

# MA-Table

## Operator's Manual (Version 1.6x)

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MA-Table is a Windows® program for atomic data, which are important for Energy Dispersive X-ray Spectrometer (EDX), like



- Energetic position of lines (line energies),
- Relative height relations between lines of a series,
- Critical excitation energies (shell energies)
- Line overlaps
- Mass attenuation coefficients (mass absorption coefficients)

The program is able to calculate excitation processes in Electron Probe Microanalysis (EPMA) and the influence of these processes to the relative heights of lines in a series. A complete spectra simulation is possible because of the built-in fundamental parameter algorithm for the characteristic radiation and Bremsstrahlung,. Furthermore the program can add to the theoretically calculated spectrum the stochastic noise and artefacts of the EDX. That is why a very realistic spectra simulation is possible. Finally the program is able to calculate Minimum Detection Limits (MDL) and analytical depth, taking into account excitation conditions, specimen geometry and special overlap situation with other elements. For demonstration purposes it is possible to simulate a real EDX-data acquisition process nearly realistic. This data acquisition depends from count rate of the X-ray spectrometer (setup value) and of acquisition time. One can watch the development of minimal detection limits with progress of current acquisition time inside a simulation of ongoing acquisition process.

All functions have access to a central data base.










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### Content:

1. Functions of Icon Bar
2. Functions of MA-Table Line Display
3. Functions of Spectra Display
4. Functions of Spectra Display Setup
5. Specimen / spectra Composer
6. Spectra comparison
7. References
8. Finally some Hints

## 1. Functions of Icon Bar



-  ... Switch between table and Icon-Bar
-  ... Display periodic table of elements
-  ... Element search with line energy position 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 of the element of choice
-  ... Move the focussed element inside table



### Table on / Table off

With this icon a possibility exists to switch between complete table and the small icon bar very fast. If MA-Table is reduced to an icon bar, the program needs very little space from the desktop and is however at any time available. But even as icon bar, one has access to all functions without any disadvantage.

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


Z	name	Ka1	Ka2	Kβ1	Kβ2	KL	KM	Ec(K)	La1	Lβ1	Lβ2	Lγ1	Li
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 overlaps with the element in the line are specified in the yellow columns (for fast orientation). The main critical excitation energy of the main electron potential (electron-shell) is marked with red colour.



**Table 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 element line energy display (see later).



**Periodic chart of elements**

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

MA-Table (Periodic System of Elements)																																													
1 H																	2 He																												
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne																												
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar																												
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr																												
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe																												
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn																												
87 Fr	88 Ra	89 Ac	104 Ku	105 Bo																																									
<table border="1"> <tbody> <tr> <td>58 Ce</td> <td>59 Pr</td> <td>60 Nd</td> <td>61 Pm</td> <td>62 Sm</td> <td>63 Eu</td> <td>64 Gd</td> <td>65 Tb</td> <td>66 Dy</td> <td>67 Ho</td> <td>68 Er</td> <td>69 Tm</td> <td>70 Yb</td> <td>71 Lu</td> </tr> <tr> <td>90 Th</td> <td>91 Pa</td> <td>92 U</td> <td>93 Np</td> <td>94 Pu</td> <td>95 Am</td> <td>96 Cm</td> <td>97 Bk</td> <td>98 Cf</td> <td>99 Es</td> <td>100 Fm</td> <td>101 Md</td> <td>102 No</td> <td>103 Lr</td> </tr> </tbody> </table>																		58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr
58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu																																
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr																																
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The  button offers a quick jump to the element line energy display (see later).



## Search for elements and overlaps

There is the possibility of looking with given line energy position for the elements, which emit lines at this energetic position (assistance to find and identify the elements accurate).

Searching for alpha- and escape- lines is the standard setting (default). It is possible to look for all lines or omit the escape lines (e.g. if the spectrum is yet escape-corrected). By changing the search window (standard +/- 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 *in commercial EDX* spectrometers are not sufficient or even *wrong (!)*.

Element	Line	Energy [keV]	Offset [eV]
19 K	Ka1	3.314 keV	- 86
50 Sn	La1	3.444 keV	+ 43
60 Nd	La1-Esc	3.478 keV	+ 77
94 Pu	Ma1/2	3.33 keV	- 70
95 Am	Ma1/2	3.41 keV	+ 9

Element	Line	Energy [keV]	Offset [eV]
19 K	Ka1	3.314 keV	+ 4
45 Rh	Lg3	3.364 keV	+ 54
46 Pd	Lg1	3.329 keV	+ 19
47 Ag	LB2/15	3.348 keV	+ 38
47 Ag	LB6	3.256 keV	- 53
48 Cd	LB1	3.317 keV	+ 7
48 Cd	LB4	3.367 keV	+ 57
49 In	La1	3.287 keV	- 22
49 In	La2	3.279 keV	- 30
50 Sn	Leta		
83 Bi	M(N3-M1)		
84 Po	M(N4-M2)		
89 Ac	Mg		
90 Th	Mg		
92 U	MB		
93 Np	Ma1/2		
94 Pu	Ma1/2		

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

3.31 keV  
Overlap (+/- 70 eV) with all lines

Legend:  
K-overlaps (green)  
L-overlaps (purple)  
M-overlaps (orange)

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## 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:

W 74 Tungsten			
Ec-K	69.525	Ec-L3	10.207
		Ec-L2	11.544
		Ec-L1	12.099
Ka1	59.318	Ec-M5	1.809
Ka2	57.982	Ec-M4	1.872
KB1	67.244	Ec-M3	2.281
KB2	69.101	Ec-M2	2.575
KB3		Ec-M1	2.82
		La1	8.398
		La2	8.335
		LB2/15	9.96
		LI	7.388
		LB6	9.612
		LB1	9.672
		Lg1	11.286
		Leta	8.724
		LB3	9.819
		LB4	9.525
		Lg2	11.608
		Lg3	11.674
		Ma1/2	1.774
		Mz1	1.381
		Mz2	
		MB	1.835
		Mg	2.035
		M(O4-M3)	
		M(N1-M3)	
		M(N4-M2)	2.315
		M(N3-M1)	2.397

The main lines of the series are highlighted with red colours.

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 menu.

W 74 Tungsten			
Ec-K	69.525	Ec-L3	10.207
		Ec-L2	11.544
		Ec-L1	12.099
Ka1	59.318	Ec-M5	1.809
Ka2	57.982	Ec-M4	1.872
KB1	67.244	Ec-M3	2.281
KB2	69.101	Ec-M2	2.575
KB3		Ec-M1	2.82
		La1	8.398
		La2	8.335
		LB2/15	9.96
		LI	7.388
		LB6	9.612
		LB1	9.672
		Lg1	11.286
		Leta	8.724
		LB3	9.819
		LB4	9.525
		Lg2	11.608
		Lg3	11.674
		Ma1/2	1.774
		Mz1	1.381
		Mz2	
		MB	1.835
		Mg	2.035
		M(O4-M3)	
		M(N1-M3)	
		M(N4-M2)	2.315
		M(N3-M1)	2.397

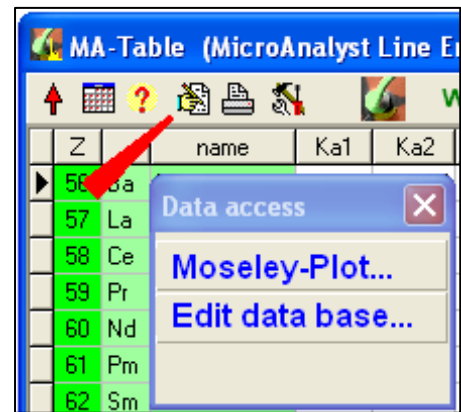
W Ma1/2 Overlap			
1.774 keV +/-		100	eV
<input checked="" type="checkbox"/>	main		
<input type="checkbox"/>	all		
<input checked="" type="checkbox"/>	Escape		
14	Si	Ka1	1.740 keV - 34
37	Rb	La1	1.694 keV - 80
38	Sr	La1	1.806 keV + 31
50	Sn	La1-Esc	1.692 keV - 82
51	Sb	La1-Esc	1.853 keV + 78
73	Ta	Ma1/2	1.709 keV - 65
75	Re	Ma1/2	1.841 keV + 66



## Edit data-base

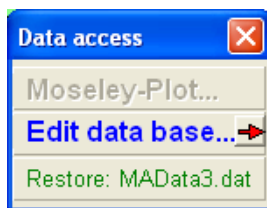
The icon has got a double functionality:

- edit of data base
- calls a Moseley-plot



## Edit data base...

There is the possibility to edit data.



