MA-Table

Operator's Manual (Version 2.xx)

MA-Table is a Windows® program to display and handle atomic data, which are important for Energy Dispersive X-ray Spectrometry (EDX or EDS), like

- Energy positions of line series (the element X-ray line energies),
- Quick possible element and line searches for selectable energy,
- Quick line overlap search to identify element coincidence problems,
- Relative height relations between lines of a series,
- Critical excitation energies (shell energies),
- Mass attenuation coefficients (mass absorption coefficients).

MA-Table is able to calculate Electron Probe Microanalysis (EPMA) excitation processes and the influence of these processes to the relative heights of the lines. Complete spectra simulation is possible because of the built-in P/B fundamental parameter model for characteristic radiation and Bremsstrahlung. Furthermore the program simulates stochastic processes of X-ray emission and also all artefacts of the EDX spectrometer which contribute finally to the usually measured spectra. A very realistic spectra simulation is finally performed.

Additionally MA-Table is able to calculate Minimum Detection Limits (MDL) and the analysis depths, taking into account excitation conditions, specimen geometry and special matrix and overlap situations with other elements. It is possible to simulate a real EDX-data acquisition process for nearly realistic demonstration purposes. This simulated data acquisition depends from count rate of the X-ray spectrometer (setup value) and of acquisition time. Alternatively the simulation is possible to switch to stable electron beam-current with changing count-rated depending from acquisition conditions. Watching the reduction of MDLs with progress of acquisition time during simulation of ongoing acquisition process is an impressive feature.

All functions have access to the central data base.

Content:

1. Functions of Icon Bar

... Switch between table and Icon-Bar

... Display periodic table of elements

... Element search with line energy input

... Edit data base *(only in licensed version)*

... Print, store and copy of data *(only in licensed version)*

... Setup, registration, demo, manual and updates

... Call spectra simulation

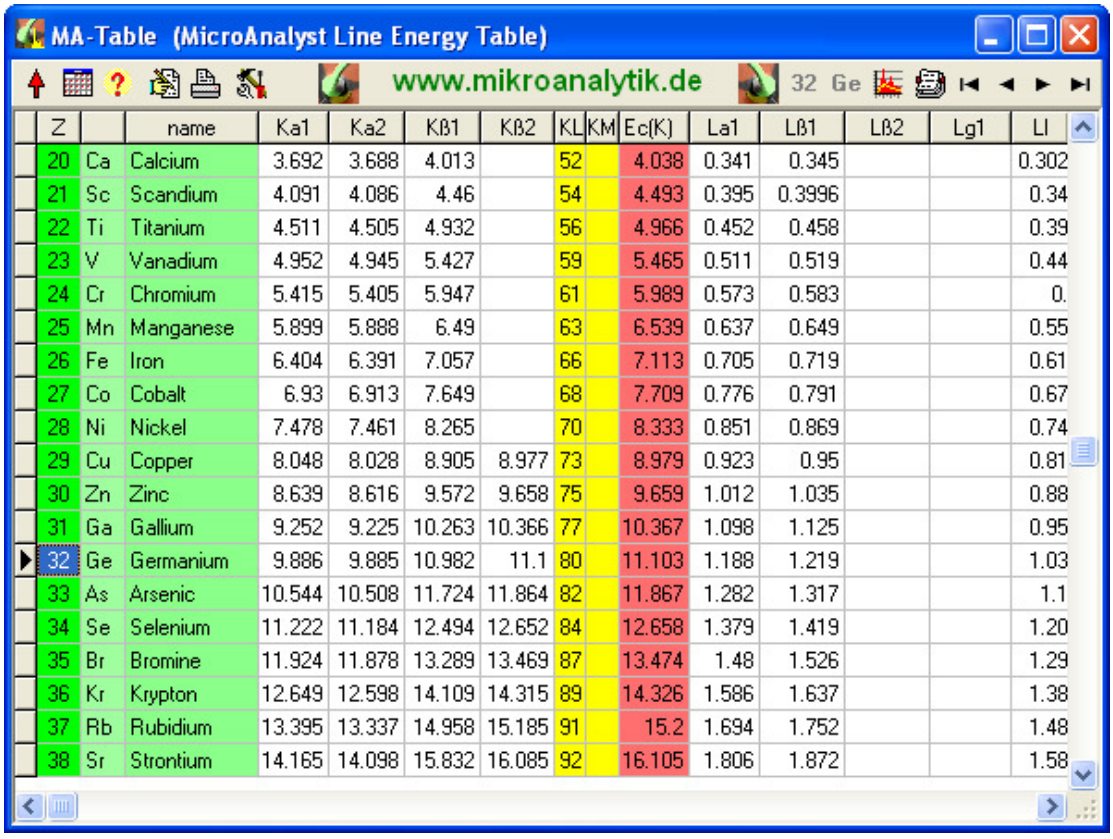
... Display all EDX line energies and data for elements of choice

... Move the focussed element inside table

Table on / Table off

This icon gives the possibility to switch very fast between complete table and the small icon bar. If MA-Table is reduced to an icon bar, the program needs very little space from the desktop and is any time available. But even in icon bar shape, the access to all functions is available without any disadvantage.

The standard MA-Table view is with complete table chart:



Z		name	Ka1	Ka2	Kß1	Kß2	KL	KM	Ec(K)	La1	Lß1	Lß2	Lg1	Ll
20	Ca	Calcium	3.692	3.688	4.013		52		4.038	0.341	0.345			0.302
21	Sc	Scandium	4.091	4.086	4.46		54		4.493	0.395	0.3996			0.34
22	Ti	Titanium	4.511	4.505	4.932		56		4.966	0.452	0.458			0.39
23	V	Vanadium	4.952	4.945	5.427		59		5.465	0.511	0.519			0.44
24	Cr	Chromium	5.415	5.405	5.947		61		5.989	0.573	0.583			0.
25	Mn	Manganese	5.899	5.888	6.49		63		6.539	0.637	0.649			0.55
26	Fe	Iron	6.404	6.391	7.057		66		7.113	0.705	0.719			0.61
27	Co	Cobalt	6.93	6.913	7.649		68		7.709	0.776	0.791			0.67
28	Ni	Nickel	7.478	7.461	8.265		70		8.333	0.851	0.869			0.74
29	Cu	Copper	8.048	8.028	8.905	8.977	73		8.979	0.923	0.95			0.81
30	Zn	Zinc	8.639	8.616	9.572	9.658	75		9.659	1.012	1.035			0.88
31	Ga	Gallium	9.252	9.225	10.263	10.366	77		10.367	1.098	1.125			0.95
32	Ge	Germanium	9.886	9.885	10.982	11.1	80		11.103	1.188	1.219			1.03
33	As	Arsenic	10.544	10.508	11.724	11.864	82		11.867	1.282	1.317			1.1
34	Se	Selenium	11.222	11.184	12.494	12.652	84		12.658	1.379	1.419			1.20
35	Br	Bromine	11.924	11.878	13.289	13.469	87		13.474	1.48	1.526			1.29
36	Kr	Krypton	12.649	12.598	14.109	14.315	89		14.326	1.586	1.637			1.38
37	Rb	Rubidium	13.395	13.337	14.958	15.185	91		15.2	1.694	1.752			1.48
38	Sr	Strontium	14.165	14.098	15.832	16.085	92		16.105	1.806	1.872			1.58

The atomic numbers of elements, which have most overlaps in regard the element lines, are specified in the yellow columns (for fast orientation). The critical excitation energy of the main electron shell is marked with red colour.

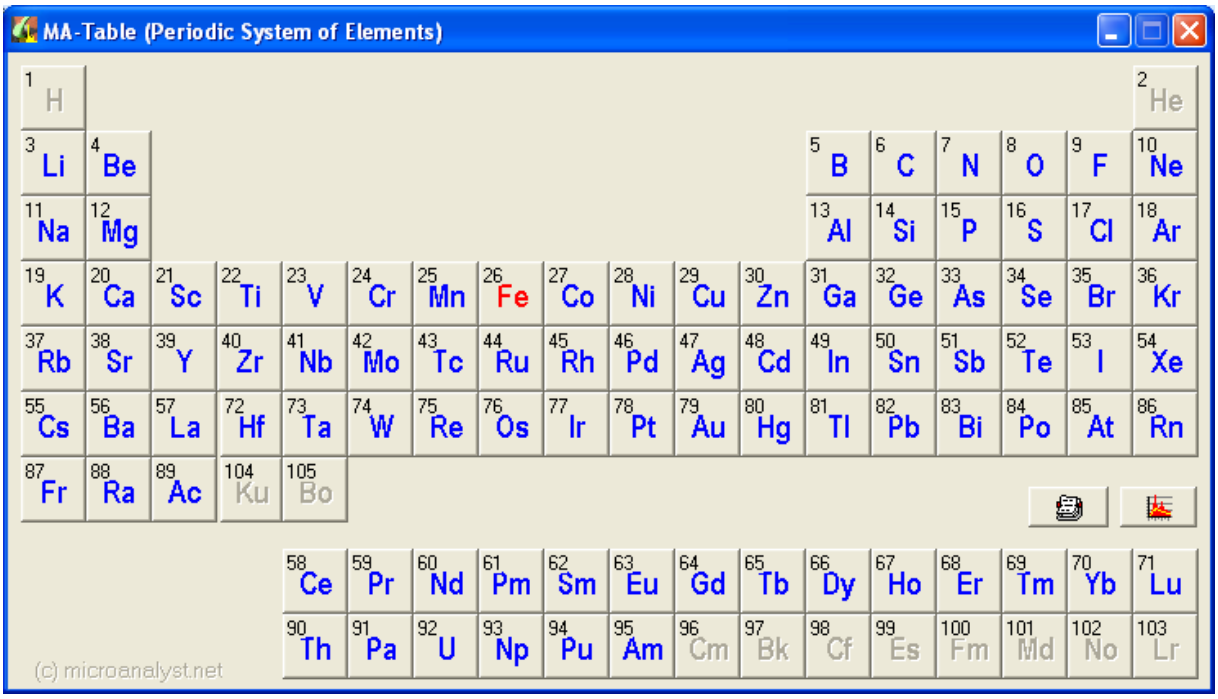
Table position focus move

You can select an element with simple mouse clicks into the chart or alternatively may move the element focus with the help of this special table function icon bar.

Then the  button offers a quick jump to the complete single element line energy data window (see later).

Periodic chart of elements (periodic table)

The operator can use a periodic table of the elements (PSE, Periodic System of Elements) with a simple mouse click to select any element of interest:

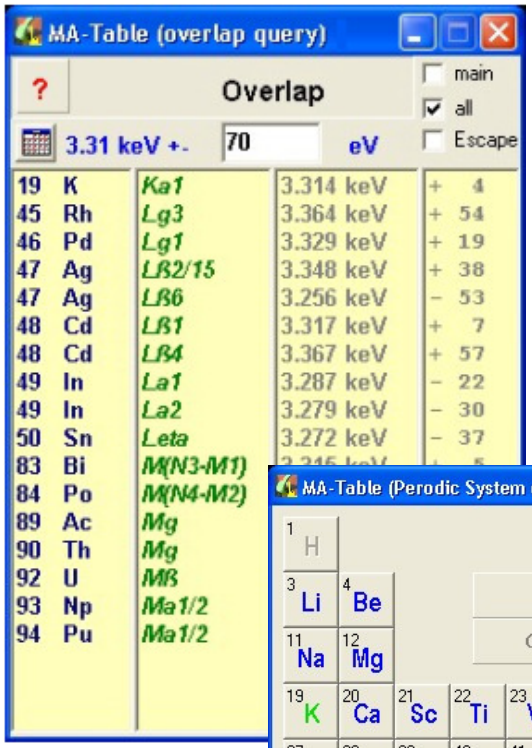


The  button offers a quick jump to the complete single element line energy display (see later).

