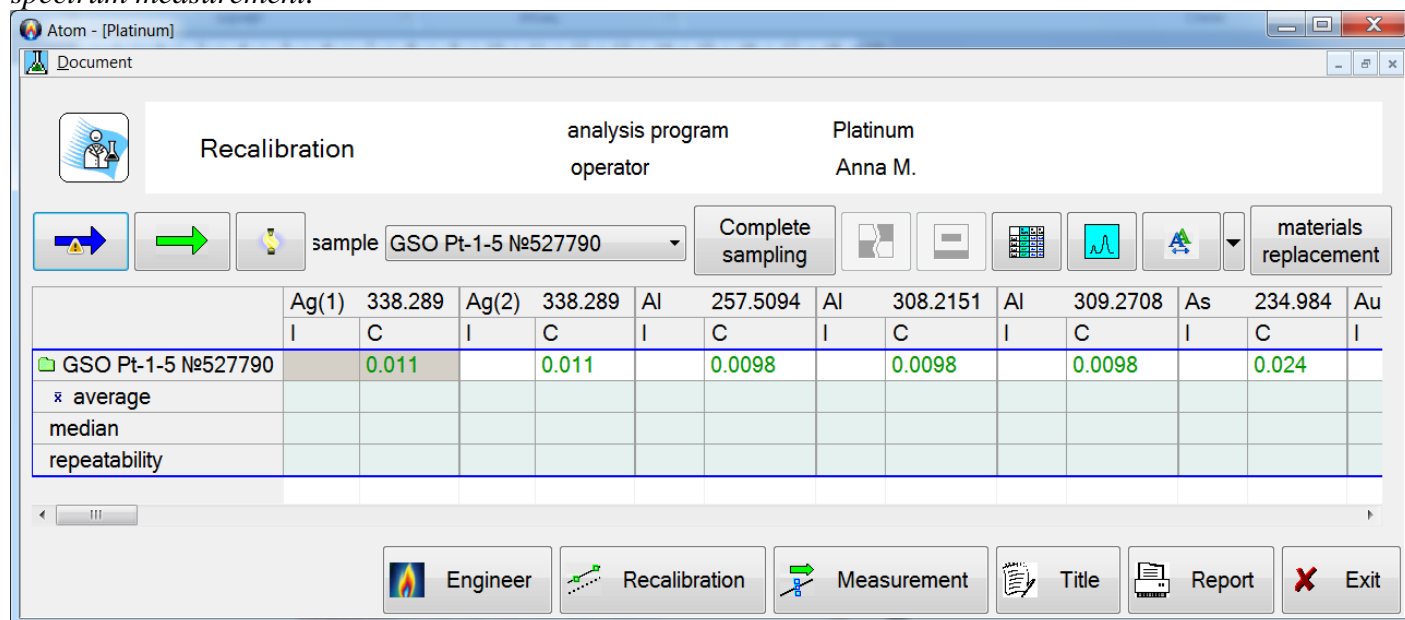
If program "with re-calibration" is selected, you can start spectrum measurements of reference samples or switch immediately to measurements of work samples.

If the engineer during analysis program development specifies that it is necessary to measure dark signal periodically, then upon expiration of the specified interval the program will prompt to measure it. If you reject, it will be possible to measure spectra; however, the program will remind continuously about this. If you specify "wait for device operating mode stabilization", the program will open the measurement dialog during the first session when switched to "Reference samples" or "Measurement" mode. The program will measure the dark signal SD until it reaches the specified level.

Recalibration

Reference samples specified by the engineer for recalibration with the entered impurity concentration values are shown in the table. Choose the current reference sample (to do so, click sample header in the table, or select name in the list above the table) and press . Selected reference sample spectrum measurement starts. Current reference sample is highlighted with a blue frame in the table. Use next reference sample upon completion of the required number of necessary parallel measurements. Perform the required number of parallel measurements of reference samples and press **"Recalibration"**.

Press remote start button connected to MAES or click "Enter" button on the sample name input box to start spectrum measurement.



Atom - [Platinum]

Document

Recalibration

analysis program Platinum

operator Anna M.



sample GSO Pt-1-5 №527790

Complete sampling

materials replacement

	Ag(1)	338.289	Ag(2)	338.289	Al	257.5094	Al	308.2151	Al	309.2708	As	234.984	Au
	I	C	I	C	I	C	I	C	I	C	I	C	I
GSO Pt-1-5 №527790		0.011		0.011		0.0098		0.0098		0.0098		0.024	
average													
median													
repeatability													

Engineer Recalibration Measurement Title Report Exit

Button  is used to discard table cells. Click cell and then click this button. Click parallel measurement header and then press button  to delete spectrum from the table.

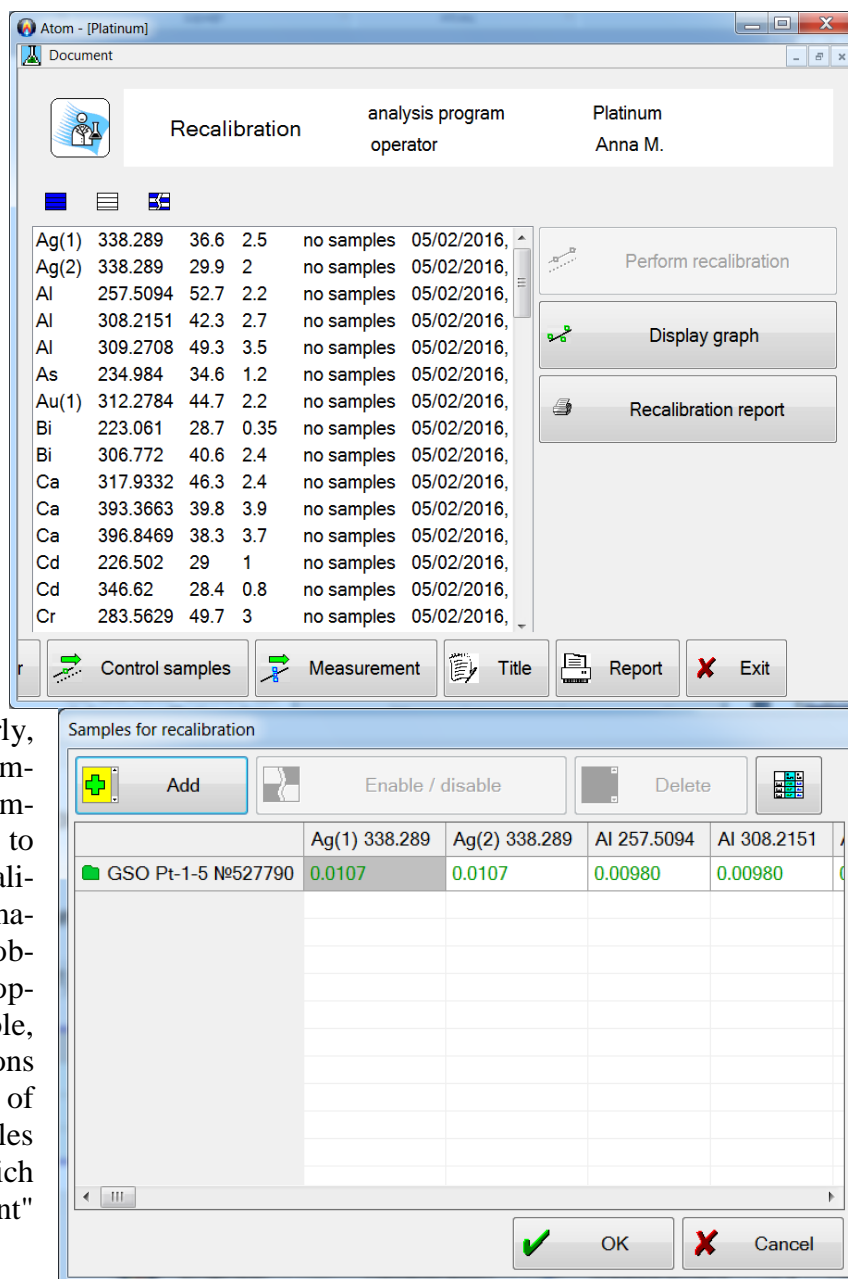
If the engineer specified during program development the maximum number of parallel measurements, a corresponding message will appear if you try to measure the excess spectrum.

If the engineer specified during program development the minimum number of parallel measurements, a corresponding message will appear when entering the "Recalibration" mode.


If "Maximum deviation of reference samples from the calibration graph,%" was specified in "Recalibration" mode during program development, and deviation is of a higher importance for a line, then "Recommended (X %)" text is displayed, where X is reference sample deviation from the graph value, in %. Select lines to recalibrate and press **"Run recalibration"**. By default the program selects all lines with "recommended" text. If the line was recalibrated, "ok" text appears next to it. Usually parallel shift of graphs is performed. If there are several reference samples, mean shift is calculated.


Replacement of Reference Samples

In case when analysis is performed regularly, and reference samples were spent completely, it is necessary to introduce new samples. Use "Sample replacement" button to open replace/add window. In case of recalibration by concentration values, the information on newly added samples may be obtained from the reference material base, copied from an existing sample in the table, filled with one value, or all concentrations may be entered manually. If recalibration of analytical signals mode is on, new samples are added from the existing ones, which spectra are registered in "Measurement" mode.

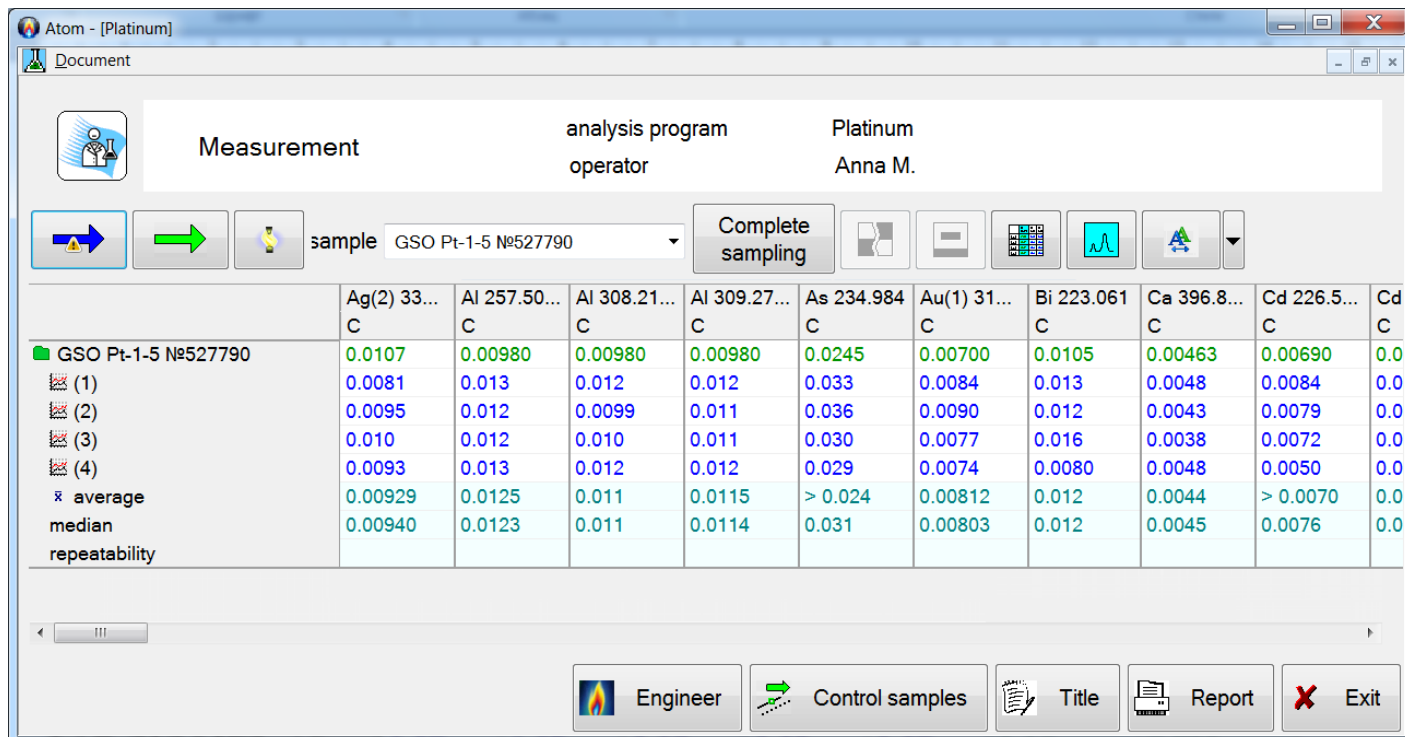


Measurement of Work Samples

"Measurement" mode is used to measure spectra of work samples. Enter new sample name in input box above the table and use button  to measure spectra of parallel measurements. Press Enter button on the keyboard or click "Start" button in MAES to enter "Measurement" mode.

Use buttons  to change whether one or several samples will be displayed on the screen as results in the table, just like in "Engineer" mode.

"Complete sample" button prepares the screen for introduction of a new sample, it instantly prints them and saves information to file. According to Save/Export settings, analysis data may be copied to a universal format file compatible with external programs and exported to the enterprise data base.

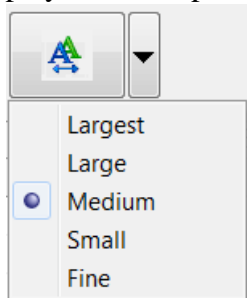


Attention! Timely measure the dark signal!

If you work in "Preset sample" analysis mode, samples and blank parallel measurements are already entered in the table. In this case the program will not allow entering a new sample name — select name in the drop-down list or in the table.

If the engineer specified a limit for the number of parallel measurements, the "preset samples" type of program, then the number of parallel measurements for each sample is checked upon measurement start command and upon completion of measurements.

Upon completion of measurements you can print the report. **"Report"** — transfer to Preview mode before printing (see "Report" mode). Warning message will be displayed, if you already printed the report in this analysis program. If you answer **"Yes"**, the program will automatically select new registered samples in the report for printing, which were not in the table during the previous print session. This message is not displayed in the "preset samples" mode. The program returns to measurements when exiting Preview mode.

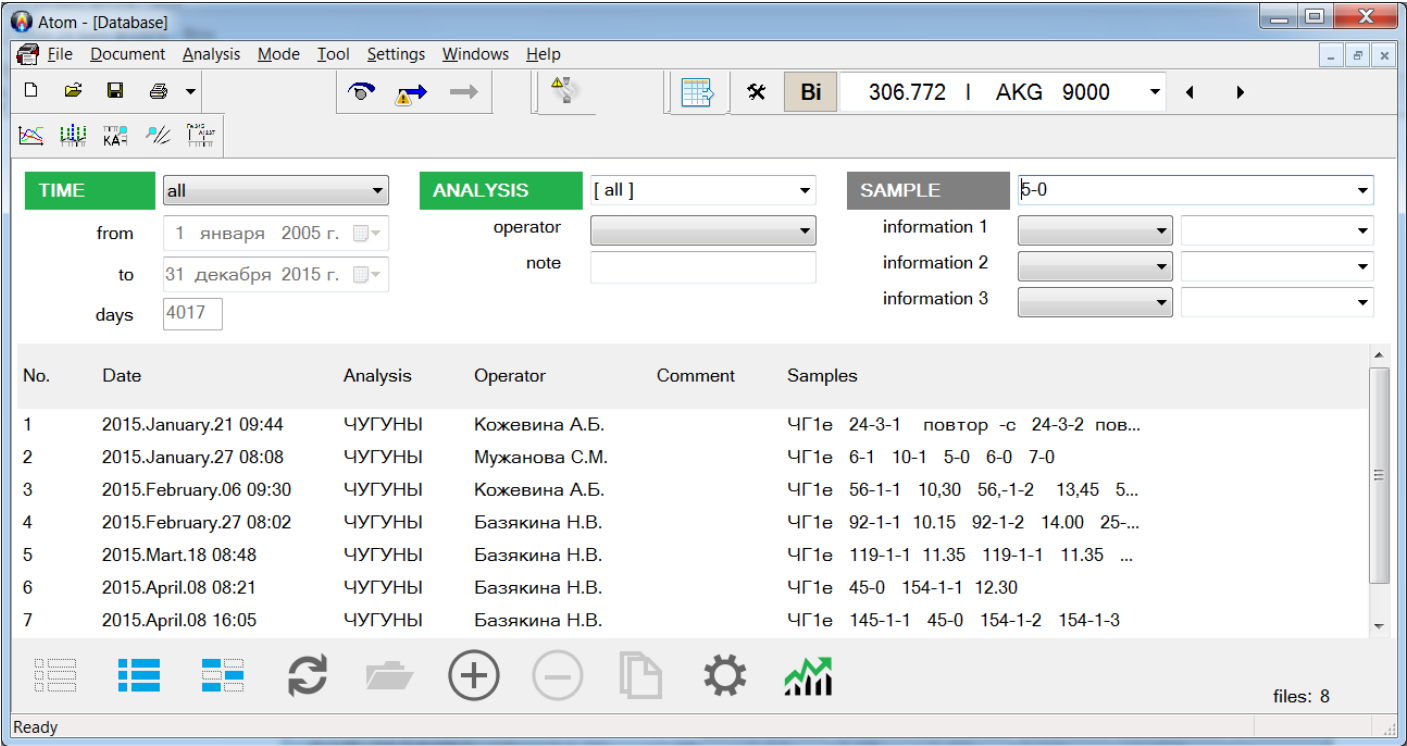


Use button with a dropdown menu to select and save font size in the analysis table.

If at least one spectrum was registered in "Measurement" or "Recalibration" mode, when exiting the program, it will automatically save the file with analysis results. It will be stored in "year/month/day" database directory, file name will include the laboratory assistant last name, program name and the sequential number of analysis during a shift. Usually, it is not necessary to search and open a file to view results received in "Assistant" mode; it is more convenient to use built-in search in "Database" mode.

During program operation it automatically saves temporary files in case of accidental interruption of operation — for example, if the computer is switched off. After restarting, these temporary files are loaded with a notification on emergency recovery without loss of measurements.

"Database" Mode



"Database" mode is used to view and analyze saved program results. All analyses performed in "Assistant" mode, are automatically saved in the database. In order to export analysis results received in "Engineer" mode to the database, select "File"/"Export to DB..." in the main program menu.

File with analysis results (*.spd file) is the database storage unit. Each line in the table corresponds to a file. "Data", "Analysis", "Name" and "Comments" columns correspond to title margins (see "Title" dialog). "Column" template includes analysis program name, where analysis was performed in "Assistant" mode.

Files meeting the current filter criteria are displayed in the table. Use controls above the table to measure filter parameters. Filter is set by default to "today" status, it displays all analysis files generated today. If several filter parameters are specified (for example, data, name, analysis), they are combined with "and" operator, i.e. all files must meet all specified selection criteria.

"Filter" — specify time period, for which analysis results must be shown: *"today"*, *yesterday*, *"this week"*, *"current month"*, *"current year"*. *"All"* means that if other filters are not set, all files available in the database will be displayed. In order to accelerate this operation, this list is limited to the first 1000 files. (Note the string *"found: ... shown ..."* above the table). *"specify..."* allows defining manually the range of dates — see **"From"** and **"To"** fields.

"Name" — specify laboratory assistant/operator name, who performed the analysis. To do so, select it from the dropdown menu or enter it (click "Refresh" button when done). List of names is generated from two sources:

- 1. names contained in "User list" dialog,
- 2. names are added from files already viewed in "Database" mode.

It is recommended to specify "Filter" field first. The program will sort out all files according to the specified dates and fill the user list, then specify "Name" field. Use this filter to define, for example, how many analyses were performed by an operator with this name within the specified time period. To do so, specify the dates first (see "Filter" field), and then the "Name"; other filters must be blank.

"Analysis" — specify analysis program name. To do so, select it from the dropdown menu or enter it (click "Refresh" button when done). Name list is generated from two sources:

- 1. names of all currently existing analysis programs,
- 2. names are added from files already viewed in "Database" mode.

It is recommended to specify "Filter" field first. The program will sort all files by the specified dates and will fill the user list. After that, specify "Analysis" field. Use this filter to define, for example, how many analyses

were performed using the specified analysis program within the specified time period. To do so, specify dates first (see "Filter" field), then specify "Analysis" field; other filters must be blank.

"Template" — similarly to "Analysis", but program runs according to the "Template" field. Specify "Template" field together with "Analysis" field, because the same program may perform various analyses. For example, to control content of a particular element individually or in groups.

Analysis queries may be received from various sources (workshops, departments, etc.) These analysis aspects may be specified in "Template" field for a more precise selection in the "Database" mode.

"Comments" — enter text and press "Refresh" button. Entered text appears in "Comment" field of the File title.

Click column header in the table to sort the files found.

Click again the header to sort column in descending or ascending order.

"Information 1,2,3" — allows searching analyses with additional fields, such as "Workshop", "Furnace", "Melt", "Time", etc.

The following buttons are located under the table for main database operations:



Select and unselect strings in the table list



"Update" — search again files that meet the specified filter criteria.



"Open" — open file from table in "Atom" program. File is opened in a new document.



"Import" — specify one or several files in "Open File" dialog to copy them to database.



"Remove" — remove selected files from data base. It is greyed when there are no selected strings.



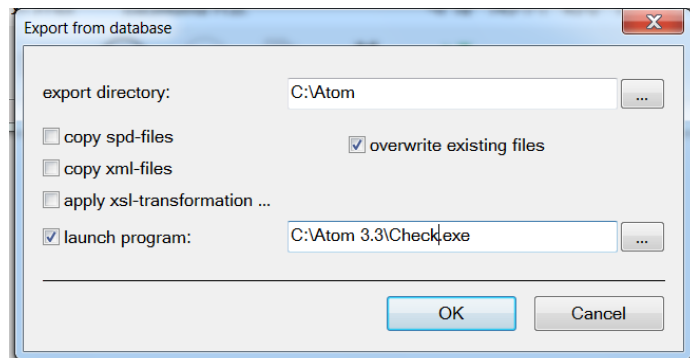
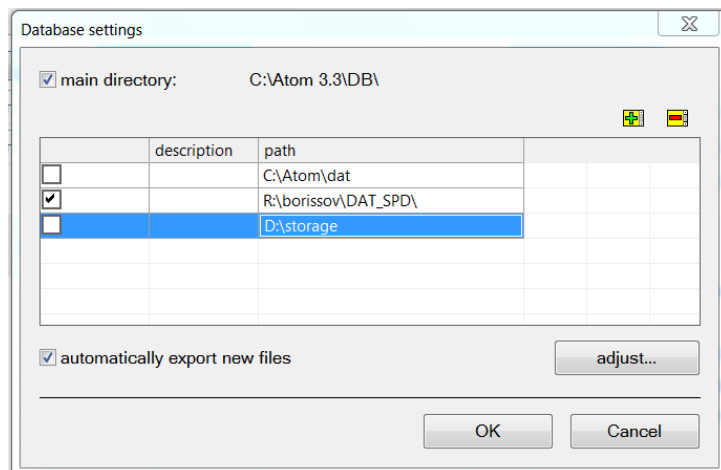
"Database setting" — "Database setting" window appears, where you can specify what exactly must be copied, and what conversion changes will be made. You can also specify destination directory here. Use this mode to create user-defined text files of report based on .xsl-files to export results to external programs.

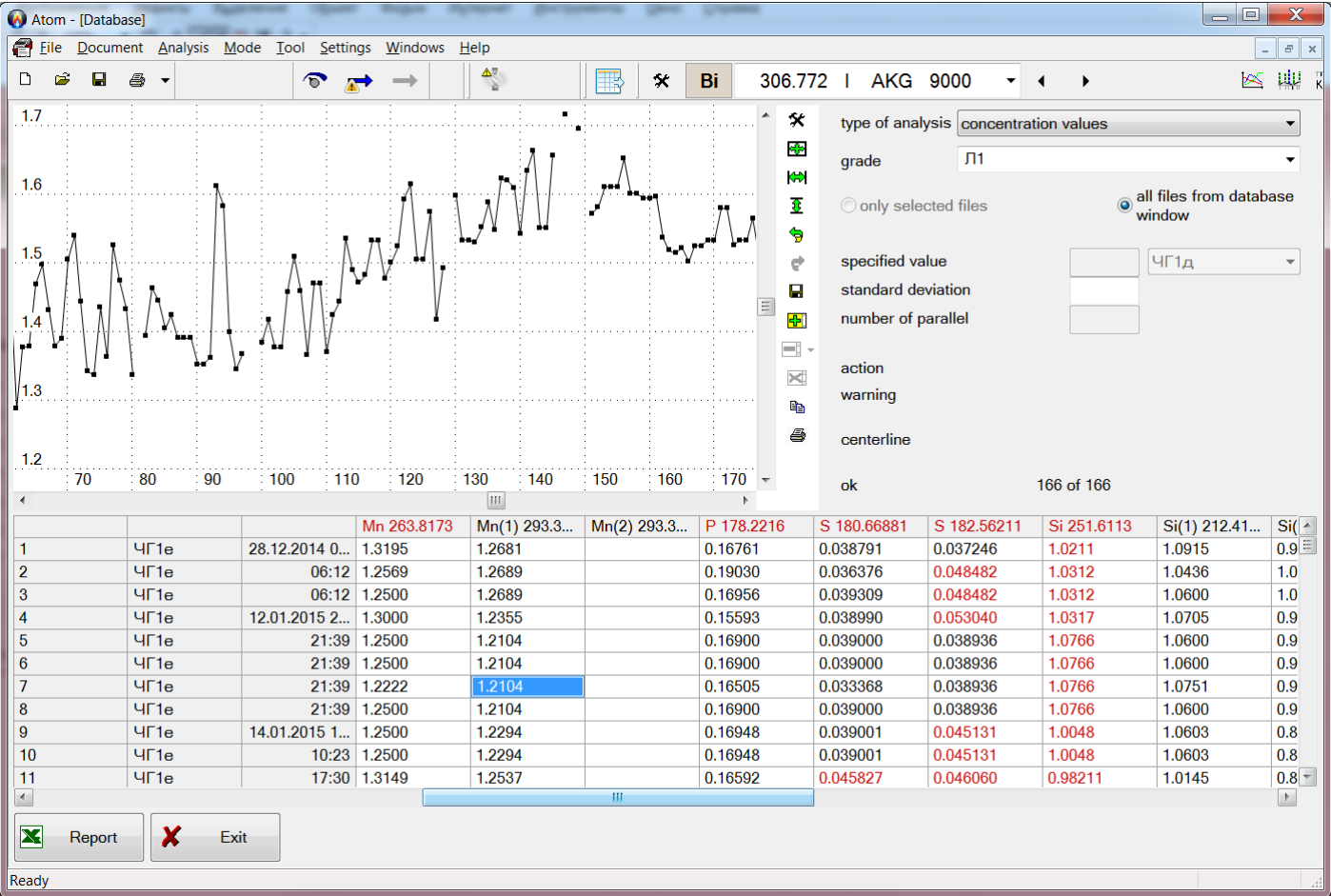
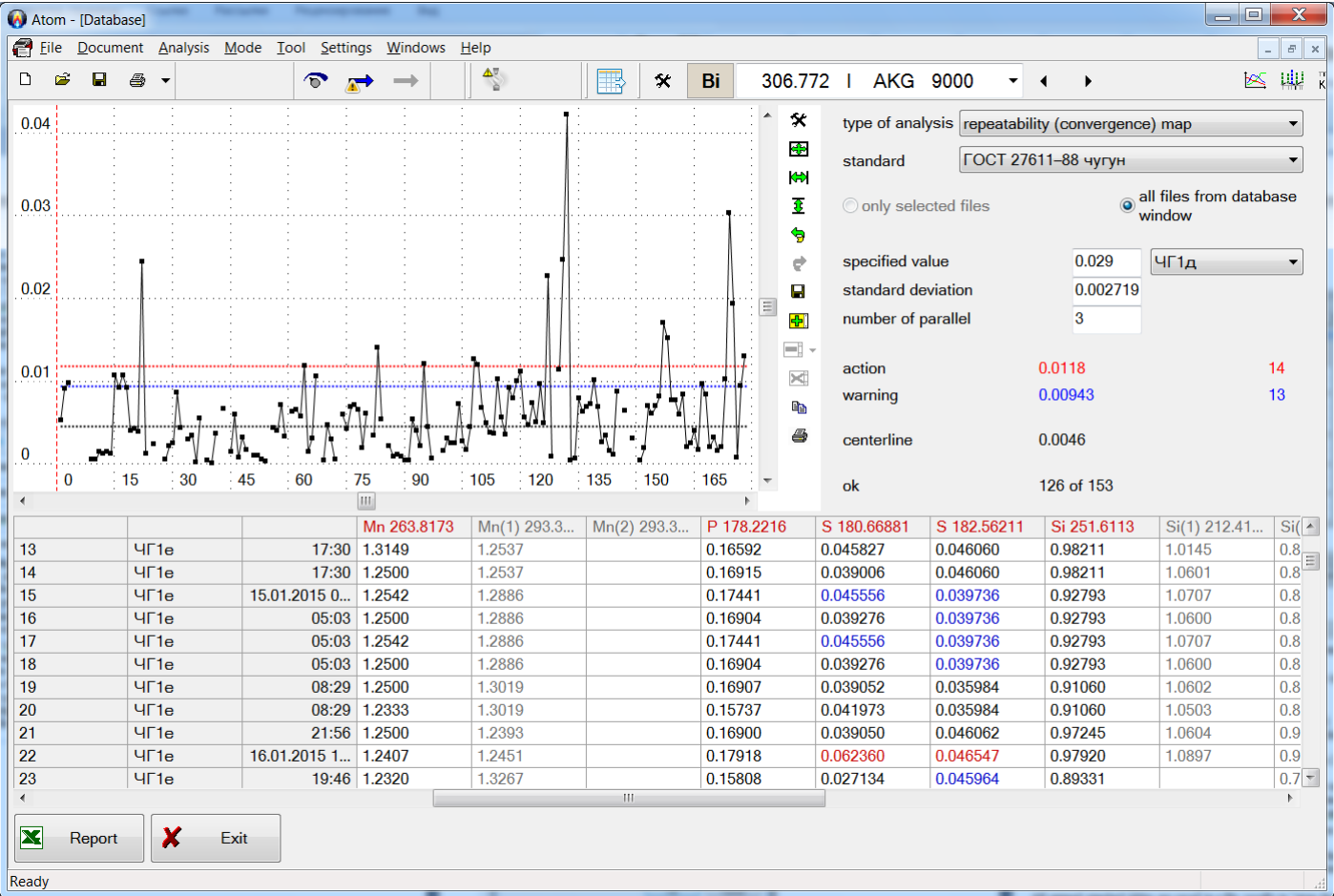


"Export" — manual export from database for selected files. Copying files and XSL-conversion could be made while conversion. It is greyed when there are no selected strings.



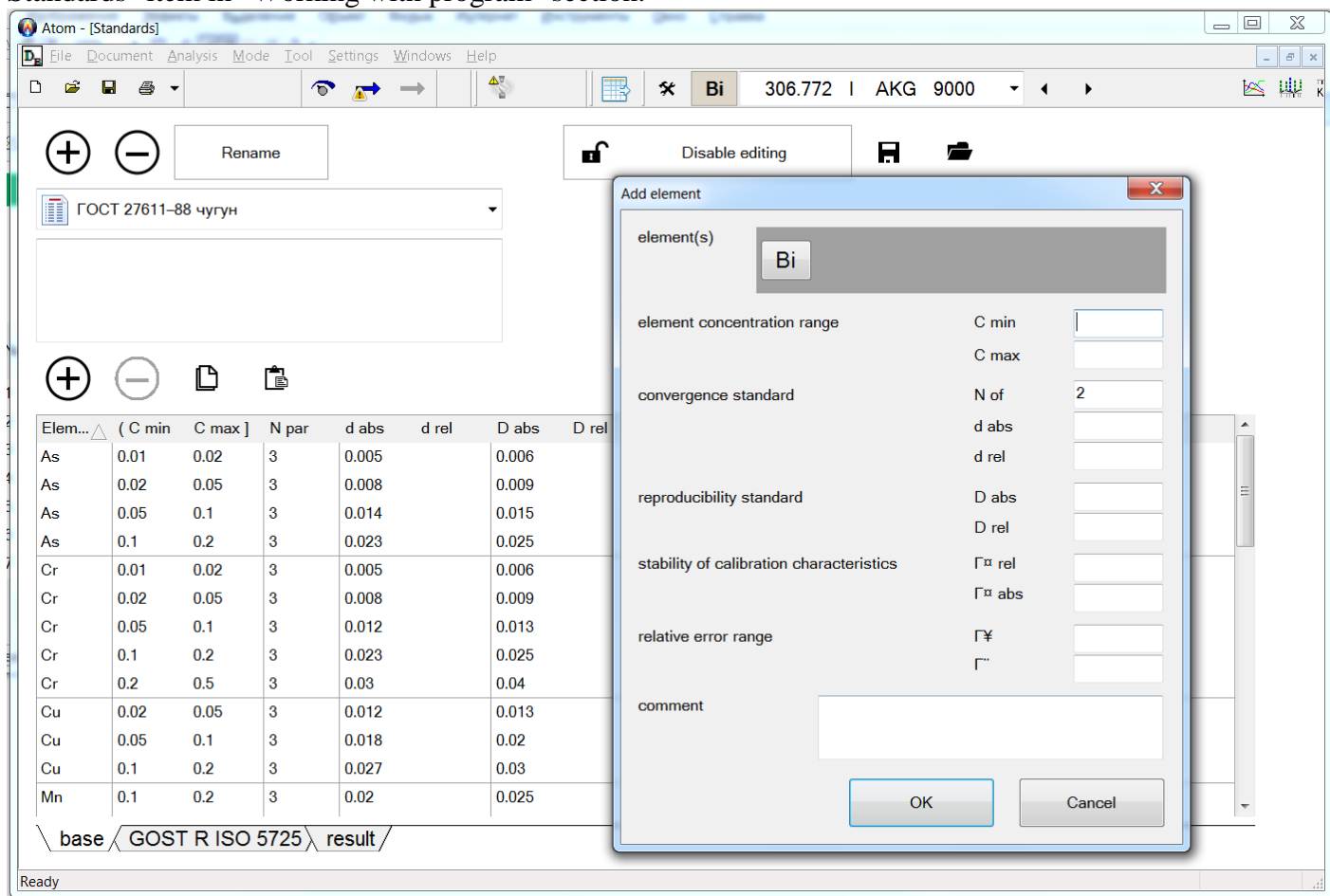
"Analysis" — view Shewhart graphs for selected analyses. In order to simplify operation, it is recommended to enter beforehand the information on reference materials into the reference sample database and the respective metrological parameters into the code of standards. Then, select necessary items from the list to create graphs of repeatability, precision and errors for each element. You can also export processed data to MS Excel for subsequent processing. Select any point using the cursor in the graphic window to select it in the table of results. Double-clicking analysis table line to open a data file that corresponds to this line in the "Engineer" mode.



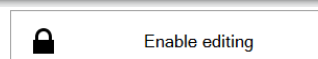


"Standards" Mode

Standards mode is used to enter and edit tables with standards for operative control of convergence and reproducibility of analysis results. This manual section describes user interface, for more details see "Use of Standards" item in "Working with program" section.



Switch "Edit" mode on to add and edit information on Standards table




. When edit-


ing is complete, save the document (button ) and press button




Names of entered standard tables are displayed in the upper part of the window. Select a name to display the list of elements with standard values of operative control (in the lower part of the table).

Press  above the list of tables and specify new table name and comments in the open dialog to add new standard table.

Tables are arranged in such a way that standard values required to execute an analysis program are located in one table. Or, in other words, a standard table (one table) must conform to each analysis program (if standards are used to execute it).

Click  above the list of elements to add new string to the table. Specify element name, concentration range (if any) and the required standard values in the dialog.

Click table name and then press  to delete it.


If some values are not used or are unknown, they may be skipped.

Difference criterion for N parallel measurements is applied to check the convergence standard according to GOST or the analysis procedure in use.


Reproducibility standard is checked as per difference criterion for 2 measurements.


Relative error limits are used to check homogeneity of reference materials and to attest procedures and commission SRM (see "SRM attestation"). All calculations are performed according to OST 95 10554.


Position cursor over the respective cell of the table to modify the entered value and enter new value.

Click the leftmost cell of the string (name of the element) and press  to delete strings from the standard table.

Click column header where you want to start sorting to modify the sorting order in the table. For example, in order to sort the table by element name, click Element column header. Click again to change the sorting order, either in ascending or descending.




All entered standard tables are saved in a file, usually in "atom.dps" file. Click button  to load another file with standards. If it is necessary to load automatically the standard file when launching the program, specify it in "Files" dialog.

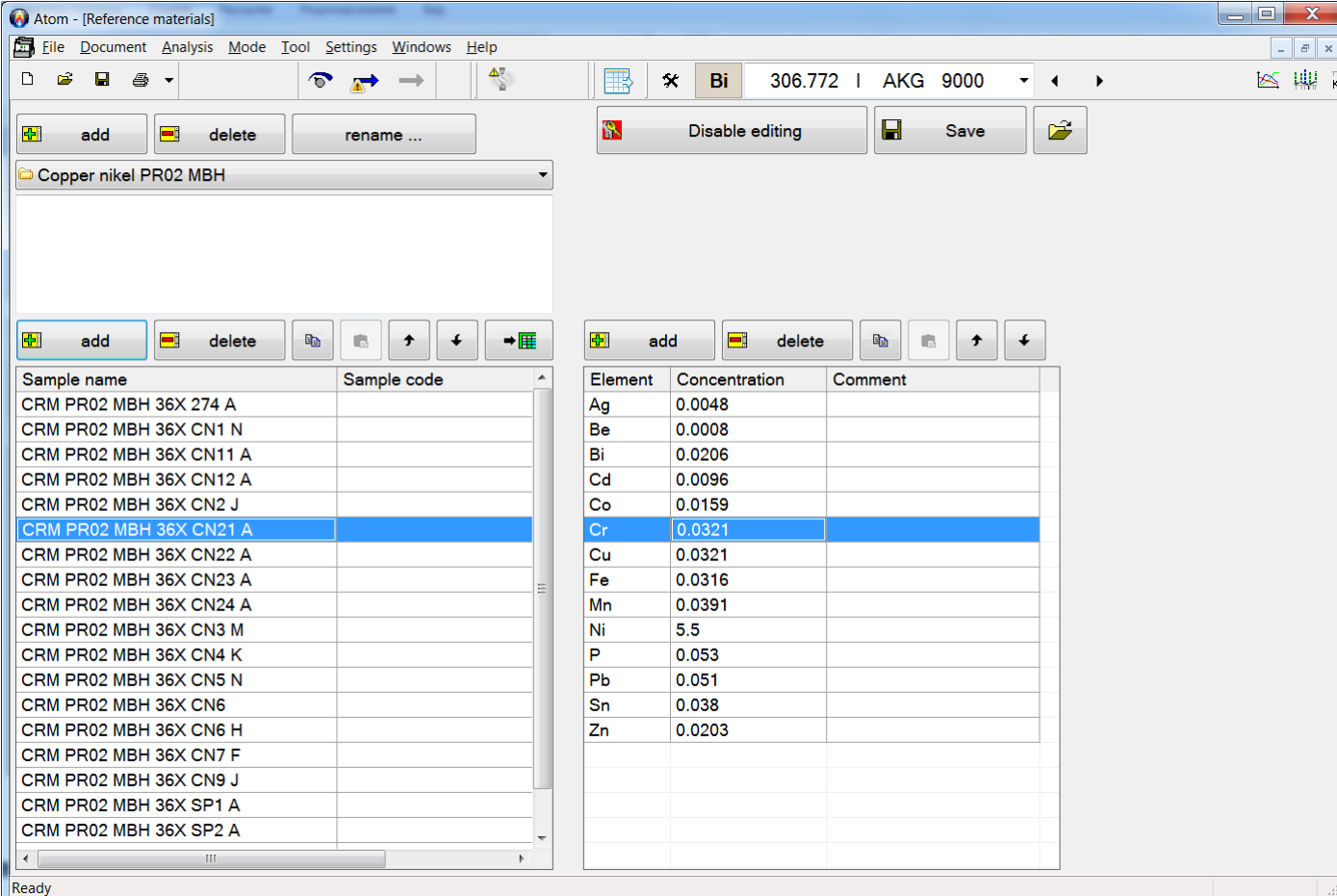
Use button  to save standards to file. If standards were edited after program was loaded, you will be prompted to save changes when exiting the program.