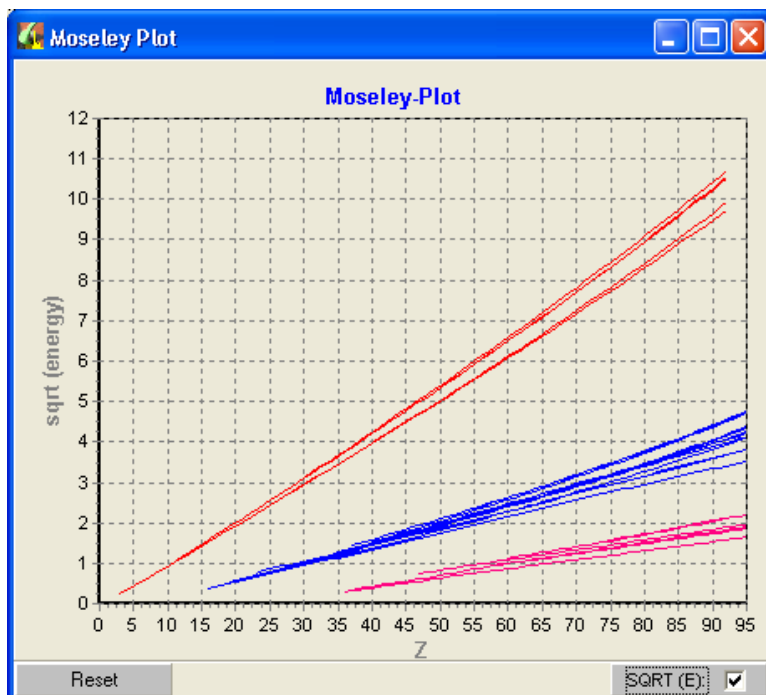
The operator has full access to both data-base files, EdxData1.DBF (first click) and EdxData2.DBF (second click). With third click one comes back to the standard view (without possibility to edit).

MA-Table (MicroAnalyst Line Energy Table) EDAX internal

ATOMIC_NR	EL_SYMB	AT_MASS	K_ALPHA1	K_ALPHA2	K_BETA1	K_BETA2	K_BETA3	K_
20	Ca	40.08	3.632	3.688	4.013			
21	Sc	44.96	4.091	4.086	4.46			
22	Ti	47.88	4.511	4.505	4.932			
23	V	50.94	4.952	4.945	5.427			
24	Cr	52	5.415	5.405	5.947			
25	Mn	54.94	5.899	5.888	6.49			
26	Fe	55.85	6.404	6.391	7.057			
27	Co	58.93	6.93	6.913	7.649			
28	Ni	58.69	7.478	7.461	8.265	99.99		
29	Cu	63.55	8.048	8.028	8.905	8.977		
30	Zn	65.38	8.639	8.616	9.572	9.658		
31	Ga	69.72	9.252	9.225	10.263	10.366		
32	Ge	72.59	9.886	9.885	10.982	11.1		
33	As	74.92	10.544	10.508	11.724	11.864		
34	Se	78.96	11.222	11.184	12.494	12.652		
35	Br	79.9	11.924	11.878	13.289	13.469		
36	Kr	83.8	12.649	12.598	14.109	14.315		
37	Rb	85.47	13.395	13.337	14.958	15.185		

Because the composer is using a condensed data base (MAData3.dat), this is important to restore 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 exampl-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 provided 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.



## 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.

MA-Table (print)

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Element	Ka1	Ka2	Kβ1	Kβ2	KL	KM	EcK	Lα1	Lβ1	Lβ2	Lγ1	L1	Lγ3	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					120	0,284											
7 N Stickstoff	0,392					122	0,401								0,01			
8 O Sauerstoff	0,525					123	0,532								0,007			
9 F Fluor	0,677					126	0,685								0,009			
10 Ne Neon	0,849					128	0,87								0,022			
11 Na Natrium	1,041		1,067			130	1,072								0,031			
12 Mg Magnesium	1,254		1,302			133	1,305								0,051			
13 Al Aluminium	1,487		1,557			135	1,56								0,073			
14 Si Silicium	1,74	1,739	1,826			137	1,839								0,099			
15 P Phosphor	2,014	2,013	2,139			140	2,145								0,135			
16 S Schwefel	2,308	2,307	2,464			142	2,472	0,1487				0,1487		15	39	0,164		
17 Cl Chlor	2,622	2,621	2,816			144	2,822	0,1826				0,1826		15	40	0,2		
18 Ar Argon	2,998	2,956	3,191			147	3,203	0,221				0,221		15	42	0,249		
19 K Kalium	3,314	3,311	3,59			149	3,607	0,2603				0,2603		16	43	0,294		
20 Ca Calcium	3,692	3,688	4,013			152	4,038	0,341	0,345			0,3027		16	45	0,347		
21 Sc Scandium	4,091	4,086	4,46			154	4,493	0,395	0,3995			0,348		17	46	0,402		
22 Ti Titan	4,511	4,505	4,932			156	4,966	0,452	0,458			0,395		17	49	0,455		
23 V Vanadium	4,952	4,945	5,427			159	5,465	0,511	0,519			0,447		18	51	0,513		
24 Cr Chromium	5,415	5,405	5,947			161	5,989	0,573	0,583			0,5		18	52	0,574		
25 Mn Mangan	5,899	5,888	6,49			163	6,539	0,637	0,649			0,556		19	53	0,64		
26 Fe Eisen	6,404	6,391	7,057			166	7,113	0,705	0,719			0,615		19	55	0,708		
27 Co Cobalt	6,93	6,913	7,649			168	7,709	0,776	0,791			0,678		10	56	0,779		
28 Ni Nickel	7,478	7,461	8,265			170	8,333	0,851	0,869			0,743		10	57	0,855		

Table Print



## Settings/Registration/Demo

Settings

**MA-Table**  
Version 1.60 (2008/12/10)

Registration

**Language**

Deutsch

Englisch

Autostart

Update

Demo

**Method**

EPMA  XRF  Elevation angle 35°

**Detector**

Window utw/slew (MOXTEK) Details

Count rate 2000 cps Resolution 130 eV

**Service links**

Manual License Forum Service MailTo

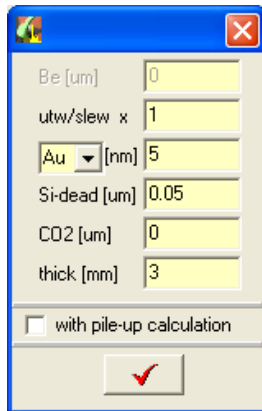
(c) microanalyst.net (2003..2008) Autor: Frank Eggert OK

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

Click at **Demo** and you you can lay back in your armchair (like in cinema), to watch the full functionality of MA-Table.

