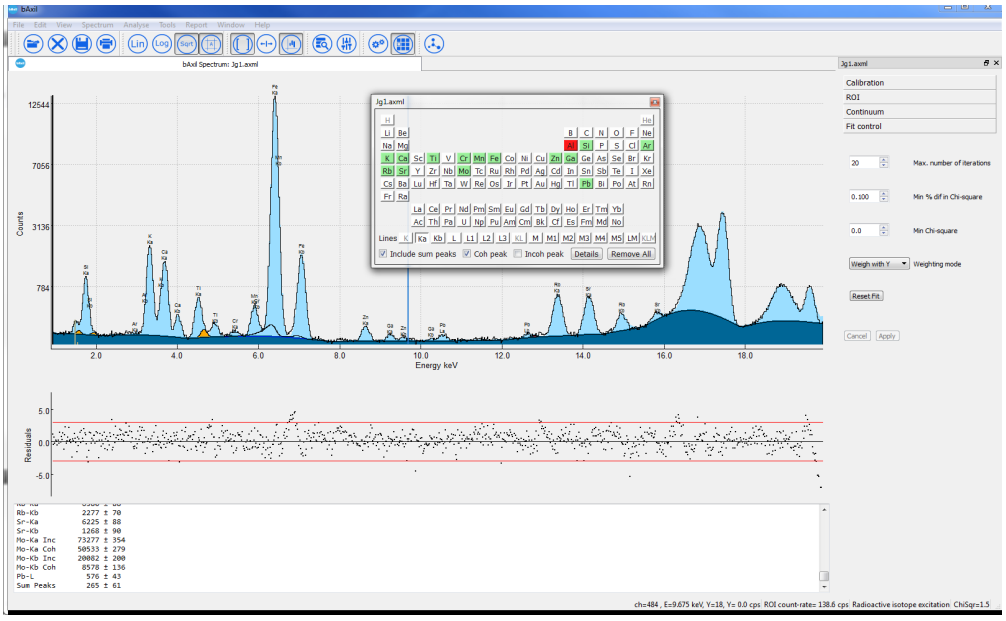
TECHNICAL SPECIFICATIONS

bAxil Software Package



INTRODUCTION

The analysis of the energy spectra resulting from a x-ray fluorescence process (ED XRF) is still the most critical step in ED XRF analytical technique due to its complexity, e.g. large amount of interference between elemental emissions, presence of spectrum artifacts (sum and escape peaks), complex continuum, excitation peaks (coherent and incoherent radiation), and many others. Furthermore, the advances of today's measurement and detection technologies imposes new challenges to the XRF spectrum analysis.

bAxil is a new software for the XRF spectrum analysis. Although it is based on the internationally well-know AXIL spectrum analysis methods, it incorporates recent developments and research in spectrum analysis and peak de-convolution. bAxil development has also taken into consideration the vast working experience and extensive operational feedback from previously developed AXIL software versions (e.g. Axil-PC, QXAS, etc.) for improving and fine-tuning its spectrum analysis steps and methods.

bAxil has been developed using the most recent and powerful software development and programming techniques. The software takes advantage of higher computer power (such as 64-bit processors), modern operating systems (bAxil is a multiplatform software), and new data structures (XML-based files).

bAxil software incorporates an special module and new algorithms for fast XRF image scanning analysis and data compression.

Additionally, the bAxil product line includes "bAxil Programing Libraries" which (as separate product) allows the user to take advantage of the powerful spectrum analysis engines and include them in their own development.

COMPONENTS

The bAxil application software package consists of the following components:

- Spectrum analysis program, which also includes:
  - MCA control and data acquisition via Topaz-X MCA
  - Macro ED XRF image scan analysis, incorporating "hybrid" spectrum analysis engine
- Quantitative analysis programs, implementing different calculation methods:
  - Using calibrations obtained via Linear Regression method derived from measured standards
  - Standard-less "Fundamental Parameter" calculation method
  - Standard-based "Fundamental Parameter" method
- A Batch module for the analysis of large amount of XRF spectral files in an unattended way.
- A tool program for creating compressed scan image data files