Button  deletes all information on standards.

"Reference Material" Mode

It is used to fill information on reference materials that are used to create calibration graphs and perform re-calibration. This information includes names of samples, reference materials, and known concentrations of elements in each sample.

Switch "Edit" mode on to add and edit information on concentrations  Enable editing. When editing is complete, save the document (button ) and press button  Disable editing.



Atom - [Reference materials]

File Document Analysis Mode Tool Settings Windows Help

add delete rename ... Disable editing Save

Copper nikel PR02 MBH

add delete

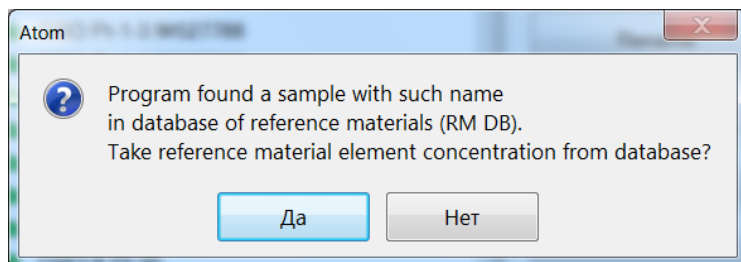
Sample name	Sample code
CRM PR02 MBH 36X 274 A	
CRM PR02 MBH 36X CN1 N	
CRM PR02 MBH 36X CN11 A	
CRM PR02 MBH 36X CN12 A	
CRM PR02 MBH 36X CN2 J	
CRM PR02 MBH 36X CN21 A	
CRM PR02 MBH 36X CN22 A	
CRM PR02 MBH 36X CN23 A	
CRM PR02 MBH 36X CN24 A	
CRM PR02 MBH 36X CN3 M	
CRM PR02 MBH 36X CN4 K	
CRM PR02 MBH 36X CN5 N	
CRM PR02 MBH 36X CN6	
CRM PR02 MBH 36X CN6 H	
CRM PR02 MBH 36X CN7 F	
CRM PR02 MBH 36X CN9 J	
CRM PR02 MBH 36X SP1 A	
CRM PR02 MBH 36X SP2 A	

Element	Concentration	Comment
Ag	0.0048	
Be	0.0008	
Bi	0.0206	
Cd	0.0096	
Co	0.0159	
Cr	0.0321	
Cu	0.0321	
Fe	0.0316	
Mn	0.0391	
Ni	5.5	
P	0.053	
Pb	0.051	
Sn	0.038	
Zn	0.0203	

Ready


The list of entered samples is specified in the left part of the window. Besides the name, "code" and "comments" may be assigned to each sample. Sample name corresponds to its name in the analysis table. "Code" may be used to enter full sample name, comments are a user-defined accompanying text.

Sample list may be divided into several directories for easy navigation. Specify directory in the "Add reference material" dialog, where the sample will be located (see below). Samples from the current directory are displayed in the list; select directory name in dropdown list above the sample list to change the current directory.




If, when adding new sample into the analysis table the program finds a sample with the same name in the reference materials list, the following message will appear:

If you answer "Yes", "SRM" fields for elements specified in reference material mode will be filled for the new sample.

Press the top left button  **add** to add information on the new sample. Fill the required fields in the open dialog and press "OK".

Description of dialog fields is provided above.

Select samples in the list and press  **delete** to delete them.

Each sample includes a list of elements with known concentrations. Click sample name to display the list. The list consists of three fields: name, concentration and comments.

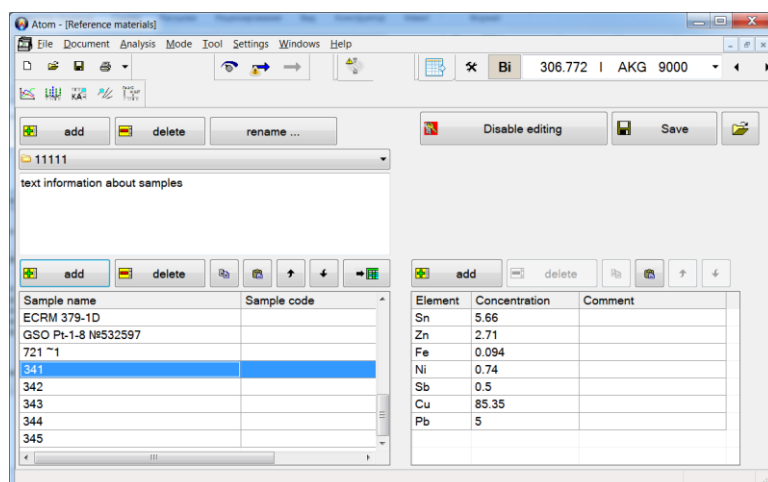
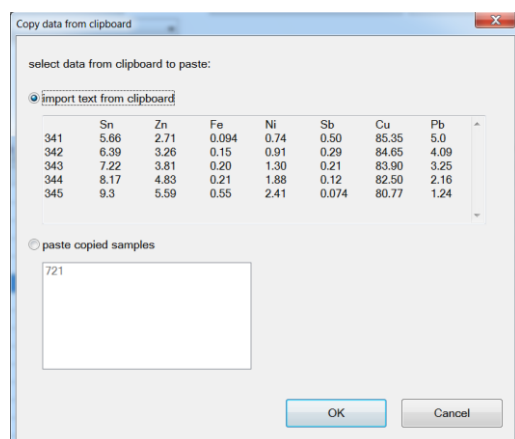
You may enter information in blocks with names of samples and elements, just like in the table:

First line must include symbols of elements

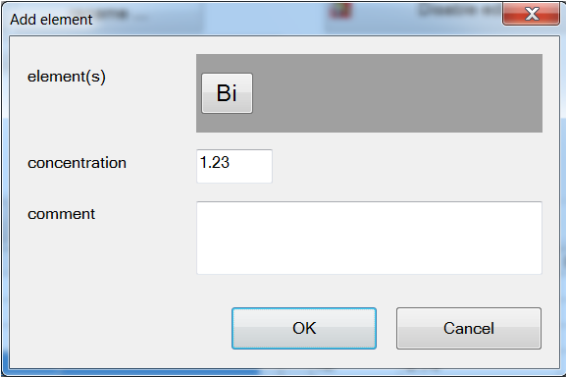
First column must include names of samples


	Sn	Zn	Fe	Ni	Sb	Cu	Pb
341	5.66	2.71	0.094	0.74	0.50	85.35	5.0
342	6.39	3.26	0.15	0.91	0.29	84.65	4.09
343	7.22	3.81	0.20	1.30	0.21	83.90	3.25
344	8.17	4.83	0.21	1.88	0.12	82.50	2.16
345	9.3	5.59	0.55	2.41	0.074	80.77	1.24


The program prompts to enter text to copy this table from Word or Excel program to Windows buffer





You may change the sorting order in lists of samples or elements. To do so, click column header to sort samples and elements by. Click again the header to change the sorting order: "ascending" — "descending".



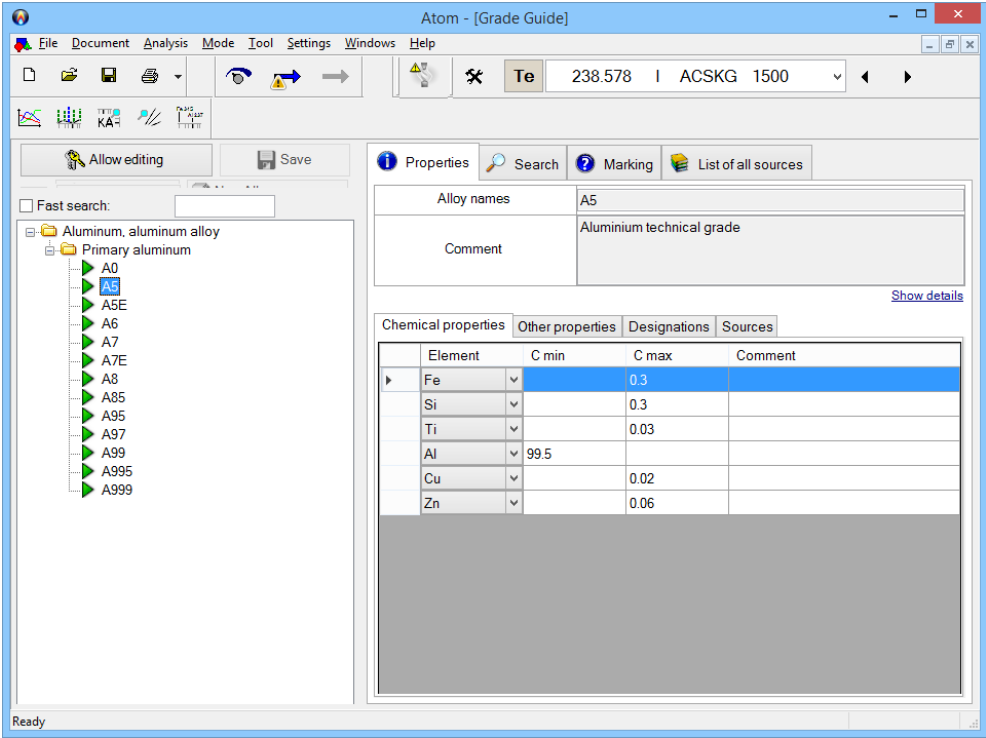
Click  **add** above list of elements to add once the element information. Fill fields in the open dialog and press "OK".

Select elements in the list and press  **delete** to delete them.
Double-click field values and edit them directly in the field to modify them.

Click  to copy information samples and concentration to analysis files
"Engineer" mode has options to copy information to analysis files also. To do so, use reference material database window button .

"Grade Guide" Mode

This mode is used to enter information for automatic grading of samples. User enters grades (of alloys) and concentration ranges of its elements.
Current version of alloy database provides information from several reference books on composition and properties of steels, cast irons, bronzes, brasses and other alloys.
Add "Alloy" column in the analysis table to display grading results. The program calculates mean concentration for each sample element and displays all grades corresponding to the entered concentration ranges based upon this data.



tion for each sample element and displays all grades corresponding to the entered concentration ranges based upon this data.

All grades are divided into several directories for simple navigation.
Activate editing mode first (use button "Allow editing") to change and add information on alloy grades, then start adding, updating and editing.
List of grades is located in the left part of the window. Each grade contains a name, code (of full name) and comments. Click "New alloy" above the list to add new grade. New record will appear in the current directory, which fields must be filled with respective information. Use "drag and drop" method to move alloys from one directory to another.

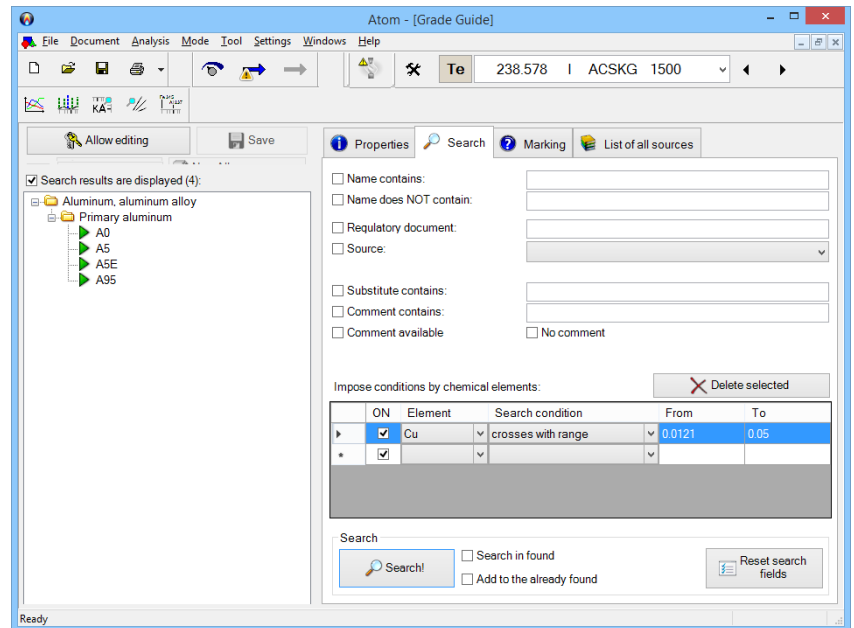
Select grades in the list and press "Delete" button to delete them.
Each alloy has a list of element concentration ranges. Information on the range includes element name, minimum and maximum concentration and comments. Press "Add" above the list of ranges to add new element; choose element and specify values. It is not necessary to enter both range limits to specify only the lower or upper limit; but at least one range limit must be entered. Select elements in the list and press "Delete selected" to delete them.
You can change the sorting order in the lists of grades and ranges. To do so, click column header to sort samples and elements by. Click again the header to change the sorting order: "ascending" — "descending".

Double-click field values and edit them directly in the field to modify them.

If you start typing text in "Quick search" window, the program starts searching among alloys and will display the list of respective alloys.

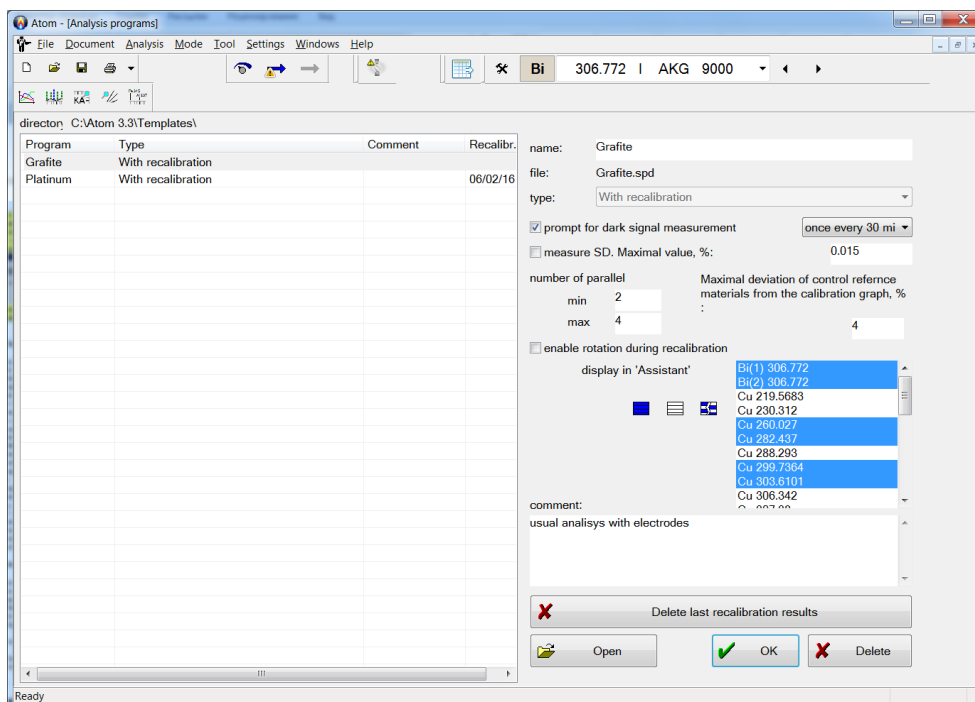
Use Search tab for a more detailed searching in the grade guide. You may specify values in any field that includes information on alloy grade, or you may specify only concentration of any element with various parameters, such as range, limit etc.

Press "Search" button to update the list of found alloy grades (meeting the criteria).



"Analysis Programs" Mode

This mode is used to display and measure some analysis program settings. Programs are used to perform routine analysis in the "Assistant" mode.



the program to initial calibration graphs.

Developing Routine Analysis Programs

This mode may be activated in "File" menu using "Develop Analysis Program..." item.

This automatic mode is essentially different from the similar procedure in the previous versions of "Atom" program. Major changes were mainly made in standard operations, which are run by the program itself through obtaining necessary information from the engineer by means of query dialogs.

Select application name in the list to the left, change necessary settings and press "OK". Or press "Delete", if you want to delete analysis program.

Double click the list of programs to open a file in the selected program in "Engineer" mode.

Press OK after online editing of analysis settings or the list of lines and columns to be displayed.

Most recent recalibration results are applied when starting analysis program in the standard mode. Press "Delete last recalibration results" to return

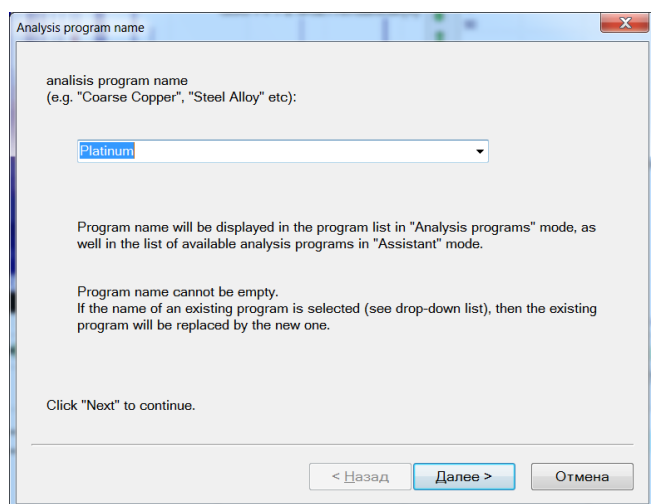
This mode is the final phase in developing the routine analysis program. To accomplish it, follow necessary and obligatory procedures for checking and preparation of several settings in "Engineer" mode:

1. usually, in order to develop a program, spectra and calibration graphs obtained earlier are used, i.e. you shall start with reading the data saved earlier;
2. if you create a completely new analysis, you shall add all analytical lines of elements and reference lines measured (as it is specified in the analysis procedure) to the analysis table; compare analytical lines with corresponding reference lines; enter all necessary parameters to calculate line intensity values, calibration graphs, concentrations; register and record reference material spectra in the analysis table to built calibration graphs; select reference lines to control spectrum position relative to the detector;
3. set "Measurement" mode, parameters for spectrum registration and generator control according to the analysis procedure — burning time, exposure (including the number of spectra when working with "Time record" parameters);
4. if constant graph method is used, analysis tables must include spectra of reference samples or reference materials, which will be used to control the calibration graphs;
5. customize the analysis table view, usually concentration column is displayed, including "Mean" and "RSD" or "difference" values;
6. customize Report view, if the laboratory assistant must print it;
7. if matrix printer with continuous or reel feeding is connected to LPT1 port of the PC, you can specify instant printing during the analysis (open dialog in the main program menu "**Settings/Log ...**", detailed information regarding this dialog is provided below).

Upon completion of preliminary operations, programs development starts, and first "Analysis program name" dialog opens (menu "**File**" > "**Create analysis program...**").

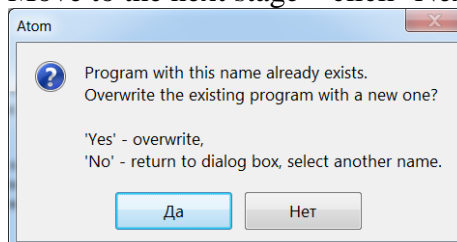
ATOM program uses Windows system windows message buttons so their caption depends on system language setting and could be in Russian or English at different computers. Here is translation for helping:

< Назад	Back	Далее >	Forward	Готово	OK, Ready
Отмена	Cancel	Да	OK	Нет	No

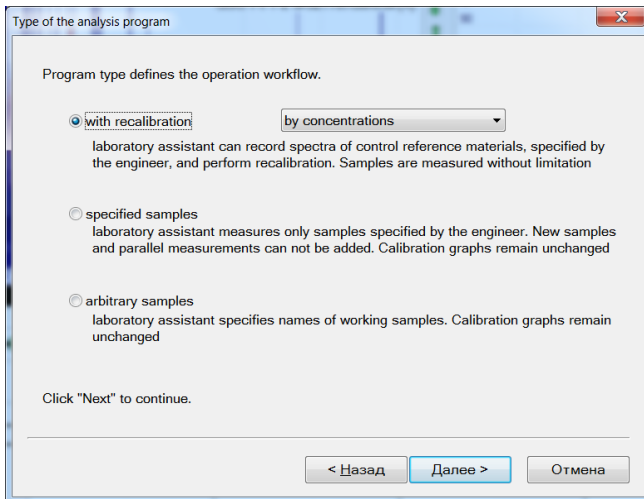


Fill program name field or select it from the list of complete programs. In this case the current program will be replaced, and the program always warns you about it by means of a confirming dialog. Specified name will be subsequently included in the list of complete programs, in the database, report etc.

Move to the next stage – click "Next" button



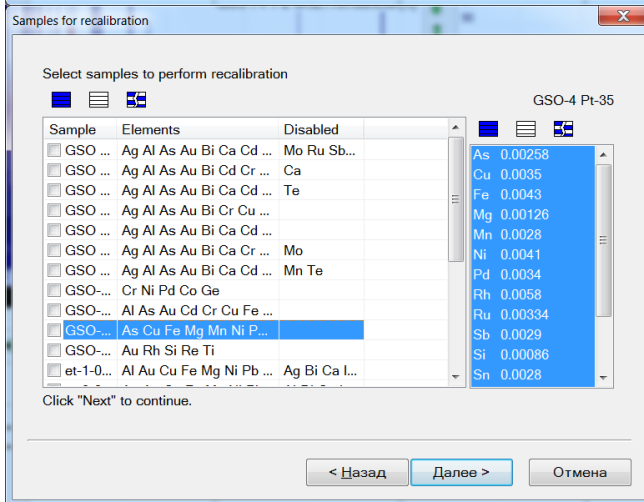
Use unique Analysis program names – existing names are checked before creation.



select program type from the following options:

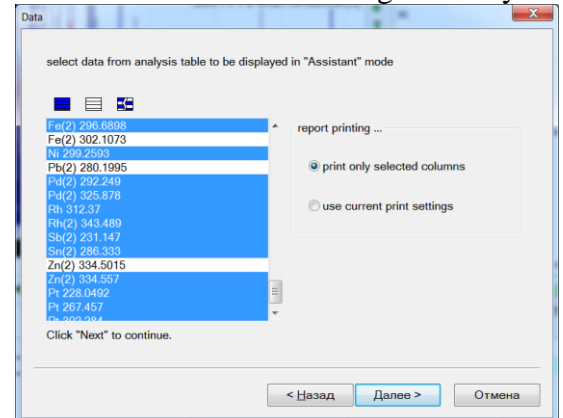
- "with recalibration" by concentration values or analytical signals;
- "specified samples" – laboratory assistant will be able to analyse samples according to the number of parallel measurements specified in the analysis table; calibration graphs are applied without recalibration;
- "user-defined samples" — the number of samples is not limited; calibration graphs are applied without recalibration.

Move to the next stage — click "Next" button.



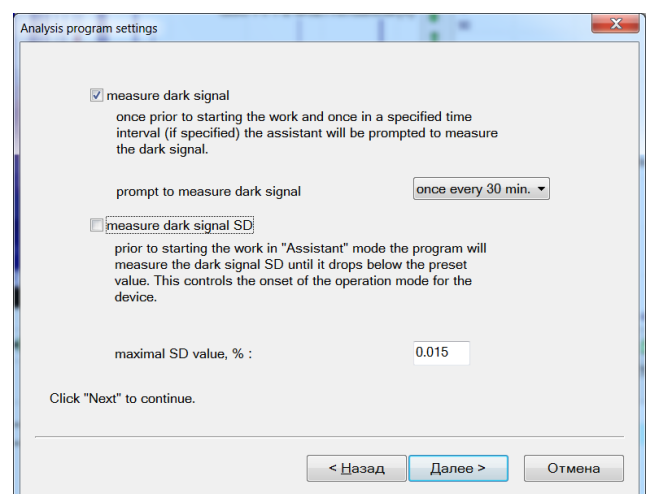
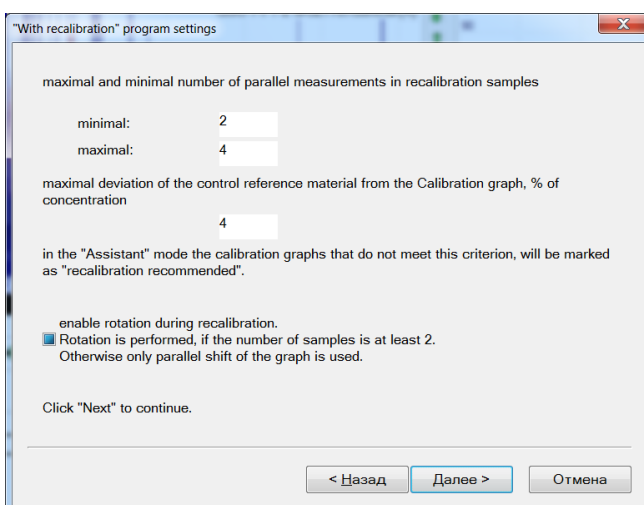
Select reference samples and specify, what elements these samples will be applied to.

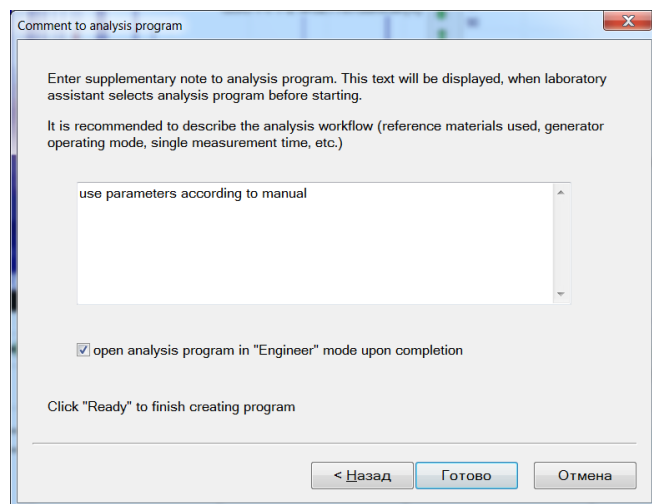
At the next stage, select lines which the laboratory assistant will view during the analysis.



Then estimate the number of measurements for reference samples and the permissible deviation, in case of excess of which it is recommended to perform recalibration. All lines will be checked.

At the next stage it is recommended to specify "Measure dark signal" and set frequency of measurement queries to 30 or 60 minutes; in addition, you may select "Measure dark signal SD" item.





Final stage is to describe program implementation features in comments, reference samples to be used, generator operation mode, single measurement period, etc.

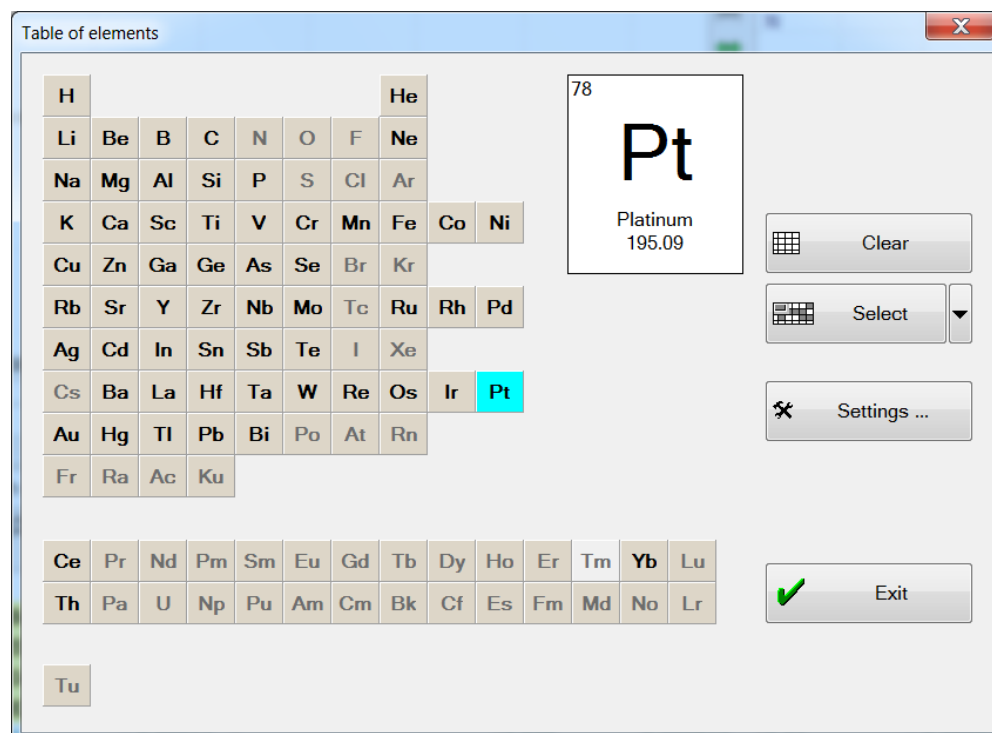
Press "Ready" and start creating the program and save it in the list of programs.

Parameters of all stages of program developing are stored in a data file. Press "Next" to repeat this procedure until the stage, where changes or corrections must be implemented, and proceed to the final stage.

Switch to "Assistant" mode to run the developed analysis program.

Description of dialogs

"Periodic table"



This dialog is displayed when pressing the active element name in the "Spectral Lines" toolbar.. It is used to select the current chemical element or several elements. One element among all chosen elements is active (it is designated with blue colour), other selected elements are black. Lines of the current element are displayed in the list of "Spectral Lines" toolbar. Lines of all selected elements are displayed in spectrum window.

Click element name to select the required element. There are two ways to select several

elements: either hold pressed "Shift" or "Ctrl" button, or press "Select several elements" button (small blue rectangle shall highlight at the top left on the button image). If one of already selected elements is clicked when selecting several elements, it will be deselected.

The following colours are used to display elements:

- blue background indicates the current element;
- black background indicates the selected elements;
- pink background highlights elements from the filter;
- names of elements, for which no spectral line is specified, are indicated with gray background.

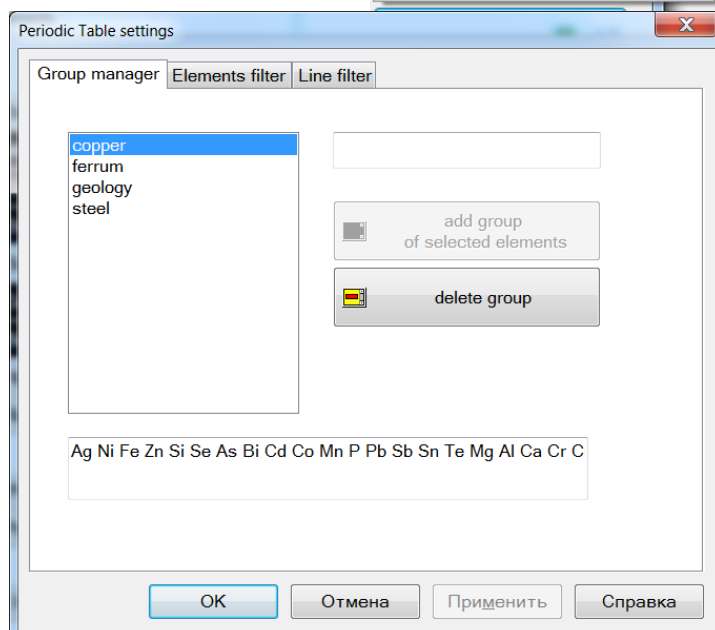
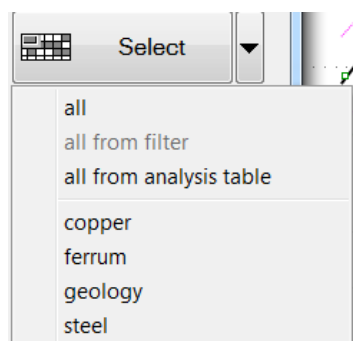
"Clear" button deselects all elements; current element remains selected.

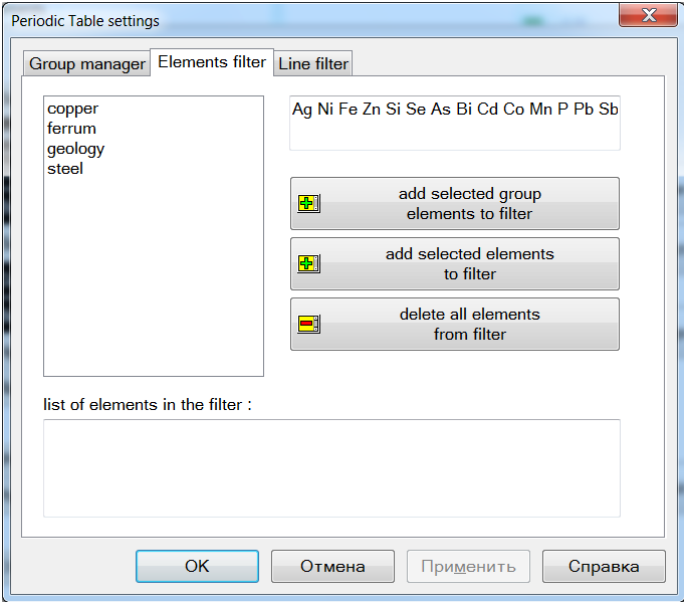
"Select several elements" button activates the mode of highlighting several elements. Click small black triangle to the right of this button to open the menu with selection options:

- "all" — select all elements in the table;
- "all from filter" — select all elements from the filter (highlighted with pink);
- "all from analysis table" — select all elements, which lines are displayed in the analysis table;;
- other menu items correspond to names of element groups. Press the name to highlight elements of a corresponding group.

Use "Setup" button to open dialogs with control options of elements.

This dialog is used to add/delete groups of elements. Groups of elements may be used later to highlight at once all elements of the group in "Periodic table"





"Qualitative Analysis" tools. Select one group of elements (the list at the top left) and press the first "plus" to add elements to the filter, or select elements in "Periodic table" dialog and press the second "plus". Press "minus" to delete all elements from the filter.

"Line Filter" bookmark corresponds to display setup dialog of spectral lines.

Use "Group Manager" and "Element Filter" to limit in advance the number of elements, which spectral lines will be analyzed by the program in "Spurious Lines" and "Qualitative Analysis" tools.

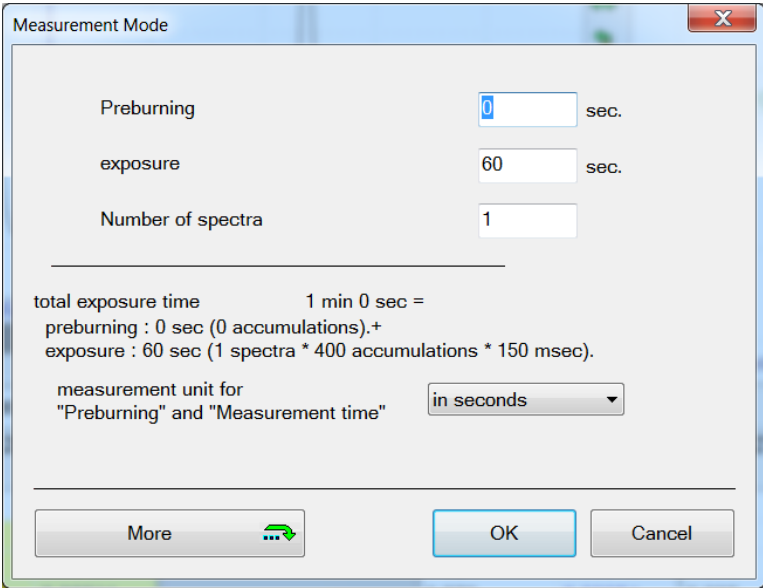
dialog or to constraint the search in "Spurious Lines" and "Qualitative analysis" tools. Perform the following actions to add new group:


1. select elements to be added to new group using "Periodic table" dialog..
2. open "Group Manager" dialog (press "Settings" in "Periodic table" dialog and select "Group Manager" tab).
3. enter name of new group in the input field (at the top right).
4. press "Add group of selected elements".

Select group name from the list (at the top left) and press "Delete group" to delete it.

Use this dialog to select filter elements. The filter may be used either to simplify the search when selecting the current element (filter elements are highlighted with pink background in the "Periodic table" dialog) or to restrict the search in "Spurious Lines" and

"Measurement mode"



Open this dialog by pressing  button located on the "Working with Device" toolbar. The program stores all settings individually for each document (file with analysis results). If several documents are open in the program with different measurement settings, change of the active document will also change the settings. Settings are saved when saving the document; settings are loaded together with the file. Various options of measurement settings are considered below depending on the spectrometer type and spectrum analysis features. Currently, operation and control of the generator start-up is supported according to different schemes –

Simple	Arc-spark excitation – Vesuviy, Fireball, UGE-4, IVS-29, etc. Pulsed laser excitation – LMA-10
Argon spark stand	DFS-51, Polyvac, SpectroLab S, etc. for vacuum spectrometers with argon feed control using electromechanical relays
Grand Expert	For spectrometers with microprocessor argon feed control. This is a series of Grand Expert, Favorit and other spectrometers.
Continuous sample feed	ICP and AAS spectrometers – ICAP-61, SpectroFlame, Kolibri, S-115, etc.

Own dialog is provided for each operating mode, where the corresponding parameters are specified.

"Preburning" — sets a pause before the measurement after the generator start-up.

"Measurement time" — duration of spectrum measurement.

"Number of spectra" sets the number of burning spectra, which shall be registered.

Depending on the mode of operation with distillation/burning spectra the measurement result will either be one spectrum with several exposures, which the program will store, or an average spectrum and separate burning spectra, which will be added to additional graphs of spectrum window, and will be stored only until new measurement. For example, if this parameter is set equal to two, then the main spectrum will appear in the spectrum window (corresponding to the whole exposure time), as well as the second and third spectra, displayed in additional graphs, corresponding to the first and the second half of exposure. If one spectrum is set, burning spectra will not be registered. Use of burning spectra is described in more detail in "Performing analysis taking into account burning of elements".

Total measurement time is equal to "Preburning" + "Measurement time" (see line of "Total measurement time" description).

The following parameters are added when using "Argon spark stand" mode, Grand Expert, Favorit spectrometer or spark sampling:

"Blowing" — sets the time of stand blowing with gas before the generator start-up.

"Register spectrum starting form preburning" – registration of spectrum and burning taking into account the generator operating mode change.


MAES analyzer for spectrometers with argon spark stand is delivered with a special control unit providing synchronization of blowing and various generator mode start-up times.

The following parameters are added in the "Continuous Sample Feed" mode:

"Measurement Delay" — sets the expected time of sample pass through the capillary to the excitation band.

"Number of parallel measurements" – the set number of spectra is automatically measured.

"Pause between parallel measurements" – pause between measurements.

Spectra are registered in two stages – press  to open "Sample Spectrum Measurement" dialog, where the operator sets the sample name and selects necessary operation. Registered spectra are automatically recorded in the analysis table with the specified name.

Change of control modes is described below.

Attention! All specified times shall be divisible by the basic exposure of the device. If a time is set, which is not divisible by the basic exposure, the program will automatically correct the discrepant values and will report about it in the yellow pop-up help window. Basic exposure value is displayed in the description line (highlighted with green colour in the figure).

"Parameter measurement unit" – allows selecting the measurement units for "Preburning" and "Measurement Time" parameters: seconds or accumulation units. One accumulation corresponds to one basic exposure of the device. When measurement unit is changed, all parameters are recalculated from seconds to accumulation units or from accumulation units to seconds.

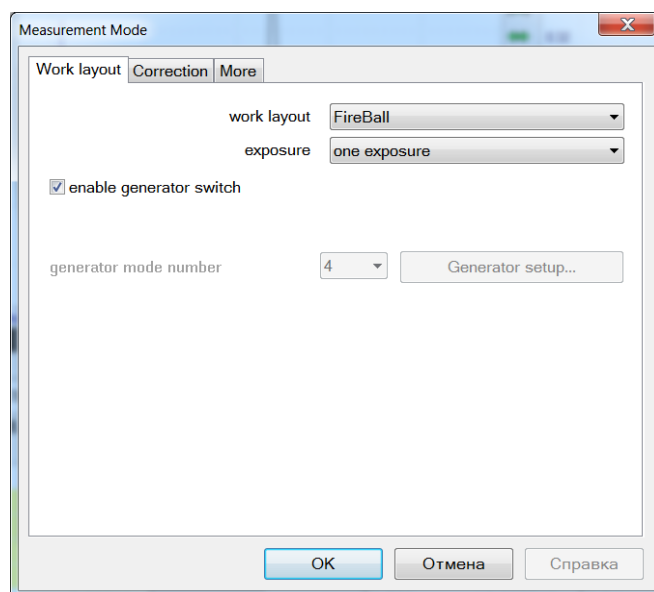
All parameters have default values. If the value of a corresponding input field is deleted, and no value is entered, the default value shall be used. Default value for "Preburning" is equal to zero, for "Number of spectra" — one spectrum, for "Measurement time" — the minimum of possible values is set — one accumulation (one basic exposure) per spectrum.