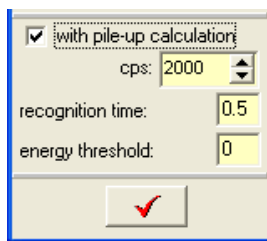
**EPMA** is standard selected. XRF is not implemented.

**Window** selects the used window of the Energy Dispersive Spectrometer (EDX). Two are available, the MOXTEK ultra thin window and a common Beryllium-window. With **Details** you can change thicknesses (for fine-tuning of spectra calculations).



Be-window thickness [ $\mu\text{m}$ ]  
 Utw-window thickness [factor to standard thickness]  
 Contact layer of the detector [nm] with material selection  
 Si-dead layer [ $\mu\text{m}$ ]  
 ... an additional CO<sub>2</sub> absorption layer on detector surface  
 detector active thickness [mm] (inside cryostat vacuum)

(able to change only with licensed version)



Check the pile-up calculation to consider this effect with each simulation, which depends from pulse processor data and from used count rate. The simulation of a pileup effect depends on the behaviour and temporal resolution of the energy threshold of the pileup detection of the pulse processor and may be covered experimentally to be adjusted.

**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, ...).

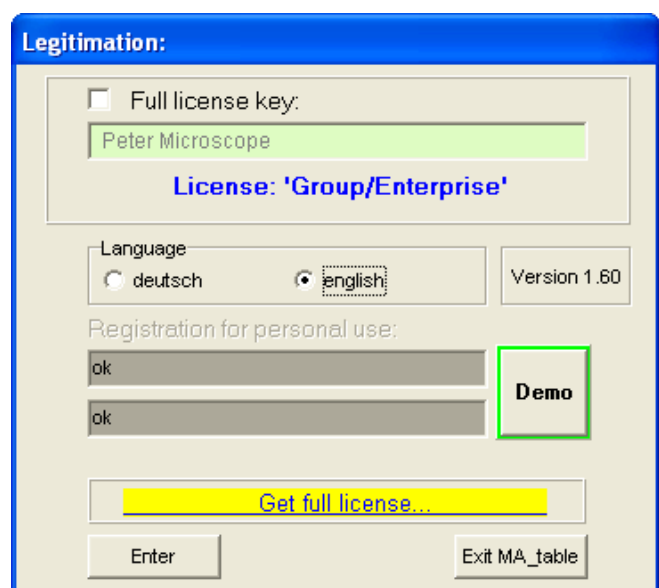
With **Resolution** you can set up your detector resolution (at Mn-K $\alpha$ ). Be care, the resolution is not dynamically changed with count rate selection (like in your real working EDX by changing the pulse processor shaping time).

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

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 anonymous). 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 for counting users. But the functionality of the free version is limited.



With **Service** several 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](http://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 realistic spectra settings)

### 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.

30	Zn	Zinc	8,633	8,616	5,974
31	Ga	Gallium	9,252	9,225	10,263
▶ 32	Ge	Germanium	9,886	9,885	10,982
33	As	Arsen			1,724
34	Se	Selen			2,494
35	Br	Brom			3,289
36	Kr	Krypt			4,109
37	Rb	Rubic			4,958
38	Sr	Stron			5,832
39	Y	Yttriu			6,734
40	Zr	Zircor			7,663
41	Nb	Niobi			8,617
42	Mo	Molybdenum	17,473	17,504	19,602
43	Tc	Technetium	18,367	18,251	20,611

Simulation

Moseley-Plot

Element chart

Settings

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WebSearch

Adv. X-ray search

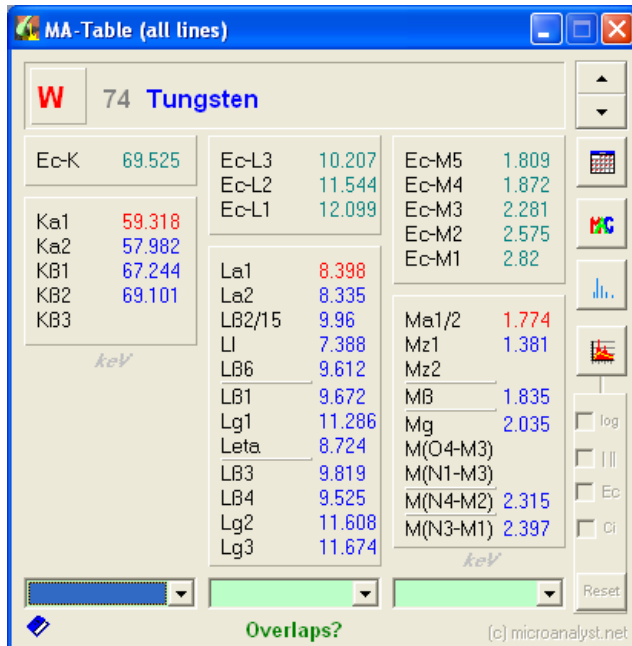
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Manual

Forum (Discussion)

Service

## 2. Functions of MA-Table Line Display



← quick change of selected element  
( $\pm$  one atomic number)