FEATURES

- Implements two types of peak shapes: "Gaussian" and "Voight profile"
- Inclusion of additional peak shape components as "Tail" and "Step" fraction functions
- Possibility to fit coherent and incoherent excitation peaks
- Capabilities to fit non-fluorescence peaks (E.g. Gamma-rays, diffraction peaks, etc.)
- Visual distinction and marking of "sum" and "escape" peaks in the spectrum plot
- Advanced graphical user interface (GUI) that can be set to user's preferences
- Great traceability, saving all information into XML-formatted files (*.axml)
- Customizable analysis reports
- Quantification via different methods:
  - "Linear regression" using calibration standards
  - Standard-based "Fundamental Parameter Method"
  - Standard-less "Fundamental Parameter Method"
- Additional module for file batch analysis in an unattended mode of operations
- **Special option for macro-XRF image scan analysis, with ultra fast "hybrid" fitting algorithm and image data compression**
- Additional tool program for creating compressed image scan data using intelligent and "spectroscopy-aware" algorithms
- The software is multi-platform and runs seamlessly under MS Windows™, MAC OS™ or Linux®

SPECTRUM ANALYSIS

The distinction of bAxil software package lies on its powerful spectrum analysis engines. They can analyze any ED XRF spectrum independently of its complexity, number of lines, type of excitation and/or detection system.

bAxil spectrum evaluation is basically based on building a mathematical model to which the analyst tries to describe the recorded experimental data (spectrum). This is done by specifying the region of interest (ROI) on the spectrum, the selection of the continuum (background) compensation method, the identification and selection of the X-ray lines (peaks) to be included in the model with their individual peak parameters, and establishing the correct values for energy calibration parameters of the spectrometer. The model also might include the conditions (excitation, type of detector, measurement setup) under which the spectrum has been recorded. The model parameters are then optimized by means of non-linear least squares method, using a modified Marquardt algorithm to minimize the sum of differences (χ^2) between the experimental data and the established mathematical model.

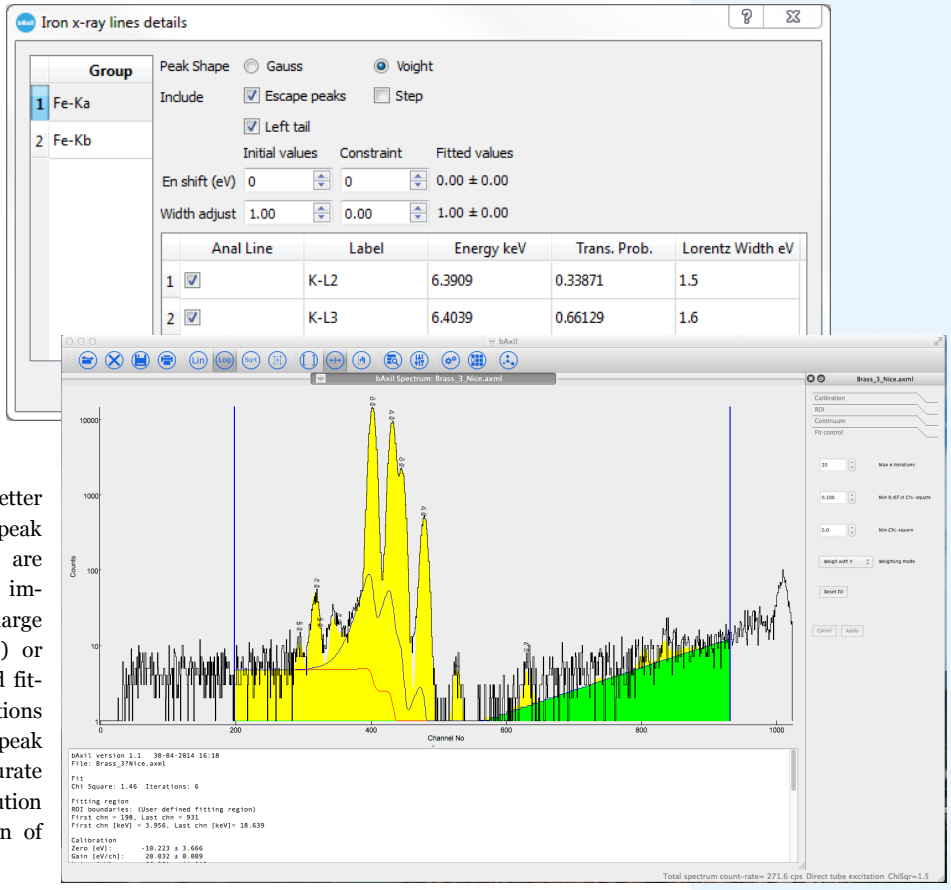
The distinction of bAxil software lies on its powerful spectrum analysis engines

