What is new in UNIFIT 2015?

Main focus of the advancement of the **UNIFIT 2015 software** was the implementation of new processing and presentation features for the treatment of a very large number of spectra of line scans and multipoint (area) scans. This requires the more efficient usage of the main memory by the software UNIFIT and an optimised presentation routine of the spectrum windows. As the result of the software optimisation the number of simultaneously processable spectra was increased from 1200 to 9000. The three new functions 'XY 3D Plot 45°', 'XY 3D Plot -45°' and 'XY 3D Colour Profile' allow the presentation of the element distribution or the plot of the distribution of the chemical components with respect to the x and y values of the recording position on the sample.

- Realization of a more efficient using of the main memory of the used computer system by UNIFIT. The loading time of projects with a large number of spectra is ten times lower.
- ii) The maximum number of simultaneously processable spectra windows was increased to 9000.
- iii) The standard-window selection dialogue was adjusted to the large number of processable spectra (see Fig. 1). The number of the selection functions has been improved.

Edit Parameters Standard	Windows - Batch parameter		Edit Paremeters Standard Windows - Batch parameter								
Select Windows											
Column 1		Column 2		Column 3		Column 4		Column 5			
🗷 W 1:	-1	🗷 W 21:	20		40	☑ W 61:	60	W 81:	80		
W 2:	1	🗷 W 22:	21	🗷 W 42:	41	🗷 W 62:	61	🗷 W 82:	81		
🗷 W 3:	2	🗷 W 23:	22	🗷 W 43:	42	🗷 W 63:	62	🗷 W 83:	82		
🗷 W 4:	3	🗷 W 24:	23	🗷 W 44:	43	🗷 W 64:	63	🗷 W 84:	83		
🗷 W 5:	4	🗷 W 25:	24	🗷 W 45:	44	🗷 W 65:	64	🗷 W 85:	84		
🗷 W 6:	5	🗷 W 26:	25	🗷 W 46:	45	🗷 W 66:	65	🗷 W 86:	85		
🗷 W 7:	6	🗷 W 27:	26	🗷 W 47:	46	🗷 W 67:	66	🗷 W 87:	86		
🗷 W 8:	7	🗷 W 28:	27	🗷 W 48:	47	🗷 W 68:	67	🗵 W 88:	87		
🗷 W 9:	8	🗷 W 29:	28	🗹 W 49:	48	🗷 W 69:	68	🗹 W 89:	88		
🗷 W 10:	9	🗷 W 30:	29		49	🗷 W 70:	69	🗵 W 90:	89		
🗷 W 11:	10	🗷 W 31:	30	🗷 W 51:	50	🗷 W 71:	70	🗷 W 91:	90		
🗷 W 12:	11	🗷 W 32:	31	₩ W 52:	51	🗷 W 72:	71	🗹 W 92:	91		
🗷 W 13:	12	🗷 W 33:	32	🗷 W 53:	52	🗷 W 73:	72	🗷 W 93:	92		
🗷 W 14:	13	🗷 W 34:	33	🗷 W 54:	53	🗷 W 74:	73	🗷 W 94:	93		
🗷 W 15:	14	🗷 W 35:	34	🗹 W 55:	54	🗹 W 75:	74	🗷 W 95:	94		
🗷 W 16:	15	🗷 W 36:	35	🗷 W 56:	55	🗷 W 76:	75	🗷 W 96:	95		
🗷 W 17:	16	🗷 W 37:	36	🗷 W 57:	56	🗷 W 77:	76	🗷 W 97:	96		
🗷 W 18:	17	🗷 W 38:	37	🗷 W 58:	57	🗷 W 78:	77	🗷 W 98:	97		
🗷 W 19:	18	🗷 W 39:	38	🗷 W 59:	58	🗷 W 79:	78	🗷 W 99:	98		
🗷 W 20:	19	🗷 W 40:	39	🗷 W 60:	59	₩ W 80:	79	🗷 W 100:	99		
1 - 100	⊚ 10	01 - 200	⊚ 201 - 3	300	301 - 400	e 4	01 - 500	● 501 - 6	600		
◎ 601 - 700	⊚ 70	01 - 800	© 801 - 9	900	© 901 - 1000	© 1	001 - 1100	1101 -	1200		
• 1 - 1200 • 1201 - 2400 • 2401 - 3600 • 3601 - 4800 • 4801 - 6000 • 6001 - 7200											
o 7201 - 8400 o 8401 - 9000											
OK Cancel All Windows No Window Every 2nd W. Every 3th W. Every 4th W. Every 5th W. Every: 6											
Sort Data	Preview	Und	o Ins	ert F	ill with	Setting:	All 3D Windows	o Nu	mber Text		

- Fig. 1. The new designed selection dialogue for standard windows
- iv) The selection of presentable curves including the 3D plots has been expanded (see Fig. 2, left). Five different curves are offered:
 - 1. Spectrum,

- 2. Modified spectrum,
- 3. Background function,
- 4. Sum curve after a peak fit,
- 5. Component curve i after a peak fit (i = 1 to n, n number of components during the peak fit).
- v) The menu for the editing of spectrum parameters has been completely refreshed. A special additional sub-menu ('Fill With' button) allows the easy manipulation of the values (see Fig. 2, right). The choice of editable parameters was expanded to
 - 1. Spectrum name,
 - 2. Batch parameter,
 - 3. x position,
 - 4. y position,
 - 5. Comment,
 - 6. Lens mode,
 - 7. Analyser Mode,
 - 8. Pass energy.