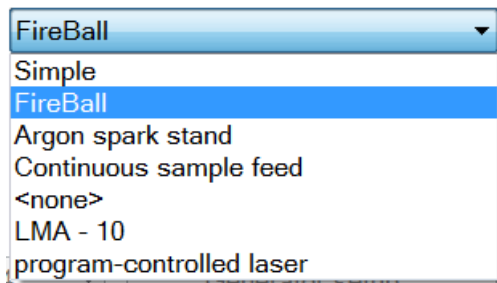
Press **"More"** button to open additional measurement settings.

"Work layout" tab

" Work layout" window defines main methods of activation (see figure).

" Work layout" dropdown list defines the main methods:





"Simple" — the simple analysis mode with one relay operated external arc/spark generator;

"Fireball" — the analysis mode with program operated external arc/spark generator Fireball-40, Fireball-250 etc.;

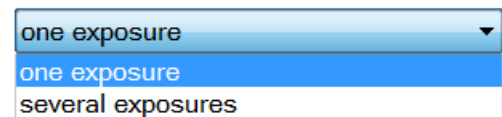
"Argon spark stand" — the complex analysis mode with three relay operated external arc/spark generator;

"Continuous sample feed" — the analysis mode with continuous sample feed via flame or ICP generator;

"<none>" — reserved for integrated programmable generator like Grand-Expert or Vesuviy;

"LMA-10" — the laser spark analysis mode with one relay synchronisation shot;

"program-controlled laser" — the laser spark analysis mode with integrated programmable shot;

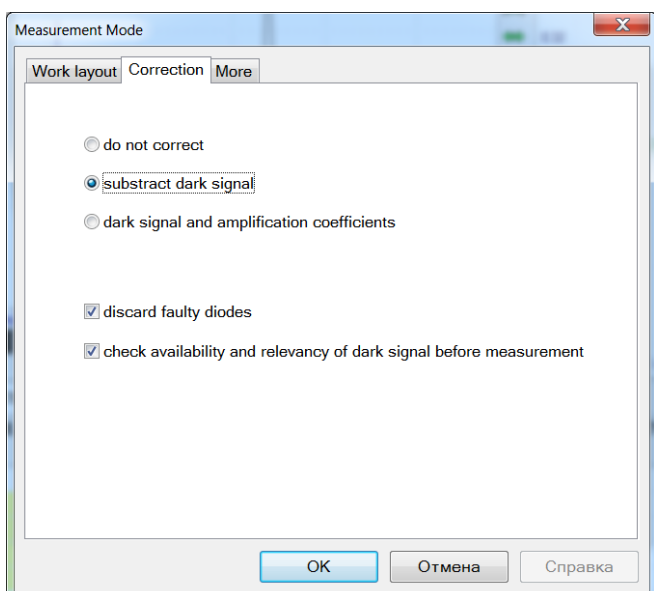


"One exposure" — all exposure in one spectrum with possible registration of several "additional" spectra (left for compatibility);

"Several exposures" — registered spectrum contains all time parts, into which the exposure was divided; it is recommended to application for all analysis techniques.

"switch on the generator" checkbox specifies, whether to switch on or not the generator for the period of spectrum measurement.

"Generator Mode Number" dropdown list is additionally defined during operation with Fireball generator and the program-controlled laser, setting one of the predetermined modes.



"Correction" Tab

"do not correct" defines that the measured spectrum shall not be corrected by sensitivity (dark shall not be subtracted and gains shall not be corrected).

"subtract dark signal" defines that it is necessary to subtract the dark signal, which was previously measured by the operator, from the measured spectrum (see "Dark Signal Measurement").

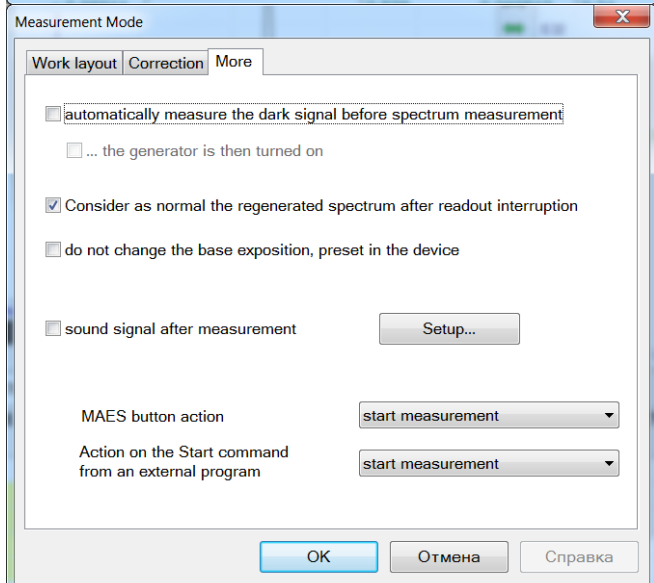
"dark signal and gains" — compensate difference of gains besides dark signal subtraction.

"leave out 'bad' diodes" — leave out previously rejected diodes from the spectrum. Spectrum is not measured in sections of left out diodes. See "Screening of 'bad' diodes".


"More" tab

"automatically take dark current reading before measurement" — the program will automatically measure dark current before each spectrum measurement.

"sound signal after measurement" allows assigning a sound file (".WAV" extension) to the program, which will be played upon completion of spectrum measurement. Press **"Customize"** button to open "Sounds" dialog: use "..." button to open standard "Open file" dialog and to select sound file (.WAV extension). Use other buttons to control sound playback.



"Add spectrum to analysis table"

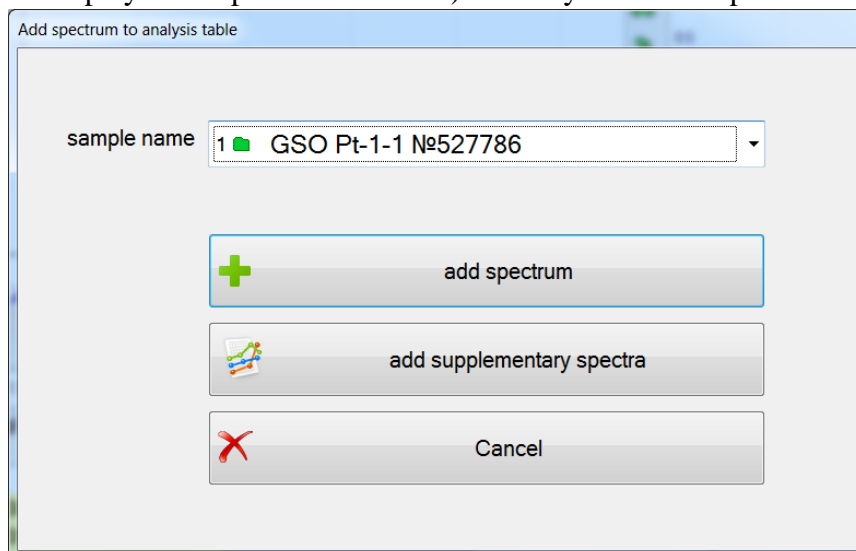
Used to add the current spectrum (which is displayed in spectrum window) to analysis table. Opens automatically after spectrum registration or by pressing button , located at analysis table toolbar.

Combined **"sample name"** list is used for selection from dropdown list (press button with black triangle to the right of input field to open dropdown list) or manual keyboard input of the name of sample to add current spectrum to. If you enter a name that is absent in the analysis table, new sample will be created with such name.

"add spectrum" — current spectrum is added in the end of the list of parallel measurements of the specified sample.

"add additional spectra" — if additional graphs are displayed in spectrum window, they will all be added to the end of the list of parallel measurements of the specified sample. Only additional spectrum is thus added (not the current spectrum!)


"cancel" — spectrum is not recorded; dialog is closed.



The program provides several options of automatic spectrum recording during the analysis – settings are displayed in "Table Window Settings" dialog of "Automation" window (see below).


Spectrum will also be recorded by pressing "Input" or "Start" button of MAES, when the dialog is open.


"Add analytic line to analysis table"

This dialog is opened by pressing  button, located in the analysis table toolbar. It is used to enter analytic lines into analysis table.

First, select chemical element (click its name in the table of elements), and then its line (the list to the right of the table of elements).

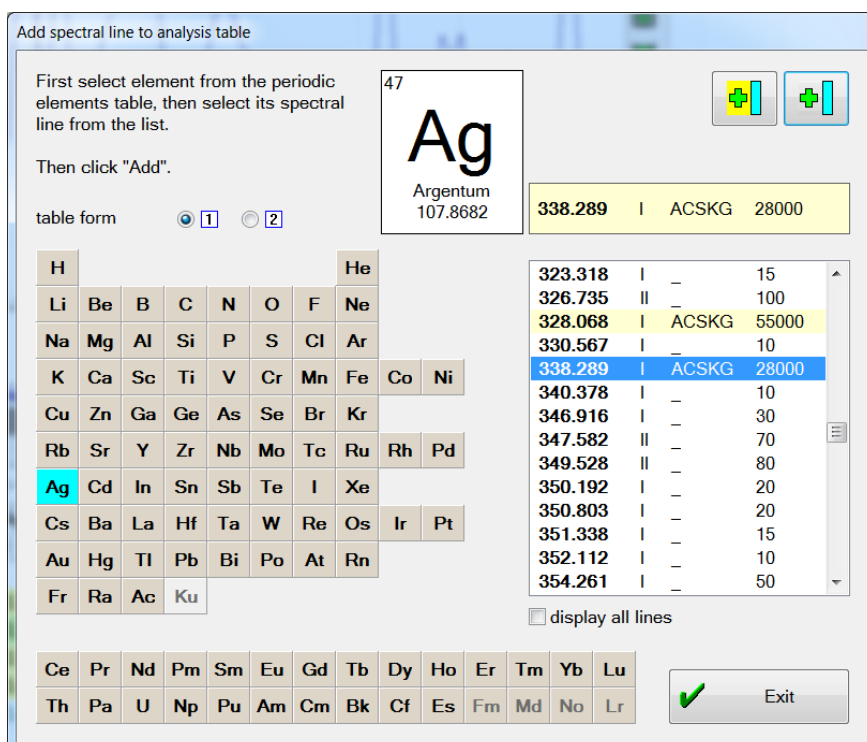
Current selected element is highlighted with blue colour in the table of elements, and its name is displayed in the dialog upper part. Selected line is drawn with a blue background in the list of lines, and is displayed in the dialog upper part.

Press  (at the top right), or double-click the line to add the selected line.

To add all lines with G key (displayed on top of the list), press .


After addition the program will return to this dialog again. Press "Exit" (at the right bottom) to exit the dialog.

"table view" switches output of the table of elements: 1) Mendeleev's table; 2) alphabetically;

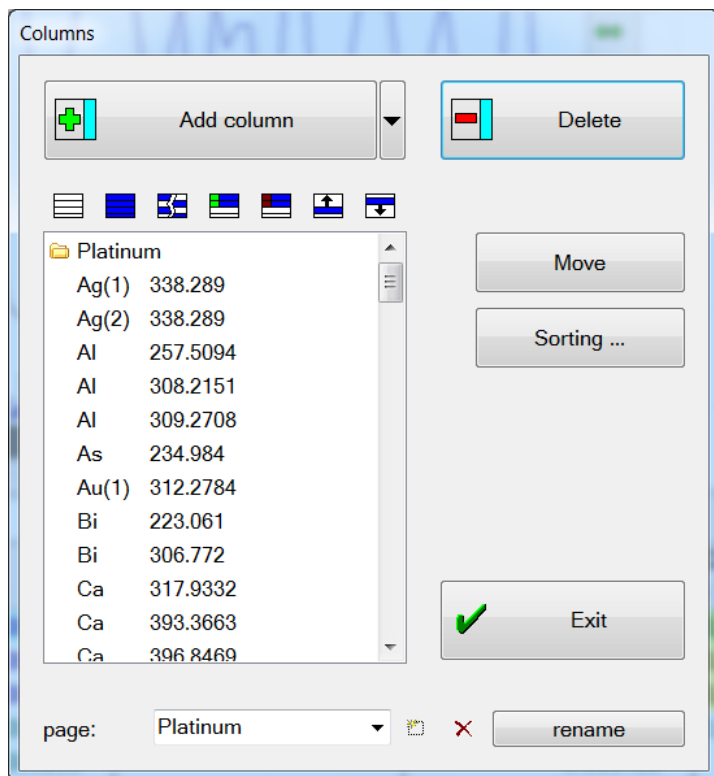



"view all lines" — if the dialog of spectral line display settings specifies to display not all lines, use this key to make the program display all lines in the list.

If reference lines are selected for the selected element (lines recommended to be used for the analysis), they are displayed at the head of the list lines against yellow background; besides, if such line is selected, its name will be displayed in the upper part of the dialog against yellow background. All reference lines may be added to the analysis table by performing the following operations:

- press button with small triangle to the right of button ;
- select "Add all reference lines" in the pop-up menu.



"Columns"






This dialog is opened by pressing  button, located in the analysis table toolbar. It performs the following operations:


- add analytic line to analysis table (press **"Add column"**). Press button with black triangle to the right of **"Add column"** text and select column type in the pop-up menu to add one additional type of columns.
- delete one or several selected columns from the analysis table. To do this, select columns in the list and press **"Delete column"**. If you press one of unselected columns, it will be selected; if it is already selected, it will be deselected. You may also use selection control button (see "Analysis Mode buttons").
- transfer the selected columns to another page of analysis table. To do so, select columns and press **"Transfer"**. Select page name in the pop-up menu.
- change order of columns in the analysis table. Select columns and use selection






movement buttons (see "Mode Analysis buttons"). You may also open "Sort columns" dialog (**"Sort"** button).


- change current page — select page name in the dropdown list at the dialog bottom. Selected page columns will be displayed in the list.
- create new page — press .
- delete page — select page and press .
- rename page — select page, enter new name in **"page"** field and press **"rename"**.

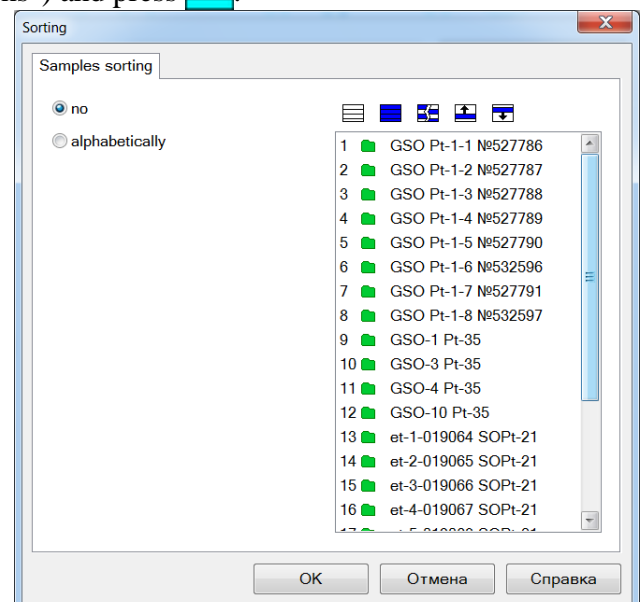
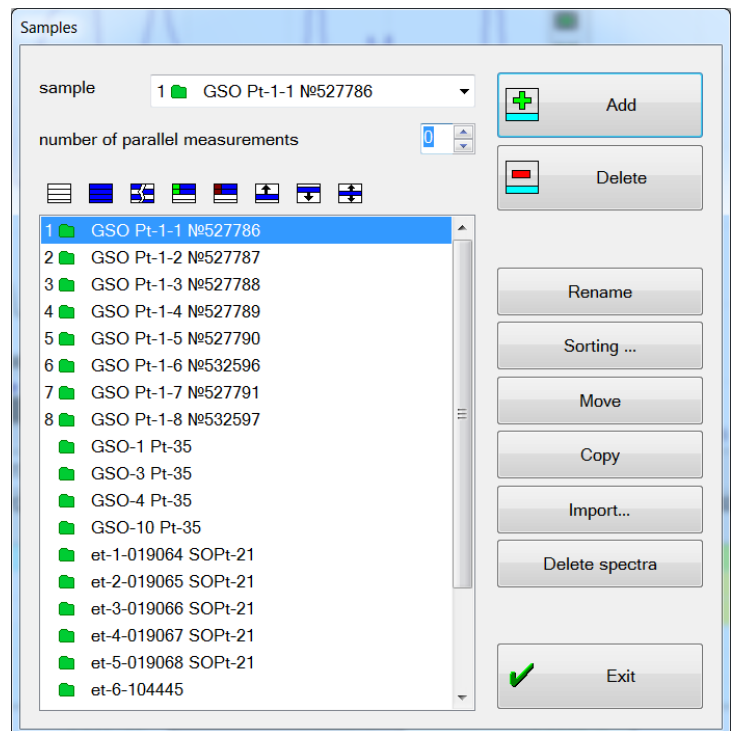
- Main selection buttons  function similarly to other dialogs, special buttons  allow selecting only lines with calibration graphs or lines displayed in the analysis table, buttons  move the selected group up or down the list.

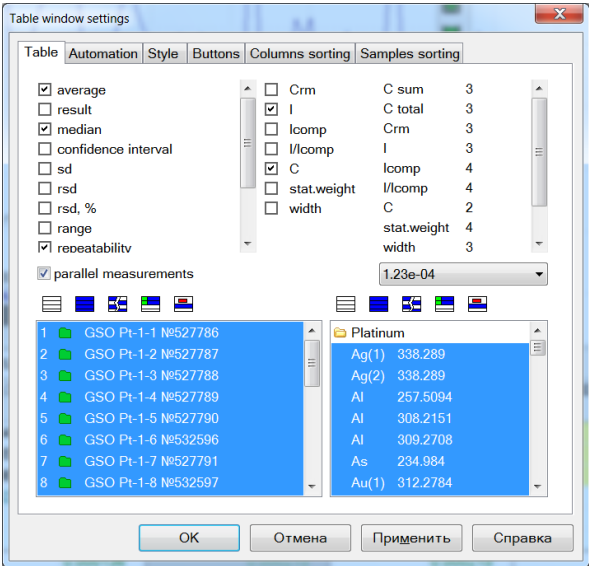
"Samples"

This dialog is opened by pressing  button, located in the analysis table toolbar. It performs the following operations:

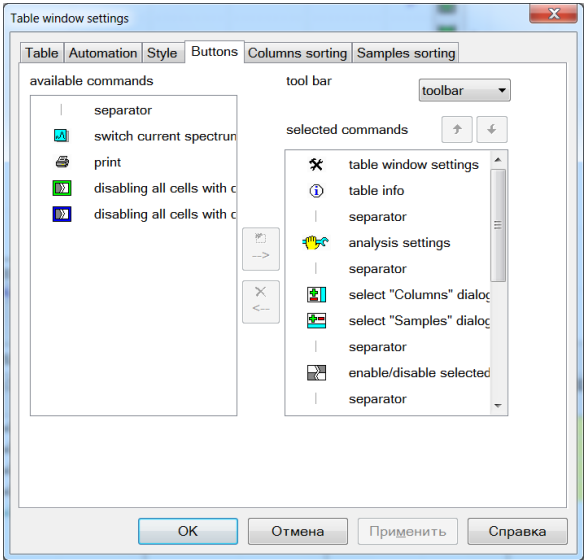
- add new sample with the specified number of "empty" parallel measurements. It is useful for initial filling of the table with names of samples with indication of the necessary number of parallel measurements for each sample; spectrum measurements are performed after that. To do so, enter new sample name in "**sample name**" field, select "**number of parallel measurements**" and press  "Add". Filling of the table with empty lines may be useful when generating analysis results file with the switched on mode of automatic spectrum addition after its registration.
- add the specified number of "empty" parallel measurements to an already existing sample. To do so, select one sample: either by using the dropdown list of "**sample name**" field (button with black triangle to the right of field), or in the sample list at the left bottom. Then select "number of parallel measurements" and press  "Add".
- delete one or several samples from the analysis table. To do so, select samples in the list at the left bottom (hold pressed "Shift" or "Ctrl" button to select several samples, or use selection control buttons located above the sample list, see "Analysis Mode buttons") and press .
- rename current sample. To do so, select sample in one of lists, enter new name in "**sample name**" field and press "**Rename**".
- change order of samples in the analysis table. Select samples in the list at the left bottom and use selection movement buttons ( ). You may also open "Sort columns" dialog (press "**Sort**" button).
- "**Transfer**"/"**Copy**" — transfers samples and spectra selected in the list to the analysis table of any open document.
- "**Import**" — loads the sample list from the text file or MS Excel table. When a camera shot is prepared in advance, this function (together with the mode of automatic spectrum recording) provides the highly automated analysis – the operator only places samples, starts spectra registration and is not distracted by input of sample names using the keyboard.

Sample name may be simple and composite. Simple name is one line. Composite name is a more flexible structure, which includes several words separated by a delimiter character. Entered name type setting is performed in "Automation" dialog window of the analysis table window settings (it is open by pressing button ).

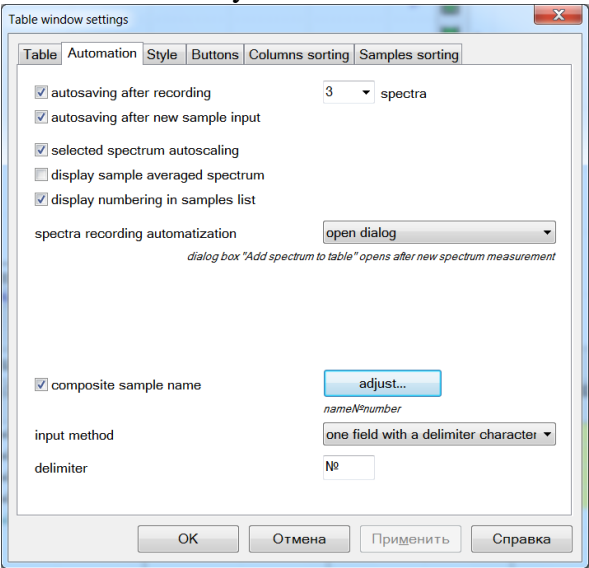




Viewing parameters windows for main analysis data table

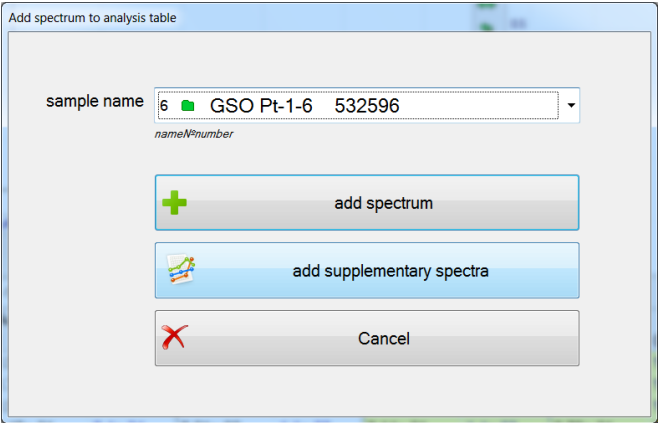


Buttons setting window for main analysis data table

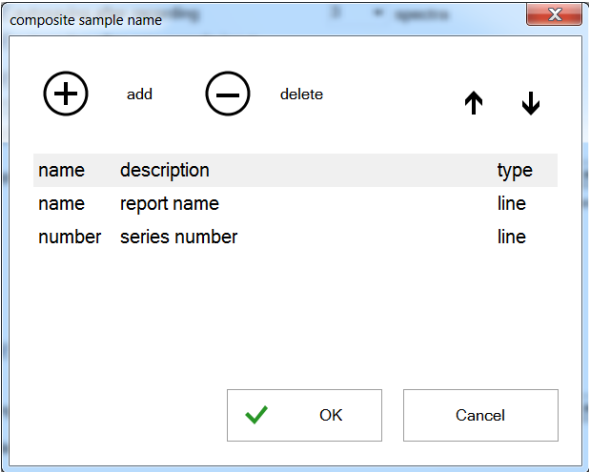


Automation parameters window

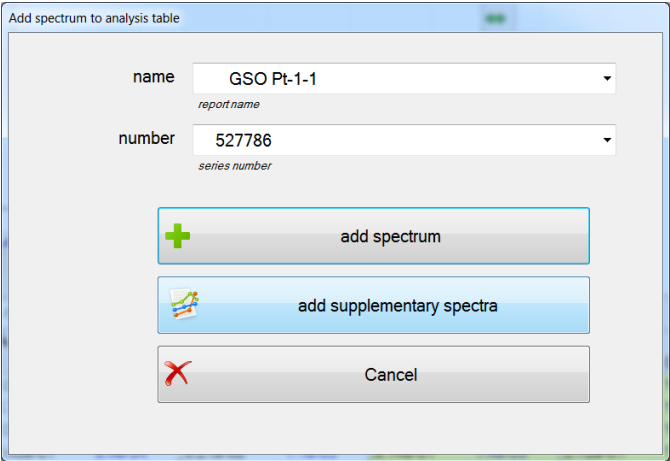
Input window of a composite sample name as one field with a delimiter character ("space" or "№" symbol). You may use any symbol, dash, comma, etc. as a delimiter character.



“One field” name





Window of composite sample name setting with individual fields




Input window of a composite sample name with individual fields

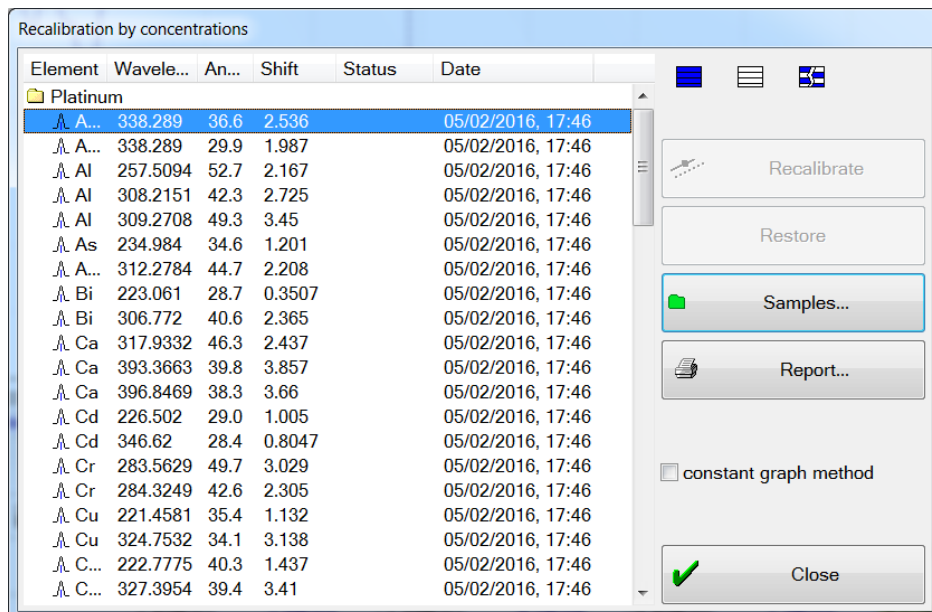
Composite sample name fields are displayed in the report as individual columns. It is recommended to use a composite sample name for well structured names, when it is necessary to select the shift, furnace, melting operation, locomotive number, engine number, warehouse number, date, sampling time, etc.

"Recalibration"

Operation using the permanent graph method is switched on by pressing button , located in the toolbar of analysis table window; when pressed, the button looks like . After that calibration graphs remain unchanged irrespective of addition/deletion of reference samples.

Recalibration dialog may be open by pressing button . The dialog allows

- recalibration of calibration graphs of selected analytic lines in the presence of control samples; calibration is always performed relative to original graphs;
- recovering coefficients of original graphs;
- switching to the report printing mode by calibration graphs.




The list of analytic lines of the analysis table, grouped by table pages, is displayed at the left in the dialog window. Only lines with calibration graphs are displayed in the list.

Select lines in the list, which shall be recalibrated (click once the line to select it; click again to deselect it; you may also use selection control buttons). Click the line to display its calibration graph in the calibration graph window. Then click "**Recalibrate**". "OK" text and correction factor value will appear by the recalibrated lines, if parallel measurements translation was performed.

Two lines — of new and old graphs (highlighted with gray colour) — are drawn in the calibration graph window after recalibration.

Click "Close" to exit dialog.

Spectral line display settings

Open this dialog by pressing button , located on the "Spectral Lines" toolbar. It is used to select the way element spectral lines are displayed in the list on "Spectral Lines" panel, in "Add analytic line to analysis table" dialog, as well as in some other lists and dialogs.

Output format

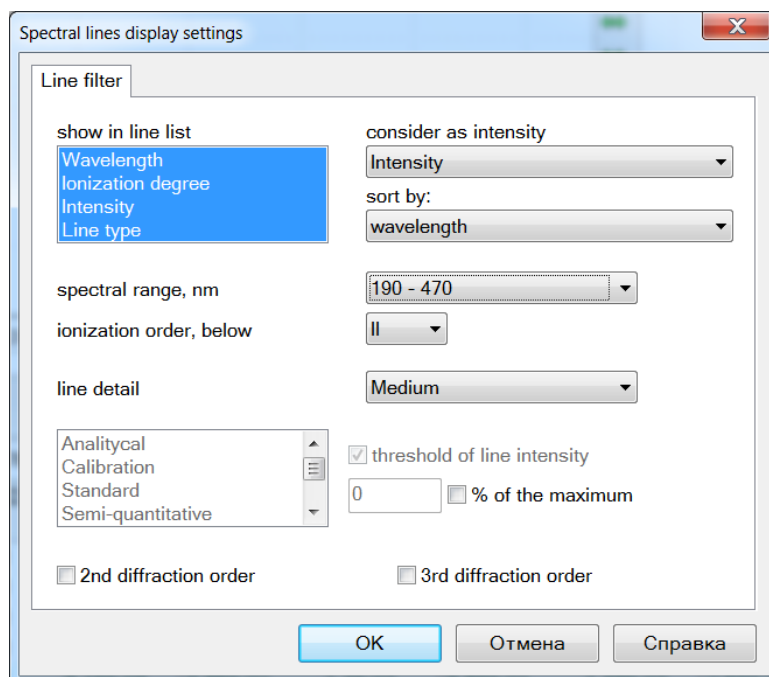
Upper half of the dialog is used to set up the output format of spectral lines:

"As 234.984 I SAKG 250"

"display in the line list" — select elements to be displayed in the line list:

"Wavelength" — this element is always selected, wavelengths are always displayed in the list of spectral lines.

"Degree of Ionization" — if degree of ionization is specified for a line, it will be displayed in the line list as symbol **I** for the first degree or symbol **II** for the second degree.



"Intensity" — if relative intensity is specified for a line, it will be displayed as a number at the end of the line (in the example provided above this number is **250**). Usually several symbolical and numerical parameters (intensity values) are specified for lines, corresponding to different types of excitation sources. Selected the intensity values to be used in "Line intensity:" list (see below).

"Line type" — several additional attributes may be specified for a line except the intensity, for example, you may specify that the line is analytical, in this case symbol **A** will appear in the line string. The list of line types — **A** – analytical, **C** – calibration, **S** – standard, **K** — line is used for qualitative analysis, **G** — line is used for quantitative analysis.

In the example provided the line describing the line type looks as **SAKG**.

"**Line intensity**" — specify in this list the possible intensity value to be used in the program. Line intensity is displayed in the line description string in line lists, as well as in the spectrum window (in the form of vertical blue lines above line names).

"*Intensity*" — intensity specified by the user

"*Arc*" — intensity of lines in case of arc excitation of spectrum

"*Spark*" — intensity in case of spark excitation of spectrum

"*Energy*" — excitation potential (eV)

"*ICP*" — intensity for inductively coupled plasma

"*PC lamp*" — for spectral lamps

"*Sensitivity*" — ...

"*Chigher*" and "*Clower*" — parameters for semi-quantitative analysis using method of line emergence and gain. If there is no line, concentration value is less than Clower; otherwise it is higher than Chigher.

"**Sort lines by:**" — specify the line sorting scheme in the list. Sorting by wave length and by intensity is possible in ascending order or in descending order.

"**Spectral range**" – restriction of the line list by wavelength, or from the current profiling, or from the specified set of characteristic values "200–400", "190–470", "170–470", "185–550".

"**Degree of Ionization**" – restriction of the line list by the degree of Ionization "all", "I", "II", "III", etc.

Line filter

The lower half of the dialog is used to limit the number of lines displayed in lists. Only lines meeting the specified criteria are displayed.

"**Level of Line Detail**" — select one of the predetermined line filters:

"*High*" — all lines are displayed without limitation;

"*Average*" — only lines with a specified intensity value are displayed;

"*Low*" – there shall be a symbol (one or several among ACSKG symbols).

"*Specify*" — manual adjustment of filter parameters (see below).

Select line types in the list at the left bottom. In order for the line to be specified in the list and be displayed in the spectrum window, it is necessary for this line to have at least one specified type from among the selected types. If all types are deselected, all lines above the intensity threshold will be displayed.

"**Intensity threshold**" — check this key, if filtering is required by line intensity values. Threshold value of line intensity may be specified in the input field in percents of the maximum intensity for each element. If zero is specified, threshold value will not be used, but filter will discard lines with unspecified intensity.

"**2nd order**" and "**3rd order**" — check these keys to view lines corresponding to the second and the third diffraction order (with a wavelength increased by two and by three, respectively).

Editing of spectral line parameters, addition of new or deletion of old lines is performed in "Spectral Line Base" tool mode.

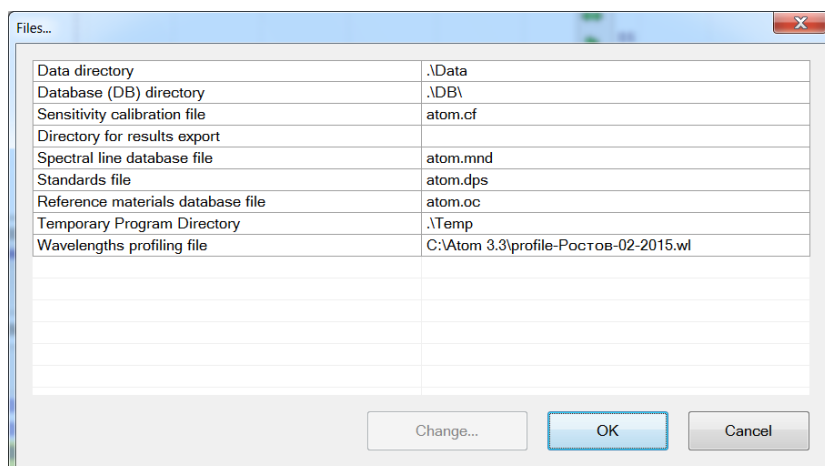
Subdialogs of program settings

"Files..."

The dialog is open using main program menu item "**Settings / Files...**" and is used to specify start-up files and directories that the program starts working with when launched. Names may be entered from the keyboard in a corresponding line or by selecting it and clicking "Change..." button – select file/directory dialog will open, where you can find the required file or directory, respectively.

The program will remember the selected element and will use it all the time until the next modification.

".\Data" designation means that this element is located in the working directory of the program. If working directory is "c:\Atom 3.3", then the full path is "c:\Atom 3.3\Data".



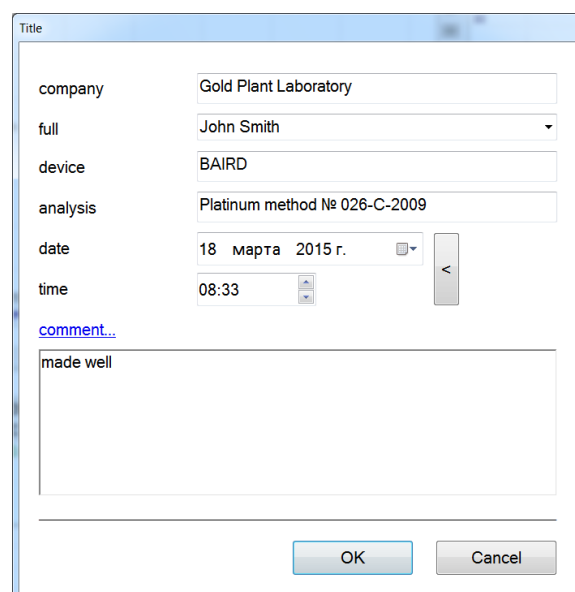
"Title"

The dialog is open using main program menu item "**Settings / Title...**" and is used to fill in the title fields. Title contents are saved in the analysis results file as additional information. The title is also used to filter database queries (see "Database" mode).

Fill in the required title fields and click "OK".

Use the dropdown list to specify the name ("**Full Name**" field). Use "User List" dialog to edit the user list..

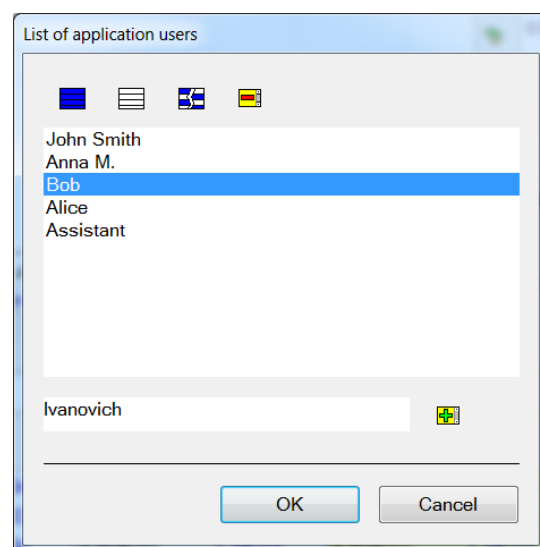
Click "<" button to specify current time/date. Use dropdown list of "**Date**" field — "Calendar" control element — to edit the date.



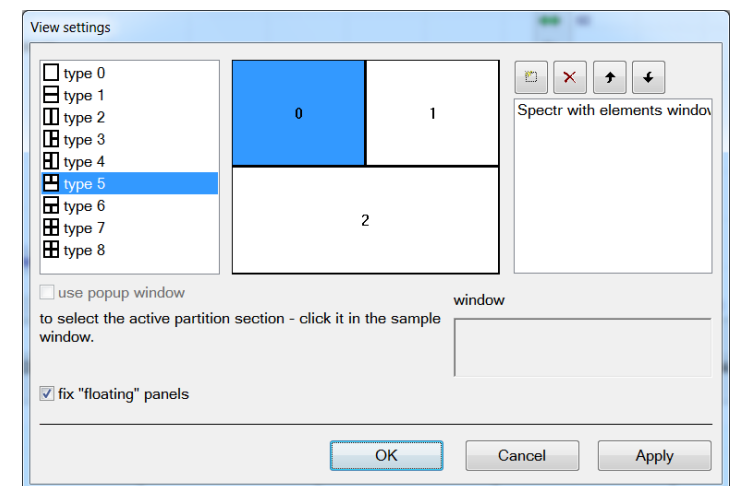
"User List"

The dialog is open using main program menu item "**Settings / User List...**" and is used to edit the list of program user names. This list is used later to speed up input in full name "Title" dialog and to select user name when entering "Laboratory Assistant" mode. To add new name, enter it in the input field at the dialog bottom ("**Petrov Pyotr Petrovich**") and click . To delete one or several names, select them in the list ("**Sidorov Ivan Petrovich**") and click .

Click the required name in the list to select it; it will be highlighted, if it has not been selected yet; otherwise it will be deselected. You may also use selection control buttons above the list of names (see "Main buttons of 'Analysis' mode"). Click "OK" to save changes.