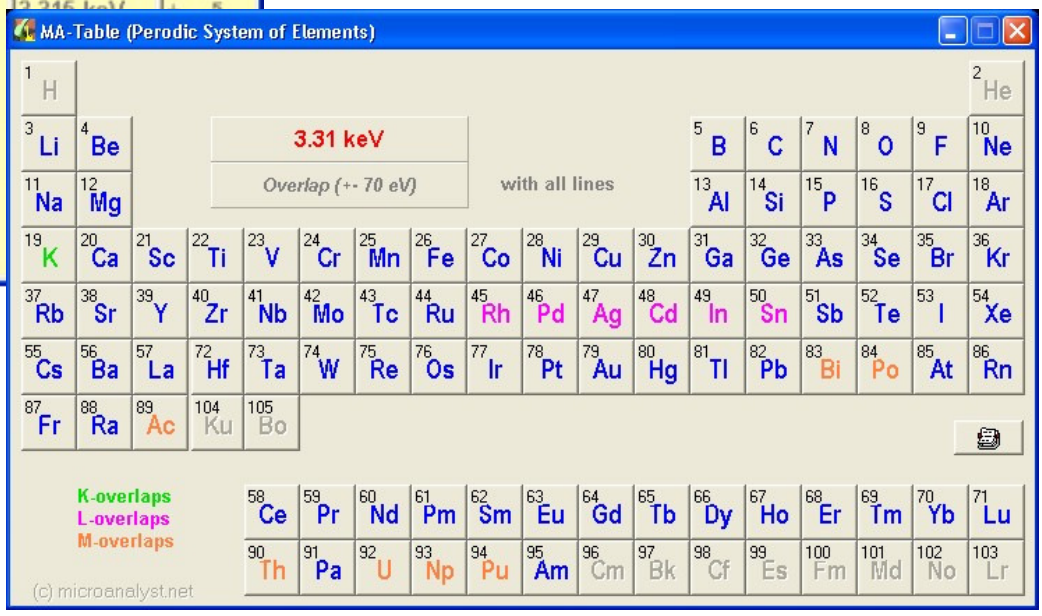
The  button offers a quick jump to spectra simulation of selected element.

Search for elements and overlaps

There is the possibility to search for elements via input of line energies. MA-Table searches for elements which emit X-ray lines at this energy (assistance to find and identify the elements accurate).
Searching for only alpha- and escape- lines is set to default. With 'alpha' is actually meant the major line, could be Ll or another one, this line which is the dominant. It is possible to search also for all lines in series ('all') or omit the escape lines. By changing the search window energy (standard is +-100 eV), the matched elements will change immediately. This search can be a valuable addition to the existing EDX, if one searches for unidentified peaks in the spectrum. Often the atomic data used even ***in new commercial EDX*** spectrometers or ***old systems*** are not sufficient correct or even ***wrong (!)***.

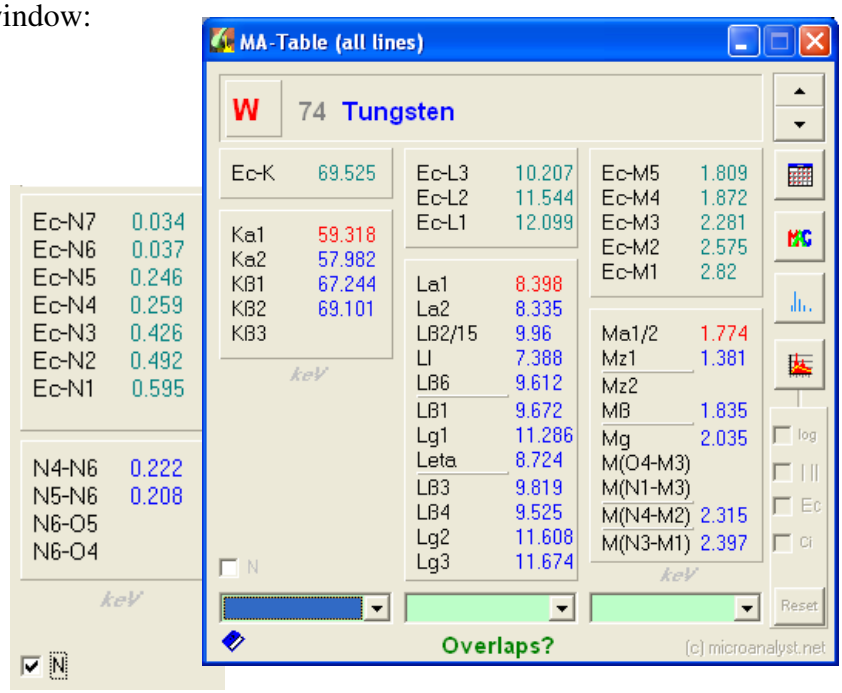


With PSE icon mouse-click one receives immediately the overview of the found possible elements in periodic system. The individual types of X-ray lines (K, L and M) are possible to distinguish by colours. It is a great assistance for the qualitative analysis (evaluation) of EDX spectra. You have the overview about the identification of elements at selected peak position (energy of the line) with a glance:



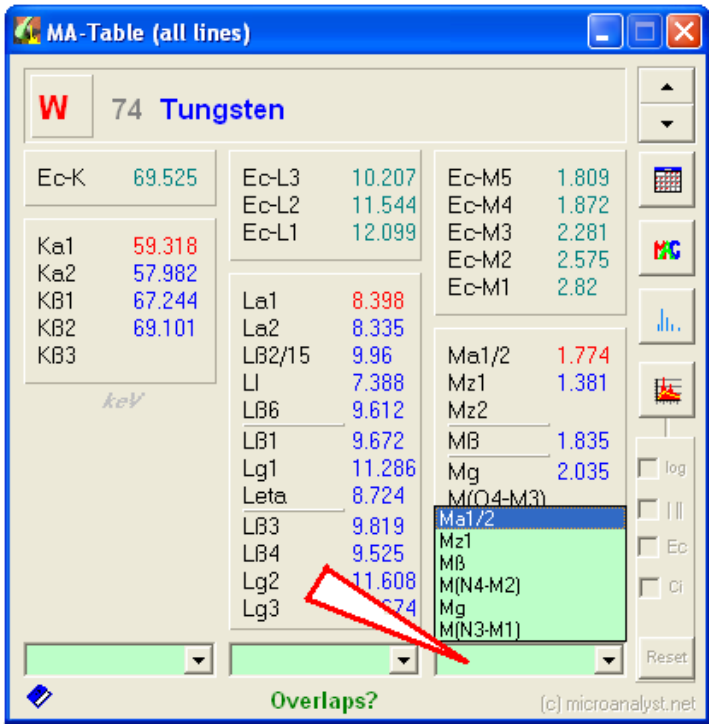
Element choice/energies

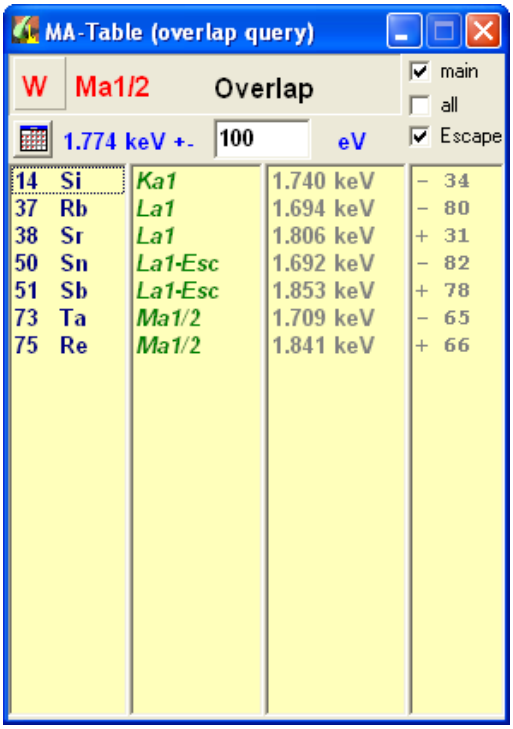
With selection of an element from table or via periodic system, the energies of all line-series are displayed in a special window:



The major line of each series is highlighted by red colours. N-lines are selectable instead K for all high atomic number elements.

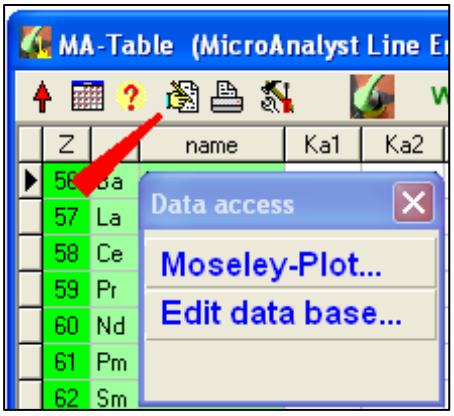
With a mouse-click at a selected line, the program starts a search for all lines of other elements, which may have overlaps with the line of interest. To do this, hit the drop-down menu via single mouse-click. Then simply select the wished line from the drop-down.





Display of all elements which have line overlaps with a selected line.

Data-base editor

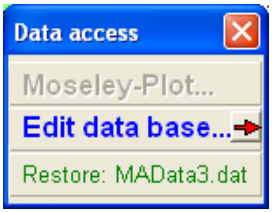


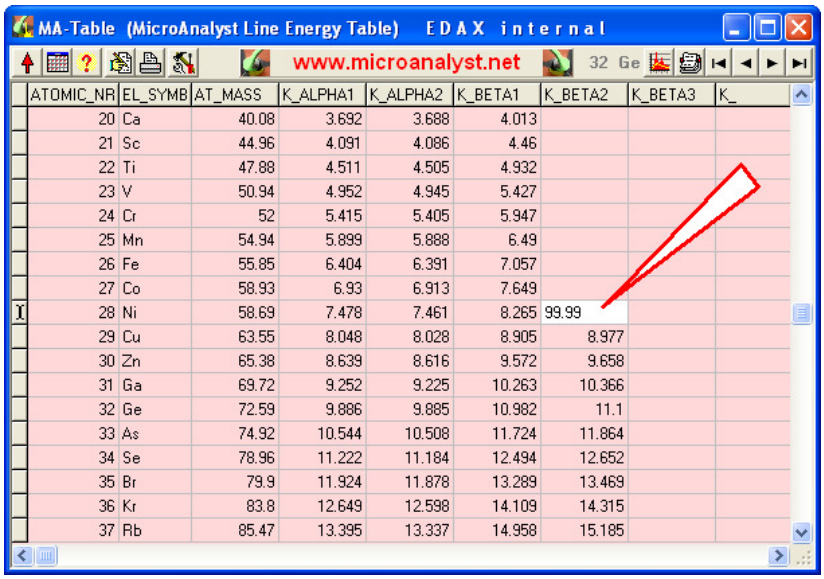
The icon has got a double functionality:

- edit of data base
- calls a Moseley-plot

Edit data base…

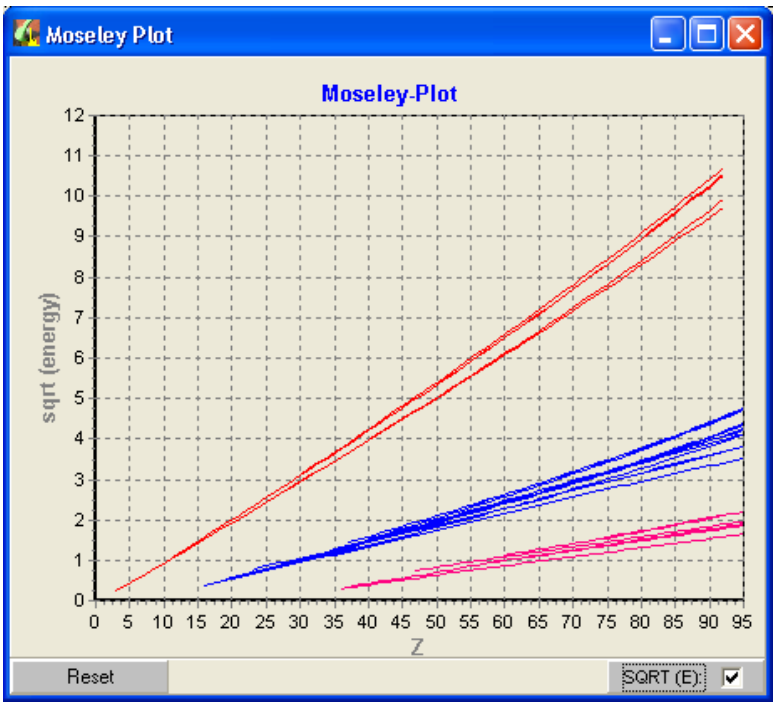
There is the possibility to edit the data.





The operator has full access to both data-base files *(only in licensed version)*, EdxData1.DBF (first klick) and EdxData2.DBF (second klick). With third klick one comes back to the standard view (without possibility to edit). Because the composer is using a condensed data base (MAData3.dat), this is important to restor after any change. If not, the operator is asking to do this with next composer use (also with a new installation and with some updates).

Please, be careful. You will change data base immediately and all calculations are possibly changed (e.g. the example edit is nonsens. If you want change, make a backup before!). If the data base is damaged, install once again.