← call periodic chart of elements for  
direct element selection

← mass absorption coefficients

→  line series intensities

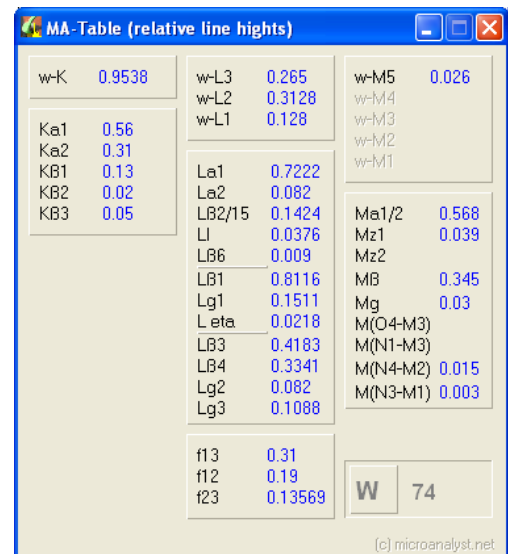
→  spectra simulation



### line series intensities

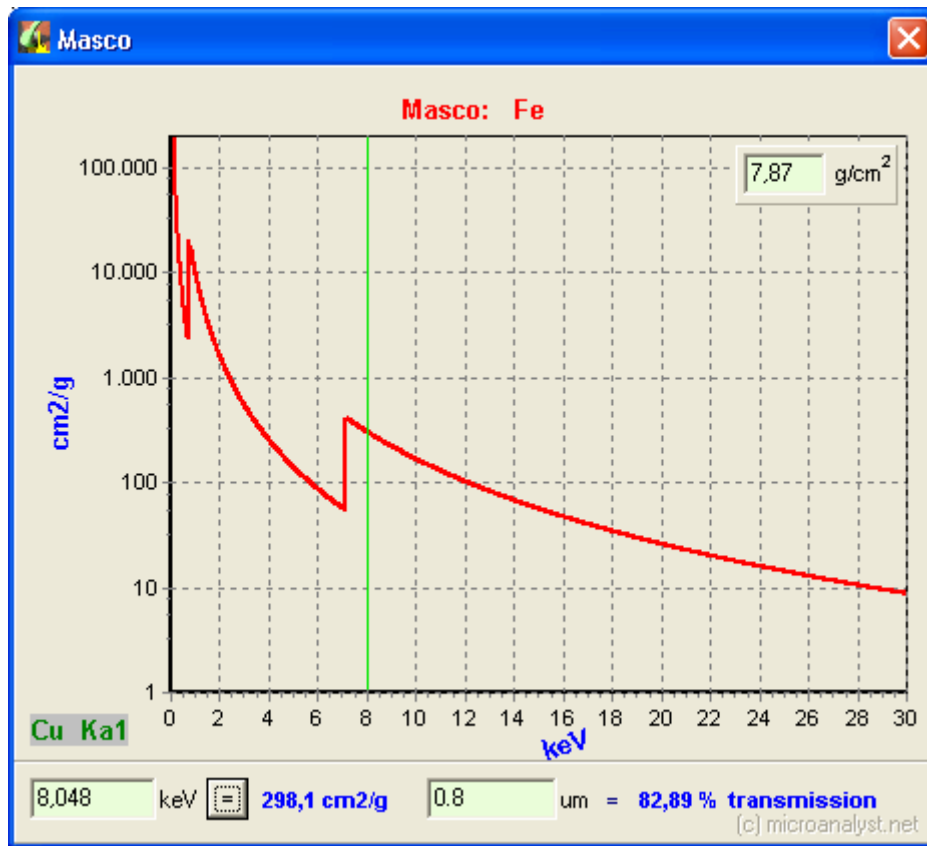
All relative line intensities of the selected element are displayed.  $w$  are the fluorescence yields and  $f$  are Coster-Kronig transition rates, both necessary for calculation the relative line series with taking into account the primary excitation energy (high voltage of electron microscope, primary electron energy). These values are stored inside data table EdxData2.DBF .

The program MA-Table takes these values for simulation calculation, all relative heights will be normalized internal (in sub-shells).





The MAC icon in element selection form is usable now. Hit the button and the mass absorption coefficient-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 density, if necessary.



### spectra simulations

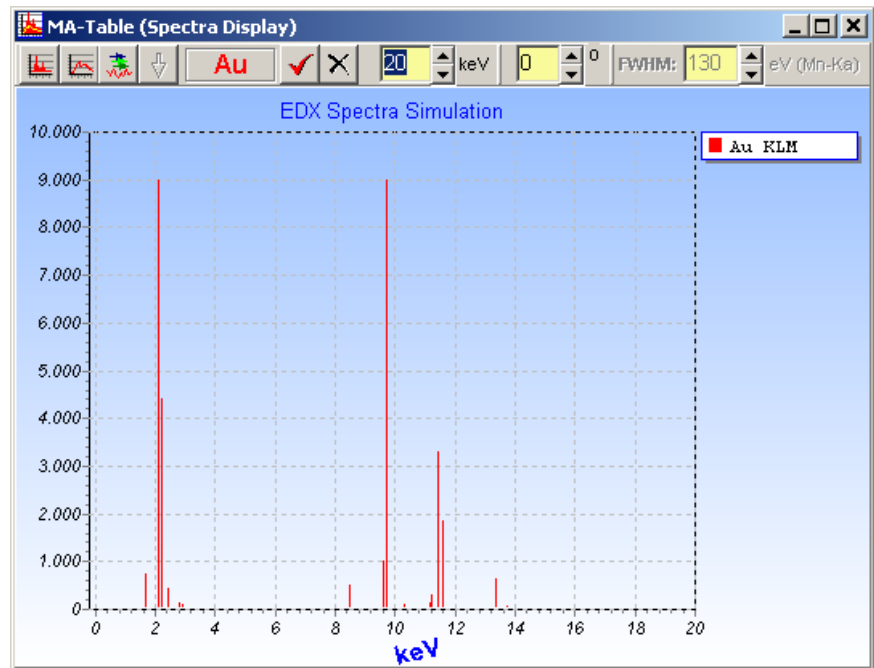
This is another way to display relative line heights. This calculation is taking into account the current excitation.

*The spectra simulation is full explained in next chapter.*

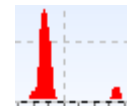
### 3. Functions of Spectra Display

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 open spectra window, after changing an element into the focus, the program is going to calculate the spectra display once more automatically (considering the selected buttons).



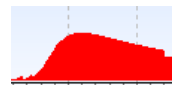
Calculation of line series taking into account detector



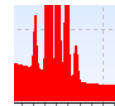
resolution



Calculation of Bremsstrahlung distribution



Complete spectra simulation (line series and Bremsstrahlung)



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



Change of estimated acquisition time

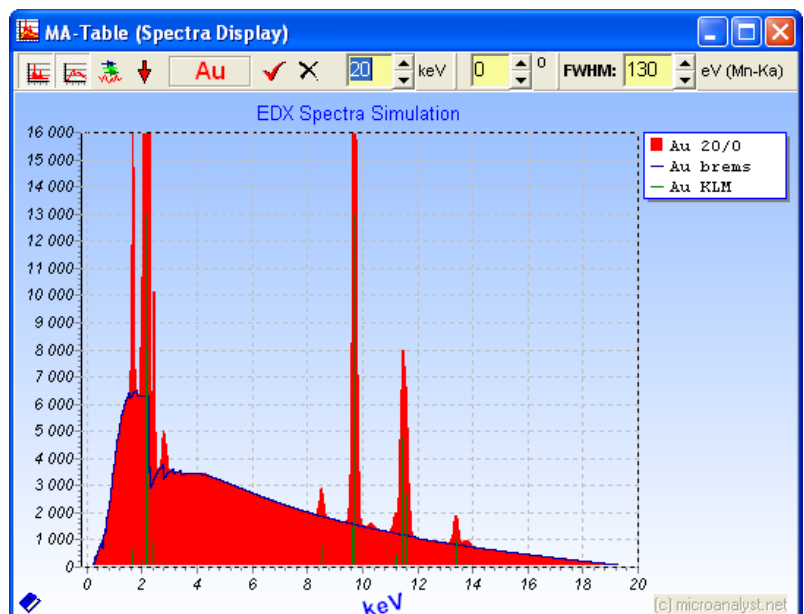


Add a spectrum for spectra comparison (maximum of 10 spectra are possible to add)



Cancel the last spectrum of comparison

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





Select primary electron energy (high voltage of scanning electron microscope)

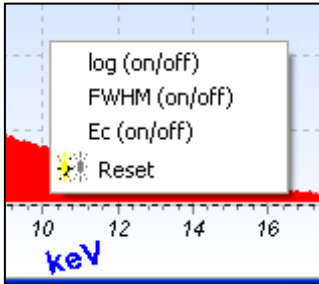


Select tilt angle of specimen



Select detector resolution

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

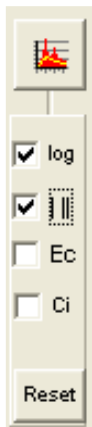


You have the opportunity to choose between:

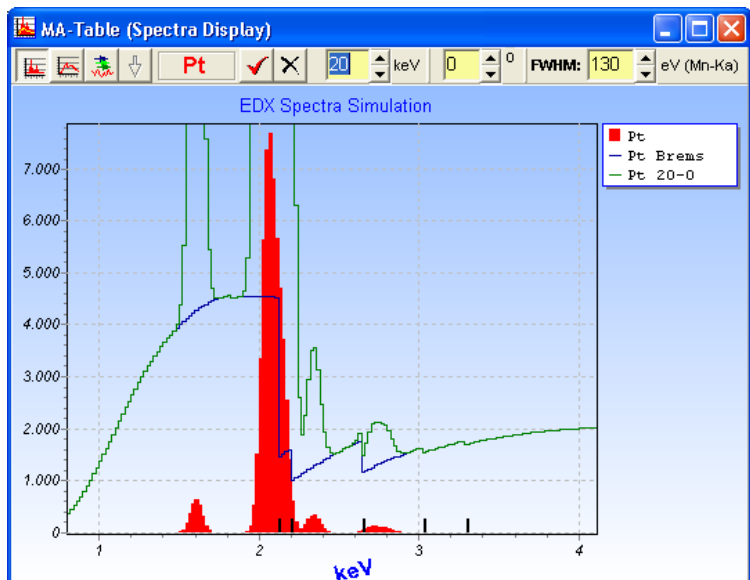
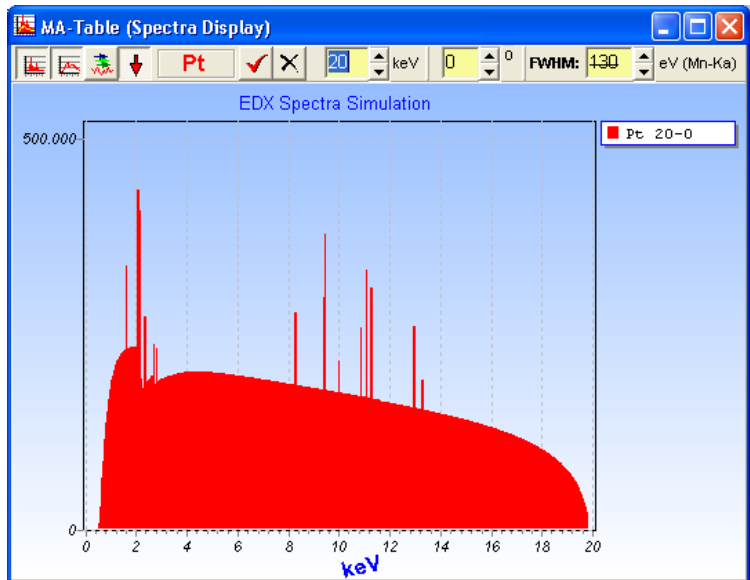
- logarithmic display or not
- taking into account detector resolution (FWHM) or not
- display of critical excitation energies or not

... Finally always the possibility for a simple and quick display-reset.

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

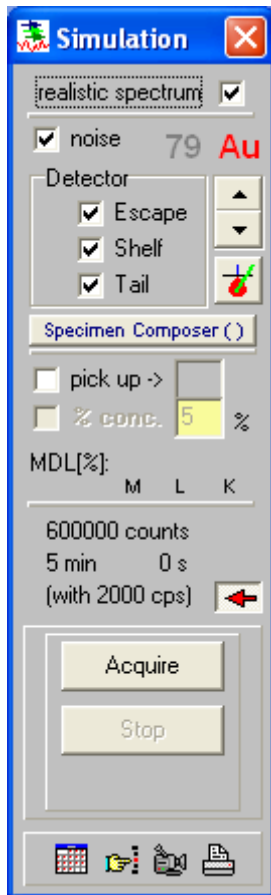


Logarithmic display without FWHM consideration

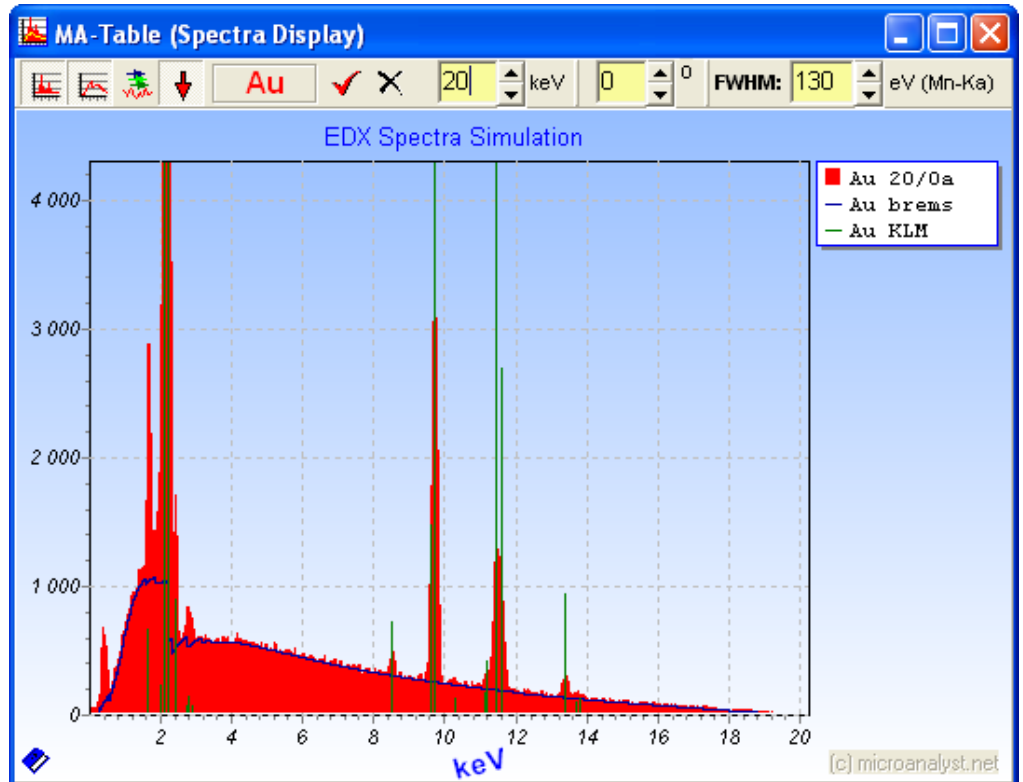


Linear display with display of critical excitation energies (shell energies) with black bars

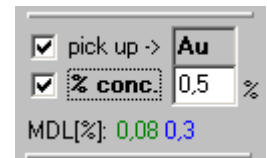
## 4. Functions of Spectra Display Setup



Select 'realistic spectrum' to add noise and detector artefacts. The simulation for the Au-spectrum is changing immediately (look to 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. Klick with mouse at 'pick up' check-box to select an element, which you want to check for overlaps with all other elements.
2. Then change an other 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 overlaped 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) and the overlaped one (green)



