



X-Ray Absorption Fine Structure

XAFS

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5th School on X-Ray Spectroscopy Methods



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1. Athena, some aspects of the program
2. How to open a data file
3. First steps in treat data
4. Extracting the signal for an iron foil fe.060
5. To do: following Bruce Ravel example on Iron
6. Linear Combination Fitting...

Our Merlin:



Bruce Ravel and his magic!

1. Athena, some aspects of the program

ATHENA is an interactive graphical utility for processing EXAFS data....

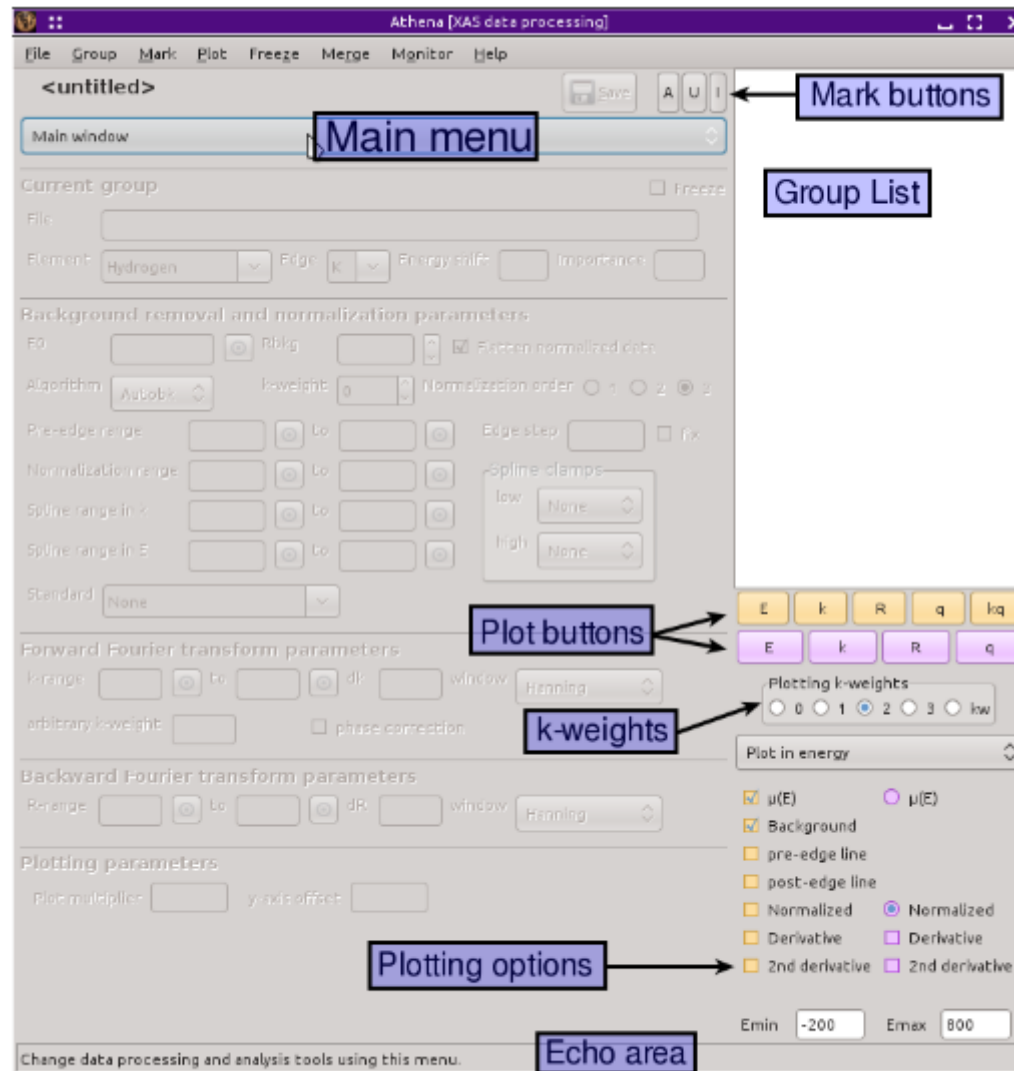


Fig. 2.1 The parts of ATHENA.