Moseley-Plot…

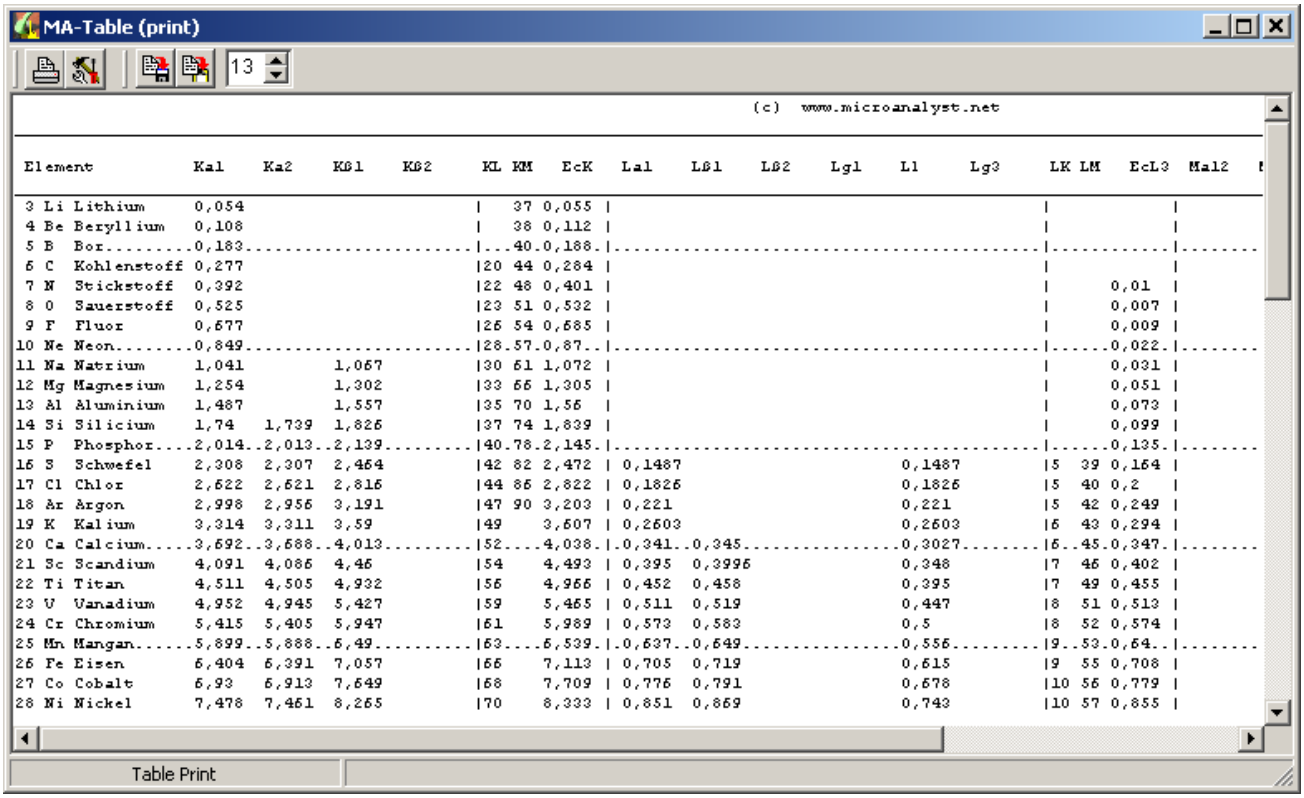
The Moseley-Plot is a proven tool, which shows very quickly possible irregularities in line energies.

A plot of square roots of line energies or the pure line energies versus atomic numbers is possible as well.

Zoom with left mouse key performing a square of wished area. Reset the zoom using [Reset] button.

Print, store and copy data

An additional window provides you with possibilities to print data, store on disc (ASCII-code) or to copy into clipboard to use in other programs. To format the printing, the character size is changeable.



Element	Ka1	Ka2	Kß1	Kß2	KL	KM	EcK	La1	Lß1	Lß2	Lg1	Ll	Lg3	LK	LM	EcL3	Ma12
3 Li Lithium	0,054					37	0,055										
4 Be Beryllium	0,108					38	0,112										
5 B Bor	0,183					40	0,188										
6 C Kohlenstoff	0,277				20	44	0,284										
7 N Stickstoff	0,392				22	48	0,401									0,01	
8 O Sauerstoff	0,525				23	51	0,532									0,007	
9 F Fluor	0,677				26	54	0,685									0,009	
10 Ne Neon	0,849				28	57	0,87									0,022	
11 Na Natrium	1,041		1,067		30	61	1,072									0,031	
12 Mg Magnesium	1,254		1,302		33	66	1,305									0,051	
13 Al Aluminium	1,487		1,557		35	70	1,56									0,073	
14 Si Silicium	1,74	1,739	1,826		37	74	1,839									0,099	
15 P Phosphor	2,014	2,013	2,139		40	78	2,145									0,135	
16 S Schwefel	2,308	2,307	2,464		42	82	2,472	0,1487				0,1487		5	39	0,164	
17 Cl Chlor	2,622	2,621	2,816		44	86	2,822	0,1826				0,1826		5	40	0,2	
18 Ar Argon	2,998	2,956	3,191		47	90	3,203	0,221				0,221		5	42	0,249	
19 K Kalium	3,314	3,311	3,59		49		3,607	0,2603				0,2603		6	43	0,294	
20 Ca Calcium	3,692	3,688	4,013		52		4,038	0,341	0,345			0,3027		6	45	0,347	
21 Sc Scandium	4,091	4,086	4,46		54		4,493	0,395	0,3996			0,348		7	46	0,402	
22 Ti Titan	4,511	4,505	4,932		56		4,966	0,452	0,458			0,395		7	49	0,455	
23 V Vanadium	4,952	4,945	5,427		59		5,465	0,511	0,519			0,447		8	51	0,513	
24 Cr Chromium	5,415	5,405	5,947		61		5,989	0,573	0,583			0,5		8	52	0,574	
25 Mn Mangan	5,899	5,888	6,49		63		6,539	0,637	0,649			0,556		9	53	0,64	
26 Fe Eisen	6,404	6,391	7,057		66		7,113	0,705	0,719			0,615		9	55	0,708	
27 Co Cobalt	6,93	6,913	7,649		68		7,709	0,776	0,791			0,678		10	56	0,779	
28 Ni Nickel	7,478	7,461	8,265		70		8,333	0,851	0,869			0,743		10	57	0,855	

Settings/Registration/Demo

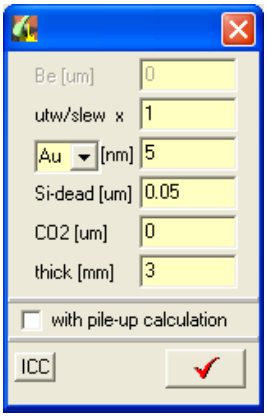
This window combines the ‚About...' functionality with version number and other program information like a 'SetUp'.

Click at **Demo** and you can relax in your chair to watch the full functionality demonstrations of MA-Table.

EPMA is standard selected for spectra simulation. **XRF** is possible to use *(version 2.00 and higher)*, but with limited functionalities. The XRF simulation is not complete quantitative, provides only a rough background and do not consider specific excitation and specimen/source geometries. Therefore the XRF simulations are not like real spectra, as the EPMA simulation is.

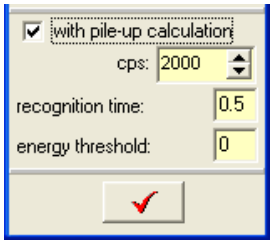
Si(Li) ←→ SDD radio buttons change the detector type with setting of some predefined typical parameters values *(version 2.10 and higher)*

Window selects the used window of the Energy Dispersive X-Ray Spectrometer (EDX). You can change thicknesses with **Details** (for fine-tuning of spectra calculation).

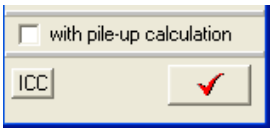


Be-window thickness [µm]
SUTW-window thickness [factor to standard thickness]
Contact layer thickness of the detector [nm] with material selection
Si-dead layer (or SiO_2) [µm]
Additional CO2 absorption layer on detector surface (inside vacuum of a Si(Li))
detector active thickness [mm]

(All is possible to change only with licensed version.)



Check the pile-up calculation to consider this effect with each simulation, which depends from pulse processor and from count rate. The pileup effect depends on the behaviour and properties of pulse processor and the built-in pile-up rejection. The two parameters are mean pulse-pair recognition time and pulse-pair energy recognition threshold. It may be covered experimentally to be proper adjusted.

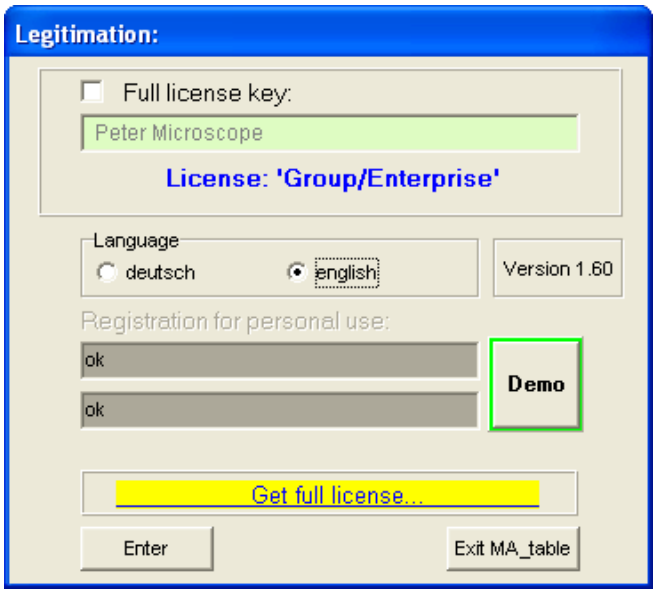


Use the [ICC] button to adjust the incomplete charge collection calculation.

Count rate defines the count rate, which you want to use for the spectra simulation. The MA-Table program is going to combine the count rate with acquisition time (for spectra acquisition simulation, calculation of detection limits, …).

With **Resolution** you can set up your detector resolution (at Mn-Ka). Be careful, the resolution is not dynamically changed with count rate selection (like perhaps in your real working EDX by changing the pulse processor shaping time).

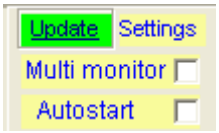
With **Registration** the operator has to input the full license user information (name and license key). In the example one can see a full licensed version (the registration key code is hidden, which is valid for the name only).



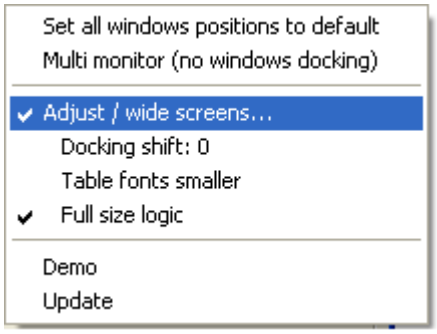
If you are ready registered, you will never need this, but for an installation of MA-Table on other computers.

'Registration for personal use:'
Alternatively the free use of MA-Table is possible via Internet based registration (free and anonymus). The program generates a code which is to type into the internet form.

The code answer is copied into MA-Table registration box. That's it. It is only to get users counted. But the functionality of the free version is limited.



With **Settings** (or right mouse pop-up) some useful extensions and adaptions are available, especially if one likes to use multi-monitor (**Multi monitor**) without the usual MA-Table windows docking. Wide screens may better to address with some useful adjustments (Table fonts, docking shift and full size logic).



With checking **Autostart** MA-Table will start with each Windows launch.

With **Service** and several other click possibilities some quick links to the **MICROANALYST.NET** home page are given. Also, you have the opportunity to send a mail to MICROANALYST.NET –service.

www.microanalyst.net **... The most rapid way to the MA-Homepage**

Spectra simulation

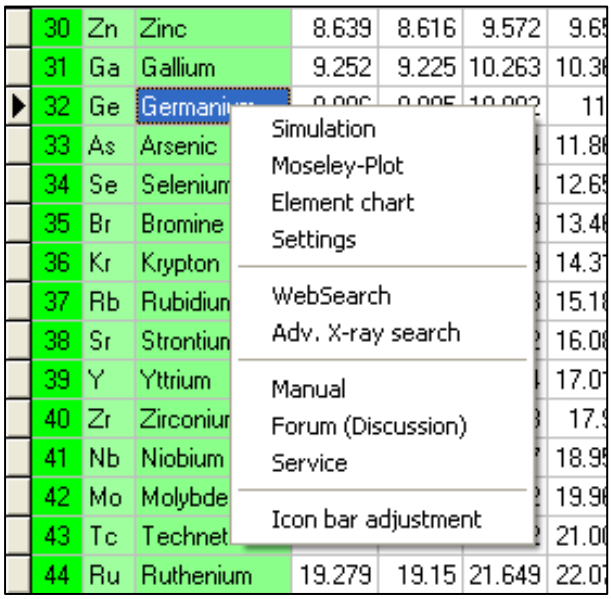
This icon of icon bar directs the operator directly to spectra simulation (with calculations of realistic spectra, see chapter 3).