- scrolling through all elements even with spectra full size display




- icon for excitation/analysis depth display



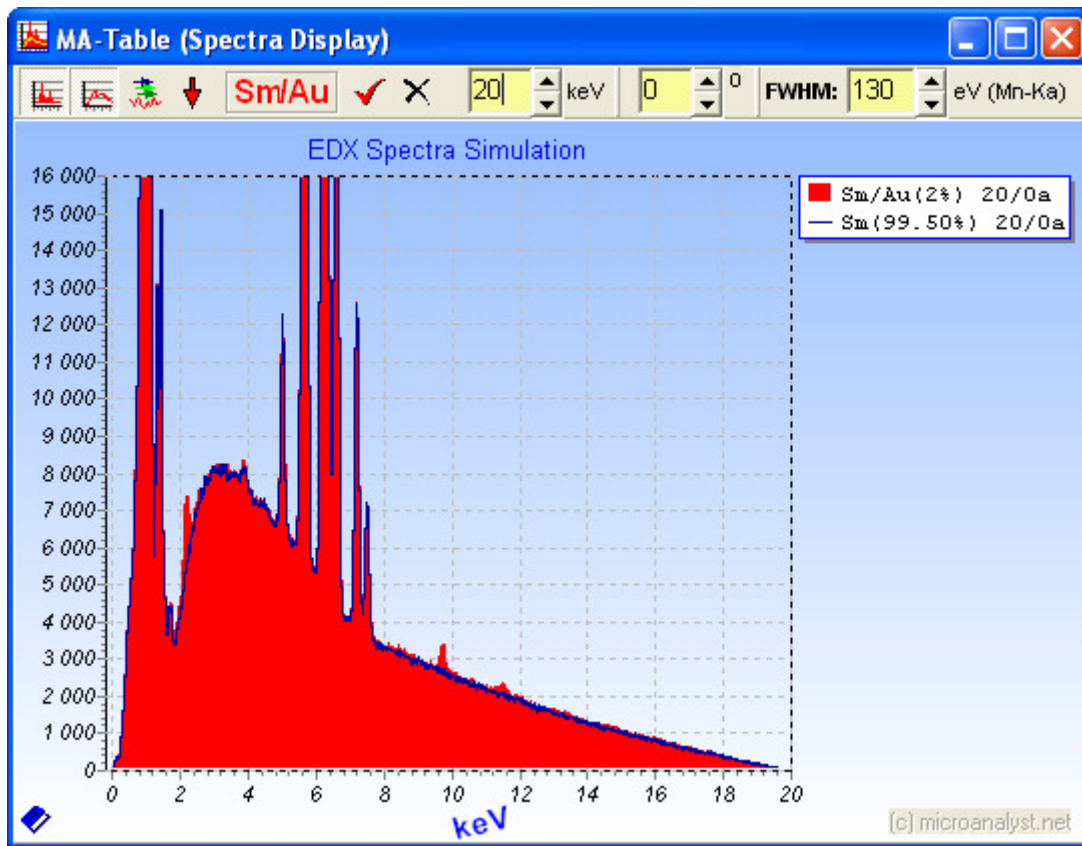
- M, L, K marks the MDL values

	0,5	0,1
M	L	K



- Calculation of detection limits with choice  
'fix beam current' or  
'fix count rate'

6000000 counts  
50 min 0 s  
(with 2000 cps) 

In the example, you will find 0.5 per cent Au in a Sm-specimen (the mean element is Sm), with 0.5 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 significant detectable. Please compare with calculated detection limits of 0.3 and 0.4 per cent respectively.

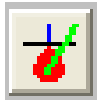


The detection limits are only calculated, if 'realistic spectrum' is selected.

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



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



## 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 ( $E_o$  too small for this line), the program will give the hint with changing to red colour for the lines values:

**Cu**

Ag	E <sub>o</sub> /E <sub>c</sub>	d
K		
L	4,5	0,38
M	>20	0,01

Au	E <sub>o</sub> /E <sub>c</sub>	d
K		
L	1,3	0,15
M	6,8	0,40

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.

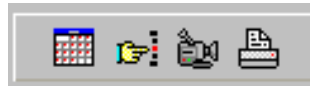
**AU**

Ag	E <sub>o</sub> /E <sub>c</sub>	d
K		
L	4,5	0,77
M	>20	0,07

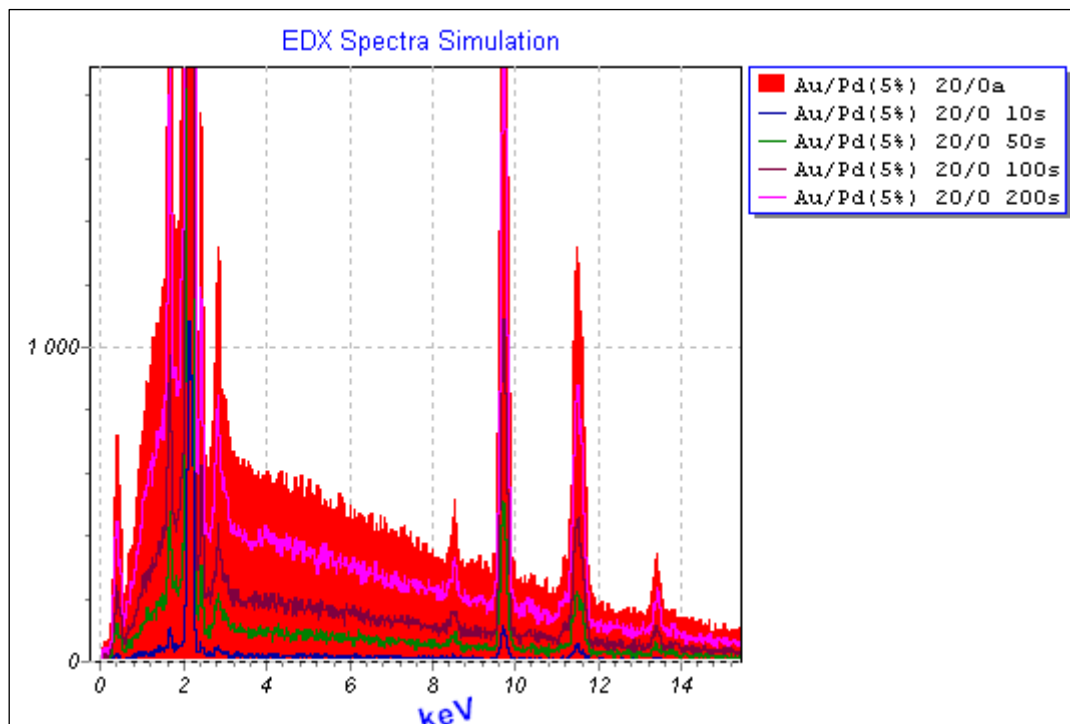
Cu	E <sub>o</sub> /E <sub>c</sub>	d
K	1,7	0,52
L	16,1	0,48
M		

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*)

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 the improvement of the detection limit with increasing measure time (live at display):

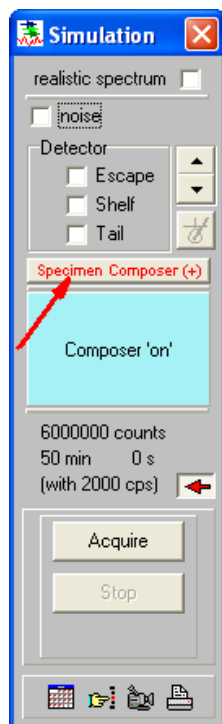


## 5. Specimen / spectra composer

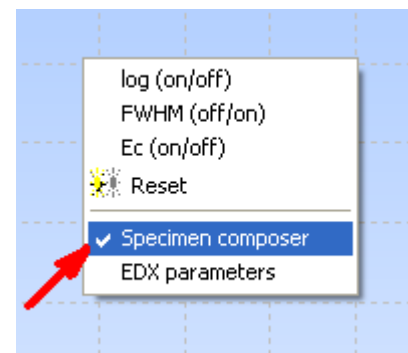
A spectra composer is implemented to simulate spectra of specimen for any element fractions (maximum of 30 elements)

It is possible to investigate the influence of excitation, specimen tilt, acquisition time, count rate, resolution and other conditions in their influence 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.

These are the ways to call the 'specimen composer':



... or hit one of these elements.