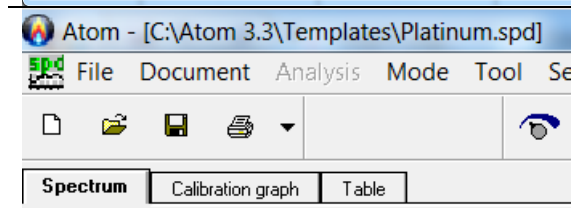


"Display View Settings"



This dialog opens using the main program menu item "**Setup / Splitting Document Windows**" and is used to set up the main window view in "Engineer" mode.

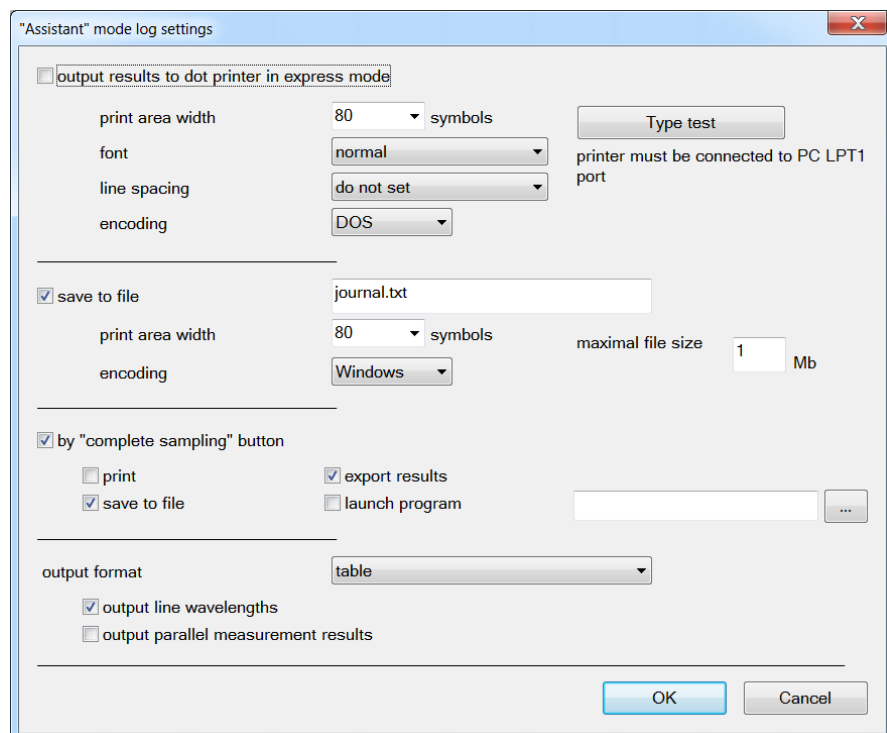
Standard main view is selected during program installation with the analysis table located below, spectrum located above at the left and the calibration graph located above at the right – **type 5**.



In a specific situation it may be more convenient to use another view, for example, of **type 0**, when windows are always maximized full screen, and switching between them is performed like between tabs in dialogs.

"Fix Floating Panels" switch is required in the following situation – to fix position of panels with buttons used to start spectrum measurement, start various modes (e.g. "Qualitative Analysis" and "Spurious Lines"). ATOM program will restore position of buttons at the start, if the switch is turned on, or will arrange them dynamically – like all standard Windows functions do.

"Log Settings..."



The dialog is open using main program menu item "**Settings / Log...**" and is used to set up express printing during routine analysis in "Laboratory Assistant" mode and/or to save results in a file, as well as to export results to an external program. Printing is performed using a matrix printer connected to LPT1 port: in continuous mode.

Program behavior is also controlled in this dialog using "Complete Sampling" button.

Example of log printout using a matrix printer

=====

'Grey iron' program
'Laboratory assistant' operator
12/09/08 11:00

dark signal measurement
09/04/12 15:20:11

		Si	Mn	Cr	Si	Mg	S	S	C
(1)	-	2.05	0.0917	0.0832	2.08	1.17	0.388	0.369	2.29
(2)	-	1.93	0.0947	0.0847	2.11	1.11	0.408	0.383	2.30
(3)	-	1.90	0.0901	0.0833	2.08	1.12	0.396	0.377	2.26
(4)	-	2.06	0.0937	0.0816	2.08	1.08	0.326	0.304	2.16
(5)	-	2.12	0.0970	0.0837	2.12	1.08	0.379	0.351	2.35
Average -		2.01	0.0934	0.0833	2.09	1.11	0.379	0.357	2.27
Difference -		0.22	0.0068	0.0031	0.037	0.098	0.082	0.079	0.18


'Grey iron' program complete
09/04/12 15:34
=====

This function is usually applied during operation with equipment that works round the clock in conditions of foundry production, where regulations provide for saving of a hard copy of analysis results.

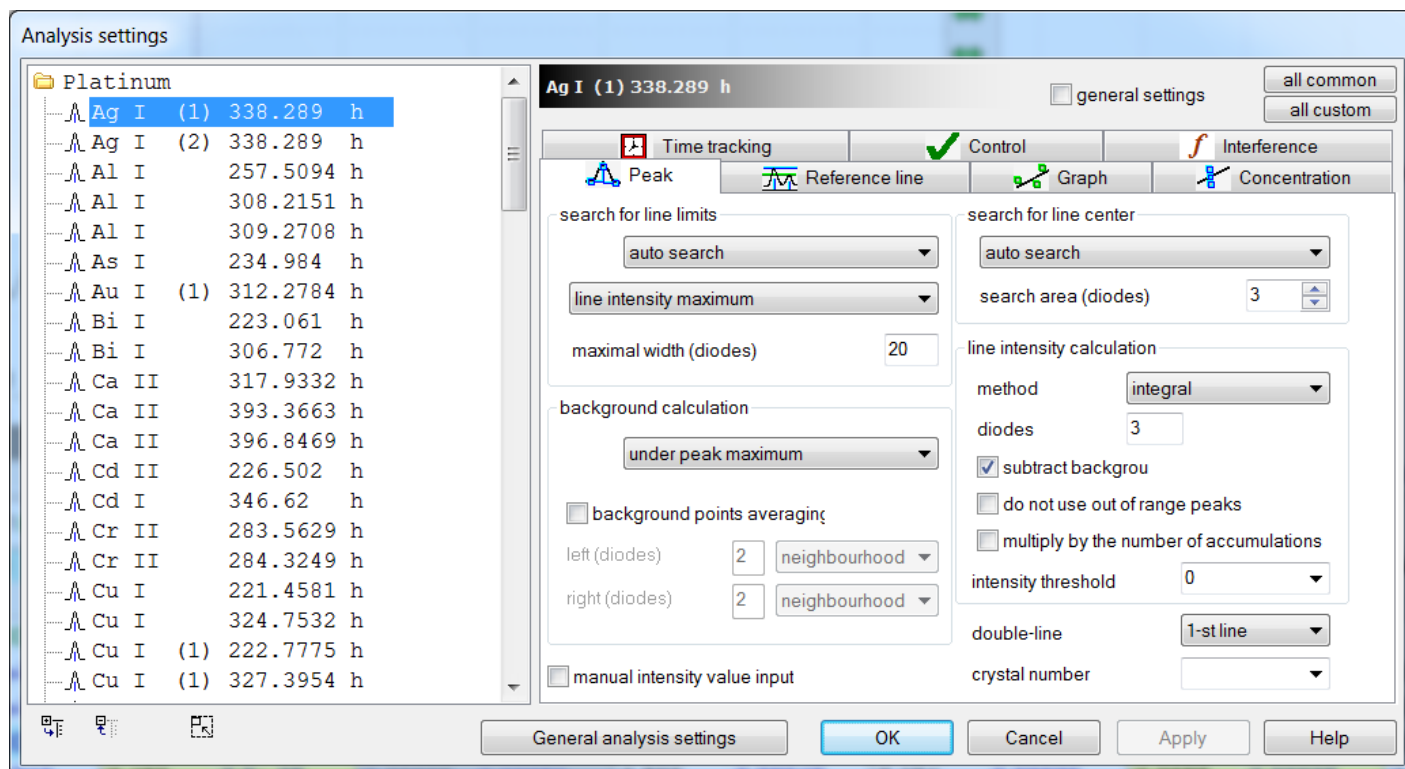
The same text results are saved to file "journal.txt" and external printer.

Special external program could be started every time as sample is finished – the program could export saved results to a local network database or laboratory information system.

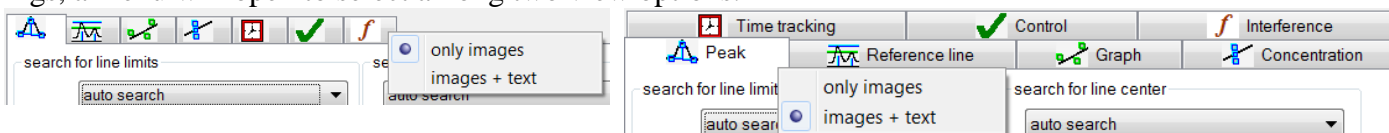
Analysis settings

Dialog is open by pressing button , located in analysis table window toolbar and is used to change analysis settings: search parameters and to calculate peaks, reference lines, create calibration graphs, calculate concentration and other values.

List of analytic lines is displayed in the left part of the dialog (including additional types of columns, e.g. "Alloy" or "Concentration Factor"), added to the analysis table. The list is grouped by table pages. In order to change calculation parameters of line values in a spectrum or another type of column, select it in this list (click left mouse button on its name). After that corresponding settings will be displayed in the right part of the dialog. Settings for the analytic line consist of several pages.



Other view of settings dialog headings is possible; to change the view, click right mouse button near headings, a menu will open to select among two view options.



Each page corresponds to a certain stage of analysis results calculations:

- **"Peak"** — search and calculation settings of line background and intensity in the spectrum;
- **"Reference Line"** — reference line for relative intensity calculation;
- **"Graph"** — calibration settings;
- **"Concentration"** — settings for calculation of concentration and statistical results of analysis;
- **"Time record"** — setting periods of time for registration of various elements.
- **"Influences"** — parameters for accounting of additive or multiplicative mutual interferences of elements.
- **"Control"** — settings for received result check conditions depending on concentration or intensity of spectral lines of other elements.

Custom settings are displayed for other types of columns:

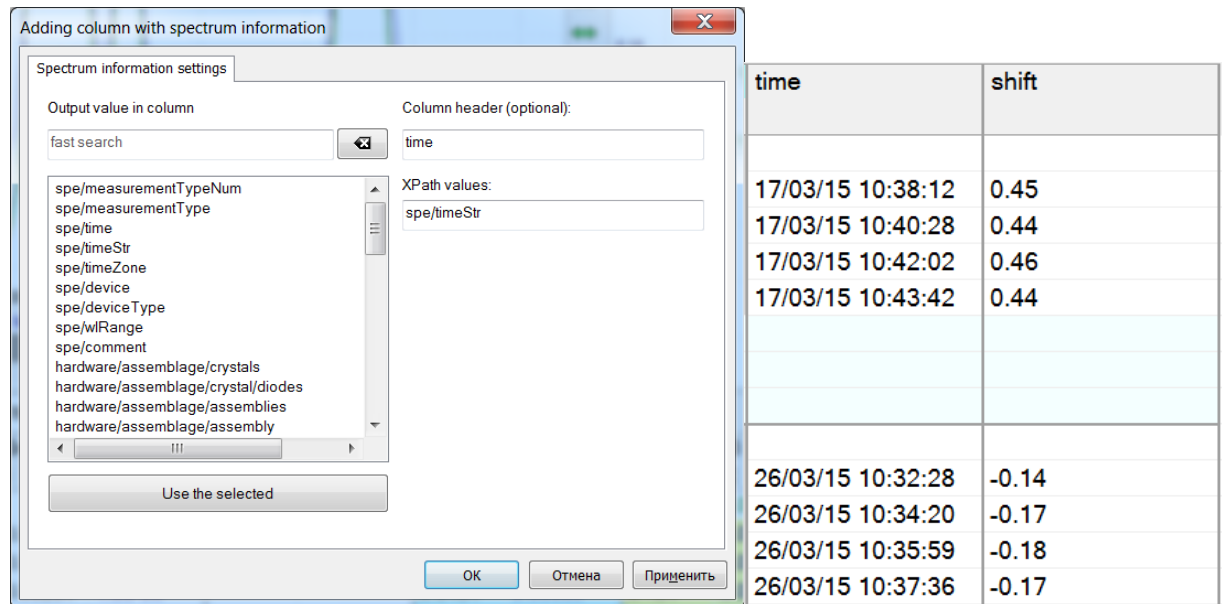
- **"Concentration by several lines"** — selection of lines used from the list of lines available in the analysis table.
- **"Sum of concentrations"** — selection of elements used from among such available in the analysis table.
- **"Concentration factor"** — coefficient type — concentration or dilution.

Each page of analysis settings ("Peak", "Graph", etc.) may have **"common settings"** and **"custom settings"**. Settings that are specified as "common" are identical for all lines. Change of analysis settings for one line will lead to change of corresponding settings of other lines that are specified as "common". If analysis settings for a line shall differ for any reason from settings for other lines, they shall be specified as "custom". Pay attention that each page of analytic line settings may have an intrinsic state — "common" or "custom". This allows specifying that the line has, for example, "common" settings "Graph" and "Reference line", but "Peak" setting is "custom". "ч" symbol is added in the list at the left of line name, which current settings page is specified as "custom". Other lines (without "ч" symbol in the name) are considered as "common" for the current settings page.

All new lines added to the analysis table have default settings corresponding to "common" settings.

"Information from spectrum" — information stored in the spectrum in the form of XML records. Such information is saved by various ATOM program modules, equipment control programs, "Fireball" generator, mathematical modules and other subprograms. Each spectrum contains a lot of ser-



vice information, which may be useful for operation control, for development of a technique and in other cases. Example below presents addition of spectrum time and position column of reference line number 1 and its view in the analysis table. It can be seen that during different time measurements are with a spectrum displacement by 1 photo diodes, which is normal.



Control elements are used to control "common"/"custom" state, located in the upper right part of "Analysis Settings" dialog:

- **"Common settings"** key specifies common or custom settings in the current settings page of the current line calculation. If this key is deselected, settings are specified as "custom"; otherwise — as "common". Upon transition to "common" state, settings are specified according to "common" settings of other lines and may change.
- **"All common"** specifies all line calculation settings as "common", and calculations of the current line corresponding to settings. It applies only to the current settings page (for example, only for "Graph" settings).
- **"All custom"** specifies all line calculation settings as "custom", and equal only of the current line settings. It applies only to the current settings page.

Upon a change of any settings, "*" symbol (at the left in the list) specifies all lines and columns, which values shall be recalculated. If line settings are changed, specified as "common", then "*" symbol will specify all other lines with common settings. If reference line calculation settings are changed, then lines, for which this reference line is a reference line, will be also specified, etc.

Values of several line calculation settings are displayed directly in the list of columns at the left. Click "+" at the left of the line name to see them. Click "-" to hide these settings. You may view/hide settings of several lines this way, by clicking "+" or "-" alternately. In order to show/hide settings of all lines, use buttons  and , located at the left under the list.

Besides calculation settings of line values in the spectrum and other types of columns, some common analysis settings are also located here, which may be displayed using **"Common analysis settings..."** button:

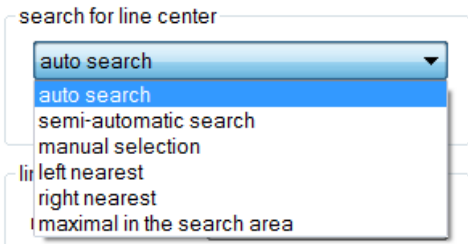
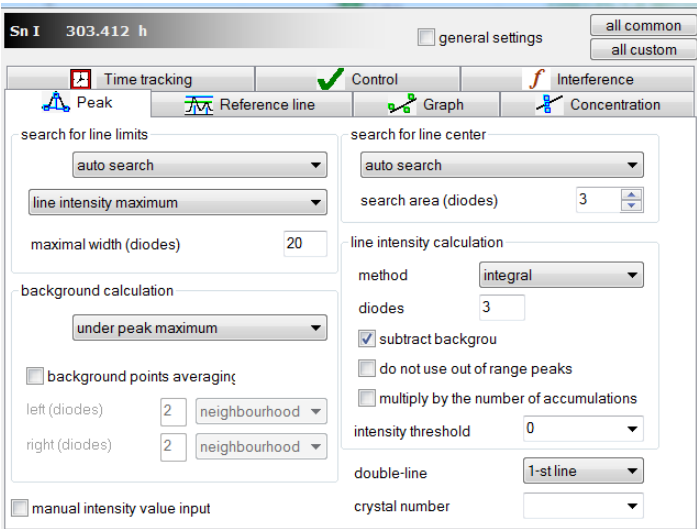
- **"Technique"**
- **"Reference lines"**

Click one of the following buttons to exit the dialog:

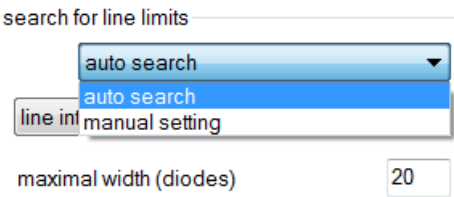
- **"OK"** — modified settings are applied, dialog is closed;
- **"Cancel"** — changes of settings are cancelled, dialog is closed;

- **"Apply"** — modified settings are applied, new values are calculated, the table is redrawn, but the dialog is not closed allowing selecting values of several settings, evaluating results of their modification, without exiting the dialog.

"Peak"



After the line maximum in a spectrum is found, left and right points of the background are searched. **"left search"**, **"right search"** – the program searches for the nearest in the left or right neighbourhood local spectrum maximum from the set reference wavelength of the spectral line. **"maximal in the search area"** – the program searches for the maximum in set neighbourhood local spectrum maximum from the set reference wavelength of the spectral line.



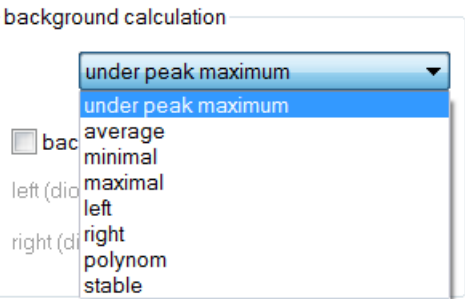
available only for "custom" settings "Peak calculation" for the spectral line (see "Analysis Settings" dialog).


"Maximum width (of diodes)" — maximum distance of the local minimum from the line center during automatic search of line borders. If the distance turns out to be higher than the specified value, the background point is set at the specified maximum distance.

Background value under the line is calculated according to the found left and right background points.

"background calculation" — select method for calculation of background intensity under the line.

- "Under the line maximum" — background intensity at the intersection of the line maximum and the straight line connecting the left and the right background points.




Dialog is open using button  on "Peak" tab, and is used to set up search parameters and to calculate the intensity of lines in spectra.

"Search for line center" — line maximum search method in the spectrum.



"Auto search" — the program searches for the nearest maximum in the set neighbourhood local spectrum maximum from the set reference wavelength of the spectral line.

"Semi-automatic search" – at first the automatic search is run. If the search was unsuccessful, it is recognized that the line maximum matches the reference wavelength.

"manual selection" — manually fix position of the line maximum using button . This item is available only for "custom" settings of "Peak calculation" for a spectral line.

"Neighbourhood of search (of diodes)" — maximum distance of the found local maximum during automatic search of the line maximum from the set wavelength. If the distance turns out to be more than the specified value, it is recognized that the peak was not found.

"Search for line limits" — select method to search line borders (left and right points of line background).

- **"Auto search"** — the program looks for the next local minima from the line center to the left and to the right.
- **"Manual setting"** — user sets the position of the left and the right background point using buttons  and . This item is available only for "custom" settings "Peak calculation" for the spectral line (see "Analysis Settings" dialog).

- "Mean value" — background intensity is equal to the mean intensity value of the left and the right background points.
- "Minimum" — background intensity is equal to the minimum value of intensity values of the left and the right background points.
- "Maximum" — background intensity is equal to the maximum value of intensity values of left and right background points.
- "To the left" — intensity of the left background point is used as background intensity.
- "To the right" — intensity of the right background point is used as background intensity.

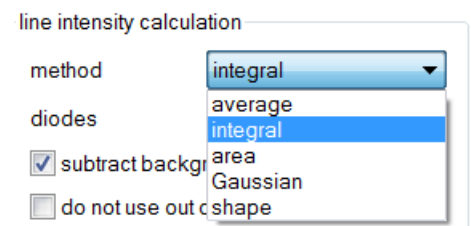
"Averaging of background points" — average intensity value of several adjacent items in the specified neighbourhood of background points may be taken as the intensity of the left and the right background points (see below).



"To the left (diodes)" and **"To the right (diodes)"** — number of the adjacent diodes used for averaging, located in the neighbourhood of background items individually for the left and the right point.

- **"To the left of point"** (for the left) and **"To the right of point"** (for the right) — the specified number of diodes is taken for averaging, including background point for the left point — to the left, for the right point — to the right of the line.
- **"Neighbourhood"** — the specified number of diodes is taken for averaging around the background point:
 - with 1 specified diode this is the spectrum value in the background point;
 - with 2 specified diodes — in background point plus 1/2 of spectrum values to the right and to the left of the background point;
 - for 3 diodes: — in the background point plus to the right and to the left of the background point, and so on.

"Line intensity calculation method" — possible options:

- **"Average"** — intensity is the mean value of intensity values of diodes in a zone, which center is located on the wavelength corresponding to the peak maximum, and width is equal to the number of diodes specified by "diodes" parameter. If the averaging zone covers a diode part, then only the corresponding part of this diode intensity is taken into account while averaging.
- **"Integral"** — intensity is the integral of intensity values of diodes in a zone, which center is located on the wavelength corresponding to the peak maximum, and width is equal to the number of diodes specified by "diodes" parameter.
- **"Area"** — intensity is the integral (area) between the left and the right border of the peak (background points).
- **"Gaussian"** — peak intensity is the Gaussian distribution intensity (see "Normal distribution (Gaussian distribution)"), which most precisely describes the spectral region between the left and the right background point. This method is recommended only when a spectral line of the base or another element is located near the analytic line of the defined element. When using this method, it is possible to specify in addition the spurious line, allowing taking into account its contribution to the analytic line intensity. To do so, switch on **"Accounting for spurious lines"** and click "...".



There are two methods to select the spurious line in the opened dialog: either as a spectral line (button ) , or as red spectrum cursor position (button ). In the first method the spurious line shall be selected beforehand as the current spectral line, and be displayed in "Spectral Lines" toolbar. Use "Spurious Lines" tool to define the element line that is spurious. In the second method it is necessary to set beforehand the spectrum cursor on the spurious line peak maximum. The algorithm currently provides accounting only for one spurious line.

"Diodes" — number of diodes for "Average" and "Integral" methods.

"Subtract background" — defines, whether to subtract background intensity or not from the line intensity value.


"Do not use out of range peaks" — intensity is not calculated, if there are points with ADC overflow in spectrum points used for intensity calculation (these are highlighted with red colour on spectrum graph).

"Multiply by number of accumulations" — the calculated intensity value is multiplied by the number of accumulations (number of basic device exposures), which the spectrum was registered with.

"Intensity threshold" — if the calculated peak intensity value is less than the preset value, it is recognized as uncalculated; it is recommended to use a small number to exclude from the analysis the random sound effects, as well as to limit, if necessary, the working range of intensity values.

"double-line" — works in spectra received by double-line analyzer MAES — it is possible to use the 1st or the 2nd line, as well as the average spectrum.

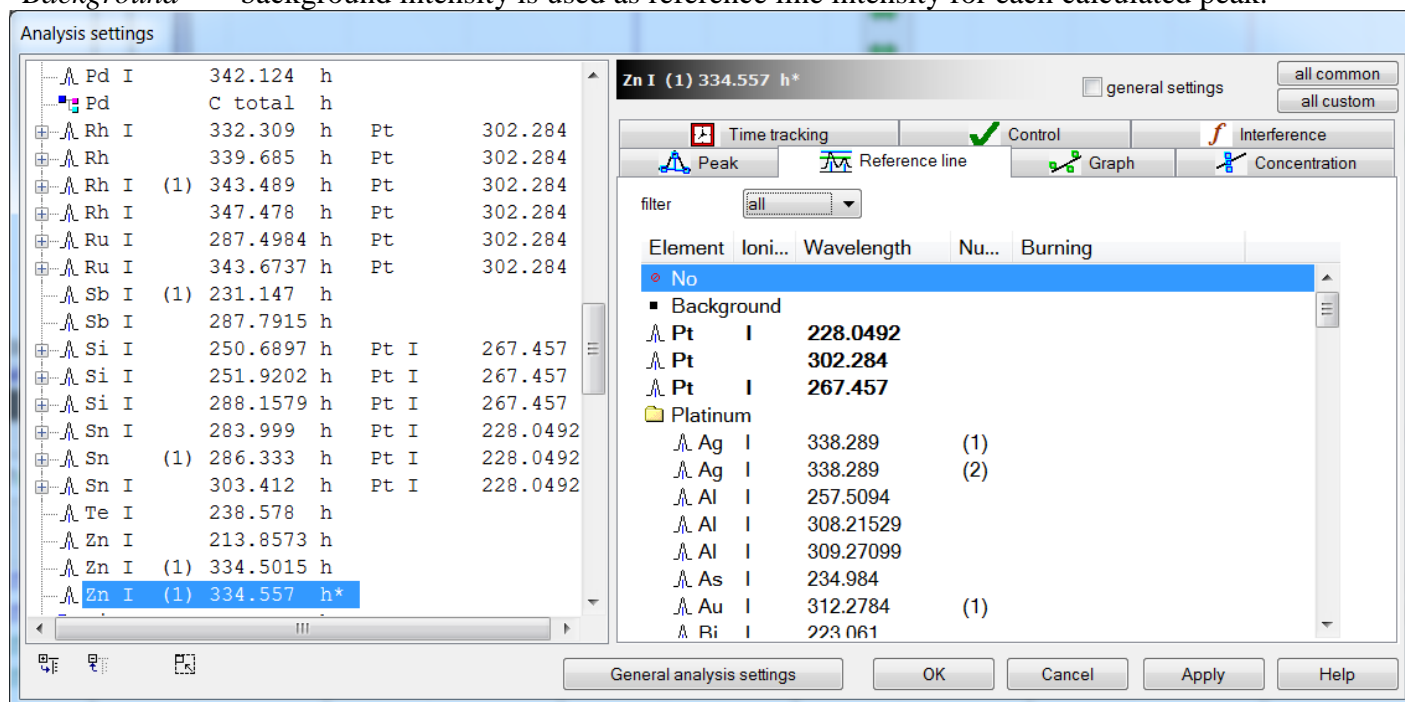
"Reference line"

"Reference line" is opened by pressing button , then "Reference line" tab. Dialog is used to specify reference line for the analytic element line.

Select reference line in the list.


"None" — there is no reference line.

"Background" — background intensity is used as reference line intensity for each calculated peak.



Division is always made by the reference line intensity; select spectral line for subtraction in intensity calculation settings. When working with techniques that use several exposures, it is necessary to pay attention to compliance of the registration time (exposure number) of analytic lines and reference lines.

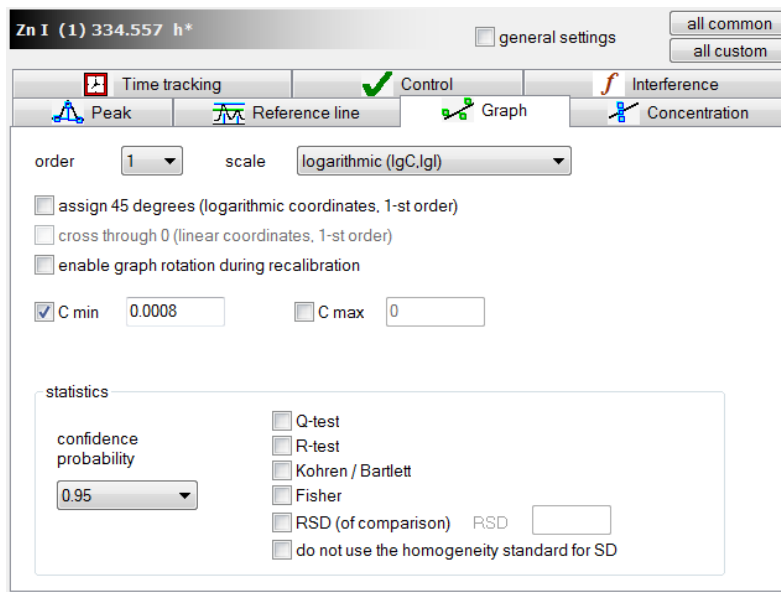
"Graph"

"Graph" is opened by pressing button , then "Calibration graph" tab. It is used to specify calibration parameters for the analytic line.

Polynomial approximant degree is selected in **"degree"** list.

Necessary calibration option is selected in **"scale"** list.

"assign 45 degrees angle for the graph" — effective, only if scale by **I** and by **C** is in logarithmic coordinates and the degree is



equal to 1. Thus the graph slope angle is always constant and equal to 45 degrees, and only the graph position (shift) is selected according to measured reference samples.

"plot the graph through 0" — effective, only if scale by **I** and by **C** is in linear coordinates and the degree is equal to 1. Thus the graph always passes through point (0,0), where zero concentration corresponds to zero intensity, and only the graph slope angle is selected according to measured reference samples.

"permit rotation during recalibration" — effective in "permanent graph" mode.

"C min", "C max" — if "C min" / "C max" value is set, reference samples (RS) with element concentration less or more than this value will be automatically disabled for this line and will not be used for calibration. It may be set only for "custom" parameters.

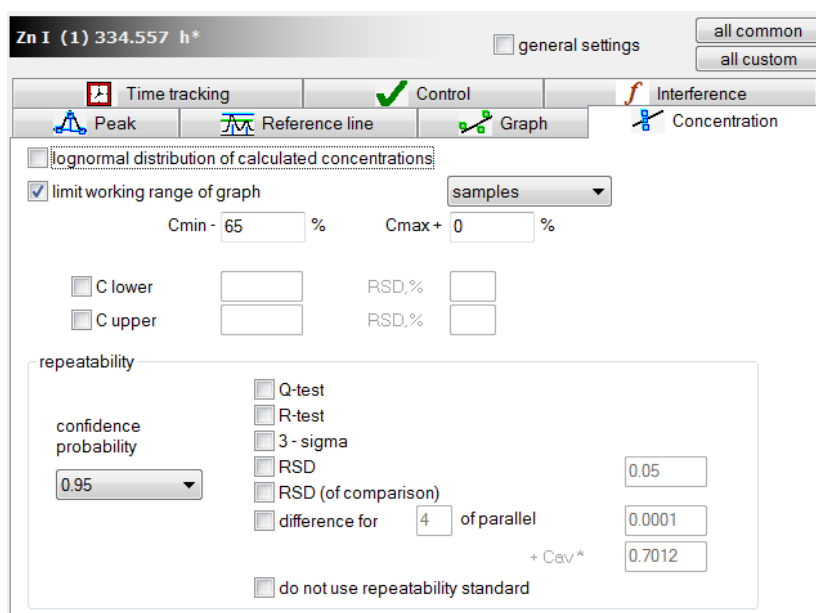
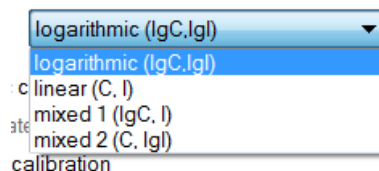
"Confidential probability" — confidential probability used to discard RS and to calculate confidential intervals. It may be equal to 0.95 and 0.99.

"Q-criterion" and "R-criterion" — discards gross errors (see "Q-criterion" and "R-criterion" in "Algorithms" section). Parallel measurements, that do not pass the specified criteria, are highlighted with red colour in the analysis table and in the calibration graph window.


"Kohren / Bartlett" — assesses RS variance according to Bartlett (if the number of parallel measurements in several RS is different) or to Kohren (if the number of parallel measurements in all RS is the same). If the calculated value of "Chi-square" parameter for Bartlett-criterion or G value for Kohren-criterion exceeds the corresponding tabular value, all RS parallel measurements with the maximum dispersion will be highlighted with red colour. See "Bartlett/Kohren criterion in "Algorithms" section ("Appendix — Algorithms for Atom calculations.doc" file on a compact disk with ATOM software). The criterion should be applied at a number of parallel measurements equal to 4 and more.

"Fischer" — assesses adequacy of regression equation according to Fischer criterion. If the calculated value of F parameter exceeds the tabular value, the calibration graph is highlighted with red colour, which means that calibration is inadequate. Besides, all parallel measurements are highlighted with red colour for the reference sample, which mean intensity value is the most distant from the calibration graph. See "Fischer criterion for assessment of regression equation adequacy" in "Algorithms" section ("Appendix — Atom software Calculation Algorithms.doc file).

"RSD (comparison)" — discards parallel measurements in RS by RSD of the calculated concentration. If a found concentration RSD exceeds the value specified in the window, parallel measurements with calculated concentration being the most distant from the mean value of the calculated concentration in a RS, is recognized as an outlier and is highlighted with red colour in the table and in the calibration graph. In case of a logarithmic scale the concentrations are calculated for concentration logarithms; otherwise — for concentration values.



"Concentration calculation"

"Concentration calculation" is opened by pressing button , then "Concentration calculation" tab. It is used to set calculation parameters of concentration and to control convergence of results.

"Logarithmically normal distribution of calculated concentration" — if you enable this key, all statistical convergence control criteria (see below) will use formulae for a logarithmically normal distribution of calculated results. For more details, see criteria description in "Algorithms" section.

"Limit reference sample graph working range" — if the button is on and the average sample concentration measured is less than the minimum or

more than the maximum concentration value in standards for the set amount of percents (which is specified in "**Admissible excess of Working Spectrum Limits, %**" field), then analysis table and report will display the uncalculated average concentration value, and "<min" or "> max" values are minimum and maximum concentration values in RS, respectively. The corresponding parallel measurements values are calculated and displayed as usual. If the button is disabled, the calculated value of average concentration will be displayed irrespective of its value.

"**Clower**" and "**Cupper**" parameters are required for visual content control of elements — impurities in working samples. Average concentration values, which are out the specified spectrum, are highlighted on the graph and in the analysis table with red colour. RSD may be also set for the lower and the upper concentration in the corresponding "**RSD**" fields. Lower limit value of spectrum will thus be equal to $\text{Slower} * (1 - \text{RSDlower})$, and upper — $\text{Supper} * (1 + \text{RSDupper})$.

Convergence control of parallel measurements

Check criteria that shall be used for discarding.

Calculations are performed for logarithms of concentration values for all criteria in case of a logarithmic scale of calibration graph concentration values, otherwise — for concentration values. Besides, if a "logarithmically normal distribution" is included, formulae are used for logarithmically normal distribution law, but not for the normal distribution.

"**Confidential probability**" is the value used to calculate statistical criteria of convergence. It can accept values 0.95 and 0.99. Value 0.99 forces the program to perform more strict control, than such for value 0.95.

"Q-criterion" and "R-criterion" — defines, whether to discard or not gross errors (see "Q-criterion" and "R-criterion" in "Algorithms" section ("Appendix — Atom calculation algorithms.doc")). Parallel measurements that do not satisfy the criterion, are highlighted with red colour when displayed in the table and on the graph.

"**3 sigma**" — discarding gross errors, see "3 sigma criterion" in "Algorithms" section. Parallel measurements that do not satisfy the criterion are highlighted with red colour when displayed in the table and on the graph.

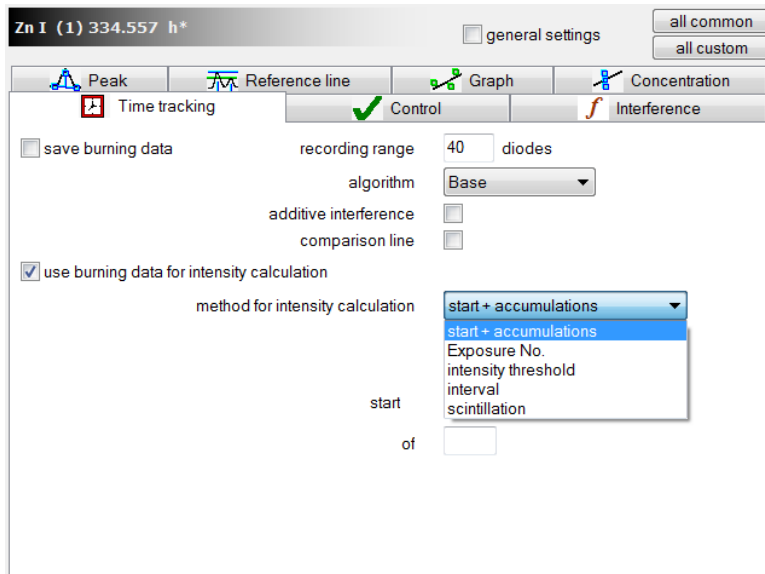
"**RSD**" — rejection of gross errors, see "Rejection of gross errors: deviation from mean value" in "Algorithms" section. Parallel measurements that do not satisfy the criterion, are highlighted with red colour when displayed in the table and on the graph. Parameter set in "RSD" field is used for discarding.


"**RSD (comparison)**" — discards parallel measurements by RSD of the calculated concentration. Parallel measurement, concentration in which is the most distant from the mean concentration value in a sample is recognized as incorrect and is highlighted with red colour in the table and on the calibration graph, if the found concentration RSD in this sample exceeds the value set in "RSD" field.

"**Difference for N parallel measurements**" — see "Convergence criterion: difference for N parallel measurements" in "Algorithms" section. Parameters set in fields located to the lower right from this criterion are used for calculations. Parallel measurements, which concentration is the most distant from the mean concentration by a sample is highlighted with red colour in the table and on the graph, if this criterion is not met.

"**Do not use the convergence standard**" — if the standard is specified in common analysis settings, which contains the data for convergence control, then all parameters specified above will be used only when this setting is active.

"Time tracking"



"Time tracking" is opened by pressing button , then "Time tracking" tab. It is used to set time record parameters for burning of elements.

"save burning data" parameter provides recording of a small spectral region corresponding to the spectral line and the background around it (30–50 diodes) from each single accumulation of the entire exposure, i.e. 80 spectral ranges will be saved in 8 seconds for a basic exposure of 100 ms. They will be used by the program to perform calculations (see histogram figure).

Depending on the mode of operation with spectra in the time record mode, it is possible to use "Start" and "Accumulation", "Exposure

number", "Intensity Threshold", "Manually" and "Scintillation" parameters.

"Start" – number of the first burning spectrum from all measured spectra. starting from which it is necessary to calculate the analytic line intensity.

"Accumulation" – number of measured burning spectra, starting from "Start", which will be used to calculate the analytic line intensity.

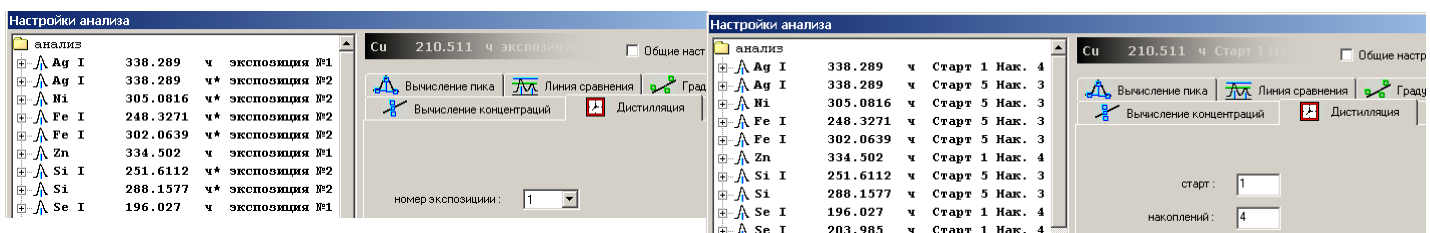


"Exposure number" – exposure selection (from 1 to 10) for intensity calculation; if a number is selected, which is absent in spectrum, the first exposure is taken into account.