Popup function menu for quicker and easier handling of all functions:

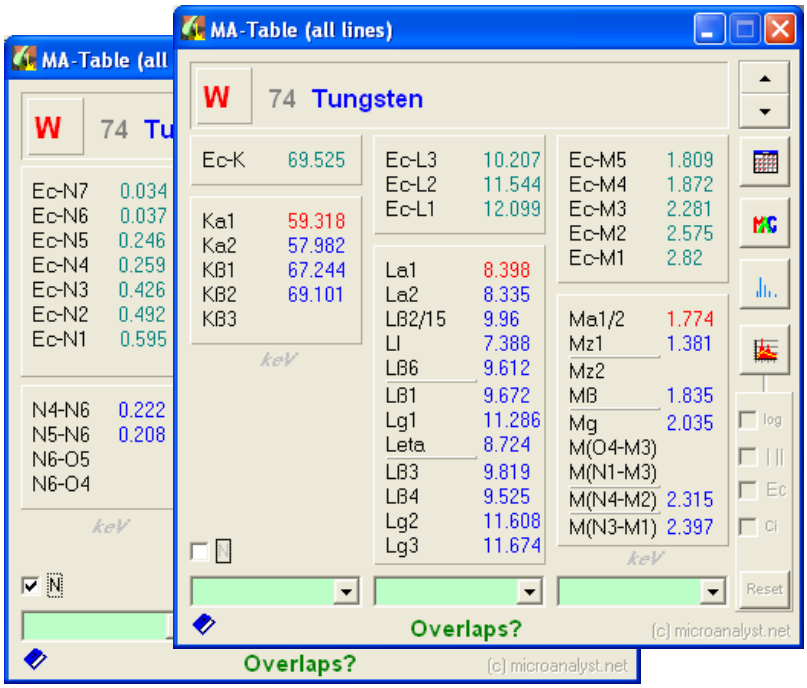
Click with right mouse key into the table or the icon bar.

You will find some functions again for quick access. Additionally there are some useful quick access points for internet search and internet links.

Use 'Icon bar adjustment' if the header of your MA-Table is misadjusted (may depend from screen resolution and Windows settings)



2. Functions of MA-Table Line Display



<— quick change of selected element (± one atomic number)

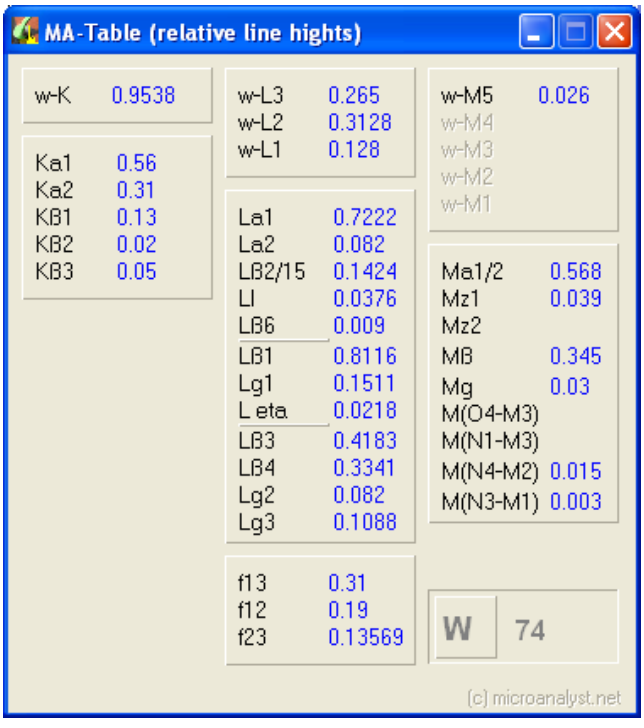
<— call periodic chart of elements (for direct element selection)

<— mass absorption coefficients

——> line series intensities

——> spectra simulation

Line series intensities

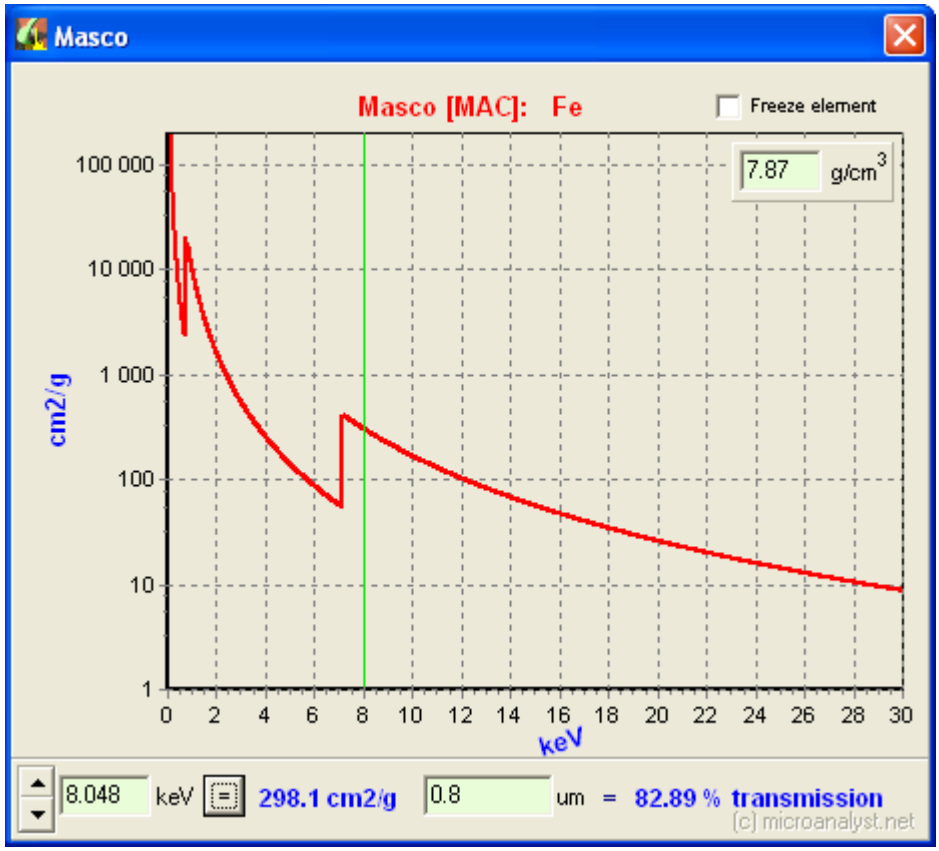


All relative line intensities of the selected element are displayed. ***w*** are the fluorescence yields and ***f*** are Coster-Kronig transition rates, both necessary for calculation the relative line series with taking into account the primary excitation energy (high voltage of electron microscope, primary electron energy). Values for N-lines are not available. All values are stored inside data table EdxData2.DBF.

The program MA-Table considers these values for all simulation calculations. All relative heights will be normalized internally (in sub-shells). M-series are assumed simplified to have no excitation dependant internal transitions, therefore normalized all to one.

Mass absorption coefficients

The MAC icon in element selection form is providing mass attenuation coefficients (mass absorption coefficients). Hit the button and the curve of current element will be displayed:



It is possible to select the energy of interest for absorption calculation directly or via selections in the line energy-form before (the same procedure as for element search with line selection). If a thickness is set, the program calculates the transmission of X-rays (selected energy or line) in a layer of the current selected element. It is possible to change the provided density, if required.

'Freeze element' keeps the selected element and you can search for line energies using entire MA-Table functionalities (e.g. scrolling to other elements with choosing selected lines which will be displayed immediately into Masco window with calculated transmission).

Spectra simulations

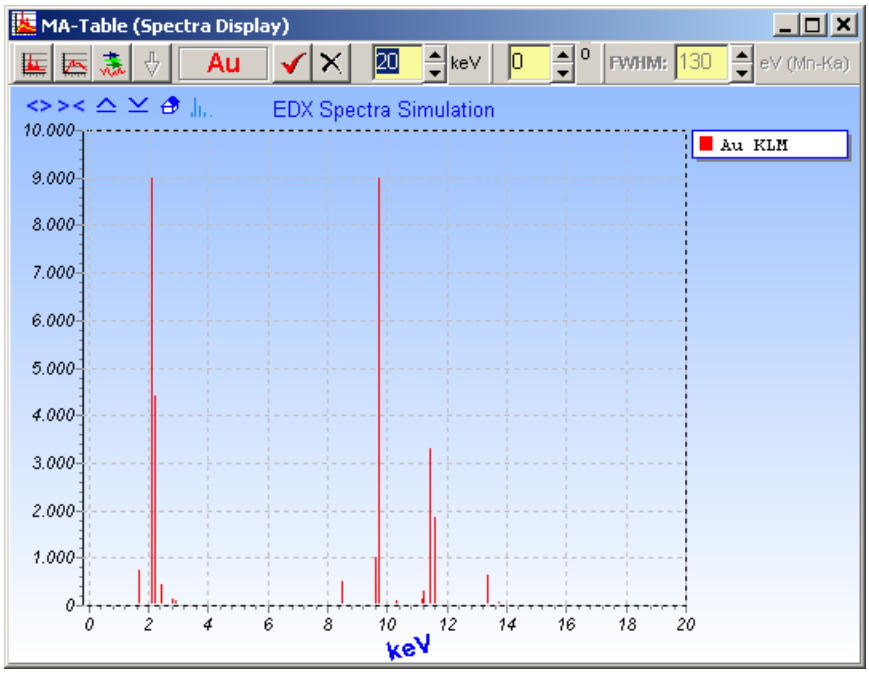
This is another way to display relative line heights. This calculation is taking into account the current excitation.

The spectra simulation is completely explained in next chapter.

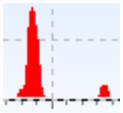
3. Functions of Spectra Display

Starting this window first time, you will always see a line-position and -heights simulation.

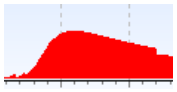
To change the element, you should use the functions in 'line series display' window. With opened spectra display window the program recalculates the spectra automatically (considering the selected buttons), if selected element was changed.

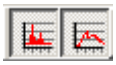


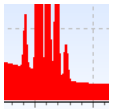
 Calculation of line series taking into account detector resolution



 Calculation of Bremsstrahlung (or XRF background) distribution



 Complete spectra simulation (line series and background)



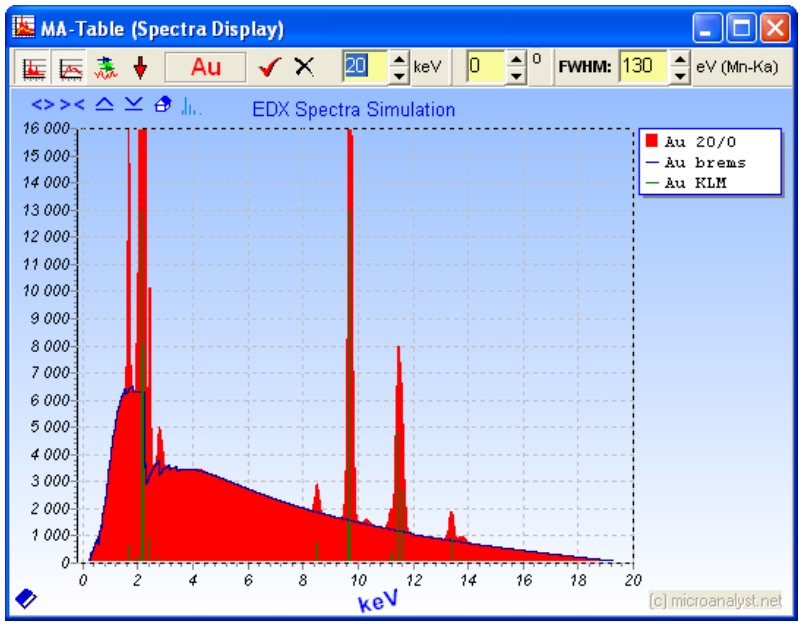
 Spectra display Setup (—> *see next chapter*)
Settings / Element overlaps / Spectra acquisition simulation

 Change of estimated acquisition time in 3 fix steps (depends from count rate setup).