1. Athena, some aspects of the program

Among ATHENA's many, many features, you will find:

- Convert raw data to $\mu(E)$
- File import plugins for reading arbitrary data files
- Process and plot multiple data scans simultaneously
- Merge data as $\mu(E)$, normalized $\mu(E)$, or $\chi(k)$
- Energy calibration
- Align data scans with or without a reference channel
- Deglitch, truncate, convolve, or smooth $\mu(E)$ data
- Self-absorption corrections for fluorescence spectra
- Compute difference spectra
- Fit linear combinations of standards to $\mu(E)$, derivative of $\mu(E)$, or $\chi(k)$ data
- Fit peak functions to XANES data
- Log-ratio/phase-difference analysis
- Background removal using the AUTOBK algorithm
- Forward and backward Fourier transforms
- Save data as $\mu(E)$, normalized $\mu(E)$, $\chi(k)$, $\chi(R)$, or back-transformed $\chi(k)$
- Save project files, allowing you to return to your analysis later
- ... and much, **MUCH** more!

2. How to open a data file

ATHENA is very versatile in how she reads in data files. Pretty much any data in the form of columns of numbers can be successfully read...

Here is an example of a data file that will make ATHENA quite happy. There are some header lines, followed by a line of dashes, followed by a line of column labels, followed by lines containing columns of data.

```
# X15B project: MT 9/23/04
# original file: STD1.001
# unpacked from original data as a sequence of 4-byte floats
# -----
# energy      I0      narrow    wide
2400.0020    60183.3008    38.5000    83.0000
2401.5088    60241.0508    41.5000    82.0000
2403.0078    60347.5508    40.0000    83.7500
2404.5039    60531.0508    42.2500    78.2500
... etc ...
```

In this example of a well formatted file, the header lines, the line of dashes, and the column labels line are all preceded by a hash (#) mark. IFEFFIT is thus able to recognize these as header lines.

2. How to open a data file

Here are some operations that can be performed as data is imported.

- Data from a multi-element detector can be summed on the fly.
- Data from a multi-element detector can be imported such that each detector channel is imported into its own data group.
- Data can be negated, i.e. multiplied by -1, or multiplied by an arbitrary constant
- A reference channel can be read from the the same file.
- Data can be preprocessed. That is, data can be truncated, deglitched, aligned to a standard, and have its parameters constrained to a standard

Here are some operations that can be handled using the Plugin architecture.

- Data can be imported as a function of pixel position on an area or linear detector.
- Conversion from wavelength to energy.
- Conversion from encoder reading or motor steps to energy.
- Conversion of data in a binary format
- Dead-time corrections using columns from the data file.
- Any math expression more complicated than sums of columns in the numerator and denominator, e.g. plugins allow you to multiply the I_f column by 7 and divide by the sine of the I₀ column, if that's what you really want.