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

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

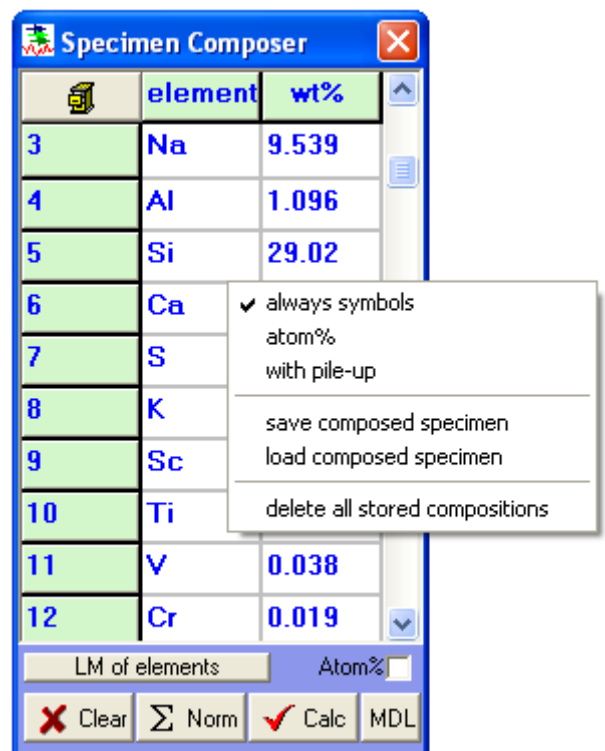
Then a form appears:

Fill out the form either with atomic number or element symbols and related weight fractions (concentrations). After each edit the [ $\Sigma$  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.

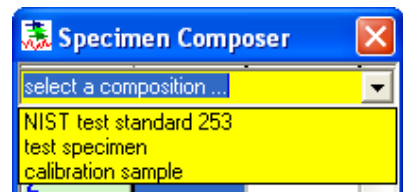
[Clear] cleans the entire form.

Check 'Atom%' if the inputs are atom% instead weight%.



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

You can save and load element sets (composed specimens) with using a pop-up menu. The file store cabinet icon is visible only with some stored compositions and possible to use like the load menu function.



[LM of elements] displays line-marks (element selection via click into table).

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

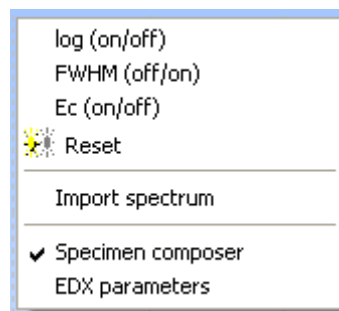
Detection limits / analysis depths / excitation						
elem.	M	L	K	M	L	K
22 (Ti)	—	0.18	0.04	—	0.17	1.3
24 (Cr)	—	0.23	0.05	—	0.25	1.3
25 (Mn)	—	0.6	0.08	—	0.22	1.3
26 (Fe)	—	0.14	0.07	—	0.25	1.2
28 (Ni)	—	0.19	0.09	—	0.13	1.2
29 (Cu)	—	0.11	0.09	—	0.14	1.1
42 (Mo)	0.13	0.03	—	0.02	1.4	—
74 (W)	0.02	0.07	—	0.8	1.0	—

EPMA     MDL [%]     analysis depth [um]

Uo (Eo/Ec)     50 min 0 s  
 best MDL     (with 1802 cps)

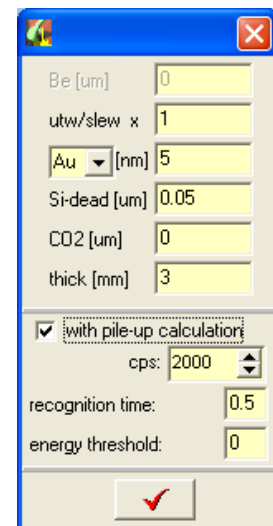
(c) microanalyt.net

You can switch on/off the specimen composer also via left-mouse click menu (pop-up menu).



This is also the way to change the detector parameter used for calculation.

It is possible to perform a simulation 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 (pulse per recognition limit). The energy threshold describes the energy which is starting sensible for pile-up rejection channel of pulse processor. An ideal

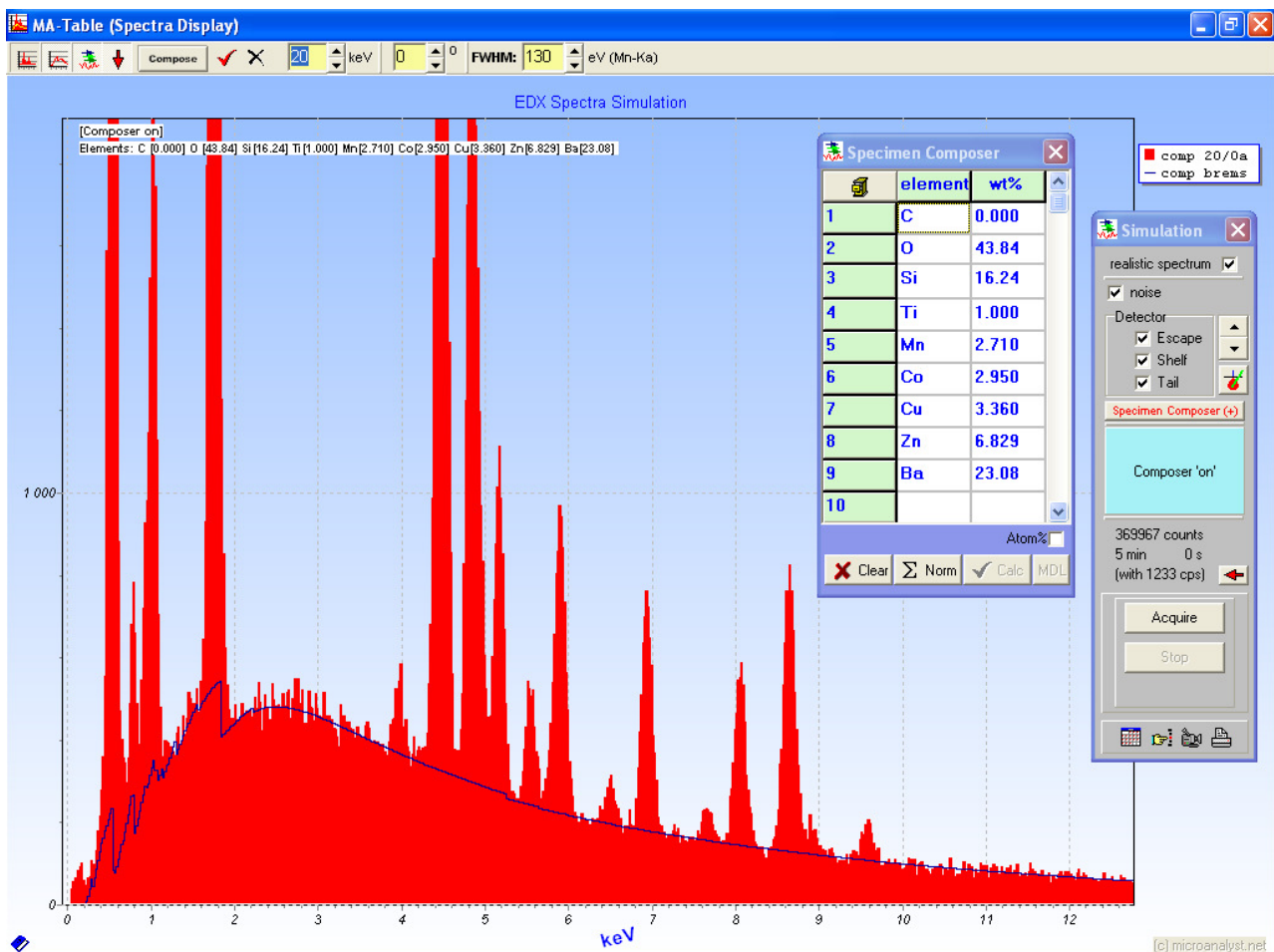


pulse processor would be a setting of zero. In praxis the fast channel is worse in energy resolution, therefore the threshold for pulse pair recognition is between 0.5 and 0.8 keV. Therefore the pulse processor pile-up rejection is blind for X-rays with energies below. This causes stocked up pulses also with higher energy quanta. The pile-up rejection is blind for low energy X-rays. This is important for high count rates an 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 makes the valleys between peaks higher, even at high energies).

