What is new in UNIFIT 2024?

Main focus of the advancement to the **UNIFIT 2024** software was the rework and new design of the definition and displaying of the preferences. The dialogue 'Programme Parameters' was redesigned and expanded. The definition of the excitation satellites was reworked completely. The pop-up and pull-down commands were improved. The setting options of the x-axis and y-axis dialogues were refreshed. New export functions were implemented.

i) The input management for the definition of the **preferences** (see Fig. 1) was completely reworked and redesigned. A new preference dialogue was implemented. Former pull-down commands of the preferences were removed. Nine groups were defined:

- a) General
- b) Display
- c) Printer
- d) Load/Define Transmission Function T(E)
- e) Peak Fit
- f) Export
- g) Import
- h) Sources
- i) Batch Processing

The operations will be carried out simultaneously. Therefore, the button 'Close' and not 'OK' leaves the dialogue. The automatic transfer of reloaded preferences to open spectra windows was deactivated. The preference 'Save Projects Automatically' was removed. The currently loaded preferences can be displayed optionally after the execution of the software Unifit 2024.

| Test Projectudy - UNITI FOR WINDOWS - D - D - D - D - D - D - D - D - D - | | | | | | | |
|---|---------------------------|---|---|--|---------------------------------------|--|--|
| 음 🔓 🗟 🖥 🛎 조 조 🇙 🔳 🖷 🖩 尤 굿 🎟 오 오 බ 🤉 🧟 🧟 🖉 🧟 🗶 🛣 🦧 🧟 🦧 🦉 🦧 🦉 🦓 🖉 🖉 🖉 🖉 🖉 🖉 🖉 🖉 🖉 🖉 🖉 | | | | | | | |
| terations: 1 C | hi ² " = 1.018 | references: C:\Users\RHesse\Documents\Unifit_2024_User_Files\presetting\presetting.set | | | | 0 X | |
| 28.00 | | General | | | | | |
| | 0 | Programme Parameters | Language | | Decimal Character Display/Printer | | |
| 24.60 | - | Number of the First Standard Window: 41 | | German | English | Point Comma | |
| ts | | Maximal Number of Reak-Fit Componente: 10 | | Unifit Project | ts | | |
| | | Maximal Number of XAS Background Steps and XPS Backgrund Funct | ons: 6 □ Save Backup Files ☑ Open with Quantification and Film Thickness Table X-Axis ws': 10 X-Rxis X-RS: Binding Energy OXPS: Kinetic Energy XAS: Photon Energy; AES/T(E): Kinetic Energy; Raman: Wave Number | | | antification and Film Thickness Table | |
| Q 21.20 | 「 | Maximal Number of Presentable Curves inside 'Plot 3D Waterfall': 200 | | | | | |
| ty / | | Maximal Number of Presentable Fit Results inside 'Plot 3D Waterfall P | | | | XPS: Kinetic Energy | |
| ັ <u>ເ</u> 17.80 | | Maximal Number of Presentable Curves Inside Parameter Plot: 20 Maximal Number of Presentable Parameter Steps inside 'Parameter P | | | | Energy; Raman: Wave Number 275 | |
| Inte | | Threshold Spike Correction: 20 | V-Avie | | | Toolbar | |
| 14.40 | - | Max. Spike Number/%: 20 | Modify | Counts | Counts per Second | Activate Toolbar Modify | |
| | ~ | Text Dialogs | | Background | XPS-Quantification Right Mr | ause Button | |
| 11.00 | - | Arial, 16, Standard, Standard, Standard | Change | Constant | ○ Linear | ○ Tougaard ○ Polynom+Shirley | |
| 54 | 44 | | | | | | |
| | | Display | | Printer | | | |
| | | Graphs Standard Window/Wagner Plot Axes/Lines/ | Text | Graphs Star | ndard Window/Wagner Plot | Axes/Lines/Text | |
| Ш 1 Ж 1 | A | 3D Plot Waterfall/XY 3D Plot/Colour Profile 3D Plot Waterfal | ll 0° Plus | 3D Plot Water | rfall/XY 3D Plot/Colour Profile | e 3D Plot Waterfall 0° Plus | |
| <u> </u> | | Parameter Plot | | Parameter Plot Print Options Dis | | □ Display Setting ===> Printer Setting | |
| terations: 1 C | hi ² " = 1.112 | | - | | | | |
| 24.00 | | Load/Define Transmission Function T(E) | Export | | Desired Observator Data | Import | |
| | | Loaded T(E): ESCALAB220_TWIN_LAXL_50EP.tm | | ages | Decimal Character Data Point | VAMAS (*.VMS;*.NPL) 155 | |
| 22.72 | | Load T(E) Define Parameters T(E) | ○ 400 dpi | 400 dpi | O Comma | ScientaSES-Spectra (*.TXT) | |
| unts | | Peak Fit | 600 dpi | O 800 dpi | Delimitation Data | SPECS Prodigy (*.XY) | |
| Ö 21.44 | - | Fit Procedure | O 1000 dpi | O 1200 dpi | Comma | | |
| × × | | Product Oconvolution Sum Sum | Text Table Im | Text Table Images O Semicolon Times New Roman, 12 Tabulator | | | |
| 1 20.16 | - | Parameters Peak Fit/XAS-Background/XPS-Background (INHOM) | Times New R | | | | |
| Iten | | Absolute O Relative | Text | Tables | Space | | |
| 드 19.99 | | Calculation of Fit-Parameter Errors | | | | | |
| 10.00 | 4 | Iterative Iterative Matrix Inversion | Sources | | | Batch Processing | |
| | | Towns and Deplement Oplandation | Al Ka | Mg Ka H | le I He II | Load Original Spectra | |
| 17.60 | <u>t</u> | Homogeneous Samples Onhomogeneous Samples | 1486.6 eV | 1253.6 eV 2 | 21.2 eV 40.8 eV | Number of Iterations per Cycle = 10 | |
| 413 Define Satellites Number of Cycles - 2 Modify | | | | | | | |
| | Display/Printer/Peak Fit | | | | | | |
| <u>i</u> 1 | A | Close Load Save Save as Tran | sfer All Win | dow O Window | ws Only Window 45 | -30 | |
| rữ -1 | | | | | | | |