"Intensity threshold" – calculation method of spectral line intensity is based on the analysis of "burning record"; intensity is calculated in each of the recorded ranges, then it is compared with threshold, all higher values are integrated or averaged. The result is displayed as a spectral line intensity value in the analysis table and is used for further calculations.

"Add burning spectra..." parameter is left to ensure compatibility with previous program versions – now we recommend using spectrum registration in the "several exposures" mode — each spectrum contains all information on burning by time, that allows recalculating intensity in this mode and adding new lines to calculation upon spectrum registration without adding new lines in the analysis table.


If it is necessary to interrupt registration of burning, "do not use distillation information" parameter will al-





low calculating the intensity and concentration by average spectra.

See ""Performing analysis taking into account burning of elements" of "Working with the Program" section as well.

"Technique"

Press button , then click button "**Common analysis settings...**". It is used to set up several parameters influencing common calculations of analysis results.

"permanent graph method" — see description in the dialog. To switch to permanent graph method, press button , located in the analysis table window toolbar. If it is switched off, any changes of reference samples (switch on/off, add/delete sample or spectrum, change analysis settings, etc.) lead to automatic calculation of new calibration graphs. Switched-off permanent graph method is recommended during calibration, and switched on — during the analysis. Press button  in the analysis table to recalibrate manually the selected lines with the switched on permanent graph method. Recalibration is performed by preliminary measured spectra of control samples.

"Identical Crm for all elements" — switch on, if all table elements have the same concentration of reference materials. Concentration value entered is set for all elements.


"use the standard..." — allows selecting the operating convergence and reproducibility control standard for the received measurement results. For more details see "Using standards" item in "Working with the program" section, as well as "Standards" mode description.

"working with distillation spectra..." — selects between work additional graphs and several exposures. The first method has parameters compatible to the previous program versions, and the second new method, allows saving, displaying and selecting several spectra exposures in one basic spectrum corresponding to one measurement — it is recommended for application when creating new analysis techniques.

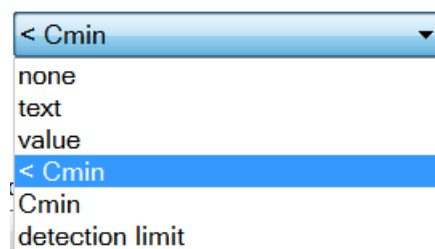
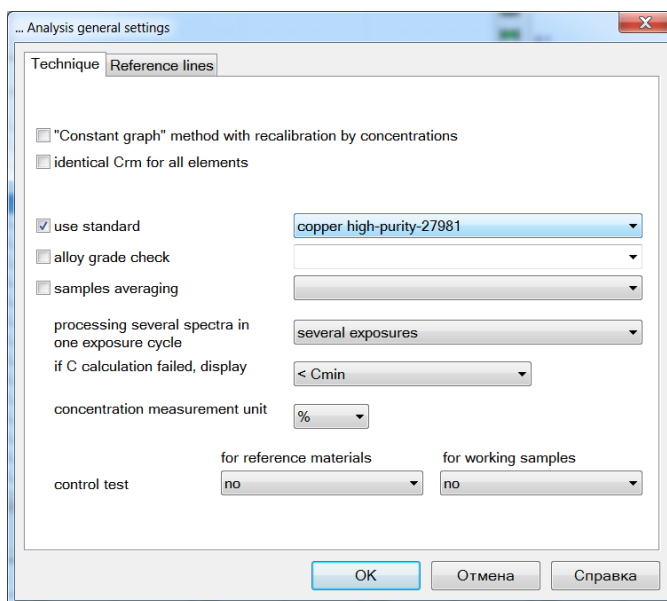
"if C calculation failed, display..." — in case when it is impossible to calculate concentration, for example, due to the absence of the analytic line, in case of a negative value in linear coordinates, etc., it is possible to select a suitable option: empty cell, text line, numerical value, Cmin value or detection limit, calculated from the calibration graph.

"Blank test" or blank sample. In several cases during the analysis it becomes necessary to compensate the constant component in intensity values of analytic lines for a number of elements, for example, during chemical preparation of samples or continuous aliasing of a molecular line or the base line, observed in all sample spectra and/or reference samples. **"Blank test"** parameter is provided for such cases. If it is set, then average intensity in **"Blank test"** is subtracted from the intensity measured in the spectrum for each analytic line. Nothing is subtracted, if average intensity was not calculated, or all parallel measurements are switched off. If necessary, blank sample may be accounted for individually for reference samples and for work samples. *For work using standard addition method it is necessary to select base accounting only for reference samples, then the base will be calculated as a sample.*

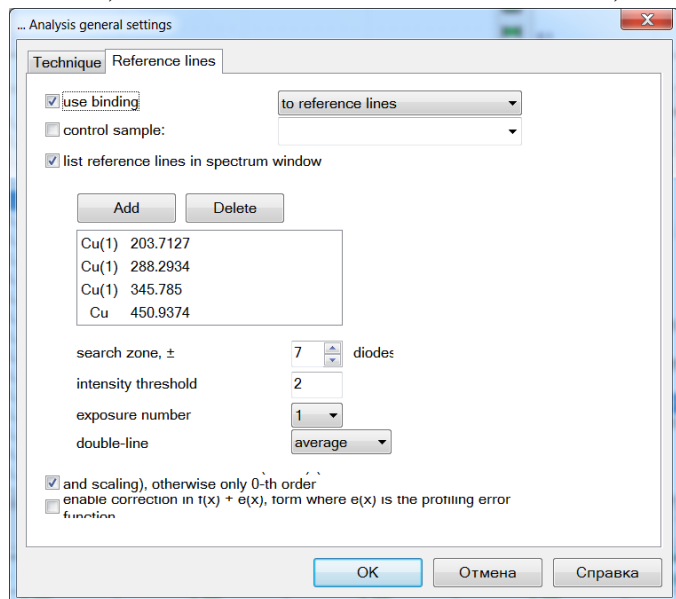
"Reference lines"

Press button , then click "**Common analysis settings...**" button and switch to "Reference line" tab. Control assignment of elements of dialog control is described in this section.

"Use binding to reference lines" — switch on/off automatic binding of spectra measured by MAES to reference lines. Measured spectrum profiling is corrected at the time of its addition to the analysis table.



"Use binding to reference element" — switch on/off automatic binding of spectra measured by MAES to the reference element. Profiling is corrected in all lines of the specified element or elements using correlation method, it works well when bases are the same, but it demands high computing power of the computer.



the maximum deviation of a reference line. The program will search a peak with the maximum intensity in this spectrum (\pm "search zone"), which, presumably, corresponds to the reference line. If the range set is too small, the program may not find the peak, if it is beyond the set range. If search spectrum set is too big, the program may not find that peak — if the shift was large, or there are intensive enough lines of other elements nearby.

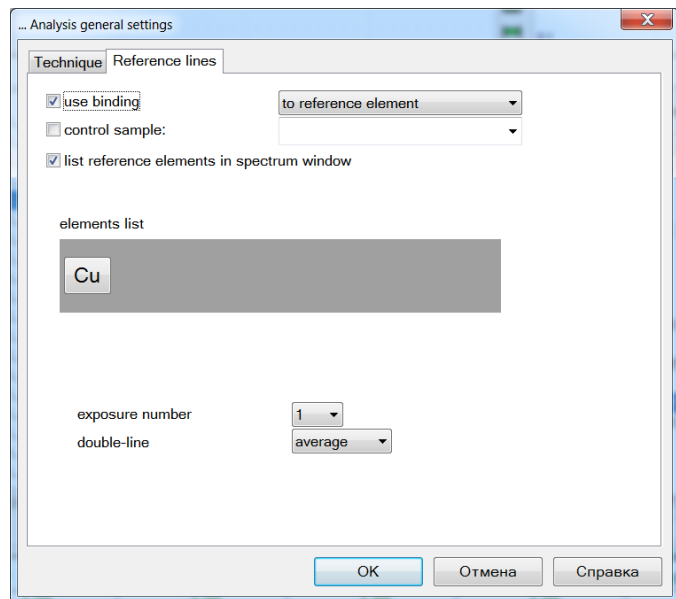
Reference line **"intensity threshold"** — sets lower limit for possible reference line intensity could be used.

"exposure number" — sets number of exposure that could be used for multi-exposure spectra.

"double-line" — sets variant number of spectrum string that could be used for double-string spectra.

"scaling" — allow profiling correction of "shift and spread" type, otherwise only the shift is selected for all reference lines. This item makes sense, if there is more than one reference line, and there is a linear spectrum distortion or a spectrum distortion of a higher degree — for example, in prismatic devices.

"enable correction $f(x) + e(x)$ " — profiling error correction by the 2nd degree polynom; $f(x)$ — profiling, $e(x)$ — error function. Profiling shift is calculated at first (or a shift and a spread, see previous item), and then error function is calculated, if this item is switched on. It is reasonable, if simply a shift or a shift and a spread correct distortions with insufficient precision.



"List reference lines in spectrum window" — if it is switched on, then in spectrum window, at the top left **"reference: line1, line2, ..."** text will be highlighted with red colour, specifying all reference lines. If it is switched off, only "reference point" text is displayed. Text with description of reference points is displayed, only if "Use binding to reference lines" is switched on (see above), and the line list is not empty.

"list of reference lines" displays lines selected as reference. Click "Add" and select line in the opened dialog to add it to the list. Only lines added to the analysis table may be used as reference lines. To delete a line, select it in the list and click **"Delete"**. The list may contain any number of lines; if necessary, the program will average the profiling correction result for all lines.

Reference line **"search zone, \pm "** — sets "(Diodes) search zone" parameter the greatest value, which sets

search zone" parameter the greatest value, which sets

"control sample" — when it is difficult to select a suitable reference line in spectra, it is recommended to apply the option with spectrum registration of a specific sample and control of profiling only in it. Correction of the next parallel measurement of this sample will be applied to all subsequent measured spectra.

"Reference element" — another algorithm for wave-length correction. Its based on many spectral lines of selected elements —there are the main components of samples usually.

After change of reference lines and/or other settings the initial profiling is restored and correction is recalculated automatically.

If profiling is divided into groups, it is necessary to set a reference line for each group — for example, for Grand spectrometer these are 280 and 420 nanometers spectrum areas, for STE-1 — 250, 320, 420 nanometers.

Reasons for using reference lines.


When air temperature and pressure changes in the working room, spectrum position relative to the detector also changes. Violation of wavelengths conformity to numbers of diodes leads to essential distortion of analysis results due to impossibility to search in the spectrum of necessary analytic lines; therefore for control of spectrum position in the window it is necessary to select reference lines from among lines specified in the analysis table. It is recommended to use individual lines of average intensity as such lines, commonly these are spectral lines of a the main sample component or the material of electrodes. Such lines shall appear in all sample and reference sample spectra, they shall have a well-defined maximum, they shall not be "off scale" or self-absorbing. It is recommended to control that spectrum region, which contains analytic lines, and to select reference lines according to the following table. There is no need to select references line located in a spectrum far from analytic lines.

Spectrometer type	Example	Number of reference lines	(Diodes) search zone	Arrangement of reference lines relative to the working spectrum
1. With a planar diffractional grating	DFS–8, 13 PGS–2	1–2	20–50	Central portion _____
2. With a concave diffractional grating	Grand MFS–4, 6, 8 DFS–458C DSF–36	2–3	10–15	Edges and center _ _____ _
3. Prismatic	ISP-28, 30	2–3	10–15	Edges and center _ _____ _


Selection of reference lines is connected with that for the first type spectrometers, which are very sensitive to temperature variation even by 1–2 °C, the change of spectrum position relative to the detector up to ±50 of diodes is corresponds well enough to the fixed bias in the entire working range; for the second type spectrometers the effect of external factors is expressed much weaker due to a relatively small size; but the changing spectrum position relative to the detector up to ±10 diodes already leads to linear discrepancy at edges of the working range, which demands application of two reference lines; for prismatic spectrometers the effect of external factors is expressed considerably when temperature changes by 3–5°C, and the change of spectrum position relative to the detector up to ±5 diodes leads to nonlinear discrepancy at edges of the working range, which frequently demands application of three reference lines for a more precise correction of concordance of wavelengths to numbers of diodes.

If MAES analyzer contains several groups of crystals (Grand, STE-1. DFS-36, etc.), the reference lines work individually for each group.

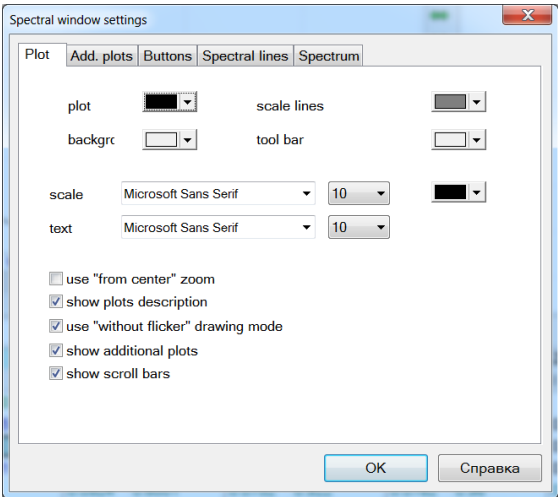
Spectrum window settings

Press  button located o the spectrum window toolbar to open this dialog. The dialog consists of several tabs; to switch to a tab, click its name in the list of tabs on top of the dialog: "Graph", "Buttons", "Home", "Spectral lines", "Spectrum"

"Graph"

It is used to control main graph settings, click button  on the graph window toolbar to open it (spectrum window, calibration graph, histogram), "Graph" tab.

- "graph"** colour — set colour of the main (not additional) graph.
- "background"** colour — set the graph background colour.
- "scale line"** colour — colour of dashed lines of the graph scale.
- "toolbar"** colour — graph toolbar panel background.



"Scale font and colour..." regulates font and colour of graph scale captions.

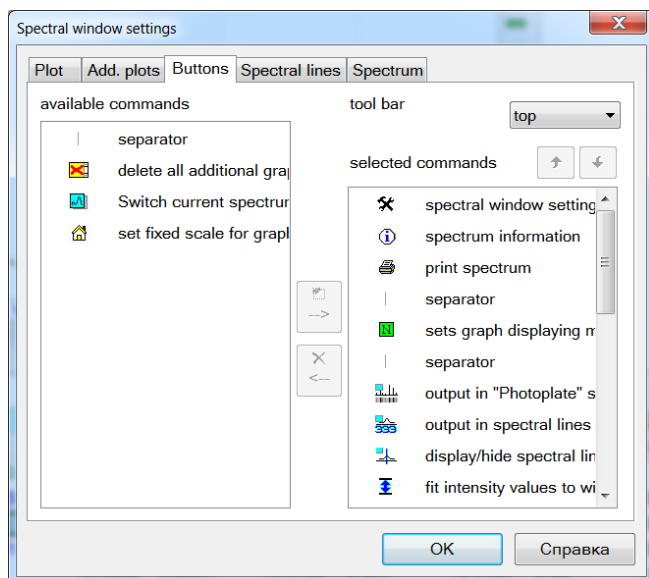
"use scaling 'from the center'" — if you set this key, then during scaling of the graph using the right mouse button (see ""Rescaling with the mouse"), scaling will be performed not from the clicked point to the point of right mouse button release, but by points located at an identical distance from the point clicked.

"display description of graphs" — controls display of graph description lines in the top right corner.


"Font for graph description..." — font for graph description lines.


"use 'smooth' graph drawing mode (without 'blinking' effect)" — in this mode the graph is drawn at first in the computer memory (the drawing process is not visible on the screen), and then the result is displayed.


"display additional graphs" — display or not the additional graphs.





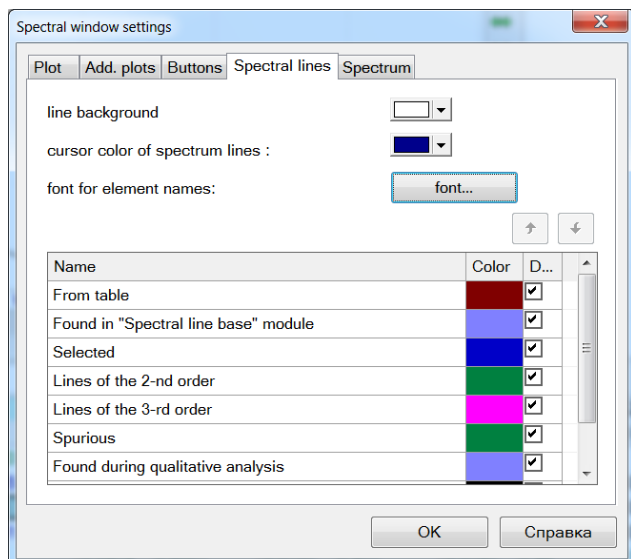
"Buttons"

It is used to control the list of buttons accessible in this window, and their arrangement on toolbars (if the window has several toolbars). Click  button on the window toolbar (spectrum window, calibration graph, analysis table, histogram), "Buttons" tab.



List of available buttons is displayed in the left part of the window. List of available toolbars is displayed in the upper right part. List of buttons of the current selected toolbar is located in the lower right part of screen. Select first toolbar, then select a button in the list to the left and press  to add this button.

Select a toolbar, then select a button in the list to the right and press  to delete this button. Each button may be added to any toolbar only once; after it is added, it

disappears from the list of available buttons. To transfer a button from one toolbar to another, first delete it from the toolbar where it is located, and then add it to the required toolbar. Use navigation buttons of the selected commands  and  to change the order of buttons in a toolbar.



"Spectral lines"

It is used to specify types, colours and the order of spectral lines display in the spectrum window. Press button  on toolbar of spectrum window, "Spectral lines" tab, to open it. You can hide/show the spectral line line button , located on the spectrum window toolbar.

At the moment the program selects the following types of spectral lines:

- **"selected"** — lines of elements selected in "Periodic table" dialog.
- **"lines of the 2nd and the 3rd order"** — lines of elements selected in the "Periodic table" dialog corresponding to the second and the third diffraction order (with a wavelength multiplied by two

and by three). These lines are available only after setting the corresponding key in the display setup dialog of spectral lines.



- **"spurious"** — current line in "Spurious Lines" tool.
- **"from table"** — lines added to analysis table.
- **"found in qualitative analysis"** — lines found in "Qualitative Analysis" tool.
- **"base lines"** — lines of elements specified in "Qualitative Analysis" tool as a "base".
- **"reference lines"** — specified in reference line settings.

"string background colour" — **"spectral lines" string** background colour.


"spectral line cursor colour" — current spectral line cursor colour in spectrum window.

"element name font" — this font is used to display names of lines in the "spectral lines" string.

In order to change colour used to display lines of a certain type, click the corresponding cell in "Colour" column and select new colour in the opened dialog. If it is not necessary to display lines of one of types, uncheck the "Display" column.

In order to change the order of display of lines of various type, select one of types and use navigation buttons for selection  and . The order of display is important, when a line corresponds to several types at the same time. For example, "table line" and "reference line". If, in this case, "reference lines" are below than "table lines" in the list, then such line will be drawn as a "reference" line and vice versa.

"Spectrum"




It is used to control additional settings. Click button  in spectrum window toolbar or the mode window, "Spectrum" tab, to open it




"set the cursor to the peak maximum" — when moving spectrum cursor, it will be automatically set to the maximum of the next peak.

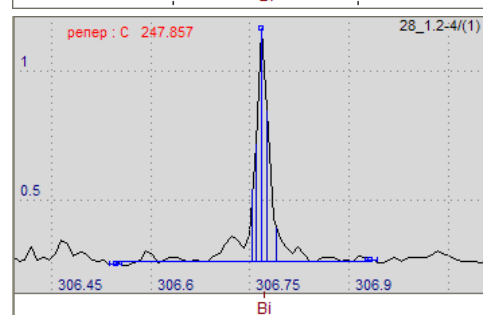
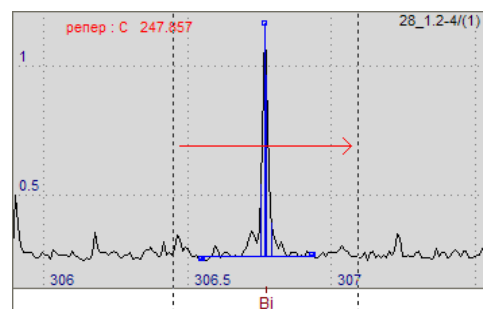
"Peak search settings..." — opens "Peak calculation" dialog to set up peak search parameters. For example, you may set the maximum distance to the next peak or a threshold intensity value of the found peak (so that peaks with too low intensity values are not searched).

"apply automatically the specified background points or the peak center to all parallel measurements in the table" — if you select a peak in the analysis table, and then use one of buttons ,  or  to specify manually background points or the peak center, then two situations are possible:


if this key is set, peak search settings of the respective analytic line from the analysis table will be changed, and intensity and concentration values for this line will be recalculated for all samples and parallel measurements.

if this key is not set, then intensity and concentration values are calculated only for the current parallel measurement in the analysis table. If you open "Peak calculation" dialog now for the current analytical line and specify "manual line border search settings" or "specify manually line center search", then points, set using buttons ,  or  will be automatically entered in the corresponding input fields, and it will be possible to calculate intensity and concentration values for the current analytic line.

if this key is not set, then intensity and concentration values are calculated only for the current parallel measurement in the analysis table. If you open "Peak calculation" dialog now for the current analytical line and specify "manual line border search settings" or "specify manually line center search", then points, set using buttons ,  or  will be automatically entered in the corresponding input fields, and it will be possible to calculate intensity and concentration values for the current analytic line.



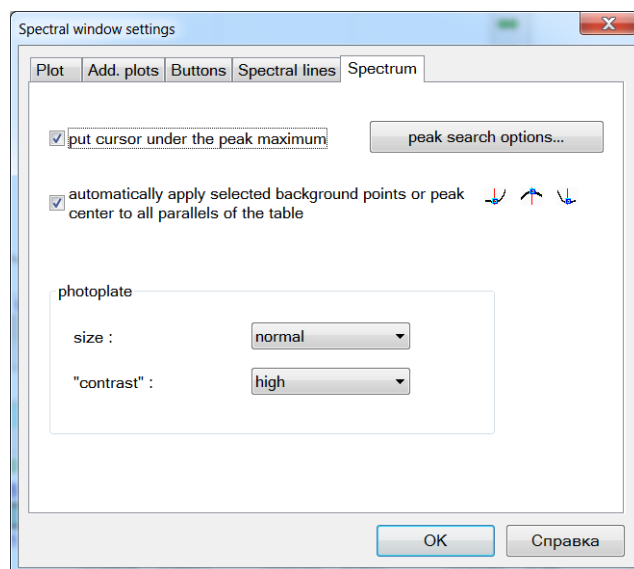
"photographic plate" — spectrum image line as a photographic plate.

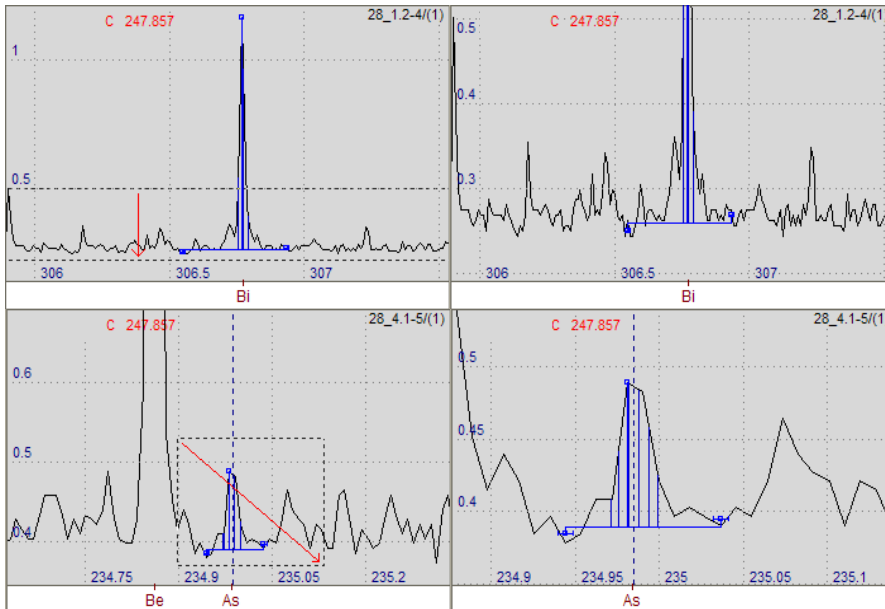
You can control line display using button , located on the spectrum window toolbar. Line display control:

- size – normal/small;
- contrast – normal/high.

Rescaling with a mouse

Graph scale may be changed both by scale selection buttons (zoom in, zoom out, autoscaling), and the right mouse button. Press the right button to start scaling operation.





Now, if you:

1) release the button, without moving the mouse, context menu will be open for the graph; scale will not change;


2) move mouse cursor horizontally, deviating in vertical direction from the point clicked for a small distance, then two dotted vertical lines will be drawn. When you release the right button, the graph will be redrawn so that these lines appear on the left and the right border of the window;

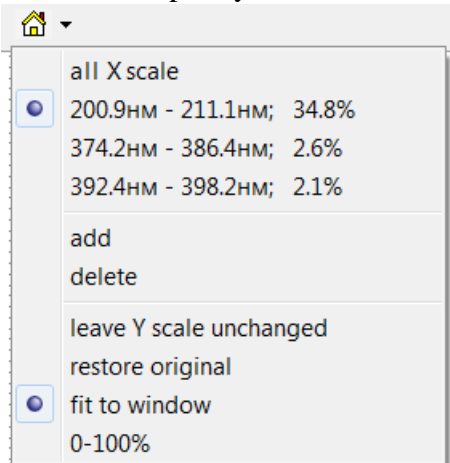
3) move mouse cursor vertically, deviating in horizontal direction

from the point clicked for a small distance, then two dotted horizontal lines will be drawn. When you release the right button, the graph will be redrawn so that these lines appear on the upper and the bottom border of the window;

4) move the mouse cursor in any direction, a rectangle will be drawn with one angle in the button clicked point and with the opposite angle — in the current cursor position of mouse. When you release the right button, the graph will be redrawn so that triangle content is stretched to the entire window;

"Home"

It is used to specify and save the scale set by button  .



The program remembers the uniform list of scales and uses in all open analysis documents. This list is also a part of the list of options when printing several spectral regions.

"**Add**" – current spectrum scale is saved; combination of coordinates is used as the name.

"**delete**" – last selected (highlighted) scale is deleted.

"do not change scale by Y" – X coordinate is restored; Y coordinate is not changed.


"**restore initial**" – all coordinates are restored.

"fit in window" – X coordinate is restored; autoscaling is performed by Y coordinate.


"0-100%" – only X coordinate is restored.


Calibration graph window settings

The dialog consists of several tabs; to switch to a tab, click its name in the list of tabs on top of the dialog: "Calibration graph", "Graph" and "Buttons"

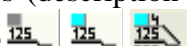
Click button , located on the toolbar of the calibration graph window, to open this dialog.

"Calibration graph"

It is used for control calibration graph elements – samples, reference samples, captions, cursors, etc. Press button  located on the toolbar of the calibration graph window, "Calibration graph" tab, to open it.

"*Reference samples*" and "*samples*" control the display and colour of points that correspond to work samples and reference samples; they are also controlled using buttons .


"*captions*" — control the display and colour of captions of statistical characteristics of the calibration graph: convergence variance, adequacy variance, calibration SD and concentration of reference samples.

"*names of samples*" — defines, whether to display or not names of samples (description of points, corresponding to samples and reference samples); it is also controlled using buttons .


"*C minimum, C maximum*" – control the display and colour (usually red) of vertical dashed lines corresponding to Cmin and Cmax parameters, defining the calibration graph working range (see "Calibration graph calculation settings").

"*Clower, Cupper*" — control the display and colour (usually blue) of vertical dashed lines corresponding to Clower and Cupper parameters (see "Concentration calculation settings").

"*RSD interval*" and "*regression confidential interval*" — defines, whether to delete or not the corresponding curves and their colour (see "Calibration graph RSD Interval" and "Confidential interval of calibration graph regression" in "Algorithms" section).

"*prevent imposition of point captions*" — when displaying names of work samples and reference samples in the calibration graph window, several texts may superimpose on one another, complicating their reading. If this key is set, the program will try to arrange captions so that they do not cross. If several texts are imposing nevertheless, it is possible to either maximize the calibration graph window (buttons with black triangles at the top right of the calibration graph window, see "Toolbars"), or to zoom in the graph scale in the place of imposition using a mouse (see "Rescaling with a mouse"); you may also use buttons .

"Graph"

It is used to control main graph drawing settings, click button  on the graph window toolbar to open it (spectrum window, calibration graph, histogram), "Graph" tab.

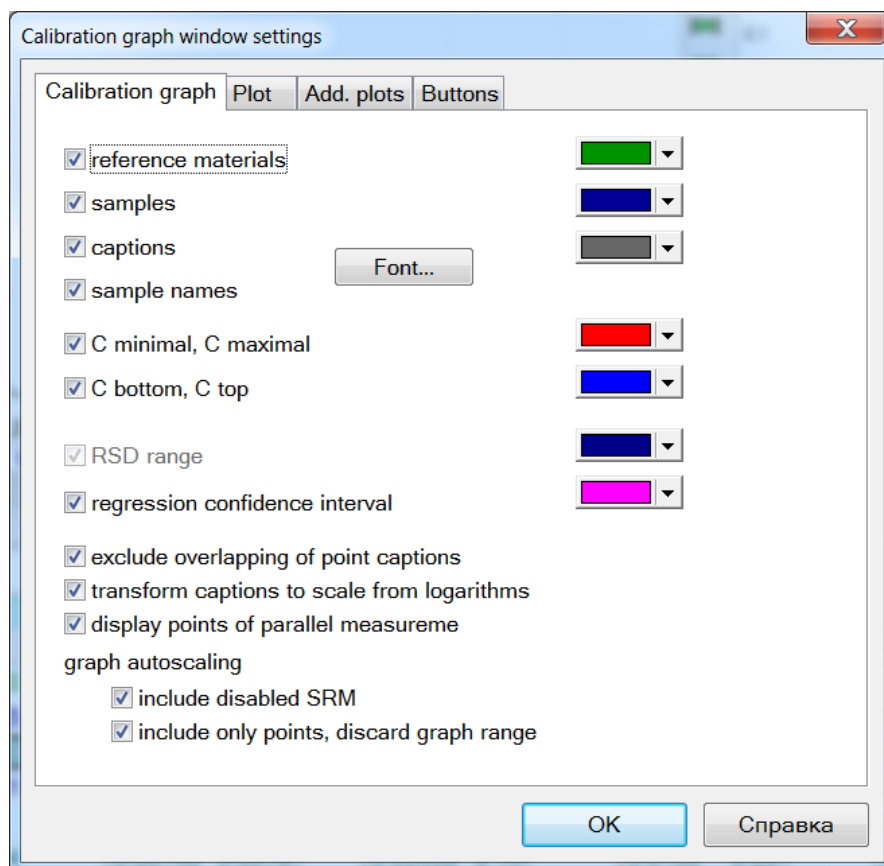
"*graph*" colour — set colour of the main (not additional) graph.

"*background*" colour — set the graph background colour.

"*scale line*" colour — colour of dashed lines of the graph scale.

"*toolbar*" colour — graph toolbar panel background colour.

"*Scale font and colour...*" regulates



font and colour of graph scale captions.

"use scaling 'from the center'" — if you set this key, then during scaling of the graph using the right mouse button (see ""Rescaling with the mouse"), scaling will be performed not from the clicked point to the point of right mouse button release, but by points located at an identical distance from the point clicked.






"display description of graphs" — controls display of graph description lines in the top right corner.

"Font for graph description..." — font for graph description lines.


"use 'smooth' graph drawing mode (without 'blinking' effect)" — in this mode the graph is drawn at first in the computer memory (the drawing process is not visible on the screen), and then the result is displayed.

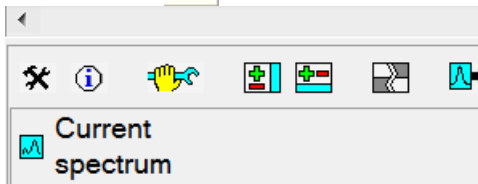
"display additional graphs" — display or not the additional graphs.

"Buttons"

It is used to control the list of buttons accessible in this window, and their arrangement on toolbars (if the window has several toolbars). Click  button on the window toolbar (spectrum window, calibration graph, analysis table, histogram), "Toolbars" tab. List of available buttons is displayed in the left part of the window. List of available toolbars is displayed in the upper right part. List of buttons of the current selected toolbar is located in the lower right part of screen. Select first toolbar, then select a button in the list to the left and press  to add this button. Select a toolbar, then select a button in the list to the right and press  to delete this button. Each button may be added to any toolbar only once; after it is added, it disappears from the list of available buttons. To transfer a button from one toolbar to another, first delete it from the toolbar where it is located, and then add it to the required toolbar. Use navigation buttons of the selected commands  and  to change the order of buttons in a toolbar.

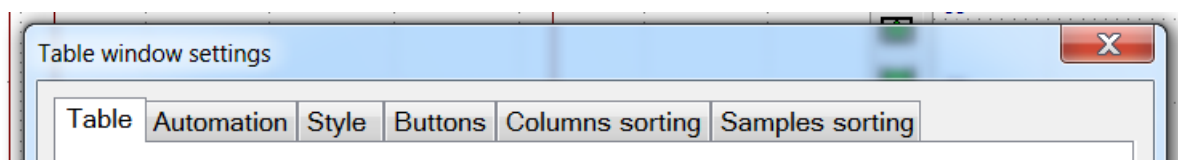
Analysis table window settings

Click button  on the table toolbar to open it.



The dialog consists of several tabs; to switch to a tab, click its name in the list of tabs on top of the dialog:

- "Table"
- "Automation"
- "Style"
- "Buttons"
- "Columns sorting"
- "Samples sorting"



Upon changing the analysis table display settings, it is possible to press one of the dialog buttons:

- **"OK"** — modified settings are applied, dialog is closed;
- **"Cancel"** — changes of settings are cancelled, dialog is closed;
- **"Apply"** — modified settings are applied, the table is redrawn, but the dialog is not closed allowing selecting values of several settings, evaluating results of their modification, without exiting the dialog.

"Table"

It is used control information display in the analysis table.

"**Statistics**" controls additional line display with the calculated values by each sample in the analysis table. Check lines, which shall be displayed in the table. At the moment such lines are as follows: mean, SD, RSD, range (difference between the maximum and the minimum value), confidential interval, median.

"**result**" line displays either the mean value, or the median value in case if convergence control parameters do not meet requirements of the analysis technique (it is calculated according to GOST R, ISO 5725-6-2002).

"repeatability" line displays the checked parameter value (RSD or range) as compared with the control limit taken from the table of standards or entered manually.


"stability" line shows for reference samples the difference between the entered certified value with the value found for calibration graph as compared against the control value of the allowed discrepancy taken from the table of standards.


"**Columns**" controls the display of columns of spectral lines in the analysis table. Check columns to display. *Deselect all lines to hide spectral line columns in the table!* At the moment the program uses the following spectral line columns: **Crm** (concentration of reference materials), **I** (intensity of peaks found), **Iref** (reference line intensity), **I/Icp** (intensity taking into account the reference line), **C** (calculated concentration values) and **stat. weight** (statistical weights of reference samples for calibration).

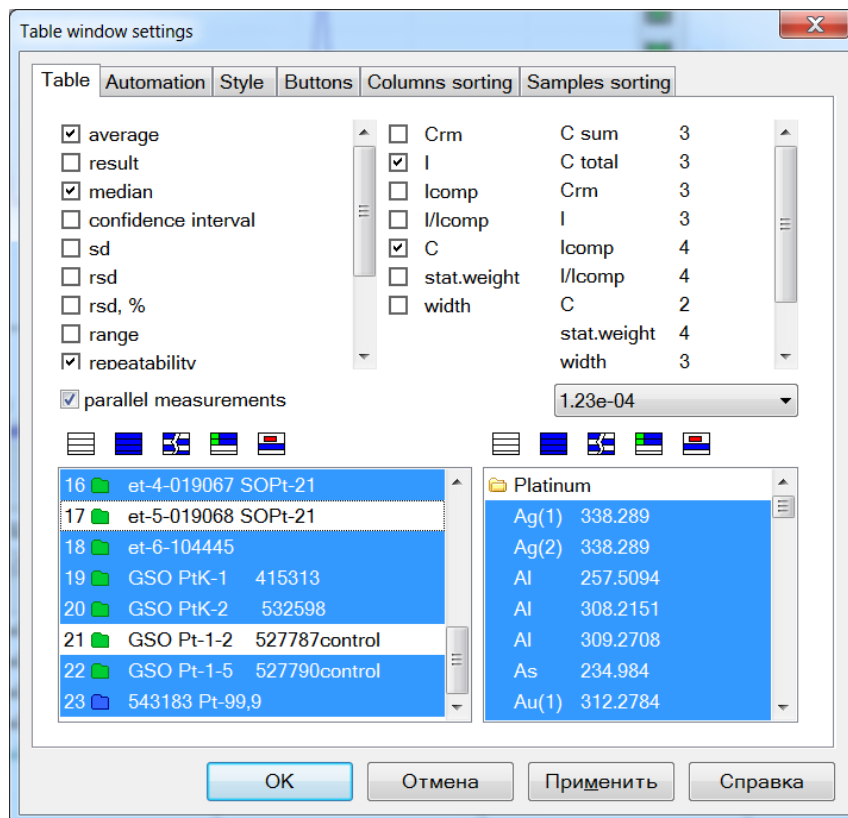
"**Number of significant**" values sets the number of significant figures of numbers displayed in the table. If, for example, it is specified that for column **I** the number of significant figures is three, then all found peak intensity values will be displayed in the table rounded to three significant figures.

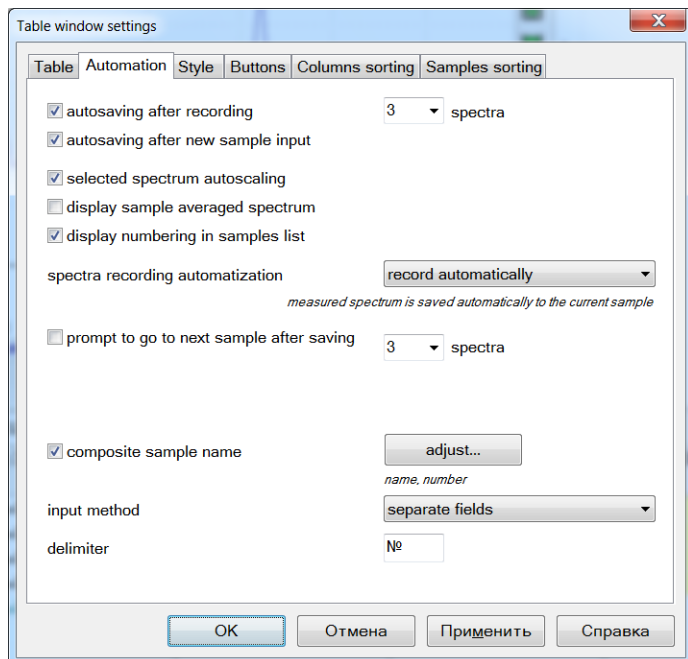
"**Number display format**" specifies the method to display a number in the analysis table. There are four options:

1. decimal fraction, or a significant part (mantissa) - order (computer format, with **e** symbol as a delimiter of mantissa and the order, e.g., "1.23e-04"). The program determines itself, when a value shall be displayed as a decimal fraction and when — with a mantissa and the order.
2. a value is always displayed in the computer format with a mantissa and the order "1.23e-04".
3. decimal fraction, or with a mantissa and the common form: "1.23•10⁻⁴" (the order is displayed as the upper index).
4. always as a decimal fraction, irrespective of the value, for example, 1234000 or 0.000001234.