 Add current spectrum for spectra comparison (maximum of 10 spectra are possible to add)

 Clear the last added spectrum from comparison

Simulation of Au-spectrum with comparison of line positions (line marks) and Bremsstrahlung. —>

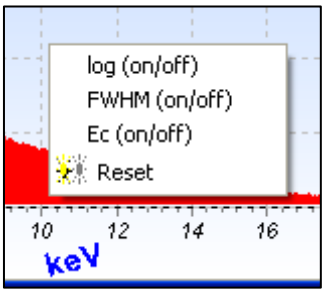


Select primary electron energy (high voltage of scanning electron microscope or tube HV with XRF selection).

Select tilt angle of specimen.

Select detector resolution.

A popup menu will be faded in with right mouse click into spectra display:

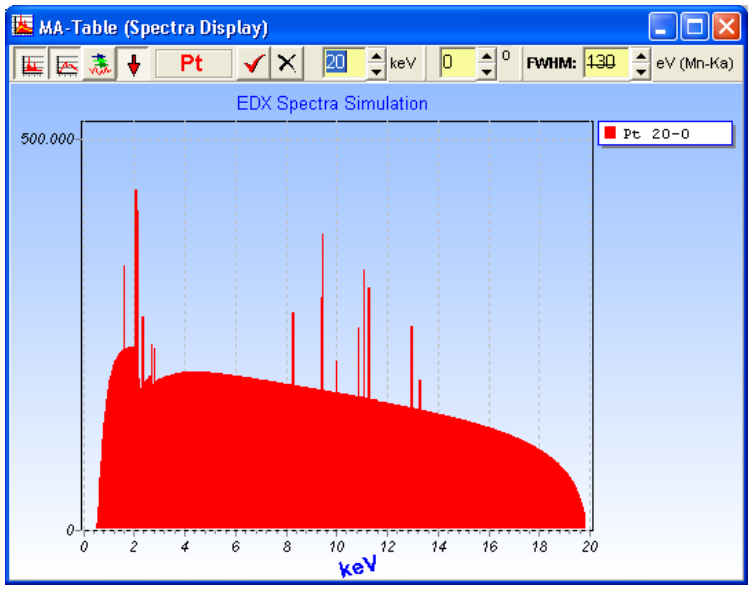


You have the opportunity to choose between:

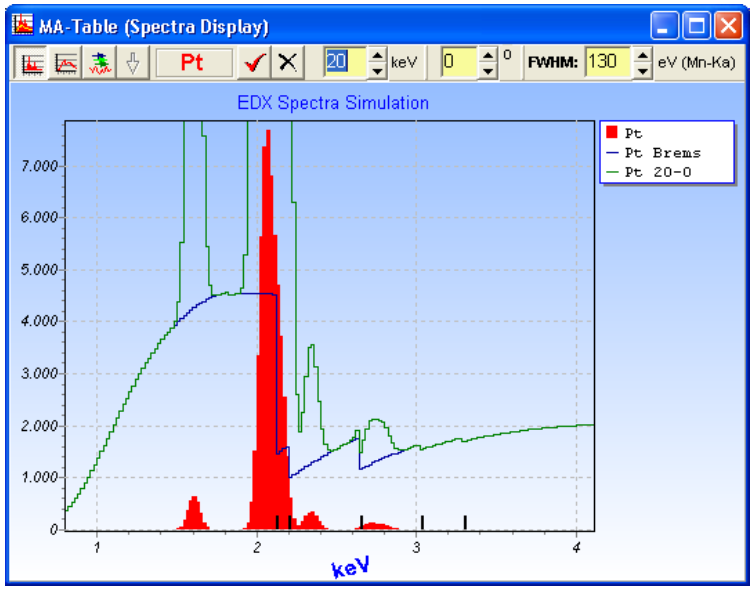
- logarithmic display or not
- taking into account detector resolution (FWHM) or not
- display of critical excitation energies or not

... and finally the possibility for a quick display-reset

The spectra display features are not only provided with the popup menu, but also selectable in single-element line energy form:



Logarithmic display without FWHM consideration



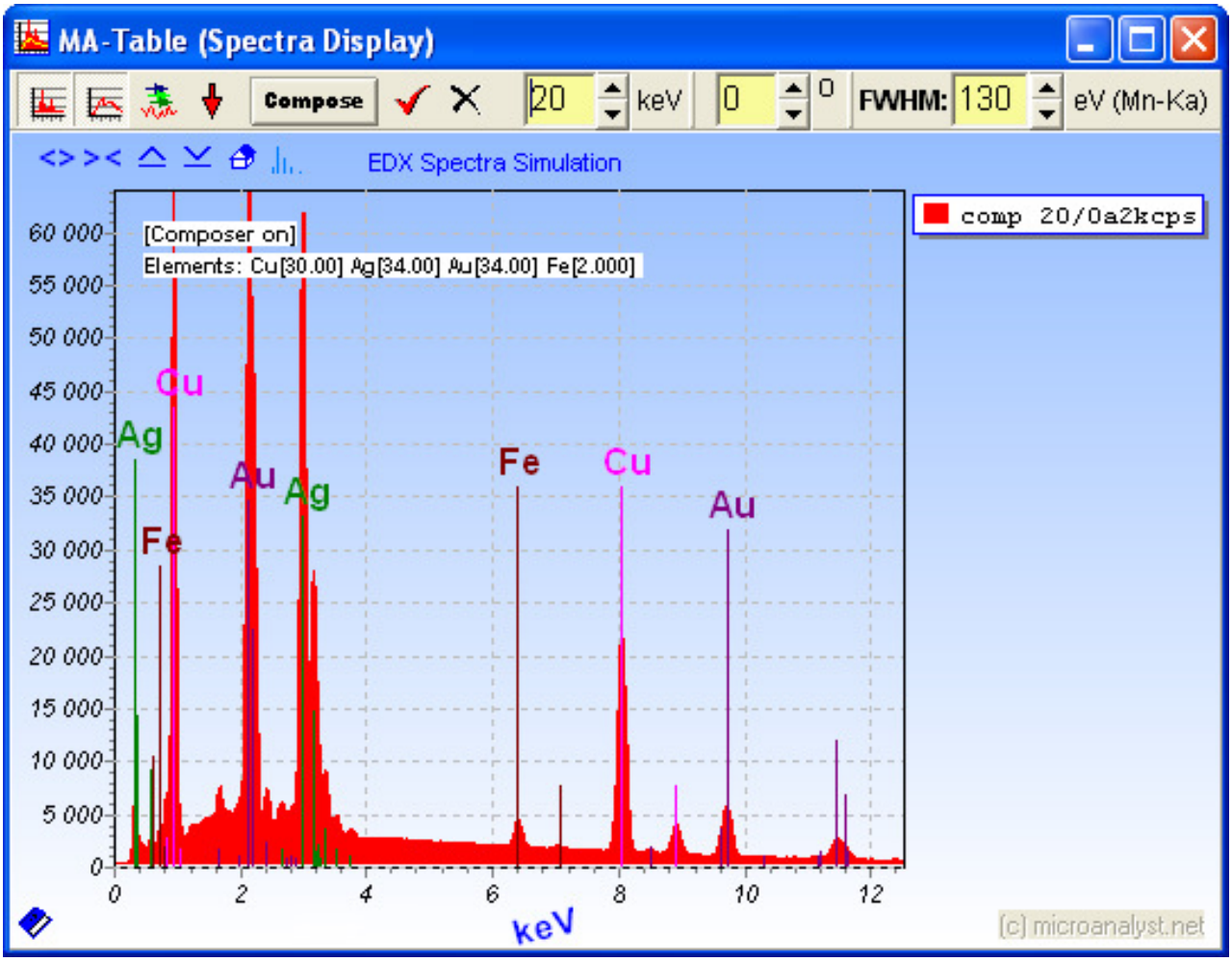
Linear display with display of critical excitation energies (shell energies) with black bars.

<> >< ^ v

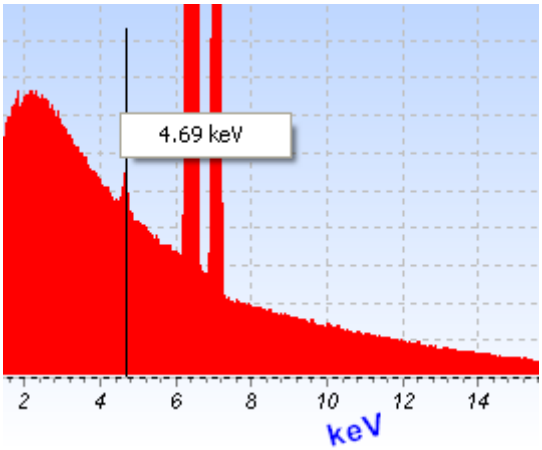
These quick spectra display icons are available always, starting with MA-Table version 2.00. It is self-explaining (see also the hints moving mouse to icon position).

Take in mind the difference of spectra display scaling up/down ^ v in comparison to icons and . These icons affect the real used acquisition time for simulations (only in 3 steps) and are therefore influencing the total counts in spectrum. Both settings are independent. It is possible to use mouse-wheel for spectrum scaling, too.

This icon is providing additionally a usual line-marker, overlaid to all spectra displayed (2 modes, hit repeated):

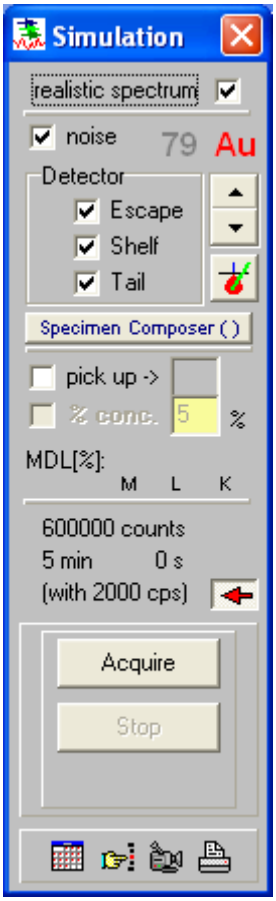


Example with specimen composer (see chapter 5)

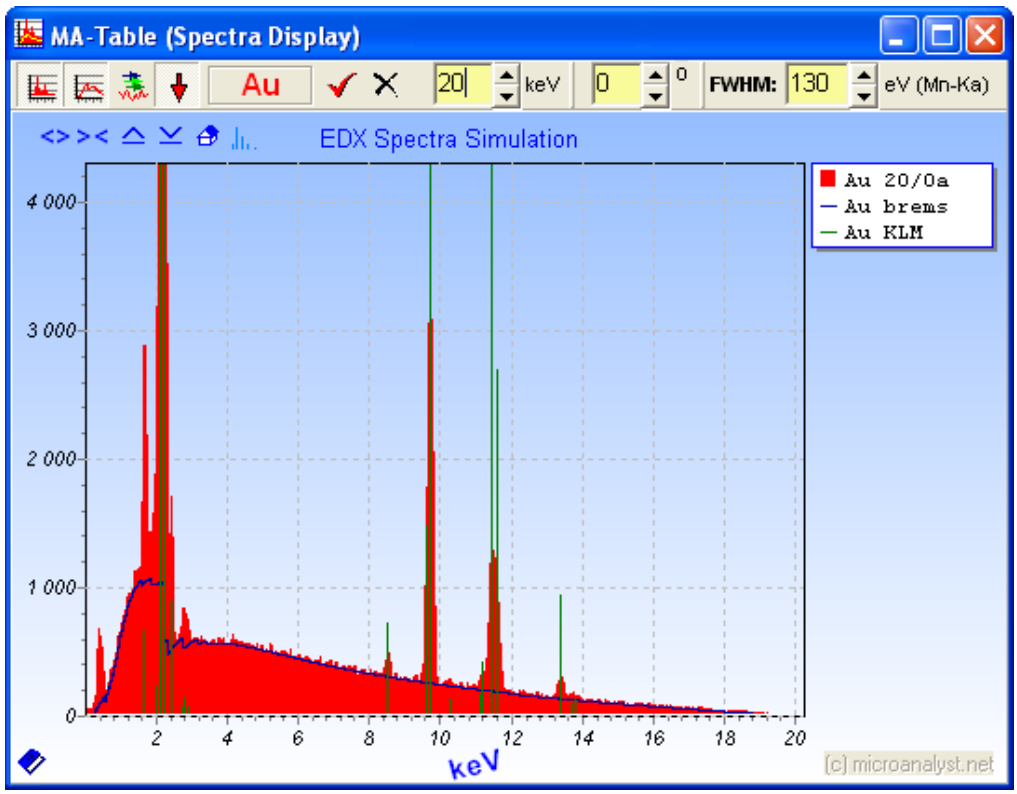


A simple mouse-click on spectrum (channel) or keV-axis is reporting the X-ray energy. With clicking the displayed flag the element/overlap search will start with this energy immediately. With each other energy selection by clicking into the spectrum, the element search will be updated immediately.