Newly, the spectrum analysis in bAxil incorporates the selection between two types of peak shapes:

- "Gaussian" peak type or, alternatively
- a Voight-profile

The latter describes better the peak-shapes resulting from high Z elemental emissions. Additionally to these peak shapes, peak components can be added as well, such as:

- "Step" fraction component and/or
- "Shelf" or "Tail" component



These peak shape components allows a better fit of peak's deviations from the selected peak shape (e.g. Gaussian). These deviations are commonly seen in today's spectra due to improved detection technology (e.g. drift charge collection, better energy resolution, etc.) or higher count-rates, etc. Peak analysis and fitting engine accounting for these deviations determine more precisely the individual peak contributions and result in more accurate peak's net area calculation, peak's contribution in a multiplet, and/or correct calculation of trace emissions in nearby large peaks.

Moreover, each peak component can be set with its own particular constraint, allowing in such a way a better fit to distorted line emissions (due to effects like scattering or diffraction). The different peak shapes and/or peak shape components can be applied to individual peaks or to all peaks in the analysis.

Additionally, bAxil has the capability to include into the fitting process peaks that do not necessarily result from the fluorescence process, such as gamma-ray or diffraction peaks. The analysis of these peaks might bring important and additional information to the sample analysis or complement the spectrum evaluation.

bAxil incorporates up to six different mathematical models for the spectrum continuum (background), which covers most of the ED XRF excitation modes and allows the software to analyze any ED XRF spectrum independently of its excitation.

The newly developed spectrum analysis methods have the capability to fit wider peaks, such as peaks resulting from multiple scattering in the sample or detector, e.g. Coherent and Incoherent peaks from the excitation. The results of such analysis can be used into more extensive calculations for the determination of the sample matrix.

SPECTRUM ANALYSIS

- Selection of a peak function from "Gaussian" and "Voight" profile
- Addition of peak shape components: "Tail" and "Step" fractions
- Fitting of scattered peaks: incoherent and Coherent excitation peaks
- Inclusion of peak analysis of non-fluorescence nature (e.g. gamma-ray, diffraction peaks, etc.).

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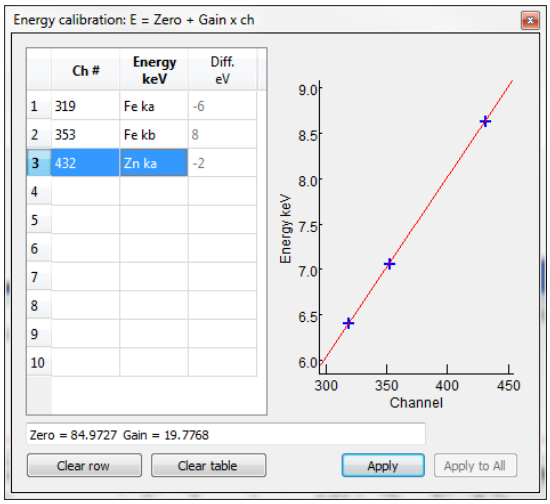
GRAPHICAL USER INTERFACE

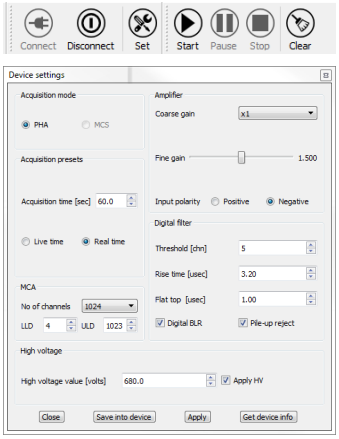
bAxil's graphical user interface (GUI) is easy-to-use, instantly accessible, intuitive, and yet a powerful tool for visual inspection of the XRF spectral data and its analysis. results The GUI is a multiple-document type and can display multiple spectra inside the common program's main window. It also uses docking widgets (e.g. for the model), which conveniently provides quick access to most model parameters and commands, allowing fast changes and instant feedback of the spectrum analysis results for the chosen conditions.



bAxil provides different functions and tools necessary for aiding with the spectrum analysis process, such as "energy calibration" and "peak search" functions. It does so in a very easy and intuitive way.

A graphical "Table of Elements", together with corresponding KLM markers, provides visual help in identifying the X-ray lines in the spectrum, as well as defining their particular peak-shape components.