"**display samples**". Select samples, which will be displayed in the analysis table. Click sample name to select it: if the sample is not selected, it will be selected; otherwise it will be deselected. You may use selection control buttons as well. Button  selects only reference samples. *If you deselect all samples, the table will not display anything!*

"**show columns**". Select columns, which will be displayed in the analysis table. Click column name to select it: if the column is not selected, it will be selected; otherwise it will be deselected. You may use selection control buttons as well. Button  selects only analytic lines with constructed calibration graphs. *If you deselect all columns, the table will not display anything!*





"Automation"

It is used to control several possibilities to automate work with the program in the Analysis mode.

"autosave..." allows selecting autosave parameters for analysis results to a file. According to the specified parameters, the program saves the file with all analysis results to "Temp" folder. In case of software breakdown or if the computer and the program are not be able complete normally their work, you will be prompted to recover the lost files during the next start.

"autoscaling the selected spectrum" — set this key to scale automatically the selected spectrum in the analysis table (click parallel measurement caption), so that entirely fits in the spectrum window.

"open 'Add spectrum to table' dialog after new spectrum measurement" — after new spectrum measurement using MAES "add spectrum to analysis table" dialog will be automatically started for sample selection, where you shall add the spectrum. This option is disabled when working with a switched on mode of automated input of parallel measurements.

"add automatically the measured spectra to the table" — upon new spectrum measurement by MAES the spectra are automatically added to the current sample (it is highlighted in a blue frame in the analysis table). If there is no current sample, "Add spectrum to the analysis table" dialog is displayed.

"offer to switch to next sample after input... of parallel measurements" – in the automatic parallel measurement input mode, if a sample already contains the specified number of spectra, then "Add spectrum to the analysis table" dialog is displayed to select another or new sample. This is convenient, if you enter several samples with the same number of parallel measurements.

"ICP..." – selects the operating mode just as in "Measurement mode" dialog for a "device with continuous sample feed".

"switch to next sample" – after a group of spectra is measured, the dialog appears to input new sample name.

"automatically assign sample names" – in case of a high flow of the same samples, they may be assigned the name, which will be added by order numbers during measurement, e.g. "sample01", "sample02", "sample03", etc.

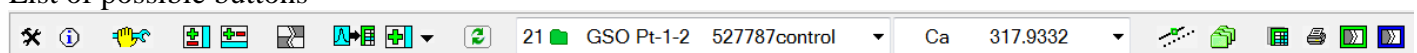
"Table view"

It is used to set up analysis table font and colours. **"Font"** dropdown list is used to select font, which is used to display the table (both for values of cells, and captions). **"Size"** sets font size for table display.

"bold font for captions" — set this key, if you want to display table captions in bold font. To adjust table colours. select colour you want to change from the **"Table Element"** list, then use **"Colour"** and **"Text Colour"** buttons. **"Restore all colours by default"** sets default values for all table colours.

"Toolbar settings"

It is used to control, what buttons from the list of buttons available for the analysis table, will be displayed. List of possible buttons –



Each button may be added to a toolbar only once; after it is added, it disappears from the list of available buttons. Use navigation buttons of the selected commands  and  to change the order of buttons in a toolbar.

"Sorting of samples"

Select "*alphabetically*" option , if you want the sample list in the analysis table to be always sorted alphabetically (by the sample name). New added samples will be sorted at once in the table.

For manual sorting of samples you may select several samples in the list (to select a sample, click its name, to select several samples, hold pressed "Shift" or "Ctrl"; you may also use selection control buttons) and selection movement buttons.

"Sorting of columns"

You may select the method of automatic sorting of table columns in the list at the left. Options – "no sorting", "alphabetically", "by wavelength", "by element number".

For manual sorting of columns you may select several samples in the list (to select a column, click its name, to select several columns, hold pressed "Shift" or "Ctrl"; you may also use selection control buttons) and selection movement buttons.

Columns of the selected table page are displayed in the list. Use the list of pages at the right top to select another page.

Samples of sorting are here:

Sorting

Columns sorting

☒ no

☐ alphabetically

☐ by wavelength

☐ by element number

Platinum

Si 250.6897

Si 251.9202

Si 288.1579

Ag(1) 338.289

Ca 396.8469

Ir 322.078

Mg 277.669

Mg 278.1416

Mg 279.5528

Cr 283.5629

Al 257.5094

Al 308.2151

Al 309.2708

As 234.984

Au(1) 312.2784

OK

Отмена

Справка

Sorting

Columns sorting

☐ no

☒ alphabetically

☐ by wavelength

☐ by element number

Platinum

Ag(1) 338.289

Ag(2) 338.289

Al 257.5094

Al 308.2151

Al 309.2708

As 234.984

Au(1) 312.2784

Bi 223.061

Bi 306.772

Ca 317.9332

Ca 393.3663

Ca 396.8469

Cd 226.502

Cd 346.62

Cr 283.5629

OK

Отмена

Справка

Sorting

Columns sorting

☐ no

☐ alphabetically

☒ by wavelength

☐ by element number

Platinum

Zn 213.8573

Cu 221.4581

Cu(1) 222.7775

Bi 223.061

Cd 226.502

Sb(1) 231.147

As 234.984

Te 238.578

Si 250.6897

Si 251.9202

Al 257.5094

Mn 259.3724

Mg 277.669

Mg 278.1416

Mg 279.5528

OK

Отмена

Справка

Sorting

Columns sorting

☐ no

☐ alphabetically

☐ by wavelength

☒ by element number

Platinum

Mg 277.669

Mg 278.1416

Mg 279.5528

Mg 280.2705

Al 257.5094

Al 308.2151

Al 309.2708

Si 250.6897

Si 251.9202

Si 288.1579

Ca 317.9332

Ca 393.3663

Ca 396.8469

Cr 283.5629

Cr 284.3249

OK

Отмена

Справка

Working with the program

Profiling

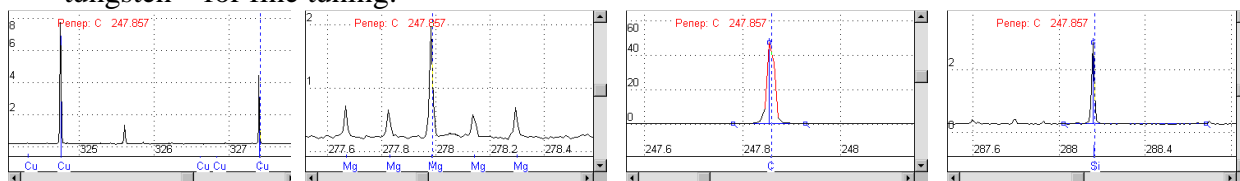
The program needs to determine position of analytic lines in the spectrum to find them; therefore prior to work it is necessary to define the correspondence rule of diode numbers to wavelengths (to perform profiling).


This section of the manual provides the list of main operations for creation of new profiling, description of buttons and dialogs is provided "Profiling Mode".



For profiling, it is necessary to measure the following spectra in the ANALYSIS mode with a small time interval between measurements and to save them in the data table:

copper, mercury, graphite, magnesium, silicon – for primary setting.

tungsten – for fine tuning.






Determine reference lines in spectra using primary setting spectra and save them to the profiling table; examples of such lines are: C 247.857, Cu 324.754, Cu 327.396, Al 308.215, Al 309.271, Si 288.159, Mg 277.983. These lines are the most intensive or give a representative pattern of lines (Mg 277.983 with circumscription). In order to save information on the spectrum line (two numbers – diode number/wavelength) in the profiling table, set the spectrum cursor in the spectrum line center (red marker), select a respective line from the table of spectral lines (blue marker) and add  this pair to the profiling table.

In order to perform complete setting, use a spectrum with a large number of sufficiently intensive, but "non-out-of-range" lines, add information about 20–30 lines for each range to the profiling table. Tungsten spectrum is usually applied for final profiling. The final stage is to save the current profiling to disk using . Further the current profiling will be assigned to each new spectrum measured by MAES. If profiling was performed or corrected by one of spectra in the data table, it is necessary to assign it to another spectra by clicking button .

It is recommended to start profiling with the minimum degree of polynom and to increase it when performing the final calculation. Depending on the spectral device type there may be one formula for the entire working spectrum (for flat diffraction gratings) or individual formulae for each range (in case of concave grids or prisms).


Correction of tungsten spectrum profiling


Correction is performed well by the spectrum of material used for final profiling (usually — tungsten). To do so, it is necessary to measure tungsten spectrum for MAES parameters settings selected earlier . Switch to Profiling mode and search all lines in the spectrum from the profiling table . Correct manually position of lines, which were not found by the program, i.e. for the selected line in the table it is necessary to set the spectrum cursor into a correct position (line center in the spectrum) and to press button .


Profiling is ready for application. All new measured spectra will have new profiling.



Analysis

Quantitative analysis is performed in the Engineer mode with the most frequent option:

1. Prepare samples and reference samples according to the analysis technique.
- 2.
3. Add analytic lines and reference lines to the analysis table according to the analysis technique().

4. Set ("Measurement mode" ) – time of single exposure, number of accumulations, as well as preburning time. It is recommended to use the minimum possible time of single exposure (usually 100 or 250 ms).

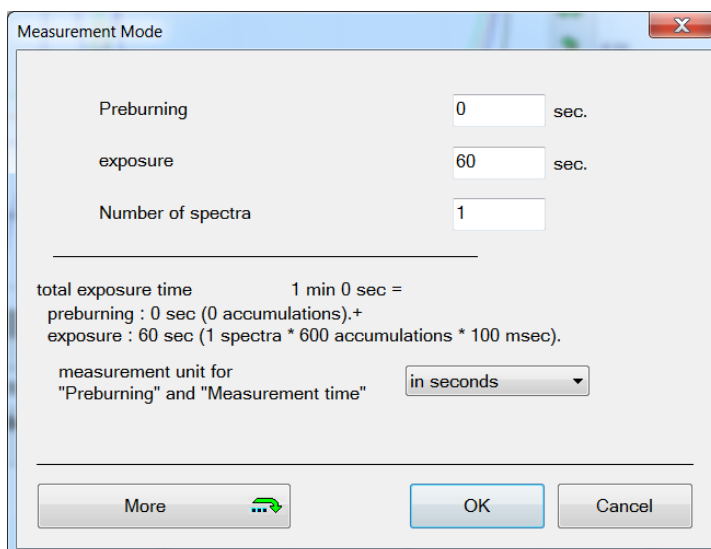
5. Measure dark current.  . Dark current shall be measured twice prior to the beginning of work and regularly every 30–40 minutes during the analysis.

6. After each spectrum measurement  it shall be saved to the analysis table with a corresponding name. Usually the program is set to ask to save spectrum measurement to the table immediately upon completion of measurement. Otherwise use button  , which opens current spectrum saving window to table.

7. Set concentration of the analyzed elements in Crm column for reference samples upon completion of measurement.

8. Check correctness of created calibration graphs for all analytic lines; if necessary, exclude "outliers" (errors) from calculation. For several analytic lines it may be required to exclude from calculation samples with "off scale" or not found spectral lines.

9. Print the report and save data to file. Saved data may be read and used later – to add new lines, to edit calculation parameters and so forth. It is recommended to save intermediate results, for example, before a measurement or editing; this will allow to return one step back, if necessary. In order to make it easier to be navigate in a large amount of files, it is recommended to include in the filename the analysis name (or its part), date, etc.



Measurement Mode

Preburning 0 sec.

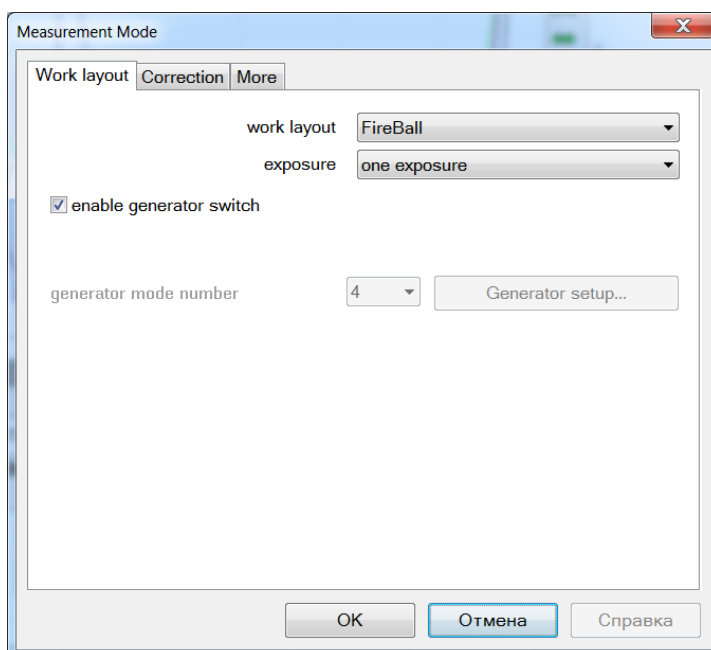
exposure 60 sec.

Number of spectra 1

total exposure time 1 min 0 sec =
 preburning : 0 sec (0 accumulations).+
 exposure : 60 sec (1 spectra * 600 accumulations * 100 msec).

measurement unit for
 "Preburning" and "Measurement time" in seconds

More OK Cancel



Measurement Mode

Work layout Correction More


work layout FireBall

exposure one exposure

☒ enable generator switch

generator mode number 4 Generator setup...

OK Отмена Справка

Intensity values are calculated for spectra measured earlier and saved to the table. Concentration values are calculated according to calibration graphs built by reference samples for respective analytic lines in the specified coordinates (for example, LgI–LgC). For the majority of spectral lines you may use common settings for calculation parameters of intensity values (Search of peaks), calibrations and calculation of concentration values. Open settings – .

Search of peaks and calculation of intensity values

For prismatic spectrometers it is necessary to set a search zone with 2 diodes and an integral with 4 diodes. For several lines with low intensity (<0.1 – 0.3) or for lines located in a range with complex spectral circumscription, individual settings may significantly improve the metrological characteristics, for example – manual setting of maximum and background points often allows improving convergence of parallel measurements for such lines.

In case when a spurious spectral base line or another element spectral line is located near the analytic line of the element being measured, then in order to reduce possible systematic errors it is recommended to switch on the mode of accounting for contribution of spurious lines (intensity calculation method — "Gaussian", to switch on "accounting for contribution of spurious lines").

Spurious lines are measured automatically whenever possible, but when lines are located very close to each other, it is necessary to select manually the wavelengths of spurious lines (click button "..."). See "Peak calculation" dialog.

Selection of reference lines

is performed from among lines displayed in the analysis table. The following information is specified in the line list: analytic line, ratio symbol of intensity values ("/" ratio, "-" difference of intensity values) and the reference line. If no reference line is set for the analytic line, then during calibration intensity values of spectrum lines are used and if a reference line is set, values of ratio (or difference) are used for intensity values of the corresponding pairs of lines

Calibration

is most often performed in logarithmic coordinates. In this case the linear approximation corresponds the most to the physical correlation between concentration and intensity values. Use of a nonlinear approximation of dependence between intensity logarithm and concentration logarithm may be substantiated, for example, in case of unremovable aliasing of a spurious spectral line onto the analytical line.

Points corresponding to reference samples are highlighted with green colour on the calibration graph. When selecting the approximation method, it is necessary to consider features of the analysis technique, amount of reference samples applied to calibration and intensity of spectral lines. You may apply several statistical parameters to control quality and correctness of calibration. Discrepancies are visually represented by a changed colour of the calibration graph and individual parallel measurements or mean values. Calibration parameters may be set up individually for each line. For example, it allows (when specifying Cmin and Cmax limits) automatically using several analytic lines of one element for work in various concentration spectra – more sensitive lines for low concentration values, and less sensitive lines – for high concentration values. When calculating the calibration graph, the program automatically excludes from calculation reference samples outside the specified spectrum. When changing the range, the switched off points are automatically restored. If it is necessary to exclude any RS from calculation, you may switch them to the status of "work samples", which allows seeing calculation of statistics and displaying these samples in the report.

Concentration calculation

It is performed upon calculation of calibration graphs for all parallel measurements, where intensity of analytic lines (as well as reference lines) was calculated. Points on calibration graph corresponding to samples will be highlighted in blue colour. Calculation settings may also be individual for each line.

Working range of the graph is defined by "Between RS" key; if it is switched on, then calibration graph will be limited to the maximum and the minimum concentration value of reference samples; if it is switched off, then, if the calibration graph exceeds the working range, concentration is calculated on a linear continuation of the calibration graph, which allows defining with a satisfactory accuracy the concentration values, that are not very far from extreme reference samples. The determined concentration values shall thus be considered

as approximate. If the mean value of a calculated concentration falls outside the calibration graph limit beyond the margin, then it is displayed in the analysis table as a higher or a lower value of the corresponding values (for example, ">0.5" or "<0.0015"), and the corresponding values of parallel measurements are calculated as usual. Results are also displayed in the report. Convergence and selection of gross errors of calculated parallel measurement concentration values may be estimated using a number of statistical criteria, including by the difference between parallel measurement results (usually specified in GOST standards for two parallel measurements, for a bigger number of measurements the admissible limit is recalculated automatically). You may also set Clower and Cupper values for visual control of impurity element content in work samples (points that are out range are highlighted on the graph in the red colour).

Performing the analysis taking into account burning of elements

In a number of analysis techniques of powder samples in a DC of AC arc with complete or partial burning of a sample material, a noticeable variation in time is often observed for intensity values of analytic lines of impurities being measured. The nature of intensity value variation usually depends directly on properties of elements, chemical composition and physical condition of the analyzed sample. The corresponding program modes are provided to control the receipt of impurities. Let us consider the most widespread mode – exposure division into two parts and calculation of element intensity/concentration values according to their time of receipt to discharge plasma (you may study the nature of intensity values variation using "Histogram" tool).

Select the number of spectra in measurement mode settings – 2. Generator parameters in this case shall be synchronized by the time of mode switching – for example, current polarity.

Select "several exposures" mode in common analysis settings ("Additional Analysis Parameters" window). In this mode the program will save the spectrum consisting of two parts – each part for its own time interval.

Then use "Time record" dialog to set the way to consider the individual nature of impurity receipt during calibration and construction of concentrations graphs for lines of the elements being measured.

Measurement Mode

Number of exposures: 2

Preburning exposure

1	5 sec.	40 sec.
2	0 sec.	40 sec.

full measurement time 1 min 25 sec =
2 exposures: 80 sec (800 accumulations).+
2 preburnings: 5 sec (50 accumulations).

measurement unit of the "Preburning" and "Exposure" parameters: in seconds

More OK Cancel

Measurement Mode

Work layout Correction More

work layout: FireBall

exposure: several exposures

☒ enable generator switch

generator mode number: 4 Generator setup...

OK Отмена Справка

... Analysis general settings

Technique Reference lines

☐ "Constant graph" method with recalibration by concentrations
☐ identical Crm for all elements

☒ use standard: copper high-purity-27981

☐ alloy grade check

☒ samples averaging

processing several spectra in one exposure cycle: several exposures

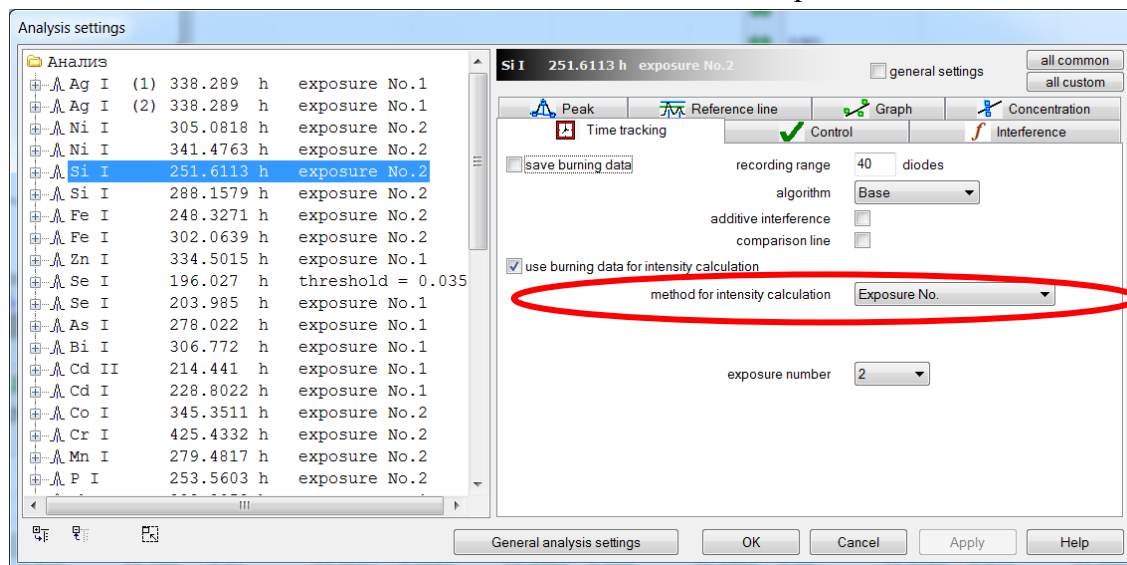
if C calculation failed, display: < Cmin

concentration measurement unit: %

control test: no (for reference materials), no (for working samples)

OK Отмена Справка

Time intervals are specified for analytic lines according to burning measurement parameters. Spectra may easily be used later for methodical development – all information is saved and may be recalculated at any time. Settings of a number of analytic lines, when determining impurity composition of the cathode copper when generator polarity is switched in the middle of exposure, are provided as an example on the figure, and accurate time frames are defined for each element to obtain optimum results.

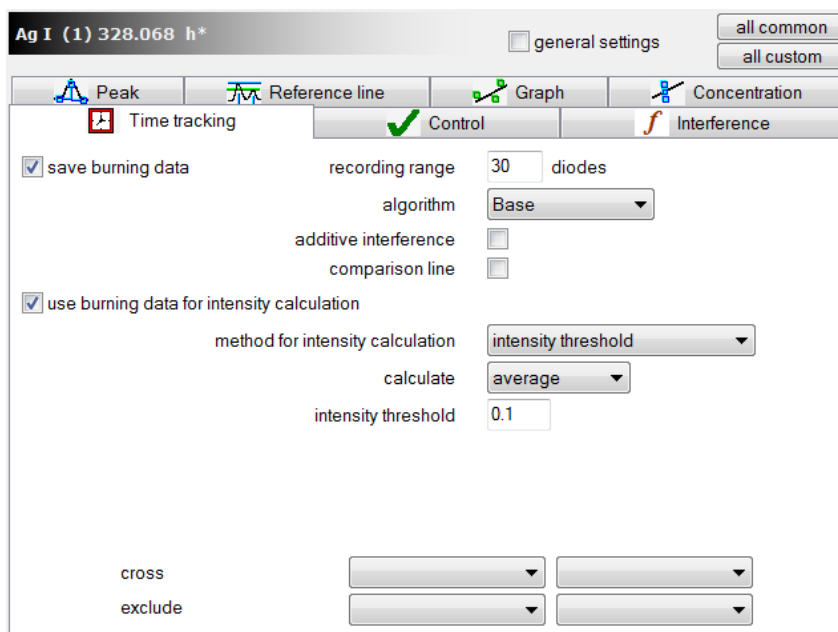


Pay attention to selection of reference lines – it is recommended to select analytic pairs from one time span. To do so, one line shall be added to the analysis table in the necessary amount and an individual interval shall be selected for each line. For example, if there are two working inter-

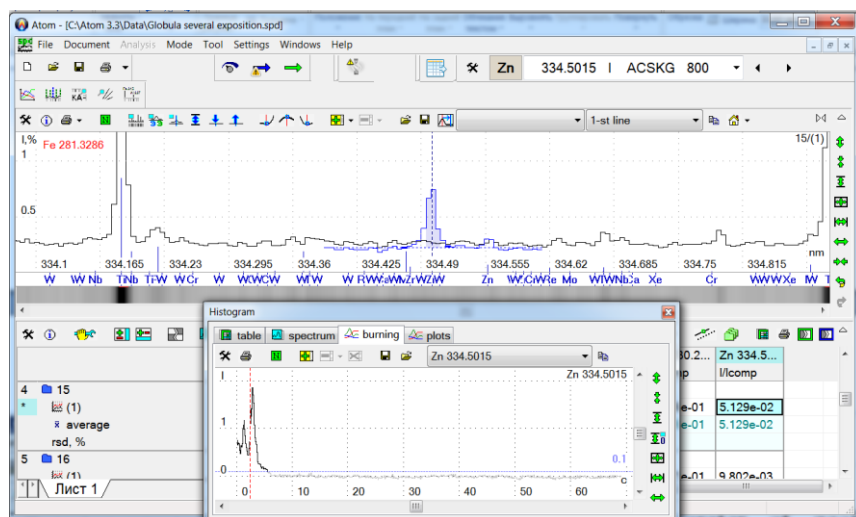
vals in the technique, the line may be required in two copies – for the 1st and the 2nd interval.

"Element burning measurement" mode is provided to monitor the receipt of elements into discharge plasma without measuring full spectra for the whole measurement period. It may be switched on for each analytic line irrespective of other lines. It provides registration and saving in the computer memory of the spectrum range in the zone where the analytic line is located, as well as calculation for each saved spectrum according to the set peak intensity calculation parameters.

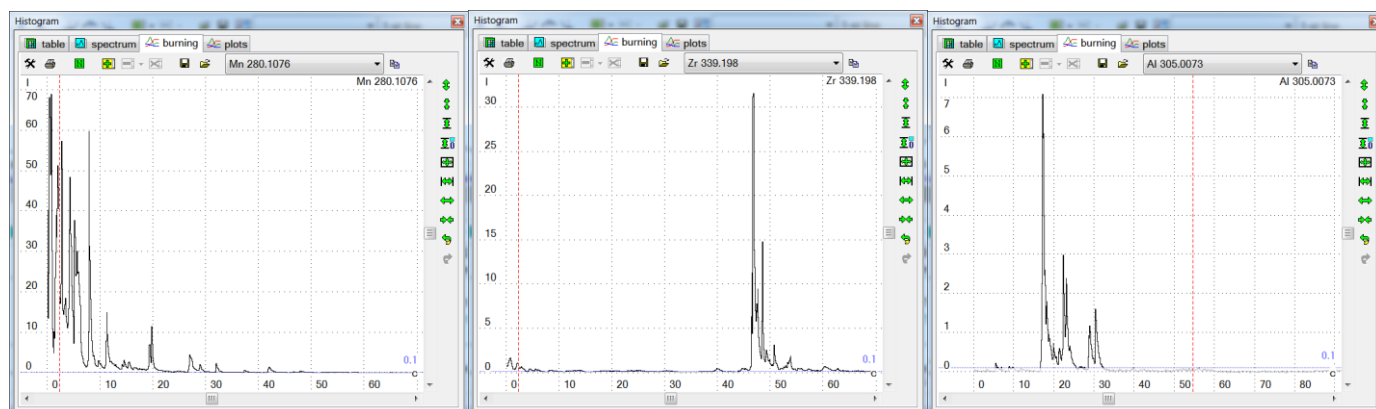
To see the saved spectrum range, select the observed range (from among three tabs) in the "histogram" window in the burning mode; a corresponding record will be displayed, highlighted in additional colour against the background of the average spectrum.



When switching on the "burning saving" and "accounting for burning for calculation" modes, the program calculates intensity values of the "saved" line in each single accumulation throughout the exposure and averages the received values. Move the pointing cursor (red dotted line) over the histogram to display in spectrum window the saved regions, which are displayed according to profiling and measurement time.



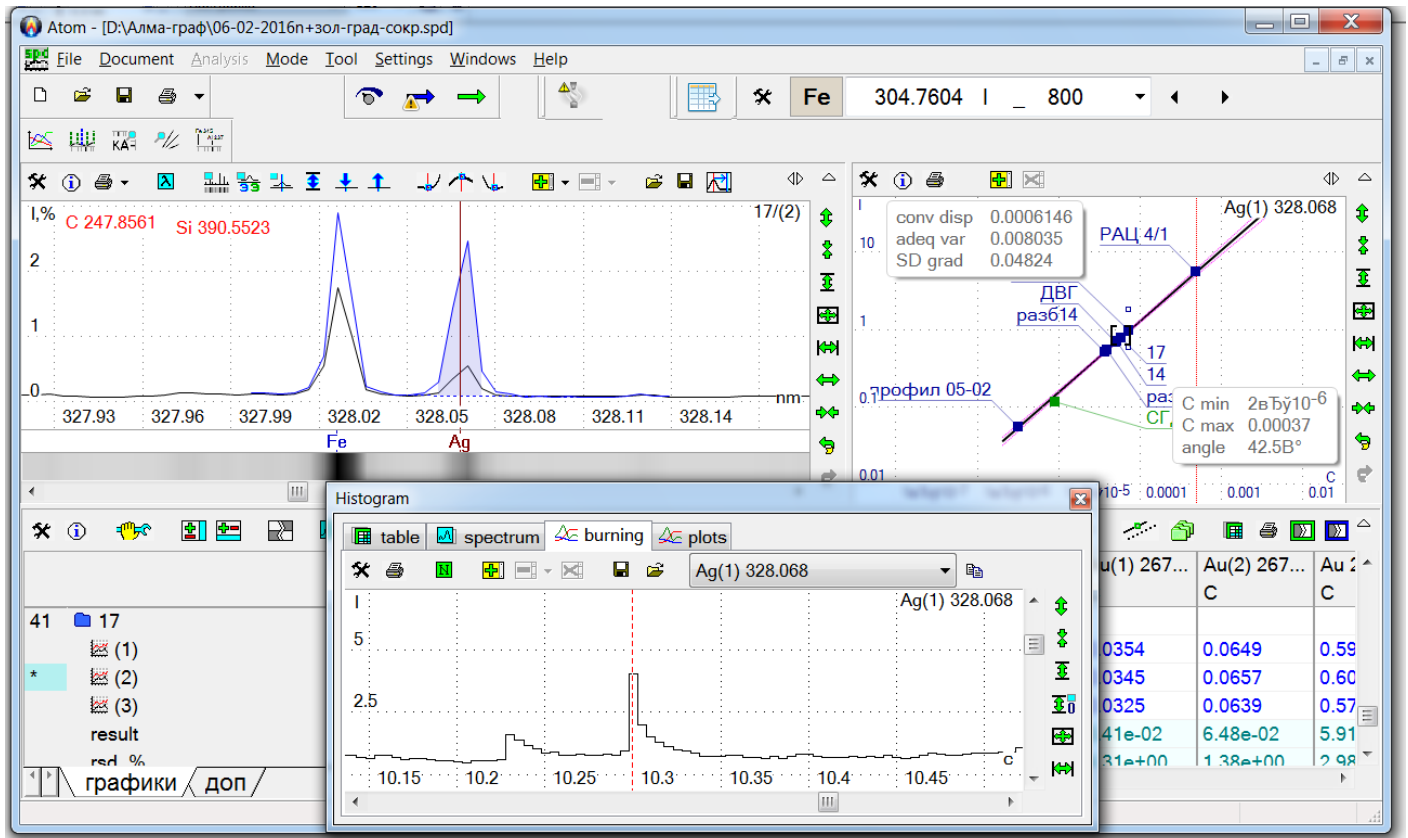
Monitoring of Zn zinc line of 334.5 nanometers at evaporation from the crater of geological sample weight with time-base sweep every 100 ms allows specifying, when this element enters the discharge at the beginning of exposure. During the entire exposure time (70 sec) the element line can be seen only during the first several seconds, and in the average spectrum its identification against a line spectrum of arc is complicated. Thus, "time record" is simple option for correct calculation of intensity values, which provides decreased detection limits, and thus does not demand additional operations when preparing samples or changing conditions of spectrum excitation.



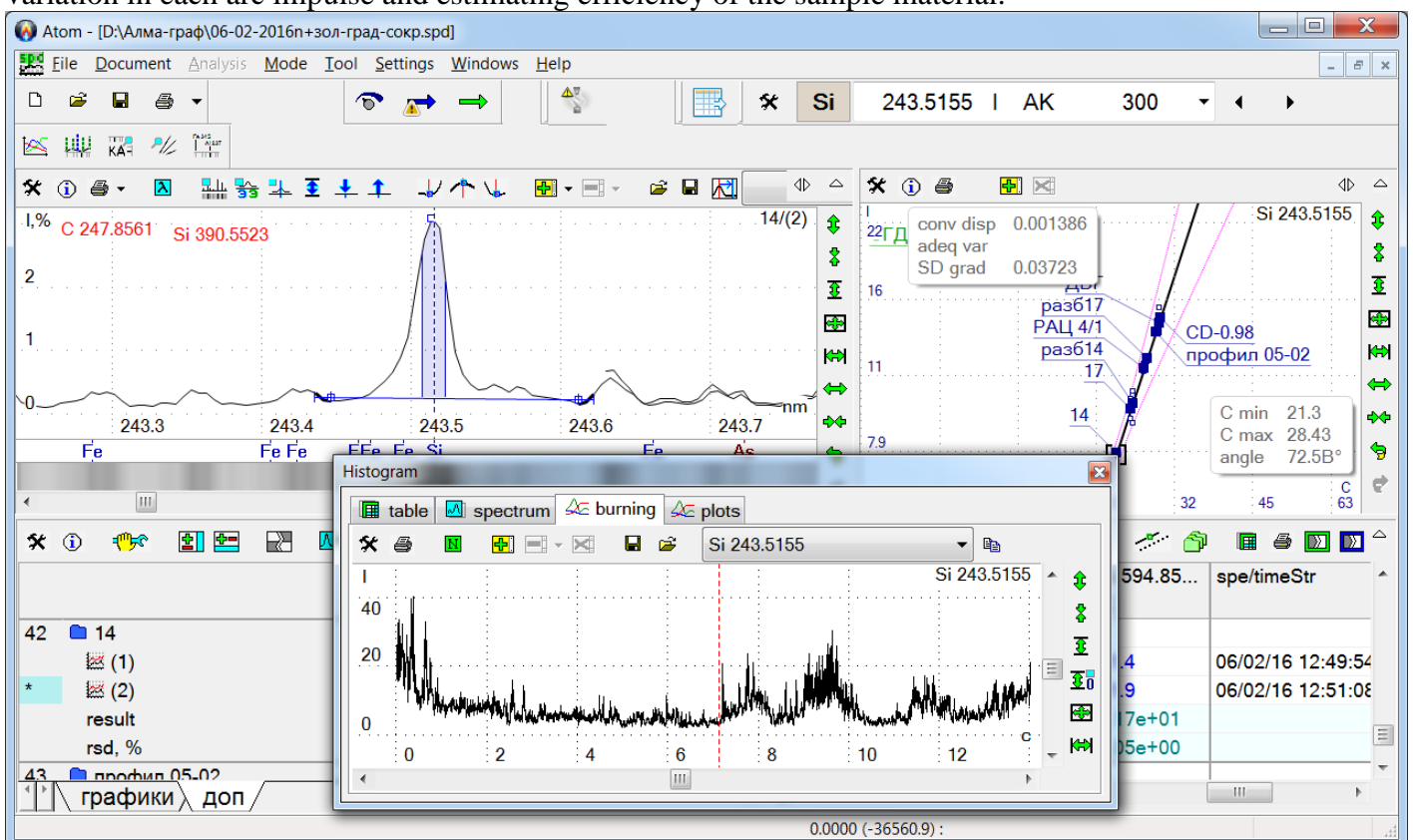
For bright lines of elements that are constantly present in plasma, almost full compliance of calculation for the average spectrum is observed for the entire exposure. Every spectral lines Mn 280.1076, Zr 339.198 and Al 305.0073 nm could be calculated with special time option for precise analysis.

For techniques with strongly marked time-dependent receipt of highly or semi-volatile elements the program may calculate and select automatically only those temporary ranges of exposures, where the analytic line of a measured element may be seen in spectra, without taking into account the "empty" spectra, and improving the "signal/noise" ratio.

For those cases when receipt of several elements is irregular relative to the overall composition — for example, when determining gold traces in natural samples using the method of spilling into arc, it is possible to significantly improve the analytic characteristics due to selection and accounting of individual flashes (scintillation method). Thus in common spectra the spectral line may be invisible due to the low average content. Monitoring the gold line Au of 267.594 nanometers with time-base sweep every 4 ms allows determining, when individual gold-bearing grains enter the discharge (seen as intensity flashes lasting for 10–50 milliseconds).



Observation over one of many lines of silicon with time-base sweep every 5 ms allows recording intensity variation in each arc impulse and estimating efficiency of the sample material.








Calculation of spectral line intensity on an automatically defined time span allows improving signal/noise ratio and lowering detection limits for several elements without additional optimization of the analysis technique.

Setting up the spectral equipment

1. Install MAES analyzer on a spectrometer according to the device design.
2. Ensure grounding of the spectrometer, MAES, MAES power supply unit and the computer.
3. Connect MAES and the interface board in the computer with an appropriate cable – the most currently widespread interface is Ethernet and TCP-IP. Computer network address in this case is always 10.116.220.1, MAES analyzers have addresses from 10.116.220.2 to 10.116.220.12. Additional devices – relay control units, Vesuviy generator, etc. have addresses 10.116.220.16 and above; they are set up automatically. Check against the table of options.

Table of compatibility of interfaces				
Operating system	TCP-IP	Ethernet	PPI-PCI	PPI-ISA
Microsoft				
Windows 7-8-10	yes			
Windows XP	yes	yes	yes	
Windows 98	yes	yes	yes	yes
Windows 3.1, 95				yes

4. Connect MAES power cable to the power supply unit and hook it up. 3 of four LEDs shall light up brightly on PU panel. Ut LED light intensity (second LED from the bottom) may increase, if room temperature increases.
5. Check settings of spectrum measurement mode using MAES ( button). Set 1 accumulation at the minimum exposure – usually 250 ms. Select in addition (using "More..." button...) "Correction"/"Subtract dark signal".
6. Measure dark current  and wait for 15–20 minutes. Repeat dark current measurement. The device is ready to work, if when measuring the signal  the average spectrum value is not negative. If the signal is positive with a closed slot, there is a flare light in the spectrometer.
7. Detect and, if necessary, eliminate the flare light. To do so, start MAES in cyclic measurement mode  with displaying of the entire measured spectrum (with a vertical scale from -1 to 1). Observing the spectrum intensity, light with a lamp the place of possible polychromator transparency.
8. Set in front of the entrance slit of the device a source of stable linear spectrum – a ball-type lamp or a lamp with a hollow cathode.
9. Open the entrance slit 2mm high and 20 microns wide.
10. Start MAES in cyclic measurement mode  with displaying of the entire measured spectrum (with a vertical scale from -1 to 10).
11. Change the position of the cassette part of the polychromator with 1 mm step, so that the peak signal from spectral lines appears on the screen.
12. Change position and slope of the entrance slit to obtain spectrum image with the "narrowest" and "high" spectral lines. Optimum width of lines for spectrometers with diffraction grating makes 3-4 diodes, and with a prism — 4-5 diodes.

Currently, the main connection interface is Ethernet, and MAES type is TCP-IP, single MAES or a composite device consisting of 2 or 3 MAES devices. In the automatic tuning mode the program defines itself the number of photo diodes and the measurement procedure.

ATOM software functions in all Microsoft Windows operating systems. ATOMS 2.05. 2.10 and ATOM 3.0–3.3 programs do not affect each other and may be used on one computer.

PPI-ISA interface board is usually used in Windows 95, 98 environment. When it is not possible to install this board, as well as on computers with Microsoft Windows NT4/2000/XP/Vista, MAES operation is ensured only by PPI-PCI and Ethernet interfaces.

ATTENTION: Work with PPI-PCI interface is not supported in Windows 95 and ME operating systems.

PPI-PCI and Ethernet interfaces are installed into the PCI connector of the computer. Drivers are installed after automatic board detection. In case of the first installation a window opens with the message –

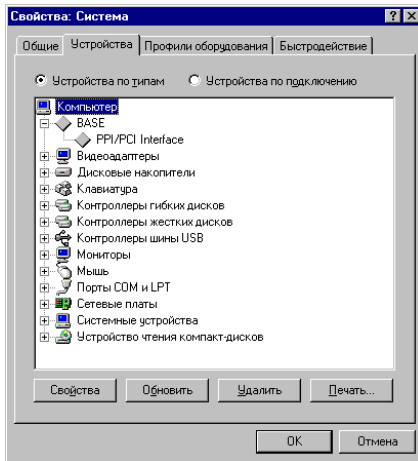
"New device found", and if drivers are already installed, no such message will appear – and in list of devices a new section will appear with "PPI/PCI Interface" subsection or, in case of Ethernet, a line with the name of the installed board will appear in "Network Boards" section ("Network adapters").