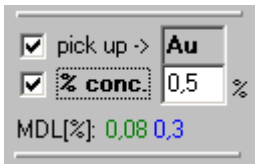
4. Functions of Spectra Display Setup



Select ‘realistic spectrum’ to add noise and detector artefacts. The simulation for the Au-spectrum (in example) is changing immediately (watch e.g. the escape peak near 400 eV).



If you like to check line-overlap situations with other elements or if you want to have a rough estimation of detection limits of an element in the matrix of another element, please work with these two check-boxes:



1. Click with mouse at ‘pick up’ check-box to select an element, which you want to check for overlaps with all other elements.
2. Then choose another element, and the minimal detection limits will be displayed (M-lines, L-lines, K-lines).
3. If you like to compare with and without the overlapped element, take the second check-box.
4. You can always change the concentration of selected element

Some additional features:

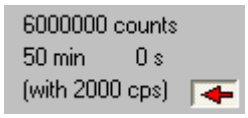
- Display of simulated main element (red) with the overlaid one (green)

- scrolling through all elements even with spectra full size display

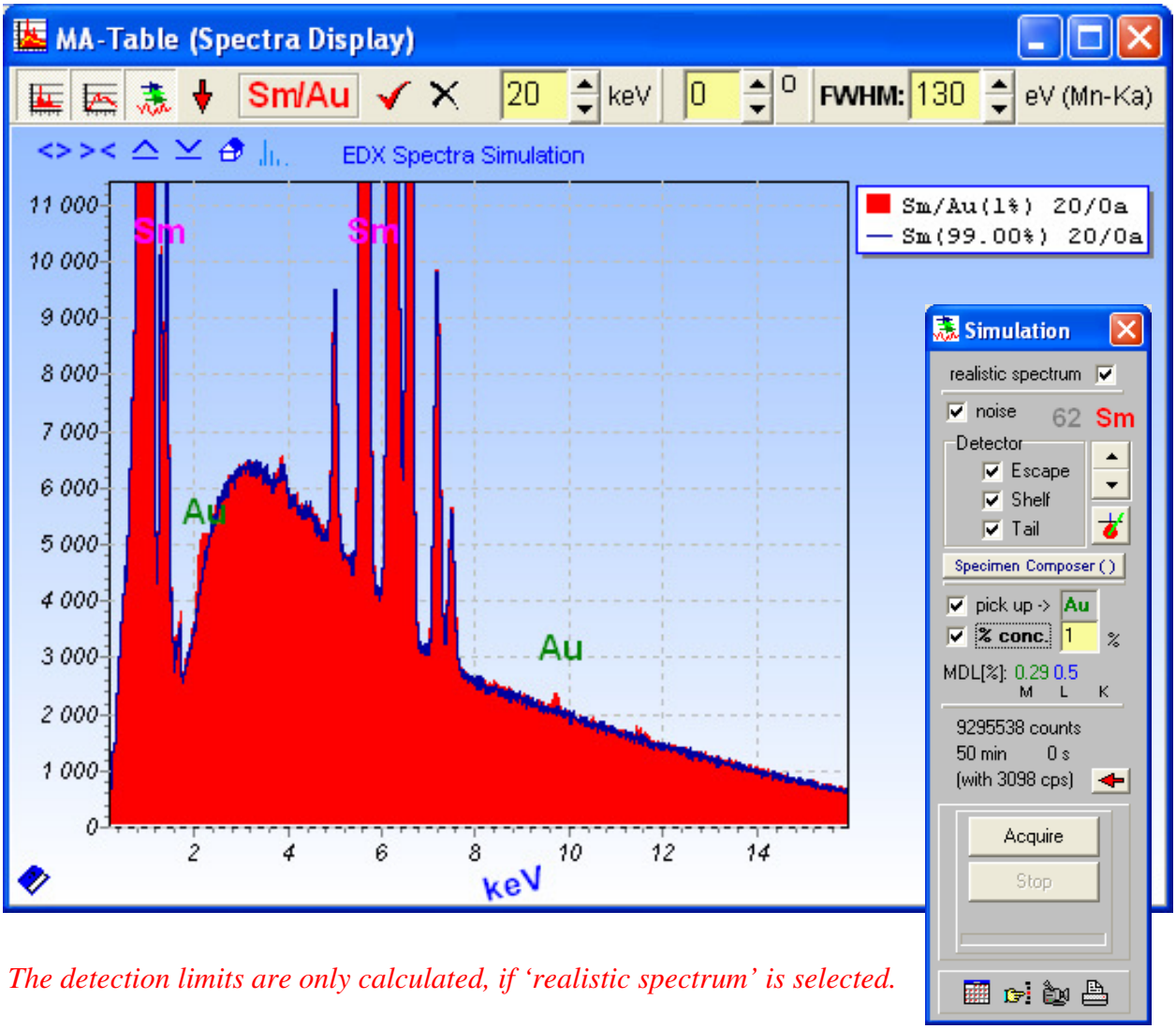
- icon for excitation/analysis depth display

- M, L, K marks the MDL values 

- Calculation of detection limits with choice
  'fix beam current' or
  'fix count rate' (if button is pushed)

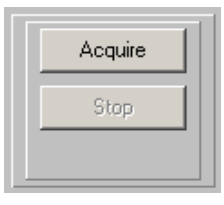


The example demonstrates 1.0 per cent Au in a Sm-specimen (the main element is Sm), with 1.0 per cent Au inside the specimen (red spectrum) and without Au for comparison (blue line). Both Au-line series (the M at 2.12 keV and the L at 9.7 keV) are significantly detectable. Please compare with calculated detection limits of 0.29 and 0.5 per cent respectively.



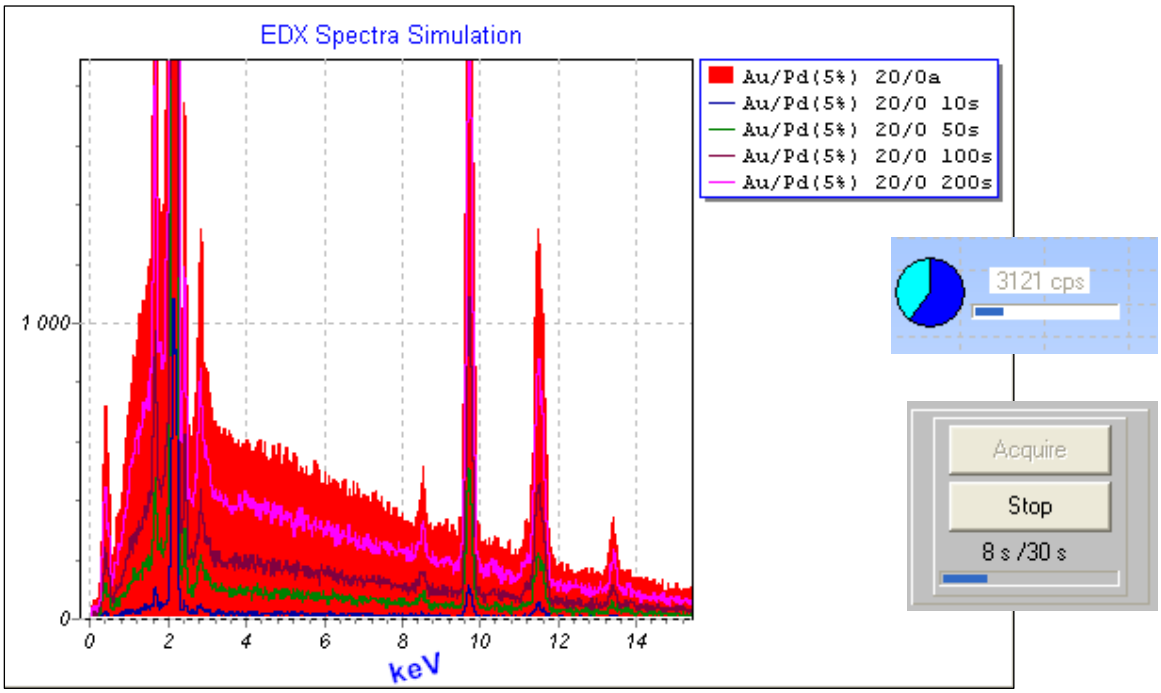
The detection limits are only calculated, if 'realistic spectrum' is selected.

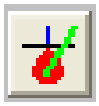
The total counts and acquisition time are not selectable free. They depend on  selection (three steps only) and pre-defined count rate of EDX system (see 'Settings/Registration/Demo'.



Hit these buttons and you are going to simulate a realistic spectra acquisition with given count rate and acquisition time.

In the example, the spectrum was frozen after 10, 50, 100 and 200 s and compared to the 3-minutes-spectrum (at 2000 cps). You can watch even the improvement of the detection limits with increasing acquisition time (live at display). Please check also the **Composer** features (next chapter).





Over-voltage and analysis depth calculation

MA-Table is able to calculate the over-voltage ($U_o=E_o/E_c$) for all lines excited. The calculation of analysis depth (d) takes into account the excitation, absorption, geometry and the mean matrix of binary specimen (the defined second element with concentration of all elements). If the excitation is critical (E_o to small for this line), the program will give the hint with changing to red colour for the lines values:

Ag K- an M-L lines with same primary electron energy but different matrix elements (Au and Cu). The analysis depth of the evaluated lines in the EPMA spectrum is changing (from 0.38 to 0.77 micron for Ag-L). The Ag-M depth is very small. Both effects are influenced strongly from the absorption processes.

The last 4 buttons are sometimes very helpful:

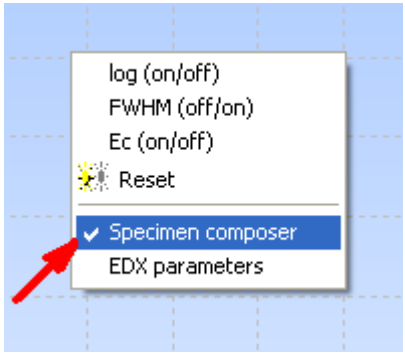
- Quick selection of elements via periodic chart of elements
- Change of spectrum display background colour *(only in licensed version)*
- Copy the spectrum into clipboard (the current image) *(only in licensed version)*
- Printing the current spectra simulation *(only in licensed version)*

5. Specimen / spectra composer *(limited use without licensed version)*

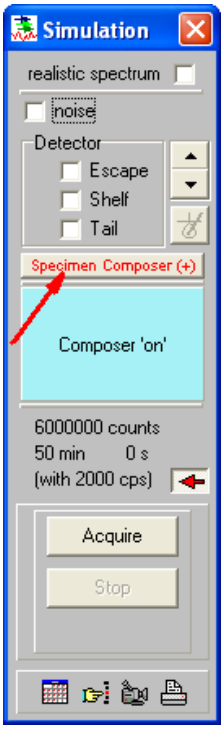
A spectra composer is implemented to simulate spectra of specimen for any element fractions (maximum of 30 elements)

It is possible to investigate the influence of excitation, specimen tilt, acquisition time, count rate, resolution and other conditions with their influences to line heights and detection limits for any specimen in Scanning Electron Microscope. The operator has only to input the estimated specimen elements with weight fractions... and the expected spectrum will be calculated. This function is valuable particularly in complex line overlap situations to optimize e.g. the specimen excitation. It is easy to estimate the expected detection limits. The influence of different pulse processor shaping times to separation of different element lines is easy to study with a change of resolution value for simulation.

