

# QXAS

## X-RAY Analysis Software

### Features:

- X-Ray and X-Ray Fluorescence Analysis Software package
- Energy-, Sensitivity- and Efficiency calibration
- X-Ray Library Manager with editor
- Complex Spectrum Fitting
- NBS Quantitative Analysis function
- AMX Quantitative Analysis function
- Example Spectrum

### Description:

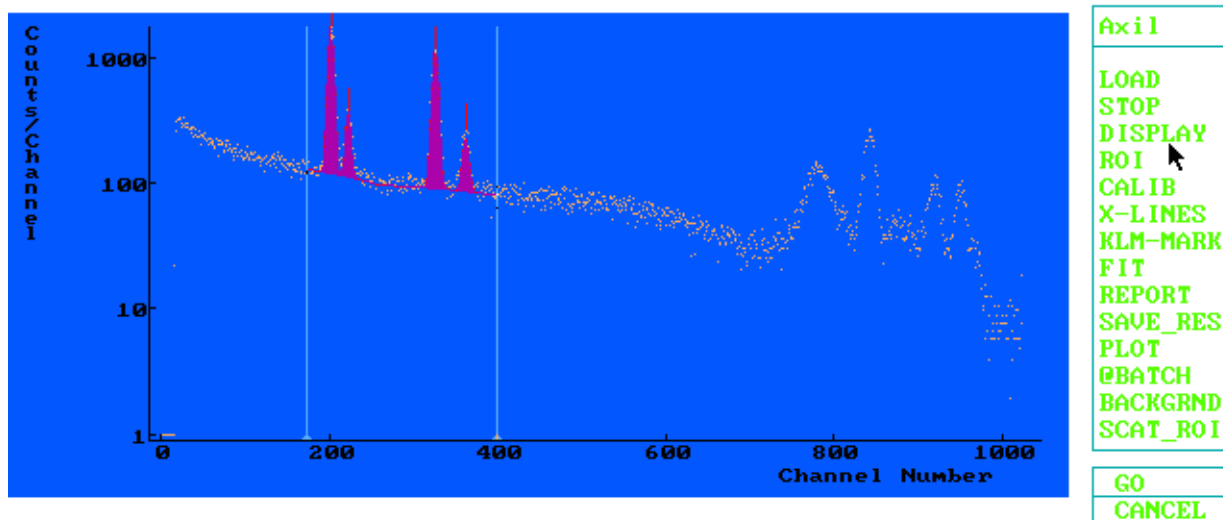
Developed under the auspices of the IAEA in cooperation with:  
 The University of Antwerp, Belgium  
 La Direccion Nacional de Tecnologia Nuclear, Uruguay  
 La Direccion General de Energia Nuclear, Guatemala  
 Ruder Boskovic Institute, Croatia  
 Instituto de Asuntos Nucleares, Colombia

The Package contains the following components:  
 Disk 1: AXIL: main programs:  
           AXFIT: spectrum fitting

AXPAR, AXRLM: parameter setup  
 Disk 2: Quantitative X-Ray Analysis of Light Matrix Materials  
           NBS Quantitative Analysis System  
           System Sensitivity and Efficiency Calibration  
           Utilities: Communication with other computers,  
                     X-Ray absorption calculations,  
                     Stability analysis  
 Disk 3: Simple quantitative analysis  
           Direct computation of count rates  
           elemental sensitivities  
 Disk 4: AMX Quantitative Analysis program v 1.0  
           Quantitative Analysis using fundamental parameters

The software is menu controled, for example the main menu contains:  
 \* System hardware setup  
 \* Execute DOS command  
 \* Spectrum analysis  
 \* Spectrum format conversion  
 \* Quantitative analysis  
 \* Utilities  
 \* Simple Quantitative analysis  
 \* Quantitative Analysis using fundamental parameters

Spectrum ALLOY1.SPE      Initial guess: ChiSquare =      4.2



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The Spectrum Analysis menu contains:

- \* Perform spectrum fitting
- \* Specify parameters for spectrum analysis
- \* X-ray library management

To perform a spectrum analysis, just specify the spectrum file (example: ALLOY1.SPE), define the fitting region and calibration, and enter the names of the lines contained in the spectrum:

ADD CR  
ADD ZN

The printout below shows the fit result obtained for the Cr and Zn K lines, This is an example of a typical report file

- To run a simple quantitative Analysis, first the calibration must be defined selecting
- \* Define Calibration and Standards and then
- \* Create new calibration file
- A form is displayed to fill all the items, using <F1> for assistance. This way a calibration file has to be made. Then standards have to be provided using
- \* Add Standards
- Furthermore, a calibration has to be made using
- \* Perform calibration of X-ray system
- As a result, a list of calculated sensitivities is made and this calibration can be optimized using
- \* Optimize calibration with Least squares fit
- The sensitivity can be plotted and a report file written.
- Finally, the unknown sample can be analysed using
- \* Analyse of Unknown Samples.

```

+-----+-----+
|          IBM-PC V3.00          |          04-04-1995   |          11:03:44
| Spectrum: ALLOY1.SPE          |                        |                        |
+-----+-----+
| Fitting Region: channels 175 - 400 |          1 iterations done
| ChiSquare = 4.2 last change = .00% |          lambda= 1.E-03
+-----+-----+
|                   CALIBRATION DATA                   |
+-----+-----+
|                   Initial estimate                   |                   Final estimate                   |
+-----+-----+
| ZERO (eV)          |          141.9 ± 200.0 |          141.9 ± .0
| GAIN (eV/ch)       |          25.961 ± 2.000 |          25.961 ± .000
| det NOISE (eV)     |          150.0 ± 50.0  |          150.0 ± .0
| FANO factor        |          .114 ± .050   |          .114 ± .000
+-----+-----+

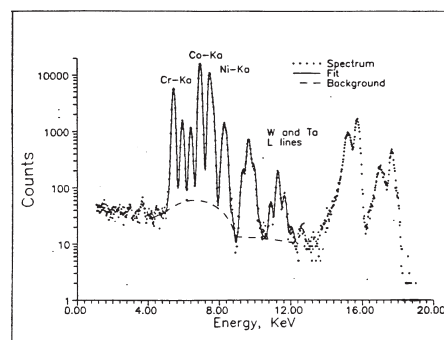
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+-----+-----+
|                   PEAK DATA                   |
+-----+-----+
| # Line            | E(KeV) | rel. int. | peak area | st. dev | chi-sq |
|                   | chan#  | fwhm (eV) | backgr    |          | tot. abs |
+-----+-----+
| 1 Cr-K           |         |           |           |         |         |
|   KA1            | 5.412  | .88264    | 16328. ±  | 0.      | 18.5
|                   | 203.000 | 188.87    | 14411. ±  | 42.     | 8.73E-01
|   KB1            | 5.947  | .11736    | 1916. ±   | 41.     | 6.8
|                   | 223.608 | 192.29    | 1644.    |         | 9.02E-01
+-----+-----+
| 2 Zn-K           |         |           |           |         |         |
|   KA1            | 8.639  | .58032    | 10858. ±  | 0.      | 13.1
|                   | 327.301 | 208.63    | 6301. ±   | 36.     | 9.66E-01
|   KA2            | 8.616  | .29832    | 3239. ±   | 36.     | 16.6
|                   | 326.415 | 208.49    | 1332.    |         | 9.66E-01
|   KB1            | 9.572  | .12135    | 1318. ±   | 38.     | 5.5
|                   | 363.239 | 214.00    | 1439.    |         | 9.75E-01
+-----+-----+
|                   FILTER BACKGROUND                   |
+-----+-----+

```

The figure below shows a spectrum and background fit of a standard high temperature alloy sample with certified concentration



Part of the spectrum of SRM 1199 sample and fitted spectrum.