In setup dialog – "Select device" use program menu item "Settings — Device — Select Device" to select interface type. "Range Parameters" window is opened by clicking "Setup" button in this dialog.

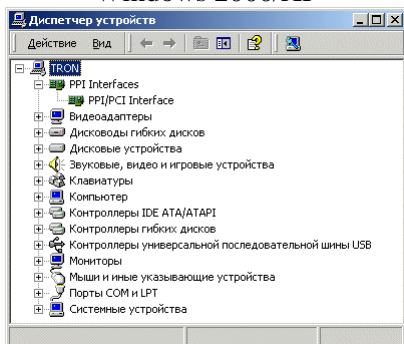
ATOM 3 program is usually installed into "c:\Atom 3.3" directory. If ATOM 3 program is installed for the first time on the computer, ATOM program was already installed before, it is necessary to perform the following operations:

1. In case of PPI-ISA interface it is necessary to check availability of BMKPPI2.386 driver (see above). In case of PPI-PCI or Ethernet, reconfiguration is usually not required.
2. Specify MAES analyzer settings according to ATOM working settings; pay attention to the number of lines of photo diodes and availability of "rotation" option.
3. Copy current profiling file from ATOM program directory (usually — "c:\Atom\atom.wl") into "c:\Atom 3.0" directory.
4. After ATOM 3 is launched, load the copied profiling, check MAES operation and conformity of positions of wavelengths in the measured spectra.

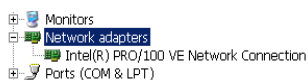
List of devices
for Windows 98



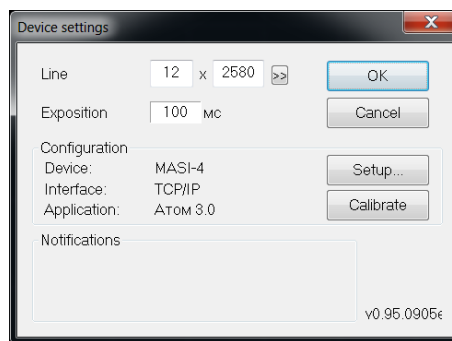
List of devices for
Windows 2000/XP



Network adapter in system properties looks as



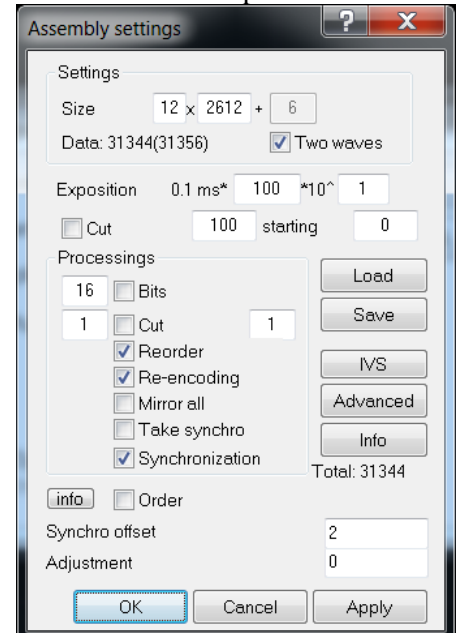
Window to select main
parameters of MAES analyzer
Size and time of one accumulation



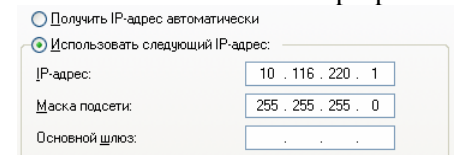
Typical settings for main types of spectrometers
(number of crystals)

Grand	12 + 5, 12 + 8
ISP-30, DFS-8	5
PGS-2, DFS-13	8 or 9
DFS-458S	8
DFS-458R	10
MFS-4...-8	8 or 12
DFS-10M, -36	12 (up to 16)
Baird, PlasmaLab	12
ICAP, Atomcomp	12 (up to 14)
SpectroLab	5 + 12
STE-1	13

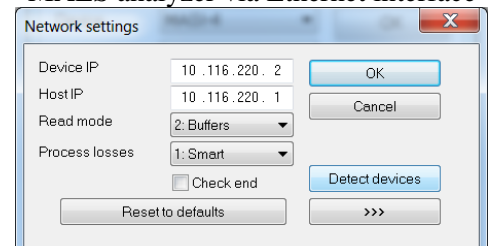
Example of detailed MAES settings
for GRAND spectrometers



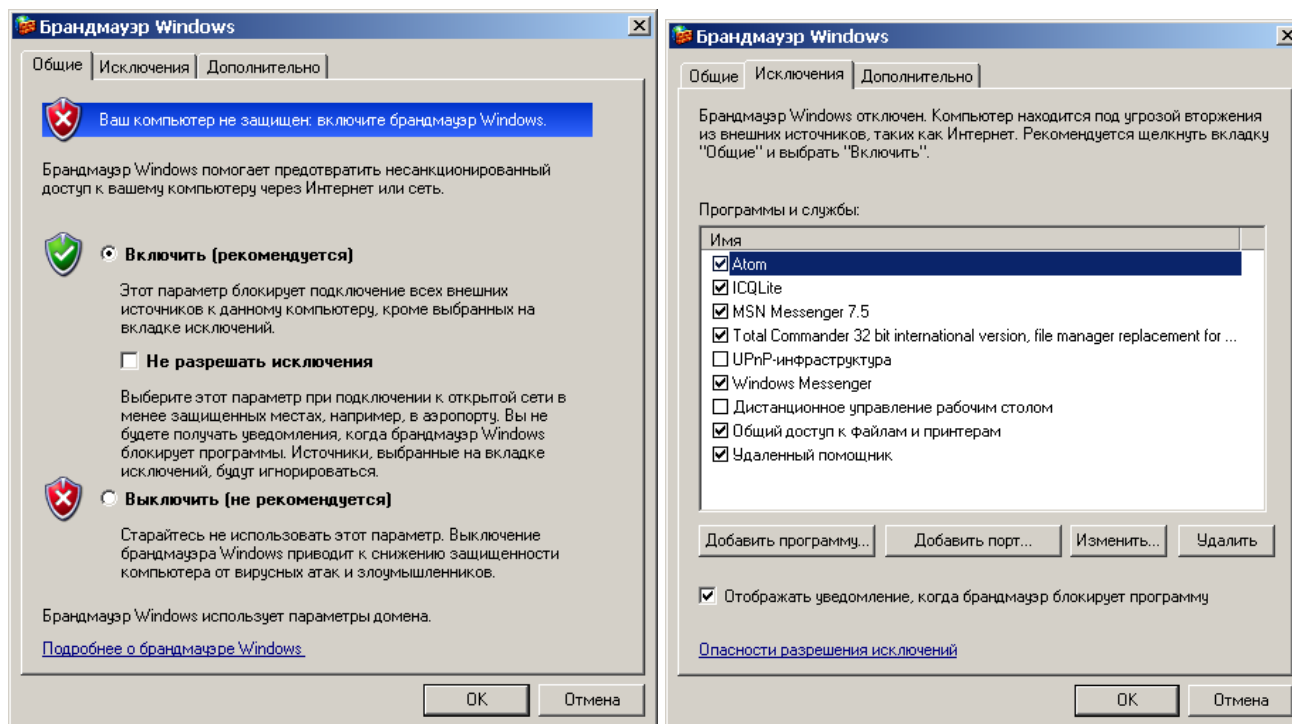
Network interface TCP-IP properties



Example of settings for work with
MAES analyzer via Ethernet interface



In case of MAES operation with Ethernet interface, when a "Firewall" control program or a or similar program is installed in the system, it is necessary to allow using the local network, otherwise the computer may block operation with MAES for safety reasons. Anti-virus program may also prevent operation



Software settings

For correct installation of ATOM program it is necessary to have administrator rights. Otherwise Windows security system will not allow correct installation of all working modules. First start of the program shall also be performed with administrator rights.

Modern Windows 7-8-10 system is completely ready for work with ATOM program, and in previous Windows XP/Vista versions for correct installation and operation of "Alloys", "MAES calibration", "Profiling" and "Spectral Lines" modules it was necessary to install the following add-ons for Windows, developed by Microsoft company and distributed free of charge:

"dotnetfx_(. NET 2.0).exe", "dotnetfx_(. NET 3.5).exe" and

«vcredist_x86_(Microsoft Visual C++ 2008 SP1 Redistributable Package (x86)).exe»

If they are not available, then during "Atom" start a message on the impossibility of their use will appear, and all other modules work normally.

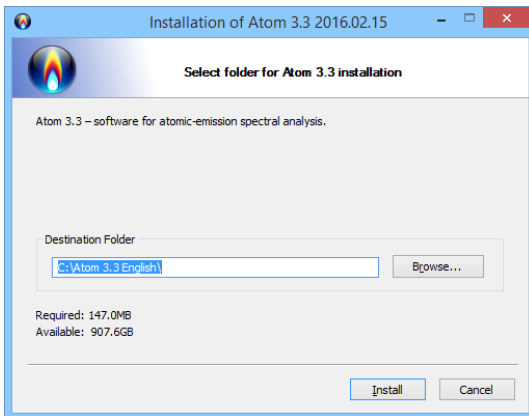
Installation of "msxml_4.0_SP2_(Microsoft XML Core Services).msi" add-on may be required for results database operation and interfacing with external programs.

For work in previous Windows versions (up to SP2) it may be necessary to install "WindowsInstaller-3.1-KB893803-v2-x86.exe" package.

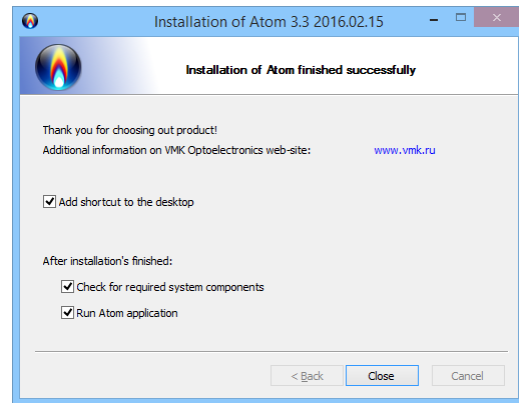
The specified files are located on the compact disk supplied with ATOM software in "Atom 3.3 setup\DEPENDENCIES\" directory, on "http://www.vmk.ru/download.htm" site, as well as on "www.microsoft.com" site.

Installation of ATOM 3.3 program is performed since November, 2011 from the single file (for example

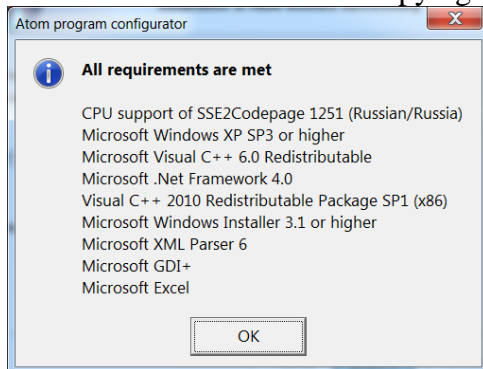
"Atom 3.3 (2012.07.27).exe"), which contains a package of all programs required for operation. "c:\Atom 3.3\Distrib\installation_logs.txt" file is created based on the results of installer operation:



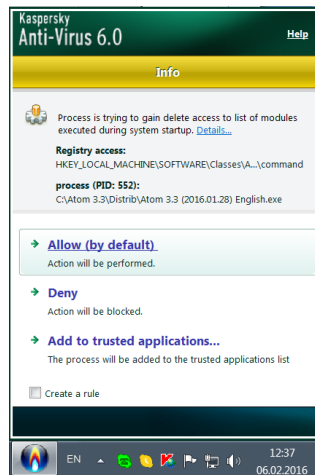
Installation starts with file copying



It is complete with system check and start of ATOM 3.3 program

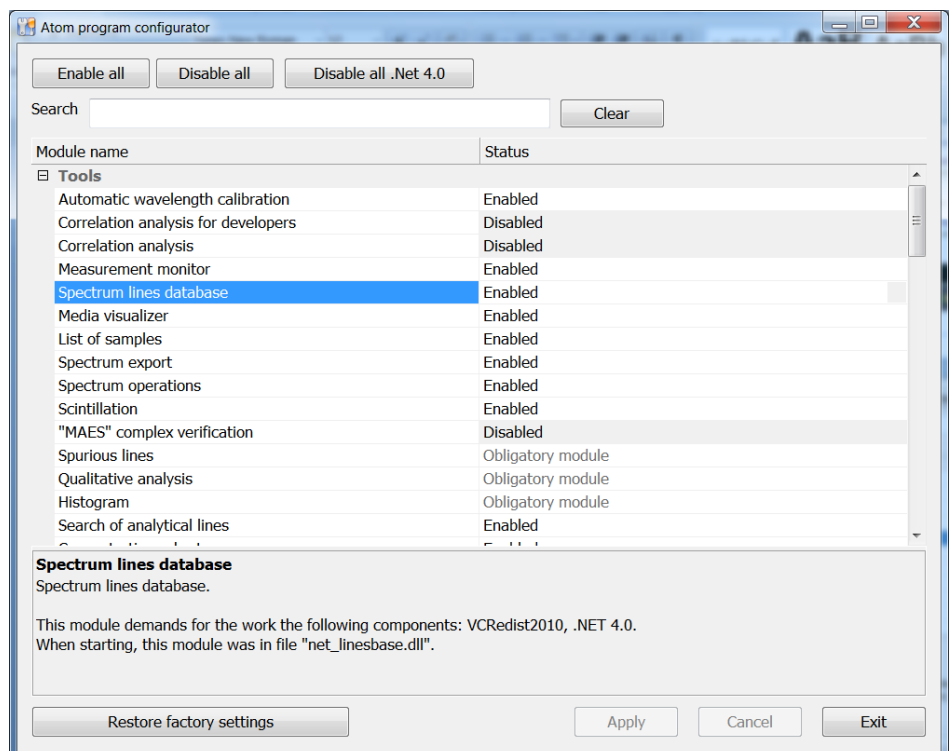


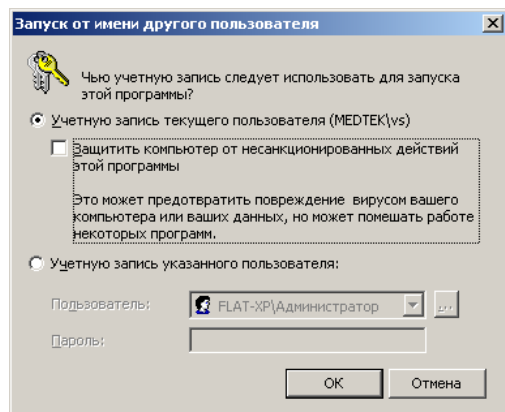
Check result — everything is OK



During the installation and first start of ATOM 3.3 program it measures several components; the antivirus program or system may, depending on security settings, require confirmation (like in Kaspersky does).

During operation it may be necessary to reconfigure ATOM 3.3 – to switch on/off program components using "Configurator.exe" program. When launched, the program checks condition of all components and displays them on the screen. You may view description for each component and switch it on/off for the period of operation.





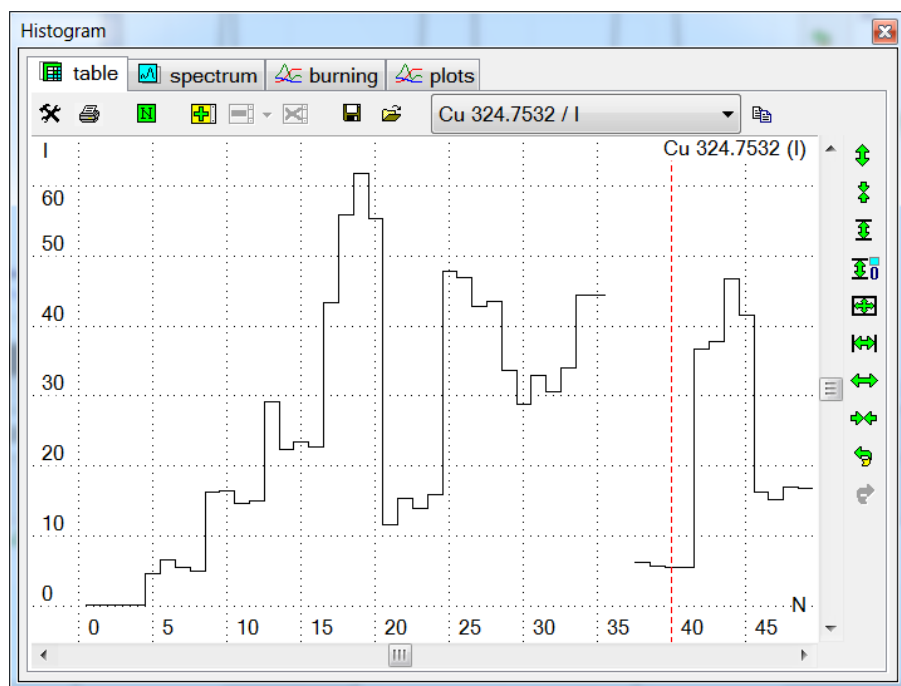
After configurator operation, during the start of ATOM 3.3 program it measures switched on components; the system may, depending on security settings, require user confirmation - such as administrative rights (like in the example for Windows XP).

Currently, the following components are usually switched off: Control of "Globula" stand, "Recording from camera", "Images", "Measurement monitor" and several other components.



For example, in case if a video camera is connected to the computer, it is necessary to switch on the "Recording from Camera" component for video recording of the analysis process, as well as "Images" component to view the recorded images.


Tools

"Histogram"




It is used to display the data slice as a graph. It works in one of the three modes: data slice by the analysis table, data slice by burning spectra and burning.

Use tabs with icons  /  to switch between modes.

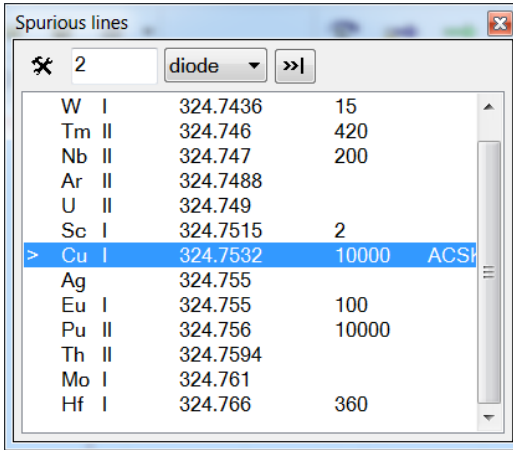
To display a data slice by the data table, click tab with icon . And then select a column in the table, which values shall be displayed in the histogram. Only values of parallel measurements are taken to build a histogram; mean values are not displayed. For example, click one of cells or column "C" caption of this line to view analysis results (peak intensity values) for "R 177.4347" line (the result is presented in the figure above).

Red dotted cursor shows the current cell position. "Double-click" the histogram window to replace the current cell in the analysis table. In order to display a data slice by a column with intensity or other values, it is necessary to make it current.

To display a data slice by the burning spectra, click tab with icon . In this case the program takes amplitudes of burning spectra as histogram values from the spectrum window in a point where red spectrum cursor is located. Move spectrum cursor to change the point of the histogram slice. In order for the histogram to work in this mode, it is necessary that the spectrum with burning spectra was displayed in spectrum window. To do so, change spectrum measurement settings so that the program will save burning spectra (see "Measurement mode" dialog, "number of spectra" parameter) and measure the spectrum.

Watch assignment of buttons located in toolbars of histogram window in "Main buttons of Analysis mode".

"Spurious lines"



W	I	324.7436	15
Tm	II	324.746	420
Nb	II	324.747	200
Ar	II	324.7488	
U	II	324.749	
Sc	I	324.7515	2
> Cu	I	324.7532	10000 ACS
Ag		324.755	
Eu	I	324.755	100
Pu	II	324.756	10000
Th	II	324.7594	
Mo	I	324.761	
Hf	I	324.766	360

It is used to determine possible aliasing of spectral lines, as well as to search lines in the specified spectral region. Lines located at a distance from the current line not exceeding the value set in the input field above the list, are displayed in the window. Element name, ionization degree, wavelength, line intensity and type are displayed. Window of spurious lines may be moved, and its sizes may be changed.

The tool works in two modes: search of spurious lines for the current spectral line (by default) and search of spurious lines round the spectrum cursor (red dashed line in spectrum window). After start the tool shows by default the spurious lines for the current spectral line (displayed on "Spectral lines" toolbar and is designated by blue cursor in spectrum window). If you change the cur-


rent spectral line, new spurious lines will automatically appear.

Double-click spectrum window to display lines under any spectrum range (around the spectrum cursor). Use this mode to define, what spectral lines will be under any peak. To do so, make sure that "set cursor to peak maximum" key is set ("Peak search" dialog), then double-click the peak. After the search around the spectrum cursor the program automatically sets the current spectral line — nearest to the cursor.

The list is display according to the line position in the spectrum: lines located above in the list are located to the left of spectrum; lines located below — to the right. Current spectral line is indicated in list by ">" symbol. Click ">>|" button above the list to change the current line (select line and press button), or double-click the line. After that spurious lines will be searched again for the current line.

If you select one of the lines in the list, it will appear in spectrum window, highlighted with green colour, which allows evaluating the degree of its possible impact on the analyzed line.

Line search spectrum may be set in nanometers or in diodes — see dropdown list. Spectrum recalculation from wavelengths to diodes or vice versa is performed and new value is displayed in the input field when changing the measurement unit.

Click button  to display search settings of spurious lines.

"Element Filter" controls elements, which lines will be used to search spurious lines:

"all" — use all elements;

"Mendeleev table filter" — use lines of elements from the filter in "Periodic table" dialog (see "Element Filter" dialog).

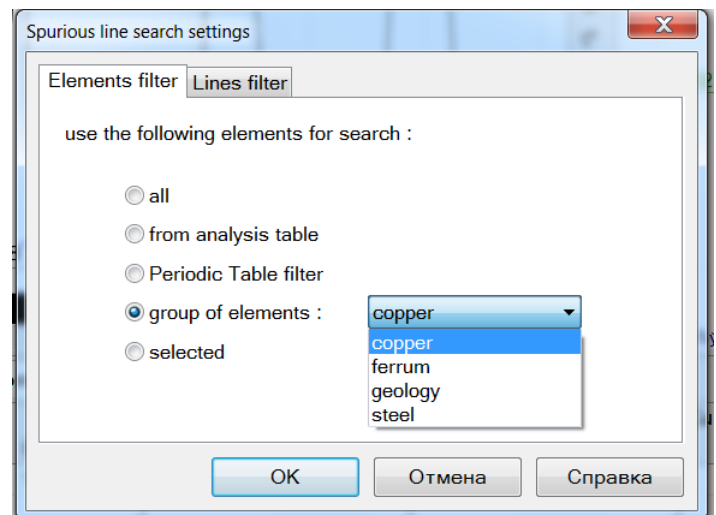
"Group of elements" — select the name of a group of elements, which lines shall be used (see "Group Manager" dialog).

"Selected" — lines of elements selected in "Periodic table" dialog will be used.

"Line filter" — controls selection of element lines:

"all lines" — use all lines

"spectral lines database filter" — use lines satisfying to the current filter of spectral lines (see "Spectral lines display settings" dialog).



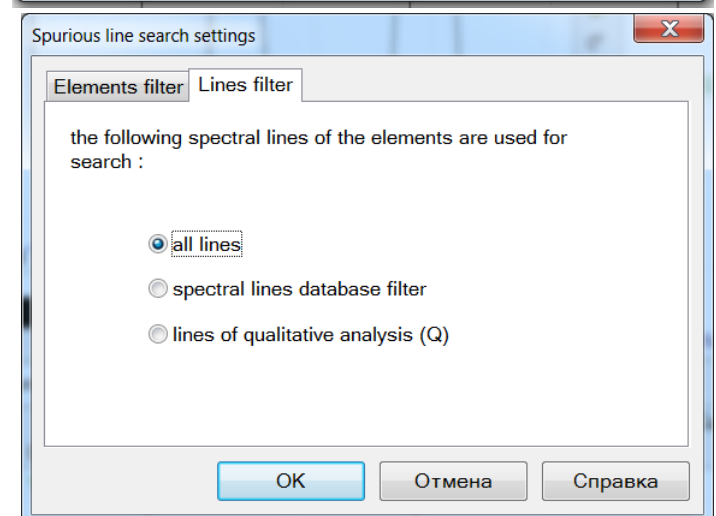
Spurious line search settings

Elements filter Lines filter

use the following elements for search :

☐ all
☐ from analysis table
☐ Periodic Table filter
☒ group of elements : copper
☐ selected

OK Отмена Справка



Spurious line search settings

Elements filter Lines filter

the following spectral lines of the elements are used for search :

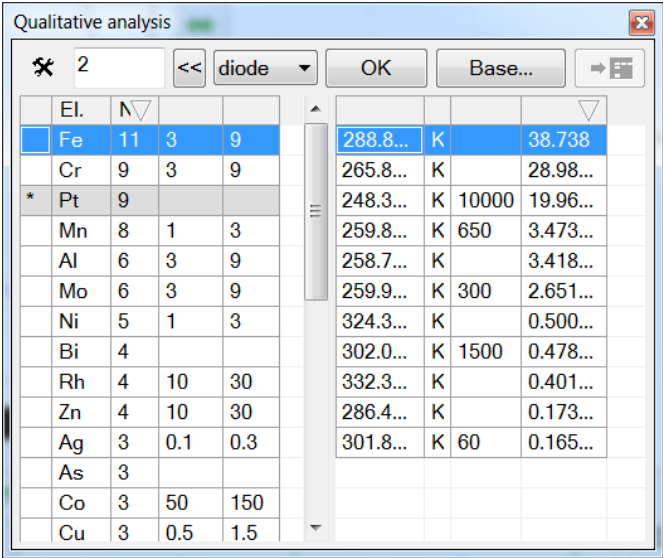
☒ all lines
☐ spectral lines database filter
☐ lines of qualitative analysis (Q)

OK Отмена Справка

"Qualitative Analysis"

It is used for qualitative and/or semi-quantitative analysis. Click OK button to start calculations and to display analysis results. The program looks for all peaks in the spectrum displayed currently in spectrum window. Analytic lines are searched for each peak found, which wavelength differs from the peak maximum wavelength no more than by the specified value. Search is performed only for elements and analytic lines set in Qualitative Analysis settings (see below). Then the number of peaks, elements and lines found, and the number of lines found for each element is displayed in decreasing order in the analysis results window. All lines found are displayed in spectrum window with gray colour.


The window consists of a toolbar located above and two lists — list of elements and the selected element line list. Qualitative Analysis window size and position may be changed.



The screenshot shows the 'Qualitative analysis' window. At the top, there is a toolbar with a settings icon (a crossed wrench and screwdriver), a field with the value '2', a '<<' button, a dropdown menu currently set to 'diode', an 'OK' button, a 'Base...' button, and a right-pointing arrow icon. Below the toolbar are two tables. The left table lists elements with columns for 'El.', 'N', and two unlabeled columns. The right table lists spectral lines with columns for wavelength, a 'K' flag, and intensity. The 'K' flag indicates a qualitative analysis line.


El.	N		
Fe	11	3	9
Cr	9	3	9
* Pt	9		
Mn	8	1	3
Al	6	3	9
Mo	6	3	9
Ni	5	1	3
Bi	4		
Rh	4	10	30
Zn	4	10	30
Ag	3	0.1	0.3
As	3		
Co	3	50	150
Cu	3	0.5	1.5

288.8...	K		38.738
265.8...	K		28.98...
248.3...	K	10000	19.96...
259.8...	K	650	3.473...
258.7...	K		3.418...
259.9...	K	300	2.651...
324.3...	K		0.500...
302.0...	K	1500	0.478...
332.3...	K		0.401...
286.4...	K		0.173...
301.8...	K	60	0.165...

Click  button to open settings dialog. Input field of the maximum deviation of the line from the peak center is located further. This value may be set either in wavelengths (nanometers), or in diodes. Use drop-down list to the right of the field to change the measurement unit; the entered value will be recalculated from wavelengths to diodes or vice versa.

"<<" button sets the maximum deviation value as the current profiling error. Click OK button to start searching and to display results.

Use "Base..." button to select base elements manually. Base elements are highlighted in the element list with "*" symbol; lines of these elements are highlighted in spectrum window with black colour. The program checks lines of each element found at the intersection with base lines; if the intersection was detected, and the checked element line is marked with "K" symbol (Qualitative Analysis line), then the element is marked with "?" symbol. Apart from the fact that base elements may be set manually, the program performs automatic detection of base elements by a heuristic algorithm.

Use button  to add lines highlighted in the list to the right to the analysis table.

List of elements found is located to the left. Element name is displayed, number of lines found for it, as well as conventional minimum and maximum concentration values, if you it is possible to evaluate them (see below).

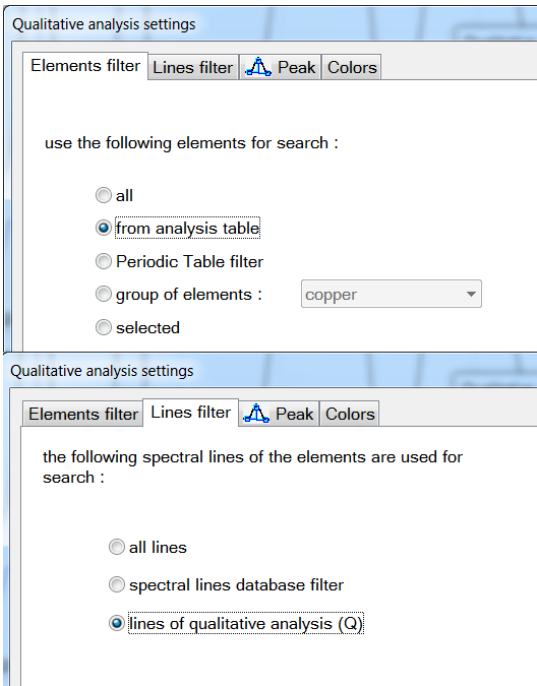
Element line list is located to the right. To display the element line list, click its name in the list of elements

located to the left. Wavelength, "K" flag for Qualitative Analysis lines, line intensity set in spectral lines database (in .mnd-file), as well as the peak intensity corresponding to the line are displayed in the list. When selecting any of the lines found, "Spurious Lines" window opens, displaying possible aliasing from the side of other spectral lines of elements found. Base lines in "Spurious Lines" window are marked with "*" symbol.


Click column caption to sort contents of the list by. Click again to change direction of sorting from "ascending" — to "descending" and vice versa.

Some lines of lists are highlighted with a different background colour. Such lines include:

- base elements;
- "totally out of range" lines of the qualitative analysis;
- lines with "self-absorption".



Background colour may be specified for such lines in "Colour" dialog of qualitative analysis settings.

Click button  to open qualitative analysis settings dialog:

"**Element Filter**" controls elements, which lines will be used for searching:

"all" — use all elements;

"*Mendeleev table filter*" — use lines of elements from the filter in "Periodic table" dialog (see "Element Filter" dialog).

"Group of elements" — select the name of a group of elements, which lines shall be used (see "Group Manager" dialog).

"Selected" — lines of elements selected in "Periodic table" dialog will be used.

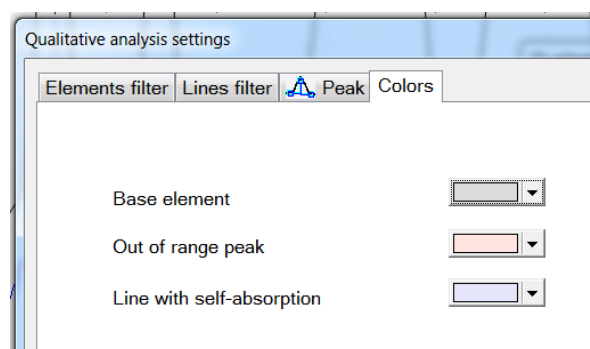
"**Line filter**" — controls selection of element lines:

"all lines" — use all lines

"*spectral lines database filter*" — use lines satisfying to the current filter of spectral lines (see "Spectral lines display settings" dialog).

"**Peak calculation**" dialog corresponds to analysis settings dialog. Use it to set calculation parameters of peak and background intensity, as well as various restrictions, for example, intensity threshold (the program uses this parameter to ignore peaks with a low intensity or to ignore the out of range peaks).

Use "**Colour**" dialog to set background colour for various lines of calculation results.

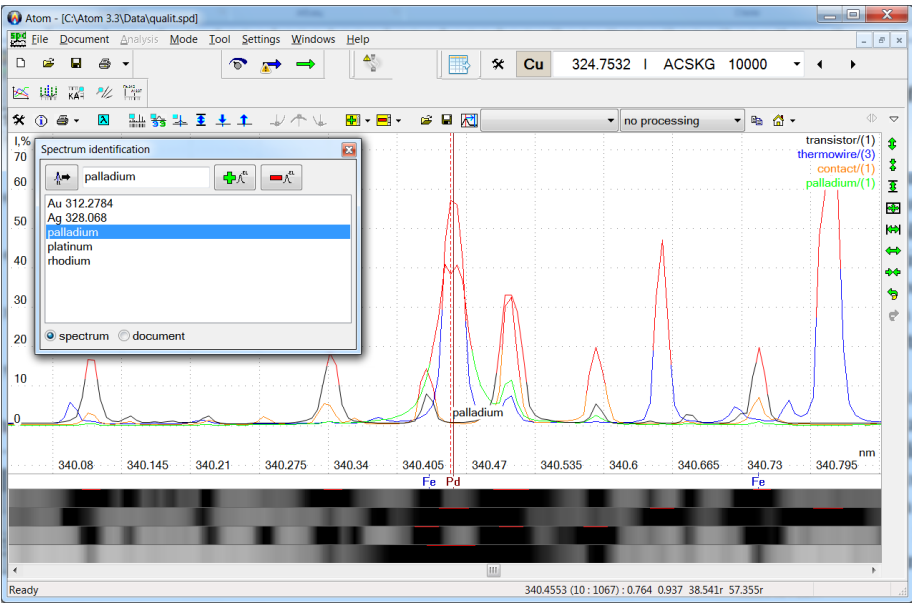


Recommendations on qualitative analysis

- Measure the analyzed sample spectrum or select the spectrum measured earlier from the analysis table. Select, if necessary, conformity of the scale of wavelengths (according to the profiling) to lines in the new spectrum.
- To set Element Filter and line filter (see dialogs "Element Filter" and "Line filter") – it is recommended to allow displaying only Analytical, Standard and Qualitative lines (to do so, set "average" resolution in "Spectral lines display settings" dialog and "Spectral lines database filter" in "Line filter" dialog) – such settings provide searching among ~1000 of the most characteristic spectral lines with various sensitivity. Switch to "Qualitative analysis" mode (item of the main program menu "Tool"/"Qualitative analysis").
- Set control spectrum in nanometers (it is recommended not to set a value more than a value for one diode, usually it is equal to 0.005–0.01 nanometers) and check "Peak search" settings, it is recommended to limit the lower boundary of line intensity values found in the spectrum and to exclude "out of range" peaks, switch on "Background subtraction", "Background averaging", intensity restriction from below 0.1; calculate line intensity as the "integral" on three central diodes, etc.
- After the settings are checked, it is necessary to start qualitative analysis by pressing OK button. After the spectrum analysis a list of elements is built (located to the left), for which the lines were found (with indication of the number of lines found for each element). Analysis is performed for impurity and main composition. For the sample analyzed the known main components may be also specified using "**Base**" button; such elements will be marked in the list with '*' symbol. Elements, for which the concentration is evaluated, with possible aliasing by lines of basic elements and lines with aliasing are marked with '?' symbol. Example of qualitative analysis is presented in the figure.
- Modern table of spectral lines contains information on Cmin and Cmax (in g/t (ppm), specified according to the book written by N.V. Arnautov, et al. "Approximate spectrum analysis...") According to this data, the program performs semi-quantitative analysis with display of the approximate spectrum of contents for the corresponding elements. Concentration spectra specified in N.V. Arnautov's book correspond to certain conditions of spectrum excitation – sample weight ~50 mg, DC arc 15–20 A, therefore assessment of the element content by spectra received in other conditions requires application of additional correction

coefficients. In any case the provided estimates may differ by several times from the real content of measured elements in the analyzed samples. Qualitative analysis requires certain skills of the analyst – he/she must have experience in performing such analyses, as well as be able to use computer capabilities.

"Identification of spectra"





For individual operation, the program allows identifying spectra of samples and performing qualitative analysis. Work is conducted similarly to identification of a photographic plate under a spectroprojector.


Due to photographic plate representation as an image, one or several spectra (together with additional ones) may be shown on the screen and printed on a printer in a form convenient for comparison and demonstration of distinctions.

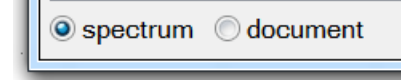
Individual spectrum lines or ranges may have any captions. The specified caption text becomes assigned to the spectrum, saved and recovered together with it. For each line in the list of captions, the program stores the position and the scale of spectrum, which are restored, when this line is selected.

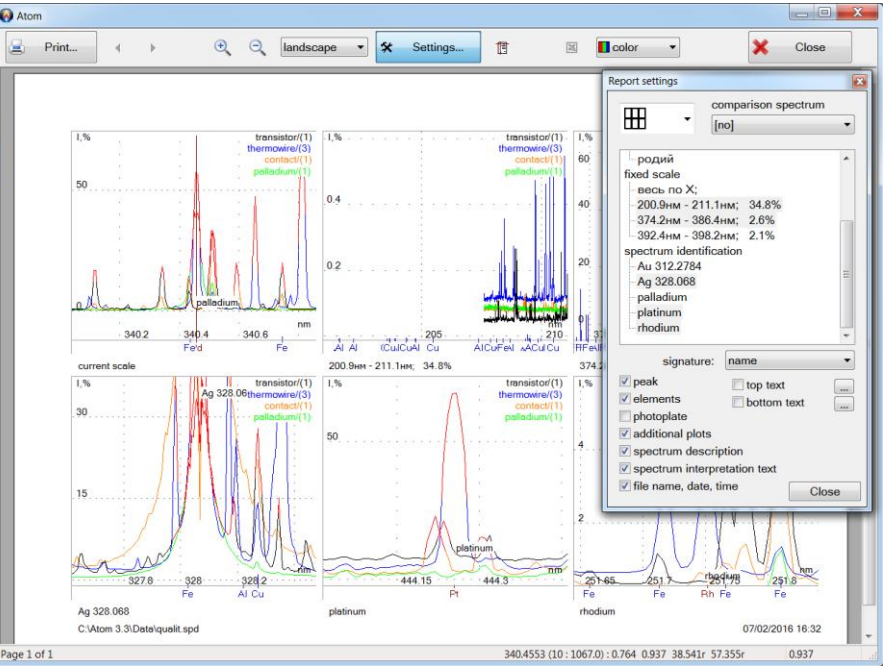
Text codes may be both specific for the spectrum (in this case they are displayed in the spectrum window) and be common for the entire document, which is convenient for the analysis of similar samples – you may define the main interesting ranges and to quickly switch between them.


Adds the current spectral line name (blue spectrum cursor) to the text line.

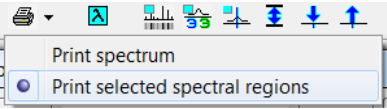

Adds text code to the red spectrum cursor location.


Deletes text code from the list.


Text code toggle switch — codes individual for each spectrum or common for the entire document.



"Print several spectrum ranges"



Report with preview for simultaneous printing of several preselected ranges of one spectrum.

A set of ranges for printing is formed from lists of captions for the document, fixed scales and the current spectrum. You may place up to 8 ranges on one page with various options of relative positioning. Display of additional information, as well as the text for the caption above/below each page, is controlled from the set-

tings window of this report.