The new bAxil GUI can easily zoom into any region of the spectrum. The components of the peak analysis (continuum, "Step" and "Tail" fraction components, etc.) can be individually displayed providing best visual feedback of the analysis results. A dedicated plot with the residuals from the fitting process helps the user to immediately spot the missed or poorly fitted regions. With a mouse click plot scales can be easily changed (e.g. to Logarithmic, Linear or Square-root) and axes set into different units (e.g. keV, cps, etc.) as well.



The spectrum plot has the capabilities to visually distinguish the peaks according to their nature, e.g. "sum" and "escape" peaks, marking and displaying them (and their exact peak contribution) in different colors.

bAxil Graphical user interface is easy-to-use, intuitive and yet a powerful tool for spectrum analysis review

The GUI also incorporates the necessary dialogs, toolbar buttons and commands to perform a data acquisition and control of a BrightSpec MCA, such as Topaz-X. It even allows to analyze this spectrum while its data is being acquired.

All the GUI components (colors, scales, etc.) and the spectrum plot can be configured to the user's preferences.

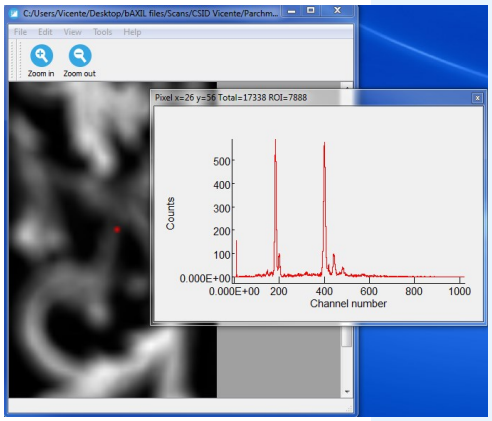
Reports can be user-defined via report templates. Report templates uses HTML-compatible scripting language together with block-structured commands for creating the reports. A set of predefined report templates (e.g. "Short" and "Long" report templates) are provided as well and ready to use.

FILES AND OTHERS

bAxil can import spectra saved under different file formats, like *.spe formatted files (QXAS), *.wax (WinAxil) binary files, and many others.

Currently, bAxil uses XML-formatted files (*.axml) and stores nearly all the information concerning the spectral data, measurements conditions and analysis results. This way of data storage provides superior analysis traceability and improves the quality control of the data results.

Spectrum analysis results can be easily exported into ASCII files (plain text files or comma-delimited *.csv files) as well.



CREATION OF IMAGE SCAN DATA

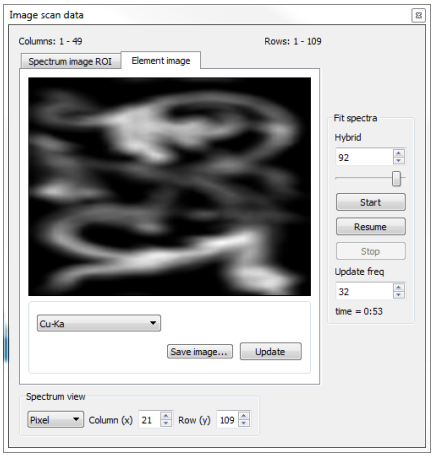
bAxil software package includes a module for creating compressed image scan data. This program uses an intelligent algorithm to compress into a single file all image-related data as well as recorded energy spectra from the object scan. Using this program a ten-fold data compression and much quick access to pixel spectra is guarantied. The resulted compressed image scan data file (*.csid) is the input for the scan image analysis module built into bAxil spectrum analysis software.

SOFTWARE PACKAGE

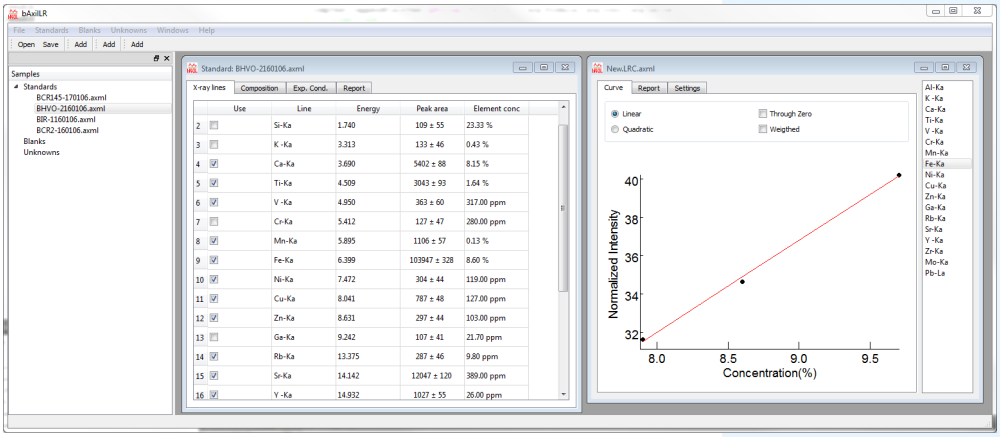
- bAxil: spectrum analysis program, which includes:
  - Image scan analysis
  - Data acquisition and MCA control of BrightSpec devices
- bAxilBatch: File Batch analysis
- bAxilConvertSID: Tool program for creating compressed image scan files
- bAxilLR: Program for quantitative calculations using Linear Regression method
- bAxilFP: Program for quantitative calculations using "*Fundamental Parameter*" method