Fig. 1 Screen shot: Dialogue for definition of the presettings of the programme handling

ii) The number of the **excitation sources** (see Fig. 2) was reduced to four. The dialogue for the definition of the satellites was redesigned and the parameters were clearly labelled. The files 'satellite.set' and 'satellite1.set' were removed. The parameters of the excitation satellites were integrated into the presetting files (*.set).

| Definition Excitation Satellites | | | | | |
|----------------------------------|------------------|--------|--------|------|-------|
| Source Name: | | Al Ka | Mg Ka | Hel | He II |
| Excitation Energy | | 1486.6 | 1253.6 | 21.2 | 40.8 |
| Peak | Peak height | 100 | 100 | 100 | 100 |
| | Displacement/eV | 0 | 0 | 0 | 0 |
| Sat. 1 | rel. Peak Height | 6.4 | 8 | 2 | 0 |
| | Displacement/eV | 9.8 | 9.4 | 1.9 | 0 |
| Sat. 2 | rel. Peak Height | 3.2 | 4.1 | 0.5 | 0 |
| | Displacement/eV | 11.8 | 10.2 | 2.5 | 0 |
| Sat. 3 | rel. Peak Height | 0.4 | 0.55 | 0 | 0 |
| | Displacement/eV | 20.1 | 17.5 | 0 | 0 |
| Sat. 4 | rel. Peak Height | 0.3 | 0.45 | 0 | 0 |
| | Displacement/eV | 23.4 | 20 | 0 | 0 |
| Sat. 5 | rel. Peak Height | 0.55 | 0.5 | 0 | 0 |
| | Displacement/eV | 69.7 | 48.5 | 0 | 0 |
| OK Cancel | | | | | |

Fig. 2 Screen shot: Dialogue for definition of the excitation satellites

iii) The dialogue '**Programme Parameters**' (see Fig. 3) was extended. Ten parameters are available:

- a) Number of the First Standard Window (1...101)
- b) Points to Average (1...19, odd)
- c) Maximal Number of Peak-Fit Components (1...30)
- d) Maximal Number of XAS Background Steps and XPS Background Functions (3...9)
- e) Maximal Number of Presentable Curves inside 'Plot 3D Waterfall' (100...300)
- f) Maximal Number of Presentable Fit Results inside 'Plot 3D Waterfall Plus' (7...21)
- g) Maximal Number of Presentable Curves inside 'Parameter Plot' (10...30)
- h) Maximal Number of Presentable Parameter Steps inside 'Parameter Plot' (30...50000)
- i) Threshold Multiplier of Spike Correction (5...100)
- j) Maximal Number of Spikes/% (5...33)

iv) The **pop-up and pull-down commands** were refreshed. The pull-down group 'Information' was renamed to 'Information/Editing'. The pull-down command 'Design - Edit Parameters...' was shifted to 'Information/Editing – Edit Parameters...'.

v) The dialogues 'Plot Energy/Wavenumber Axis' (see Fig 4) and 'Plot Intensity Axis' were refreshed (see Fig 5).

vi) Two new options were implemented in the **export of fit parameters** (see Fig 6). Now the absolute and relative peak area can be exported, too.

vii) The satellite subtraction can be carried out for the active window and optionally for all standard windows without the batch processing operation.

| Setting of Programme Parameters | |
|--|--------|
| | |
| Number of the First Standard Window (1101): | 41 |
| Points to Average (119; odd): | 3 |
| Maximal Number of Peak-Fit Components (130): | 10 |
| Maximal Number of XAS Background Steps and XPS Backgrund Functions (39): | 6 |
| Maximal Number of Presentable Curves inside 'Plot 3D Waterfall' (100300): | 200 |
| Maximal Number of Presentable Fit Results inside 'Plot 3D Waterfall Plus' (721): | 10 |
| Maximal Number of Presentable Curves inside 'Parameter Plot' (1030): | 20 |
| Maximal Number of Presentable Parameter Steps inside 'Parameter Plot' (3050000): | 50 |
| Threshold Multiplier of Spike Correction (5100): | 20 |
| Maximal Number of Spikes/% (533): | 20 |
| Show Spectra of Spike Correction after Laplace operation | |
| OK Cancel Values to Minimum Typical Values Values to M | aximum |

Fig. 3 Screen shot: Dialogue for definition of the general programme parameters

| Plot Energy/Wavenumber Axis | | | | |
|-----------------------------|--------------------------------|---|--|--|
| Binding Energy / eV | | | | |
| from: | 413 | | | |
| to: | 392 | | | |
| Number of Increments: | 7 | | | |
| Fixed Decimal Places (m | ax 4): | 0 | | |
| Decimal Places fix | | | | |
| ■ Non-equidistant Scaling | g | | | |
| □ Plot Energy - Paramete | □ Plot Energy - Parameter Area | | | |
| ☑ Labelling of Scale Lines | | | | |
| □ Grid Lines | | | | |
| □ Setting: All Std. Windows | | | | |
| □ Save as Preferences | | | | |
| XPS | | | | |
| Ebin/eV | Ekin/e\/ | | | |
| | | | | |
| Number of Points x2 | | | | |
| Original | Original Preview | | | |
| OK | Cancel | | | |
| | | | | |

Fig.4 Screen shot: Dialogue 'Plot Energy/Wavenumber Axis'

| Plot Intensity Axis | | | | |
|---|---------------------|--|--|--|
| Intensity / kCounts R(E) | | | | |
| from: to: Number of Increments: □ Scaling for All Window | 17600 24000 5 | | | |
| Fixed Decimal Places (max 4): 0 Decimal Places fix | | | | |
| All ⊠ Show Zero Lines | None | | | |
| Show Residual Plot Energy - Intensity Area Labelling of Scale Lines Grid Lines Setting: All Std. Windows Save as Preferences | | | | |
| • Counts | Counts per Second | | | |
| Original | Preview | | | |
| ОК | Cancel | | | |

Fig.5 Screen shot: Dialogue 'Plot Intensity Axis'

| Select Fit Parameters | |
|--|--------|
| Fit Parameters | |
| □ Peak height □ GP-FWHM/eV □ Position/eV | |
| □ LP-FWHM/eV □ Asymmetry □ abs. Area | |
| □ rel. Area □ Fit Background | |
| OK | Cancel |

Fig.6 Screen shot: Dialogue 'Export Fit Parameters'