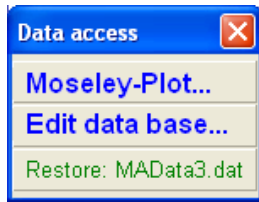
The best way to determine the needed values for simulation is to compare simulation with an acquired spectrum at high count rates. Adjustment of the parameters will make the goal (first recognition time for sum-peak adjustment, then energy threshold for dirty spectrum components).

*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.*

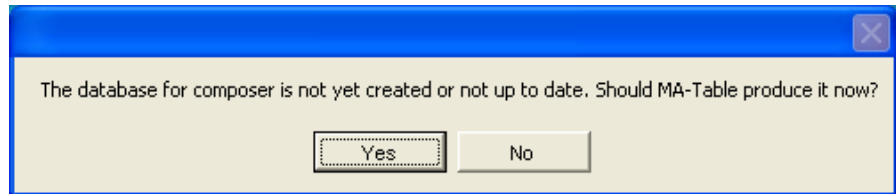
Finally the spectrum will be displayed with a simulation, which is using the element contents of the 'Specimen Composer' form. A change in concentrations, keV, tilt or Fwhm will affect the calculation.



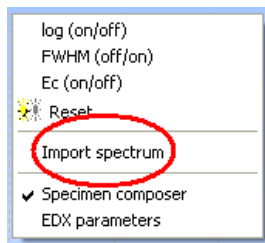
In case of a change of data-base also the condensed data file for fundamental parameter calculation machine of spectra composer is to change (MADData3.dat, a copy of the editable data-base for better machine language access). You can manage this automatically with hitting the button [Restore: MADData3.dat]:



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



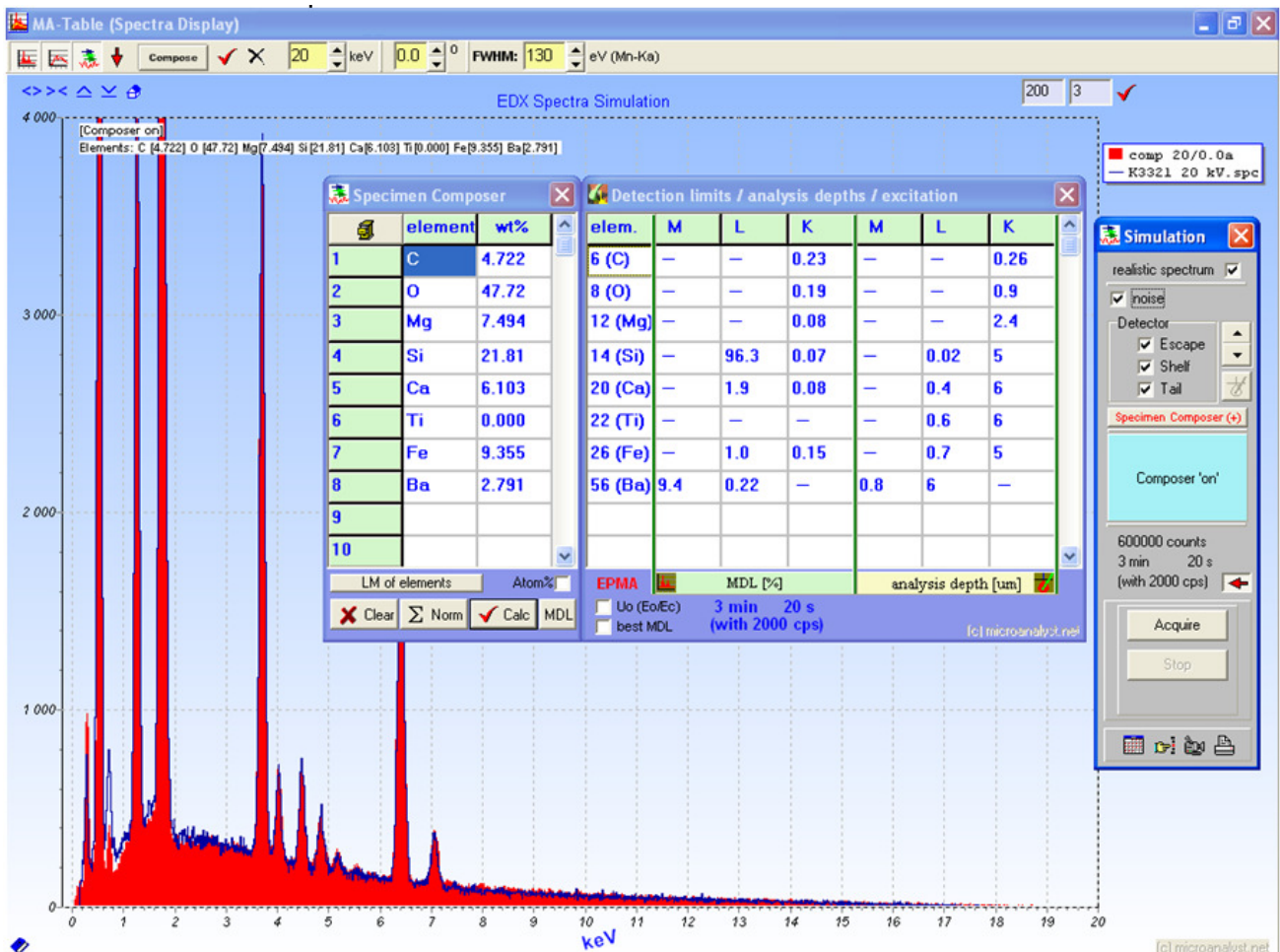
## 6. Spectra comparison

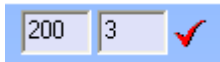


(only available with licensed version)

Two spectra formats are possible to import, EMSA-Code (different extensions and EDAX \*.spc spectra files.

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 possible to change now free (after spectra import only). 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 of acquired spectrum.

Also an additional tool bar is visible after spectrum import (only after this).



This is self explaining and very useful for usual spectra display manipulations to assess the simulation in comparison to the acquired spectrum.

*Attention! The simulation mostly 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 Röntgenspektalanalyse", 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...

## **8. Finally Some Hints**

- Often one would like to manipulate the spectrum representation to make details visible. That is always possible in MA-Table:

Zoom:

In order to select a cut out, the left upper corner of the cut out is to be selected with mouse. Hit the left mouse button. Now move the mouse to the right lower corner of the desired cut out (do not release left mouse button!), then the rectangle of the coming spectrum cut out is stretched. Now the mouse button is to be only released, and the spectrum representation is going to change automatically to the desired cut out.

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").

Scroll of the spectrum representation:

Press the right mouse button within the spectrum representation and move the mouse with pressed right mouse button back and forth.

- 
- You want to work in other programs directly with the Windows<sup>®</sup>-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. In the free version of MA-Table there are restrictions. A restriction is that 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 the 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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