ANALYSIS OF IMAGE SCAN DATA

bAxil program integrates an essential new engine in the spectrum analysis process: the image scan analysis engine. Using this module the user can open an image scan file (which contains multiple spectra) and interactively analyze and review them. The new graphical interface creates an elemental image out of the spectrum analysis of each individual spectrum (pixel) of the scanned area or object. Besides creating the elemental image map, it provides an interactively way of reviewing each pixel results.



Most importantly, bAxil features a new "hybrid" calculation engine for this particular and singular analysis. In this mode, the program combines the standardly used non-linear square fit with linear fit and parameters optimization methods. This results into analysis of large amount of spectra in very short time; e.g. million of spectra in less than few minutes.



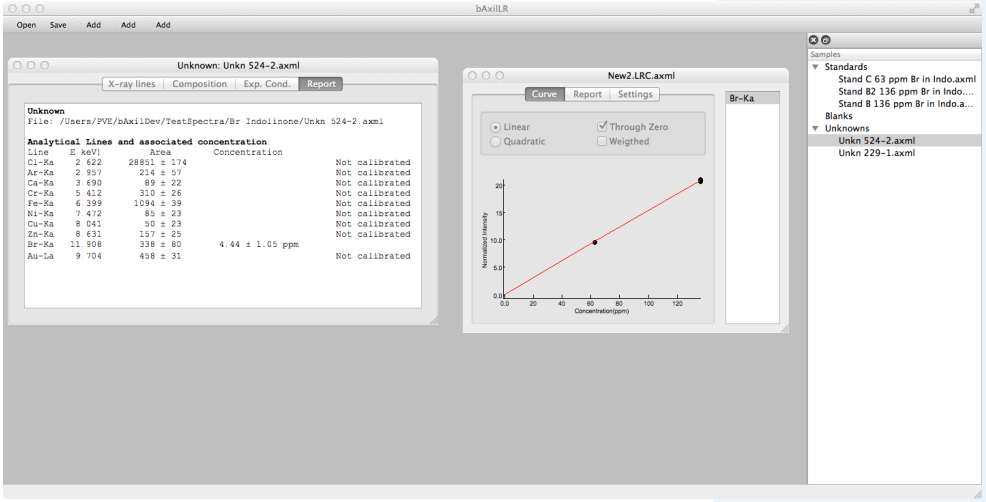
QUANTITATIVE ANALYSIS

bAxil calculates the elemental concentrations in the sample using several methods. The choice of the quantization calculation method is up to the user and can be switched quickly and easily for achieving best results.

The implemented quantitative calculation methods are:

1. Calculation of calibration functions using "Linear regression" method obtained from the analysis of the measured standards
2. Standard-based "Fundamental Parameter" method
3. Standard-less "Fundamental Parameter" method

Additionally, the quantitative calculation methods have the capability to correct for "instrumental" or "blank" concentrations .



REQUIREMENTS

bAxil is a multiplatform software and runs on the following OS:

- Microsoft Windows XP™, Windows 7™ and Windows 8™
  ⇒ 32-bit or 64-bit processors
- MAC OS®™
- Linux® OS

ORDERING INFORMATION

1. bAxil application software. Single license
2. bAxil application software. Network license.
   - A single network key with a requested number of licenses activated
3. Any of above configurations, but with the addition of the printed User's Manual.
4. bAxil package: Includes full bAxil software (single license) + Topaz-X MCA

ADDITIONAL INFORMATION

The bAxil product line includes the "bAxil Programming libraries", which are offered as separate product. Please contact us for more details on using "bAxil programming libraries" and its license options.

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