This is the ways to activate the 'specimen composer':



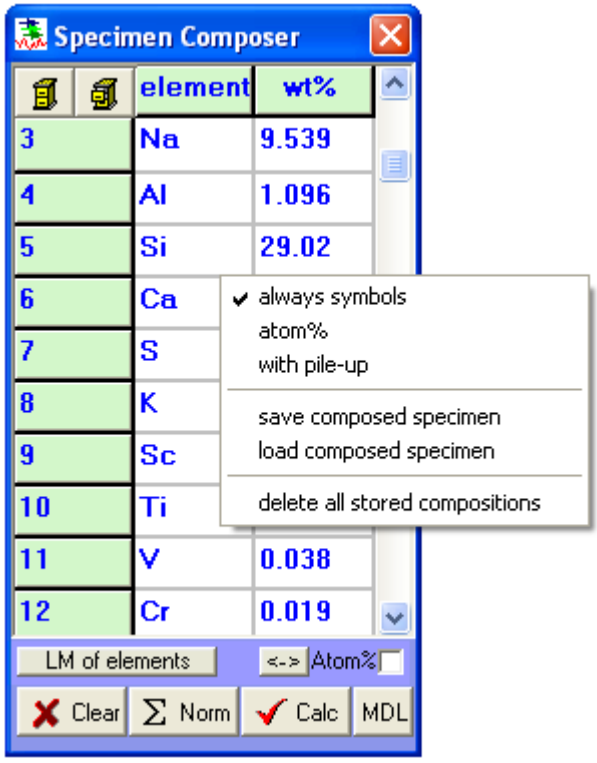
Hit right mouse-button and choose 'Specimen composer' function.



… or hit one of these elements.

You can come back into standard operating mode (no composer) using same ways.

Then this form appears:



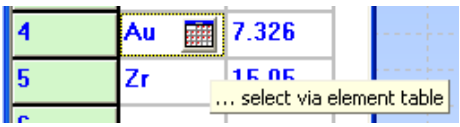
Fill out the form either with atomic number or element symbols and related weight fractions (concentrations) or atom%. After each edit the **[Σ Norm]** button must be hit once again (to be sure, that the sum of all contents is 100%).

With button **[Calc]** the spectrum calculation is started and the result is displayed immediately.

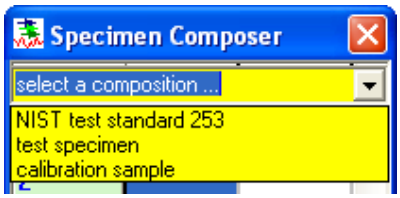
[Clear] cleans the entire form.
Check 'Atom%' if the inputs are atom% instead weight%.

Element symbols and atomic numbers can be entered, even mixed. If 'always symbols' has been chosen, all entered atomic numbers automatically converted into element symbols with normalization. The spelling is not important in regard of capital or no capital letters.

Alternatively the element selection or change is possible via element chart icon click, which will be faded in with each click into 'element' column (or placed at right side, if the number of elements is higher than 10):



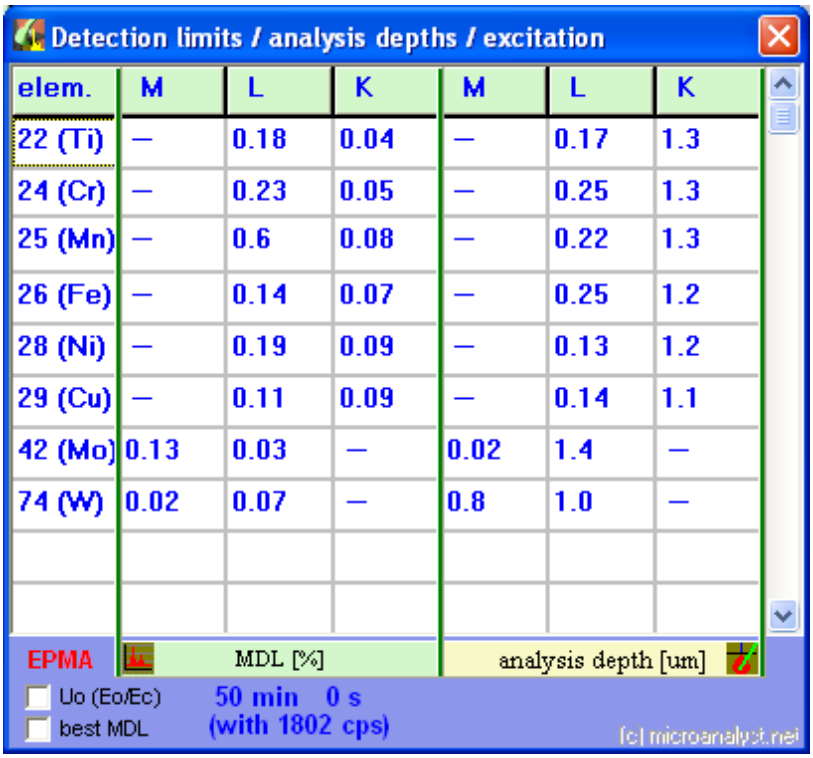
You can save and load element sets (composed specimens) with using the pop-up menu. The file-store cabinet buttons are possible to use similar:



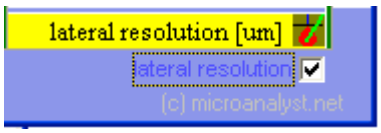
Use this button for a convenient way to calculate mass% (usually wrong named weight% or wt%) into atom% For entire composition and vice versa:

[LM of elements] displays all line marks of the elements in comparison to calculated spectrum, the current specimen excitation and absorption situation is considered. Then it will be possible to view line marks also with/without absorption to compare.

With **[MDL]** a form will be displayed with minimum detection limits (MDL) and analytical depth for the used conditions:

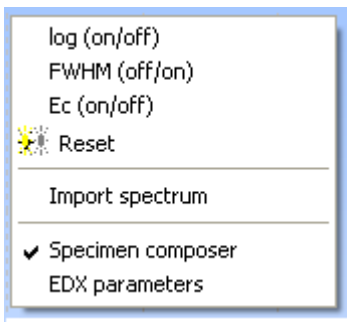


With version 2.10 it is also possible to change the 'analysis depth' columns into 'lateral resolution':

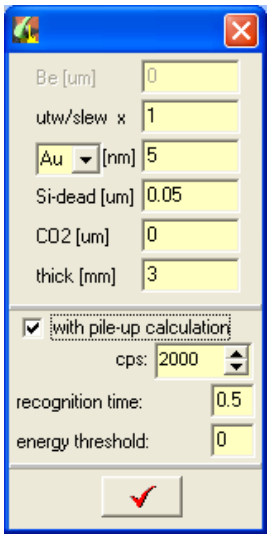


It can be much different for very soft X-rays.

You can switch the specimen composer on/off also via left-mouse click menu (pop-up menu). This is also the way to change the detector parameters used for calculation (EDX parameters) →



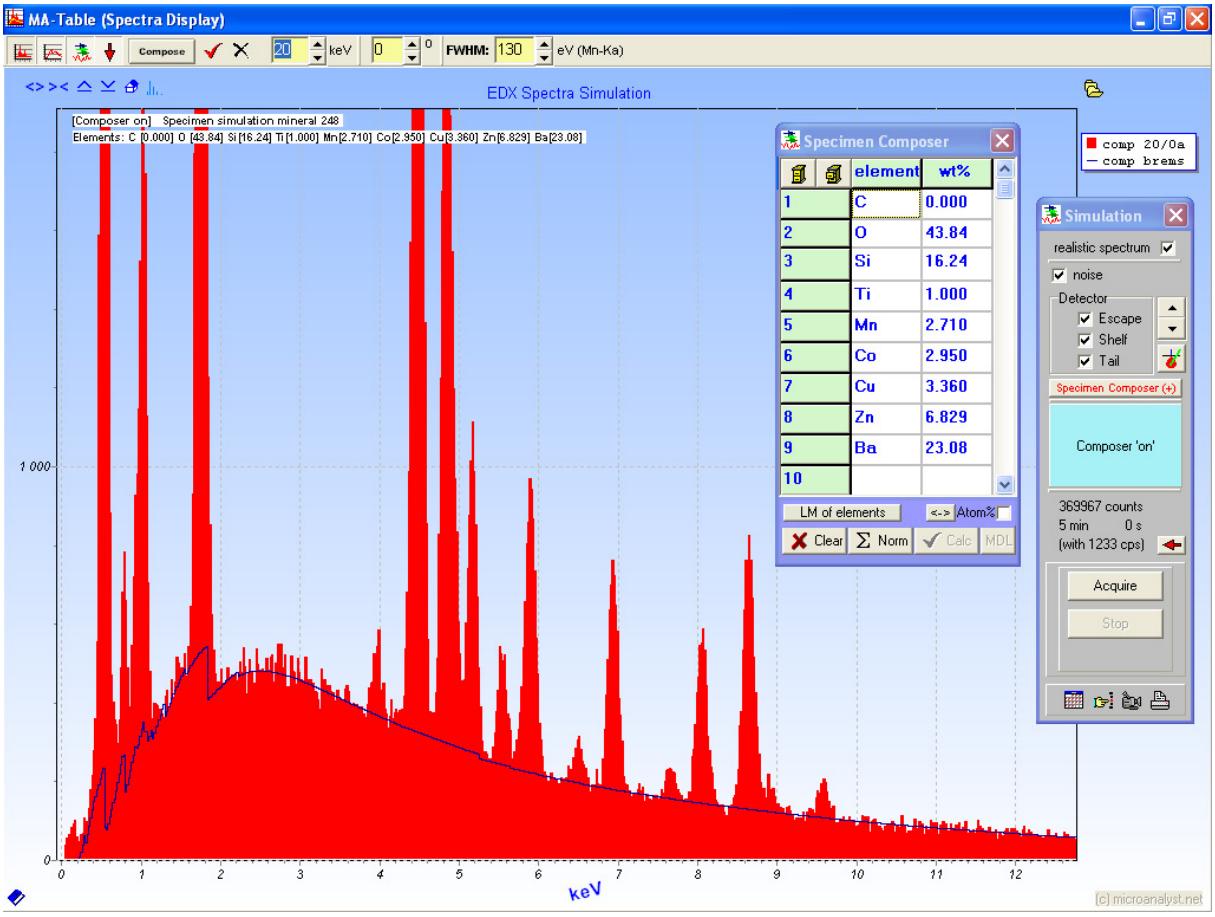
The simulation is possible to perform with or without pile-up effects. For the pile-up simulation machine some parameters are needed to know. The recognition time is the time resolution of the pile-up recognition channel. The energy threshold describes the energy which is starting sensibility for pile-up rejection channel of pulse processor. An ideal pulse processor would have a setting of zero. In praxis the fast channel is worse in energy resolution, therefore the threshold for pulse pair recognition is between 0.5 and 0.8 keV. That is why the pulse processor pile-up rejection is not recognizing X-rays with energies below. The pile-up rejection is blind for low energy X-rays. This causes stocked-up pulses also with higher energy quanta. This is important for high count rates and disturbs the spectrum (e.g. stocked up pulses with elements C or O or low energy L- and M-lines with all other element lines; continuous pile-up fills the valleys between high peaks, even at high energies).



The best way to determine the needed values for simulation is to compare simulation with an acquired spectrum at high count rates. Adjustment of the parameters will make the goal (first recognition time for sum-peak adjustment, then energy threshold for dirty spectrum components).

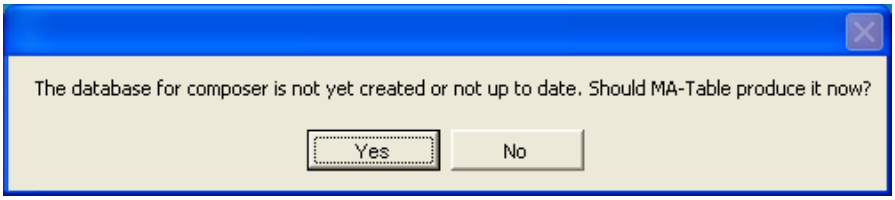
Modern pulse processors use more than one fast channel for pulse-pair recognition. Also the thresholds are not very sharp. Therefore all is a reality-near simulation.

Finally the spectrum will be displayed with a simulation, which is using the element contents of the 'Specimen Composer' form. Any change in concentrations, keV, tilt or Fwhm will affect the calculation.