The communication with external programmes via the copy-paste function was improved.

vi) The acquisition parameters x and y of line scans or multipoint scans can be used as abscissa of the parameter plot.

Curve Selection		1
Spectrum	○ Curve Component 14	Define/Calculate Items
 Modifyed Spectrum 	○ Curve Component 15	Number of selected Items: 576
Background Background Second Secon	Curve Component 16	First Item: Si2p
Sum Curve	Curve Component 17	Last Item: Si2p
Ourve Component 1 Ourve Compone	Curve Component 18	Fill with
Ourve Component 2	Curve Component 19	 First Item;
○ Curve Component 3	Curve Component 20	● Last Item:
○ Curve Component 4	Curve Component 21	 Equidistant Steps
Ourve Component 5	Curve Component 22	◎ Item + OP:
© Curve Component 6	Curve Component 23	● Item * OP:
	Curve Component 24	● Item / OP:
© Curve Component 8	Curve Component 25	Sin(Item) (RAD)
⊙ Curve Component 9	○ Curve Component 26	○ ln(ltem)
© Curve Component 10	○ Curve Component 27	o e^ltem
Curve Component 11	Curve Component 28	● Item*e^OP
Curve Component 12	Curve Component 29	
○ Curve Component 13	Curve Component 30	
· · · · · ·	· · · · · · · · · · · · · · · · · · ·	Insert Original
ОК	Cancel	Close

- **Fig. 2.** Left: curve selection dialogue of standard windows for the 3D plots, two components were fitted, right: manipulation and calculation sub-menu of editable spectrum parameters
- vii) The quantification table was adjusted to the large number of spectra.

- viii) The layout of the controls has the common Windows design. The so-called manifest of the Unifit2015.exe was accordingly modified. Additional design features were implemented.
- ix) The useable and currently used main memory of the Unifit software can be displayed via an additional information function.
- ix) The direct activation of the spectrum windows was changed and adjusted to the large spectra number.
- x) The menu points 'Close Windows', 'Close Standard Windows', 'Charge Correction' and 'Original/Accept Preferences' apply for all windows or for a number of selected windows only.
- xi) The three new functions 'XY 3D Plot 45°', 'XY 3D Plot -45°' and 'XY 3D Colour Profile' allow the presentation of the distribution of the elements or chemical components with respect to the x-y position for the measurement of the sample. Five different display options are offered:
 - 1. Maximum of the intensity of the spectrum,
 - 2. Minimum of the intensity of the spectrum,
 - 3. Background-free area,
 - 4. Area of the sum curve after a peak fit,
 - 5. Area of the chemical component i (i = 1 to n, n number of components during the peak fit).

The Fig. 3 and 4 show a 'XY 3D Plot 45° ' of Si and SiO₂ of a multipoint scan (26x26 points) of a untreated Si sample, respectively. The Figs. 5 - 7 show the same sample after sputtering. The sputter crater can be found on the left side (Fig. 5). The position x = 0 and y = 0 is the normal recording position. The zero intensities represent the measurements without x-ray excitation (x-ray source was switched off). The Fig. 5c and 6c show the corresponding 'XY 3D Colour Profiles' of Fig. 5b and 6b, respectively.

- **xii)** The appearance of the colour-scale bar of the '3D Colour Profiles' is optionally and the position variable.
- **xiii)** Now the software can use more than 3 GByte main memory. The 'Large Address Flag' of the UNIFIT.exe was settled.



Fig. 3. 'XY 3D Plot 45°' of the area of the Si component after the peak fit of a untreated Si sample, plot created using UNIFIT 2015 and inserted in this document



Fig. 4. 'XY 3D Plot 3D 45°' of the area of the SiO₂ component after the peak fit of a untreated Si sample, plot created using UNIFIT 2015 and inserted in this document



Fig. 5a. 'XY 3D Plot 45°' of the area of the Si component after the peak fit of a sputtered Si sample, areas with zero intensities show the measurement with the condition: X-ray source switched off, plot created using UNIFIT 2015 and inserted in this document



Fig. 5b. 'XY 3D Plot 45°' of the area of the SiO component after the peak fit of a sputtered Si sample, reversed presentation, areas with zero intensities show the measurement with the condition: X-ray source switched off, plot created using UNIFIT 2015 and inserted in this document



Fig. 5c. 'XY 3D Colour Profile' of the area of the SiO component after the peak fit of a sputtered Si sample, corresponding presentation of fig. 5b, areas with zero intensities (white colour) show the measurement with the condition: X-ray source switched off, plot created using UNIFIT 2015 and inserted in this document



Fig. 6a. 'XY 3D Plot -45°' of the area of the SiO₂ component after the peak fit of a sputtered Si sample, areas with zero intensities show the measurement with the condition X-ray source switched off or removed SiO₂ coverage, plot created using UNIFIT 2015 and inserted in this document



Fig. 6b. 'XY 3D Plot 45°' of the area of the SiO₂ component after the peak fit of a sputtered Si sample, areas with zero intensities show the measurement with the condition X-ray source switched off or removed SiO₂ coverage, plot created using UNIFIT 2015 and inserted in this document



Fig. 5. 'XY 3D Colour Profile' of the area of the SiO₂ component after the peak fit of a sputtered Si sample, corresponding presentation of fig. 6b, areas with zero intensities (white colour) show the measurement with the condition X-ray source switched off or removed SiO₂ coverage, plot created using UNIFIT 2015 and inserted in this document