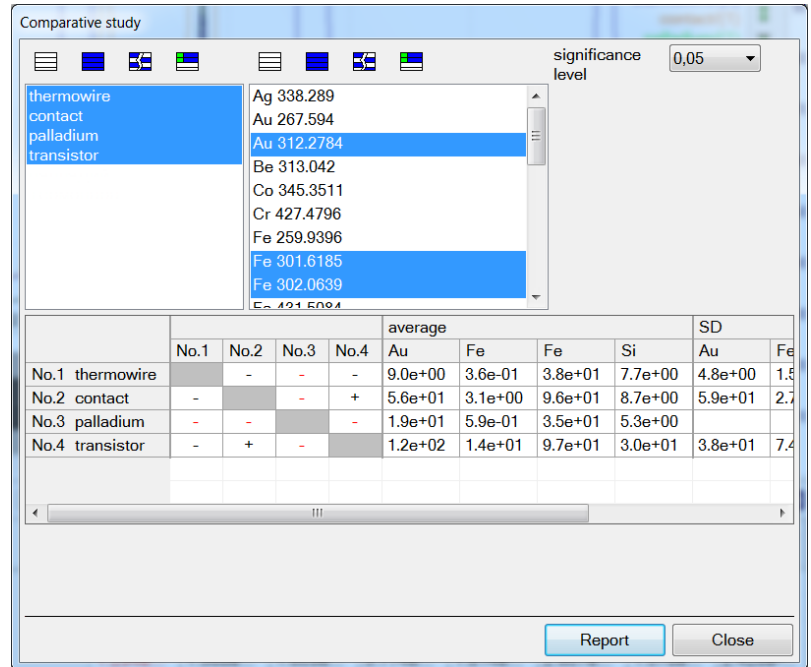
Application of this report allows optimum presentation of reports and/or performances without additional processing of individual images.

"Comparative research"

Use Tool menu to open the tool for comparative research using algorithm of the modified Student test for average intensity values and their reproducibility. It allows selecting various options and combinations of sample and element comparison. In the absence of significant discrepancies in the comparison table, "+" sign is specified; if there is at least one element, for which a significant difference is observed, "-" sign is specified. Comparison table may be exported to Excel as a report and supplemented with necessary comments.

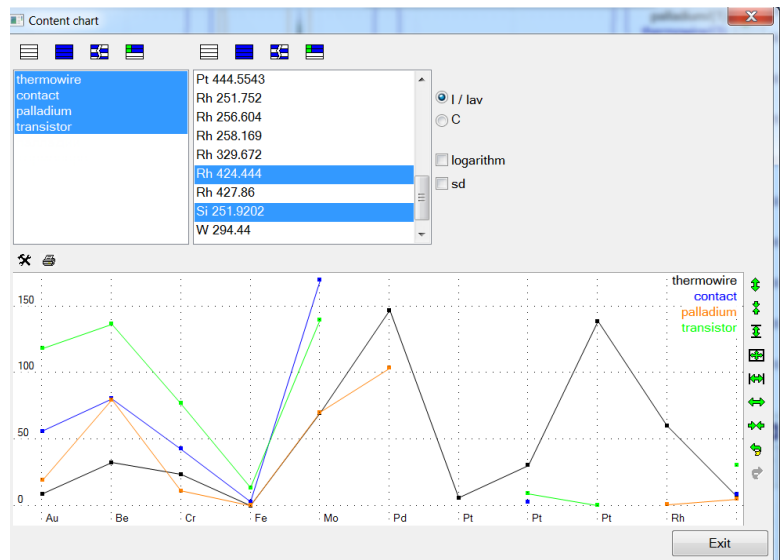
Relative intensity values are checked as the reference parameter for spectral lines, and directly entered values are checked for columns with any number, which allows checking the mixed data, also considering, for example, all samples.

Use of this tool accelerates spectrum analysis data processing and reduces the risk of errors during manual calculations in expert research laboratories.



"Content diagram"






Tool for comparative research through visual control of contents or relative intensity values of elements; it is useful for online comparison of the same samples with the aim to detect values, which are out of the common range, as well as for high-quality comparison of various materials and for searching of coinciding elements. Graphs are represented in linear or logarithmic coordinates. SD-spectrum may be displayed for relative intensity values to assess overlapping of content intervals.



"Quick tool panel"



The panel is opened through "Windows" – "Toolbars" – "Tool" menu. The program remembers panel position and status, and restores them after restart. List of tools is provided in the table.

	Fetching histogram window		Fetching spurious lines window
	Fetching qualitative analysis dialog		Fetching dialog to search pairs of analytic lines
	Fetching spectrum identification window		

"Search of analytic pairs of lines"

Search for analytical reference lines

Selection

Settings

Analytical lines

filter

180 pcs.

Ag

176.5538

178.975

184.7092

196.674

201.596

203.398

206.117

10

75

20

100

150

200

Reference lines

all lines

730 pcs.

Pt

175.561

175.5906

175.7523

175.8346

176.2127

176.3613

176.3995

II

II

II

II

I

I

I

an. line	comp. line	angle	adequ...	convergence	calibrati...	Ic...	R...	F...
Ag I 338.289	Pt II 357.7197	29.2	1.90e-02	2.54e-03	7.81e-02	9.59	8.19	-
Ag I 338.289	Pt I 331.5042	29.8	2.05e-02	2.60e-03	8.05e-02	84.1	10....	-
Ag I 338.289	Pt I 347.6747	29.4	2.07e-02	2.49e-03	8.02e-02	54.2	9.58	-
Ag I 338.289	Pt I 324.0196	30.0	2.13e-02	2.53e-03	8.12e-02	58.4	10....	-
Ag I 338.289	Pt I 325.9731	29.9	2.14e-02	2.52e-03	8.12e-02	73.1	10....	-
Ag I 338.289	Pt I 354.8814	29.3	2.14e-02	2.38e-03	8.05e-02	16.5	7.34	-
Ag I 338.289	Pt I 325.1979	30.2	2.16e-02	2.56e-03	8.17e-02	113	10....	-

36 pcs.


Searching...

Add

Exit

Tool for automatic search of analytic pairs of lines is opened from the "Tool" menu. It allows selecting various options of combinations of analytic pairs and selecting individual calculation settings of spectral line intensity values.

Search is performed in all specified spectral lines and their combinations with reference lines, by calculating linear calibration graph in logarithmic coordinates and checking of its parameters on compliance with the set values.

Search results are displayed in the table. Click caption of a column to start sorting. Select line in calibration graph window to display the corresponding image. Suitable analytic pairs may be added to Analysis table using "Add" button. Lines will be saved in the "Search analytic lines" sheet.

In order to decrease the number of options checked and to reduce the operating time, it is recommended to set reasonable limits for parameters of line intensity values, calibration graphs and mutual arrangement of analytic lines and reference lines in line search settings. If search does not provide acceptable results, it is necessary to gradually weaken the control – for example, by cutting limits or the limit intensity of spectrum lines, or by excluding extreme points on the calibration graph from the search.

Selection

Settings

Analytical lines

180 pcs.

Ag

Ag

Al

As

Au

Ba

Bi

C

Search for analytical reference lines

Selection

Settings

exposure number

1

analytical line peak search settings

155

reference line peak search settings

453

maximal deviation from 45°

20

618

maximal RSD of reference line, %

100

distance to reference line, nm

20

2

only meeting the Fisher ratio test

☐

identical ionization degrees

☐

numbers of lines, discarded according to the corresponding parameter, is highlighted with red colour

an. line	comp. line	angle	adequ...	convergence	calibrati...	Ic...	R...	F...
Ag I 338.289	Pt II 357.7197	29.2	1.90e-02	2.54e-03	7.81e-02	9.59	8.19	-
Ag I 338.289	Pt I 331.5042	29.8	2.05e-02	2.60e-03	8.05e-02	84.1	10....	-
Ag I 338.289	Pt I 347.6747	29.4	2.07e-02	2.49e-03	8.02e-02	54.2	9.58	-
Ag I 338.289	Pt I 324.0196	30.0	2.13e-02	2.53e-03	8.12e-02	58.4	10....	-
Ag I 338.289	Pt I 325.9731	29.9	2.14e-02	2.52e-03	8.12e-02	73.1	10....	-
Ag I 338.289	Pt I 354.8814	29.3	2.14e-02	2.38e-03	8.05e-02	16.5	7.34	-
Ag I 338.289	Pt I 325.1979	30.2	2.16e-02	2.56e-03	8.17e-02	113	10....	-

36 pcs.

Searching...

Add

Exit

The program allows se
 Search area may be limited both using a specific list of reference samples, and by

lecting only elements with the specified concentration in reference samples. additional limiting conditions — these may be the value and convergence of spectral line intensity values, calibration graph slope, its conformity to Fischer ratio test, distance between the analytic line and the reference line in nanometers, as well as the matching ionization degree. You may select a specific exposure number for the corresponding analysis techniques.

After the search you may select a suitable pair in the table of results. Full information is displayed for the selected line in calibration graph window.

Data control in the analysis table

Additional control elements for selection from the list of visible samples and lines/columns in the analysis table. Displaying of these elements must be enabled in "Table window settings" dialog in the analysis table toolbar in order to use them.

Dropdown lists with names of samples and the complete list of spectral lines provide fast access to samples and lines without the need to scroll through the entire analysis table.

Start typing text in the header line of the list of lines or samples, the program will start searching for a match and will display all lines/samples with the entered text. Just select necessary line/sample from the list to navigate to it — use "up"—"down" keys or the mouse cursor.

Use one of standard Windows combinations to copy to clipboard (Ctrl-C and Ctrl-Ins) to open window of data transfer from Analysis table to Windows clipboard with the possibility to control the copied information.

A text appears in the window as a table in the corresponding selected area of the Analysis table. If the cursor is currently positioned in the first line of the first column, the whole table will be selected.

Hold down Shift key and press "up"—"down" keys or use mouse cursor to select an individual group of cells – they will be highlighted in the table with light blue colour (by default).

Example below presents text from clipboard after copying of the selected range of the Analysis table.

The screenshot shows the software interface with a dropdown menu open for 'Platinum'. The menu lists various elements and their corresponding values. The analysis table below shows data for 'Cr 280...' and 'C 87'.

Sample	Cr 280...	C 87	SS-CRM 487/1	CRM 187A	YF 87
88 YF87	0.260	0.260	0.258	0.258	0.258
89 YF88	0.474	0.474	0.468	0.455	0.455

The dialog box 'Copy from Analysis Table to clipboard' is shown. It has options for 'copy' (selected fragment), 'number delimiter' (set in Windows), and checkboxes for 'amend' (row headers, column headers) and 'exclude' (statistics, samples, parallel measurement). A preview table is shown at the bottom.

	Cd 226.502	Cd 346.62	Cr 284.3249
22 GSO Pt-1-5 №527790control	6,90e-03	6,90e-03	1,16e-02
(1)	5,12e-01	4,6e-03	3,24e-01
(2)	5,76e-01	5,7e-03	3,24e-01
(3)	4,85e-01	4,2e-03	3,18e-01
(4)	5,82e-01	5,8e-03	3,73e-01
average	5,39e-01	5,1e-03	3,35e-01
median		5,2e-03	4,0e-03
repeatability			

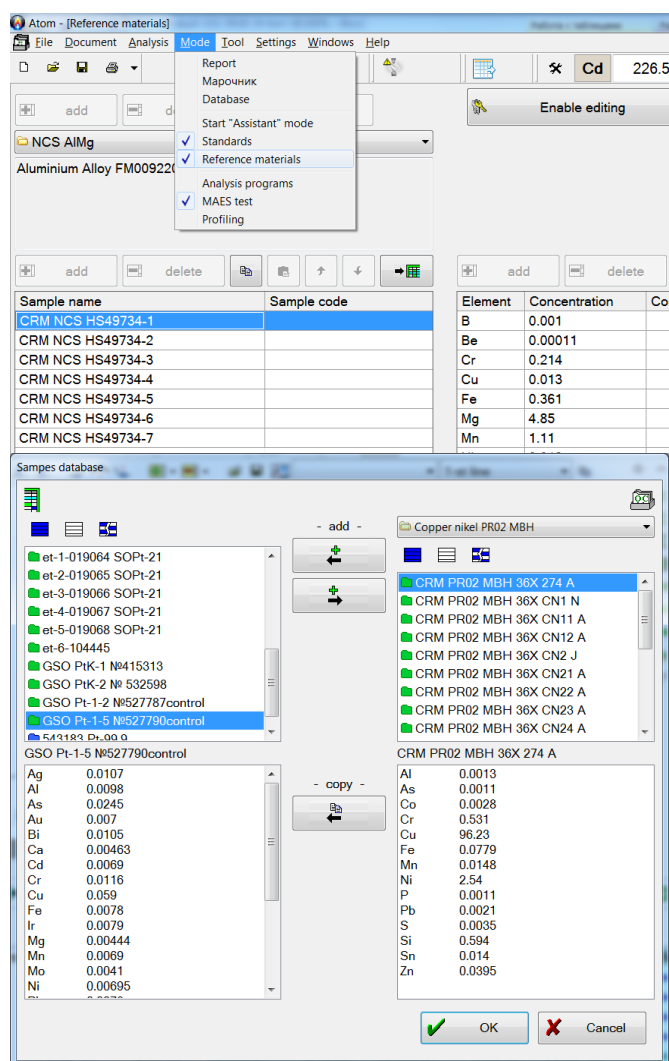
		Cd 226.502		Cd 346.62		Cr 284.3249
	I	C	I	C	I	C
22	GSO Pt-1-5 №527790control	6,90e-03		6,90e-03		1,16e-02
	(1)	5,12e-01	4,6e-03	3,24e-01	4,0e-03	3,59e+00
	(2)	5,76e-01	5,7e-03	3,24e-01	4,0e-03	2,49e+00
	(3)	4,85e-01	4,2e-03	3,18e-01	3,9e-03	2,44e+00
*	(4)	5,82e-01	5,8e-03	3,73e-01	5,2e-03	3,31e+00
	average	5,39e-01	5,1e-03	3,35e-01	4,3e-03	3,0e+00
	median					
	repeatability					

median	5,2e-03		4,0e-03		1,0e-02	
repeatability						
23 543183 Pt-99,9						
(1)	6,53e-03	1,8e-06	9,87e-02	4,4e-04	2,98e-02	6,9e-05
(2)	8,29e-03	2,7e-06	6,73e-02	2,2e-04	2,56e-02	5,8e-05
(3)	6,69e-03	1,9e-06	6,52e-02	2,1e-04	2,99e-02	6,9e-05
(4)	1,05e-02	4,2e-06	7,15e-02	2,4e-04	3,32e-02	7,7e-05
average	8,0e-03	< 2,5e-04	7,6e-02	< 1,0e-03	3,0e-02	< 9,7e-05
median	2,3e-06		2,3e-04		6,9e-05	
repeatability						

As we can see – selected data are copied from data table to text via clipboard:


Current spectrum	Ca 393.3663	Cd 226.502	Cd 346.62	Cr 284.3249	Cu 221.4581
	I	C	I	C	I
22 GSO Pt-1-5 №527790control		4.63e-03	6.90e-03	6.90e-03	1.16e-02
(1)	5.10e+01	2.6e-03	5.12e-01	4.6e-03	3.24e-01
(2)	4.45e+01	2.2e-03	5.76e-01	5.7e-03	3.24e-01
(3)	4.58e+01	2.3e-03	4.85e-01	4.2e-03	3.18e-01
(4)	6.01e+01	3.2e-03	5.82e-01	5.8e-03	3.73e-01
average	5.0e+01	2.6e-03	5.39e-01	5.1e-03	3.35e-01
median		2.5e-03		5.2e-03	
repeatability					
23 543183 Pt-99,9					
(1)	7.46e+00	2.6e-04	6.53e-03	1.8e-06	9.87e-02
(2)	6.85e+00	2.4e-04	8.29e-03	2.7e-06	6.73e-02
(3)	8.07e+00	2.9e-04	6.69e-03	1.9e-06	6.52e-02
(4)	1.07e+01	4.1e-04	1.05e-02	4.2e-06	7.15e-02
average	8.3e+00	3.0e-04	8.0e-03	< 2.5e-04	7.6e-02
median					
repeatability					

Using the base of reference materials



"Reference materials" mode used to input information is described in appropriate section of this manual.

Data already entered (element concentrations) by samples may be "transferred" by opening the reference samples database control window in the current (open) document (in the Analysis table). To do so, go to

Click button  to open Reference materials database control window, which is used to connect concentration/information by reference samples with samples in the analysis table. It is possible to copy/add information to both parts, which allows (by means of RS DB) transferring information about element concentrations between data files.

Element concentration values may be entered into RS DB both manually and by "extracting" them from the data file by copying all necessary samples.

Besides, in this window you may see the compact list of elements and the specified concentration values.

Concentration from RS DB will be stored in sample, even if there are no analytic lines of elements in the Analysis table. When adding a spectral line to the table, saved concentration values will be immediately specified for it.

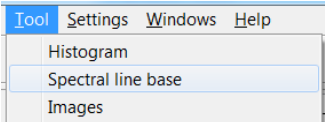
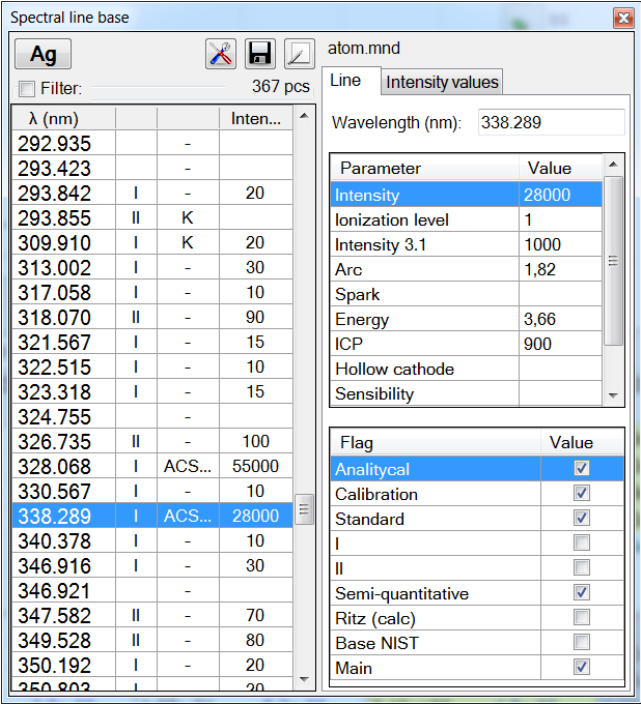
For fast access to information on concentration in reference samples you may use drop-down menu, which is activated on the sample/parallel measurement caption.

repeatability					
3	GSO Pt-1-3 N527788		3.40e-03		3.40e-03
*	(1)	Disable	2.7e-03	3.69e-01	3.1e-03
	(2)	Hide parallel measurements	2.8e-03	3.60e-01	3.2e-03
	(3)	Rename	3.7e-03	4.79e-01	4.1e-03
	(4)	Statistics	3.8e-03	4.46e-01	4.2e-03
	average	Move	3.3e-03	4.1e-01	3.6e-03
	median	Delete	3.3e-03		3.6e-03
	repeatability				
4	GSO Pt-1-3 N527788	Consider as a reference material	2.01e-03		2.01e-03
	(1)	Consider as a working sample	2.3e-03	2.76e-01	2.7e-03
	(2)	Reset individual peak parameters	1.9e-03	2.61e-01	2.3e-03
	(3)	Working with samples database	1.3e-03	1.68e-01	1.7e-03
	average	take RM values from samples database			
	median	save sample to database ...			
		add sample from database			
			4.6e-01		

Use this menu to "switch on/off" the whole sample/parallel measurements or only Crm. Reference sample with switched off Crm value (items of "To be considered as the work sample" menu) is considered by the program as the work sample, concentration is calculated for it, and the corresponding statistical control is performed.

This mode is useful during the methodical work, when selecting modes and calculation parameters of calibration relationships. Item "To be considered as the reference sample" menu "switches on" the switched off earlier Crm value.

Base of spectral lines



- click main window menu "Tool"- "Spectral line base" for using the subprogram.
- tool used to edit and view the base of spectral lines, to add new parameters, correct and add existing parameters. Use "Tools" menu to open it as a "floating" window in the "Engineer" mode.
- subprogram in "Intensity values" section provides the service on automatic input of values based on the current spectrum.



- click button before editing or adding new spectral line. The button enables manipulation with spectral line database.



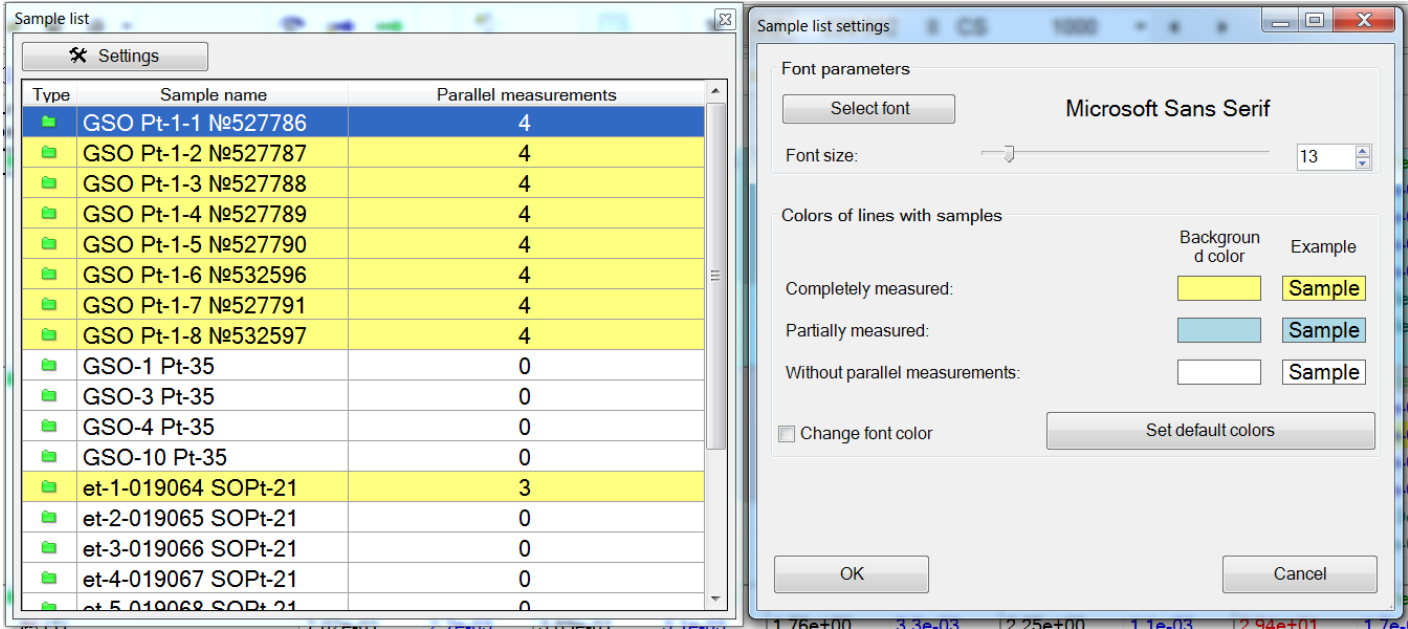
- click button to save spectral line database in external file.

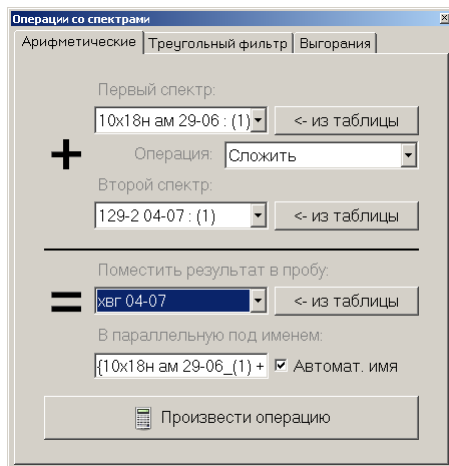


- click button for checking some editing and viewing options.

Sample list

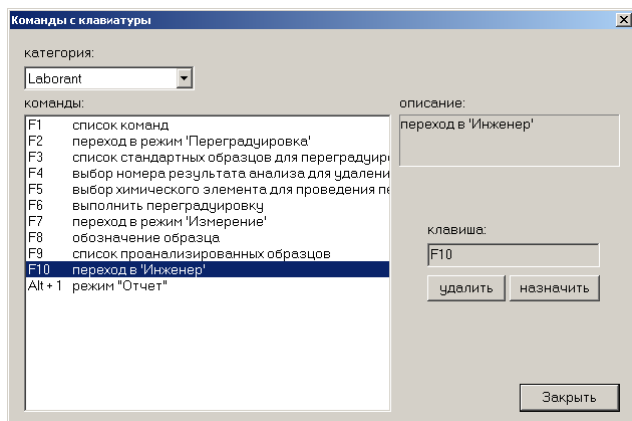
Additional window for simplification of navigation according to the analysis table in the "Engineer" mode; settings allow line font size and colour adjustment for samples with spectra and without them. Sample selected in list becomes the current sample in the analysis table.





Operations with spectra

Researcher's tool provides basic operations with spectra – pixel-by-pixel addition and subtraction, multiplication and addition/subtraction of the number. It allows checking assumptions on spectral aliasing or to subtract directly the blank test spectrum.



Keyboard Commands


"Shortcut" window settings for the most popular functions. Allows reducing the necessity to use the mouse and allows using only keyboard buttons when working both in the routine analysis "Assistant", and in the "Engineer" mode.

Add-on modules

ATOM software package may contain add-on modules ensuring operation of peripheral devices. Currently, operation of "Vesuviy" generator, "Globula" stand, vacuum spectrometer with argon spark stand is supported.

"Recording from camera"

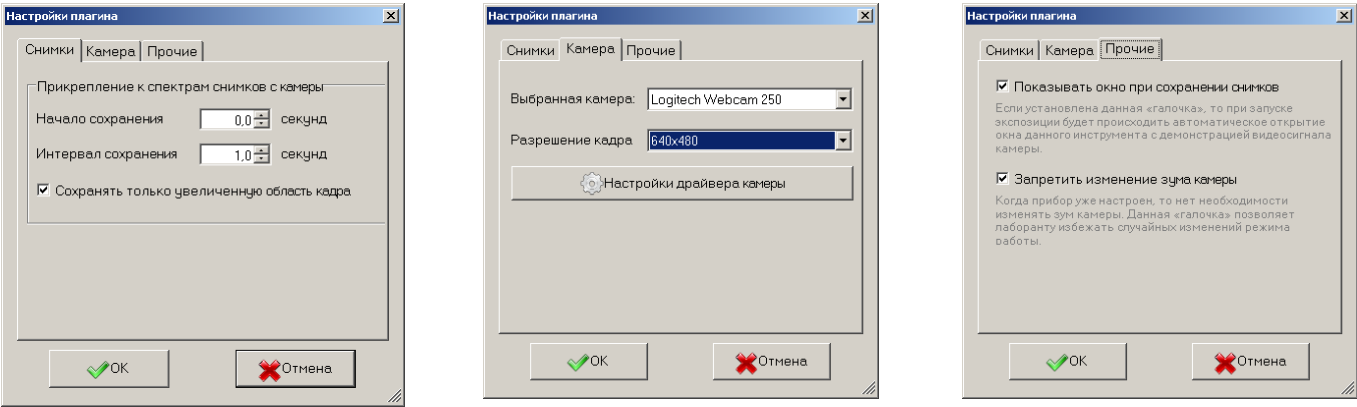
It is started in "Tools" menu or by clicking but-

ton  on the control panel.

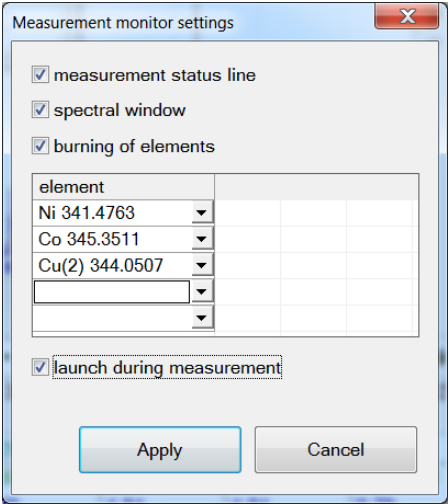
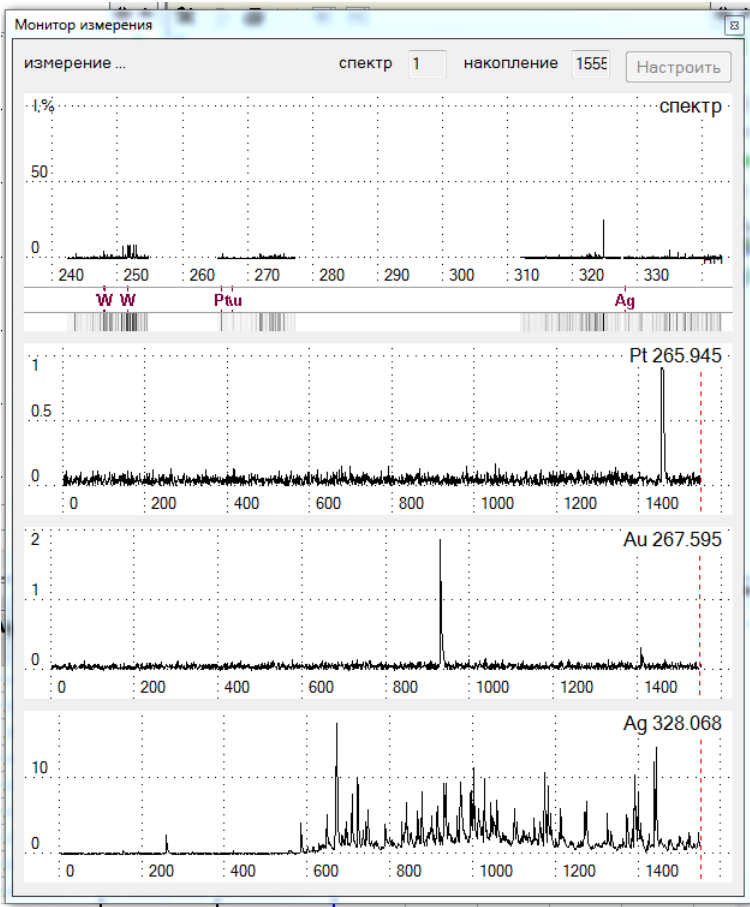
Video camera images are saved in the current spectrum and are automatically transferred to the analysis table. Information fields — recording time, time elapsed from measurement start, parameters of the saved image are applied to the image; you may also provide comments for images.

Use this tool, for example, to save desktop status or to save information of analogue instruments with time registration relative to the start of each measurement.





"Measurement monitor"




The tool is used for real time monitoring in the program window of the exposure process, the current spectrum and the receipt of preselected elements. Select in settings window up to 5 spectral lines of elements from among such displayed in the analysis table. During data acquisition from MAES analyzer the program processes it "on the fly" and displays burning records for the specified spectral lines.

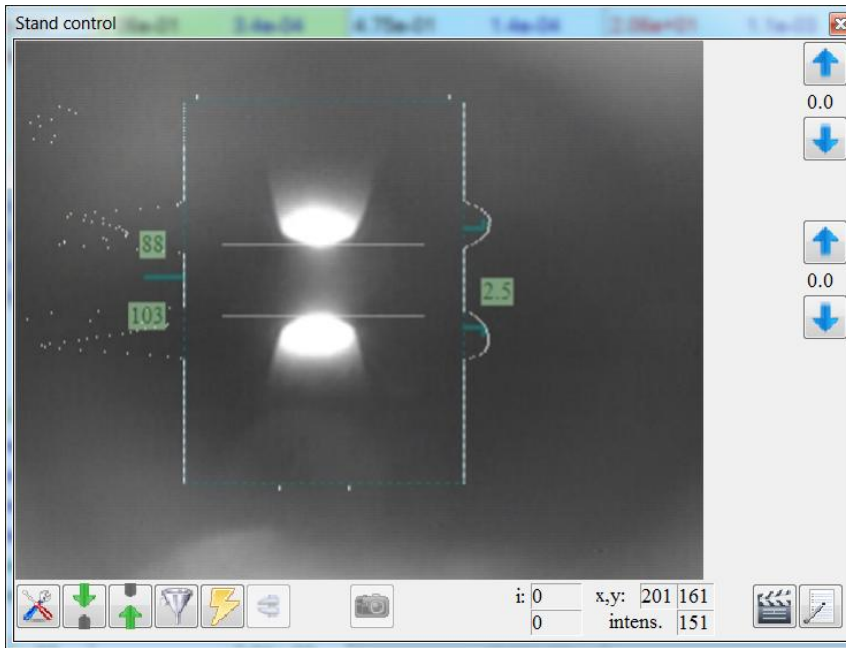
Tool settings allow selecting the time interval for data saving, video camera type (if there are several cameras in the system), as well as other parameters.

More detailed description of tools related to equipment control is provided in respective manuals.

Globula stand control

Click  button to open module window.

If there is no connection with the stand, the button will look like: 



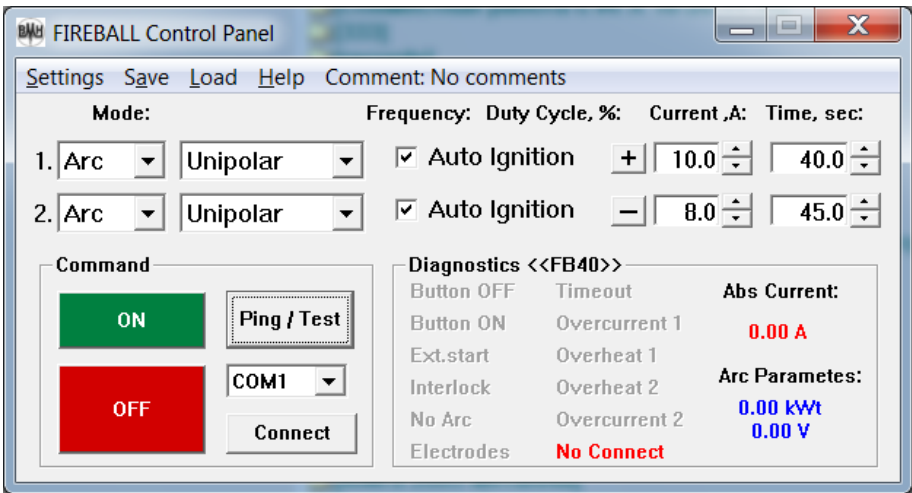
During the exposure you may enable saving of the video images and values of current, interelectrode gap, etc.; saved information remains assigned to the spectrum and may be later viewed by the operator, printed, saved to a file, etc.

All information is saved to a data file together with spectra and may be used later to control, register and check the analysis.

Saved video images may be viewed later using main window menu item "Tool" — "Images".



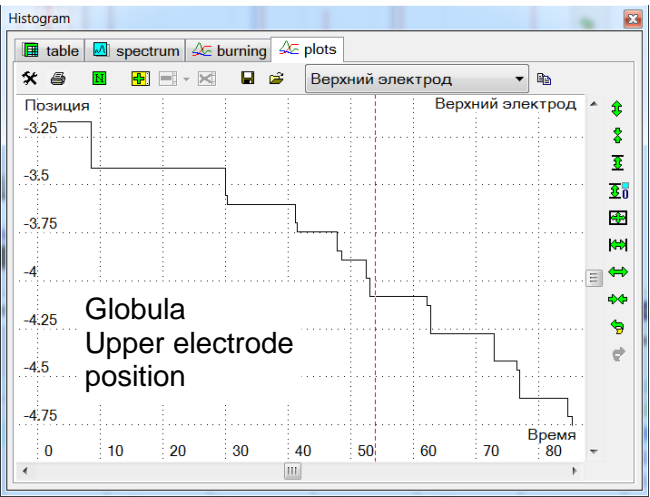
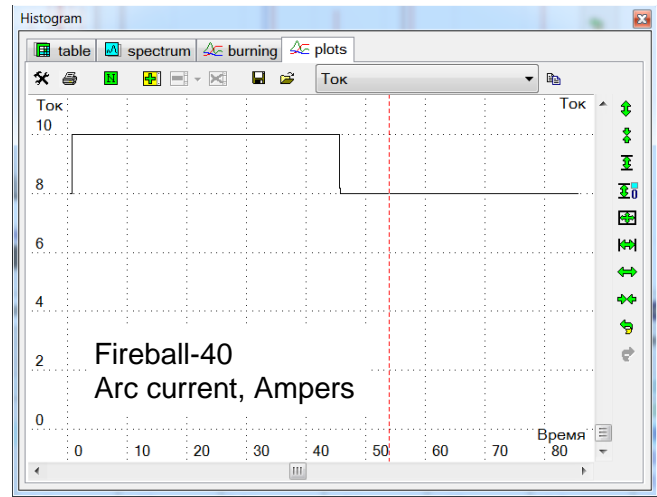
Fireball generator control



Fireball generator control program
External program “duga_shm62_oscil_eng.exe”
Discharge current is displayed in the measurement window during the exposure.

Saving equipment parameters

Modern versions of control programs for Globula stand and Fireball generators, as well as other subprograms allow saving information on values of current, voltage, etc. in relation to each spectrum.



Values of current and other values, varying during the exposure, may be viewed later for any spectrum in "Histograms" — "Graphs" display mode. Make sure the dropdown list — control element "List of sources" is enabled in settings.

Software package and licensing information

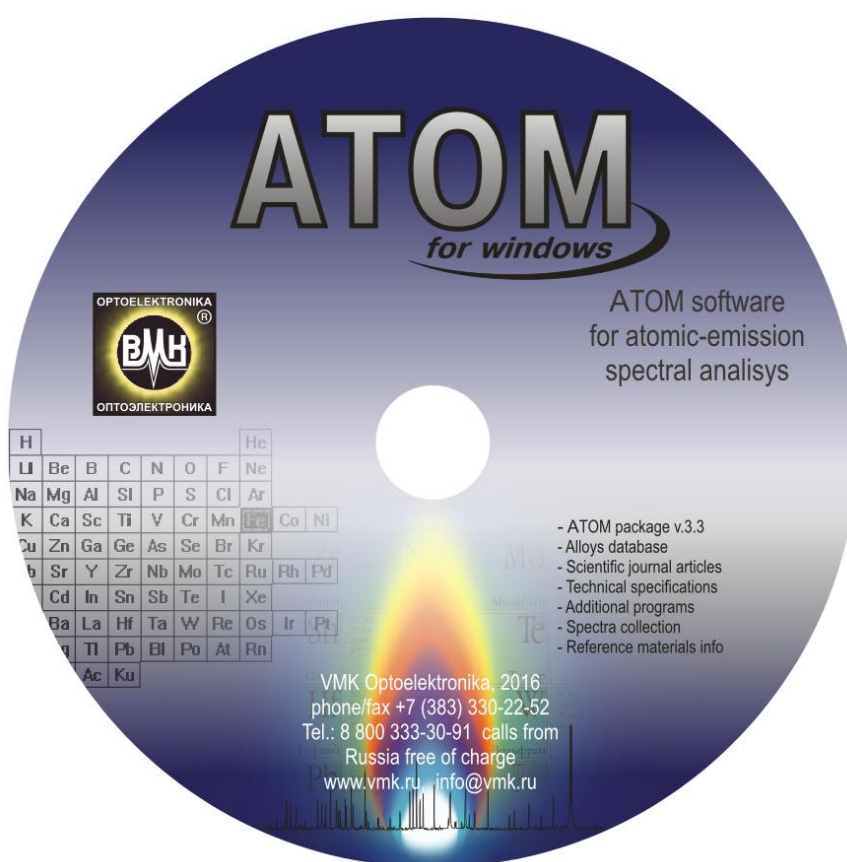
"ATOM" software package is a special tool for atomic emission spectral analysis. It works with analyzer MAES, spectrometer Grand, Globula stand, Fireball generator and many other spectral devices that VMK Optoelektronika produces.

The "ATOM" software could be used for educational purposes without charge.

The "ATOM" software should be downloaded from official site <http://www.vmk.ru>, copied from compact-disk from installation package of analyzer MAES and must be used in legal purposes only.

Reverse engineering is strongly prohibited.

ATOM package CD and DVD compact disk are labelled with special image:



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"ATOM" software User Manual total

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number

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Signature