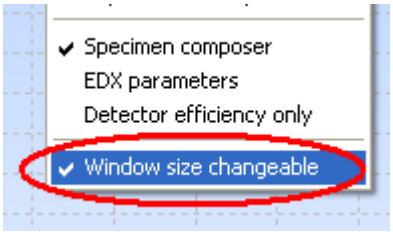
In case of a changed data-base, also the condensed data file for fundamental parameter calculation machine of spectra composer is to change (MAData3.dat, a condensed object of the editable data-base; for better machine language access). You can manage this automatically with hitting the button [Restore: MAData3.dat]:

If not, the program will give you always a reminder before next using of the composer:

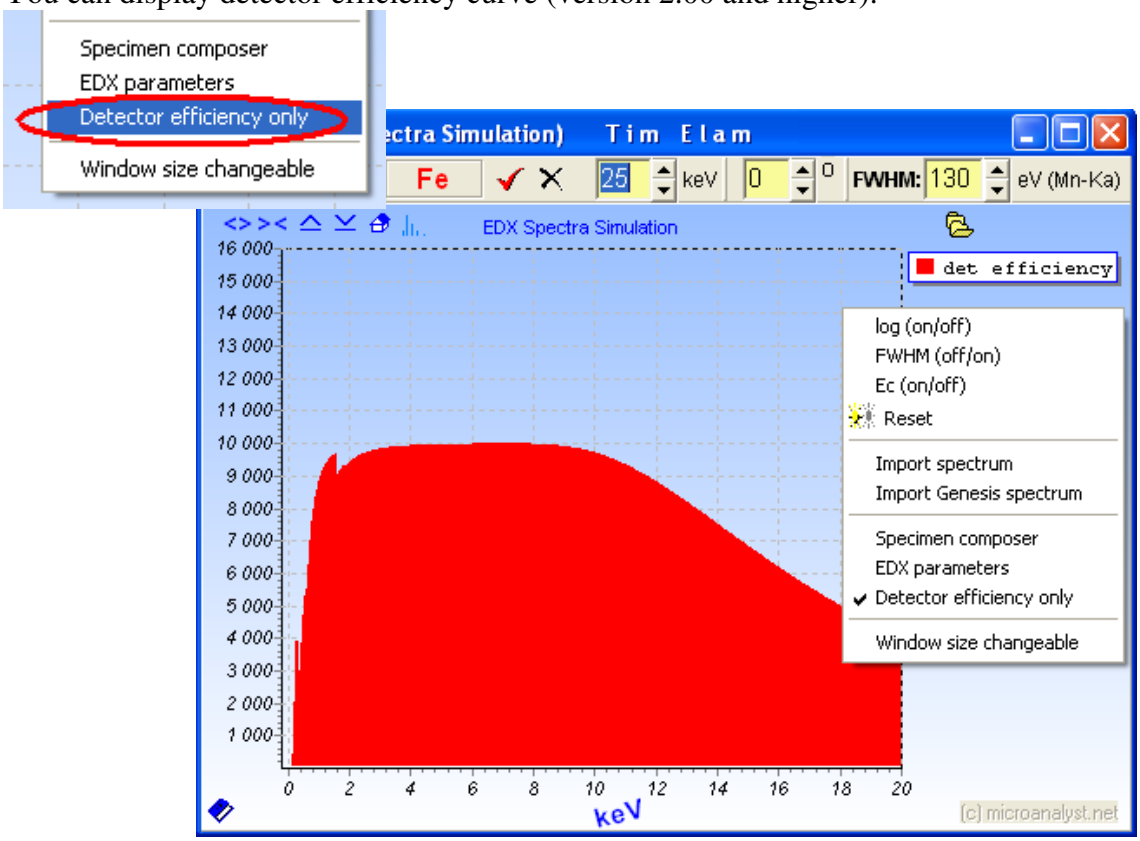


Tips:

If you like another size oft spectrum window, use this additionally (version 2.00 and higher, only licensed) function in pop-up menu:

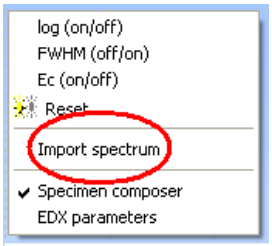


You can display detector efficiency curve (version 2.00 and higher):

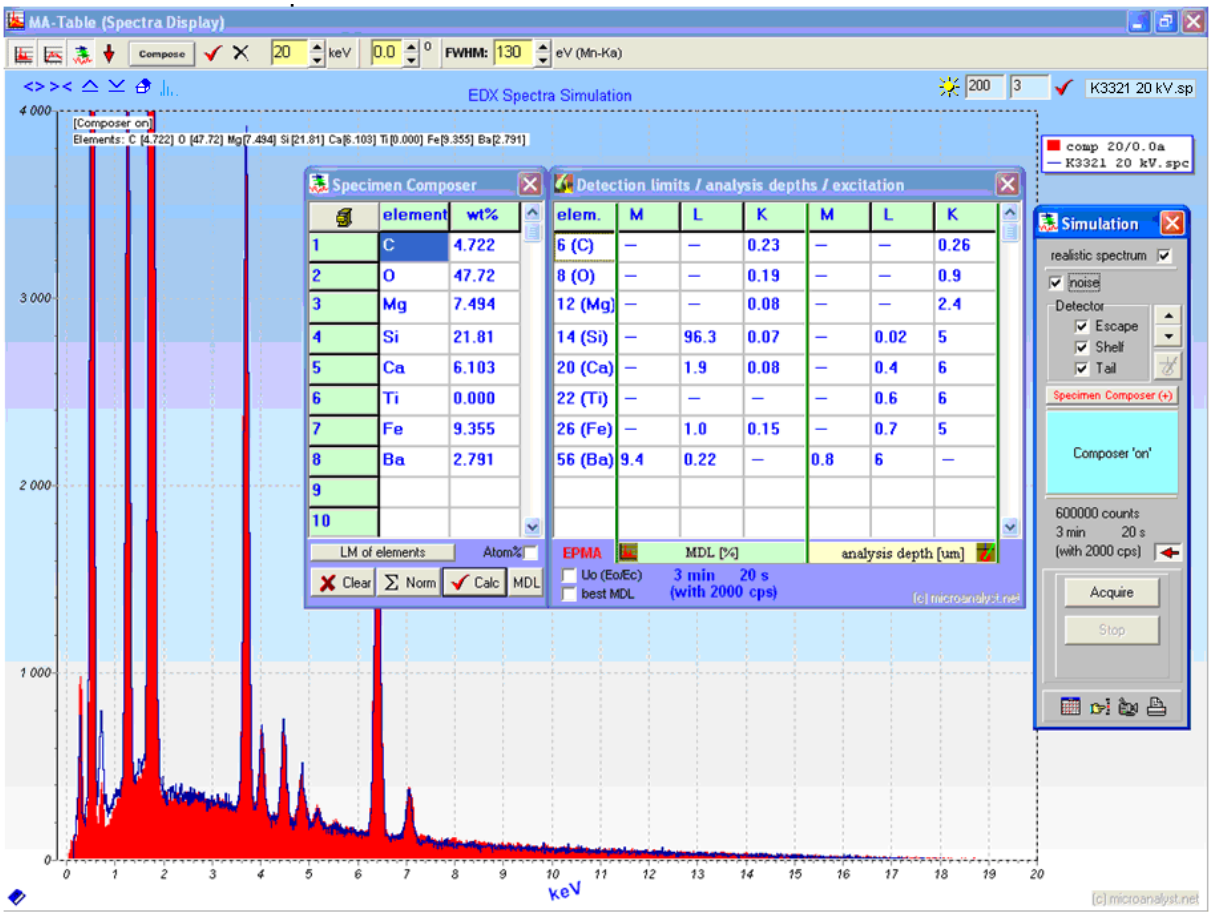


6. Spectra comparison

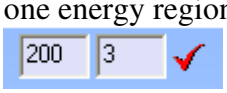
(only available with licensed version)



Two spectra formats are possible to import via pop-up menu or using the icon, EMSA-Code and EDAX *.spc spectra files (different extensions). After the loaded spectrum name is displayed right top, you will be able to load alternative spectra also by click there.



The original spectra acquisition time is used for simulation and the acquired spectrum is fit at one energy region, default with 3 keV, but possible to change:



First window: acquisition time in seconds | second window: fit energy

Please be careful with detection limits calculation. Check the count rate, because this is not imported together with the spectrum.

Also the acquisition time is now possible to change (only after spectra imports). Therefore you can calculate detection limits and other parameters just for the original acquired spectrum. Change the acquisition time, the fit energy or both, then hit the hook button and the changed values will be active for simulation and fit with acquired spectrum.

With this icon the simulated spectrum is possible to switch off/on for comparison purpose options with the real measured spectrum.

The additional tool bar is self explaining and very useful for usual spectra display manipulations to assess the simulation in comparison to the acquired spectrum (explained already):

Attention! The simulation below the energy of 1 keV is very critical and depends from the performance of the detector. There could be a lot of influences, e.g. detector icing, contamination and different behaviour in incomplete charge collection. Also not homogenous specimen or contaminations (coatings) have visible influences. Last but not least, the atomic data and ability of proper calculation of specimen excitation and self absorption is charged with more errors than usual with higher energies.

7. References

The data are blend of common used tables, new papers and 20 years personal EDX-experience:

J. A. Bearden, “X-Ray Wavelengths,” *Rev. Mod. Phys.* 39, 78 (1967)

McMaster Tables, Lawrence Livermore National Laboratory Report (1969)

M. O. Krause, J. Phys. Chem. Ref. Data. 8, 307(1979)

G.Zschornack, "Atomdaten für die Röntgenspektralanalyse", Verlag f.Grundstoffind.- Leipzig (1989)

M.Wendt, Microchimica Acta 139 (2002) 195-200

A.Aßmann, M.Wendt, Spectrochimica Acta, Part B 58 (2003) 711-716

The data base is open to improve (if necessary) and enlarge with new experience and more recent results.

The spectra simulation basics were described and published:

F.Eggert , Microchim Acta 155 (2006) 129

8. Finally Some Hints

- Often one would like to manipulate the spectrum representation to make details visible. This is also always possible in MA-Table, additionally to icons use:

Zoom:
In order to select a part of the spectrum display in detail (cut out), the left upper corner of the interested area is to select with mouse. Hit the left mouse button. Now move the mouse to the right lower corner of the wished area (do not release left mouse button during move!). Now the mouse button is only to release; and the spectrum representation is going to change automatically to the wished selected part.

Zoom cancelling:
Proceed as above with the zoom shot, only from right down to the left up. The selected cut is here no matter, since the spectrum representation returns in each case again to the start situation. The other way is to use right mouse pop-up menu (function “reset”) or ‘house’ icon.

Scroll of the spectrum representation:
Press the right mouse button mouse outside the red spectrum, but within the spectrum window and move the mouse with keeping right mouse button pressed, move to left or right.

- You want to work in other programs directly with the Windows®-clipboard (to copy, to paste). Or you want to use functionalities, which use the clipboard indirectly and the MA-Table is opened...
... and some of these functions do not work:

That is correct. The free version of MA-Table comes with restrictions. One restriction is the represented data and computed spectra cannot be copied. In order to use the clipboard in other programs, the complete MA-Table program does not have to be terminated. It is sufficient, if the opened MA-Table windows are closed and the program is transferred into the initial state (start situation: Table or Icon bar).

- MA-Table produces automatic pop-ups (on top), in free version only. If you are working with other programs (MA Table is not in the foreground), then these advertisement windows can disturbing you frequently:

One does not need to terminate the MA-Table program, in order to avoid the pop-ups. It is sufficient to reduce the program for Icon bar and to close all opened MA-Table windows, if you do not work actively straight with it. Thus the MA-Table features are permanent 'standby' and the advertisement pop-ups constantly disturb nevertheless not when operating other software.

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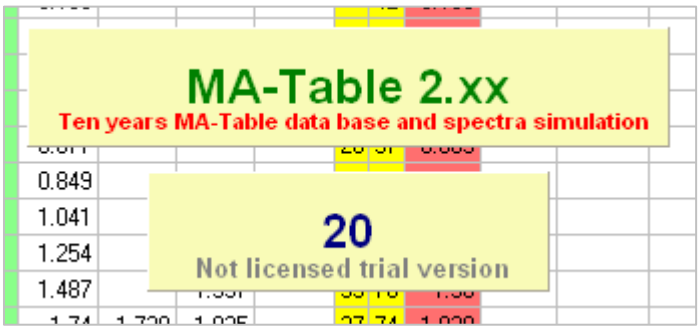
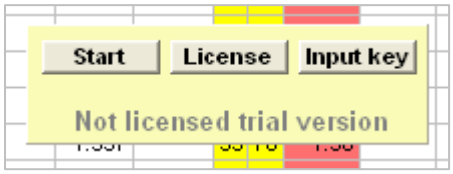
9. Version 2.xx Start

MA-Table counts down 20 seconds with each start, if the version is not full licensed:



After the count down is finished, 3 options will be possible to select:



Usually use [Start] to start the program. If you like to know how to get full licensed, select [License] (Internet connection required to get the information).

If you have already a full license key:
Select [Input key] and you will be directed immediately to the form where the license-key input is possible. The license key input is required only once (e.g. after installation using another computer), then the 20-seconds counting will be not with each next program start.