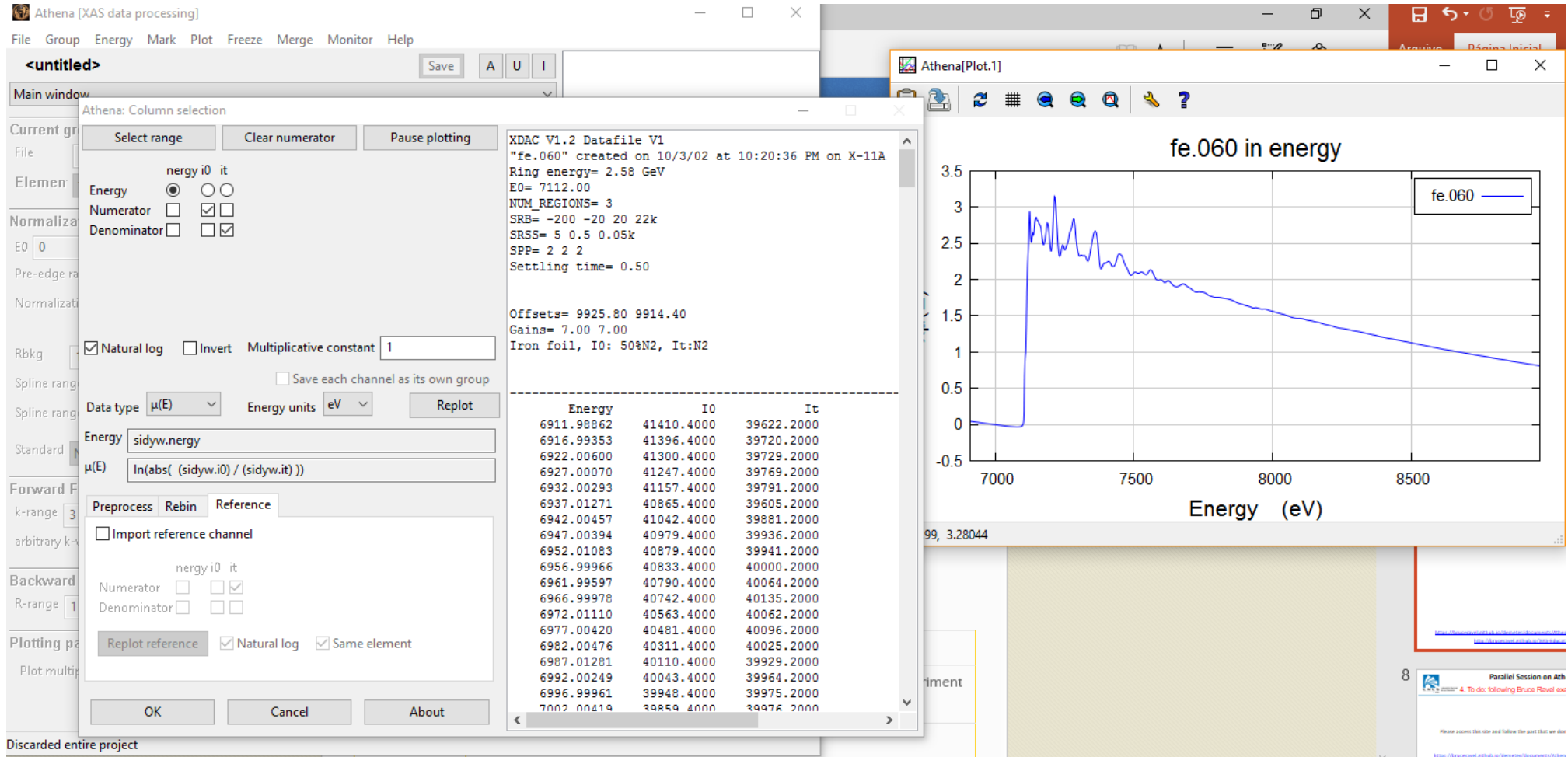
If some of the criteria for the data file format are not met, for example if there is text following the data columns or if you need to perform one of the operations not yet supported, you will need to process you data before trying to import into ATHENA.

3. First steps in treat data

1. Calibration
2. Pre-edge fitting
3. Post-edge normalization
4. E0
5. Extraction of the signal
6. Fourier Transform
7. Rbkg
8. K-weight
9. Selection of the region of interest
10. Save the file!

4. Extracting the signal for fe.060

0. Import data



The screenshot shows the Athena software interface with the 'Athena: Column selection' dialog box open. The dialog box contains the following information:

XDAC V1.2 Datafile V1
 "fe.060" created on 10/3/02 at 10:20:36 PM on X-11A
 Ring energy= 2.58 GeV
 E0= 7112.00
 NUM_REGIONS= 3
 SRB= -200 -20 20 22k
 SRSS= 5 0.5 0.05k
 SPP= 2 2 2
 Settling time= 0.50

Offsets= 9925.80 9914.40
 Gains= 7.00 7.00
 Iron foil, I0: 50%N2, It:N2

Energy	I0	It
6911.98862	41410.4000	39622.2000
6916.99353	41396.4000	39720.2000
6922.00600	41300.4000	39729.2000
6927.00070	41247.4000	39769.2000
6932.00293	41157.4000	39791.2000
6937.01271	40865.4000	39605.2000
6942.00457	41042.4000	39881.2000
6947.00394	40979.4000	39936.2000
6952.01083	40879.4000	39941.2000
6956.99966	40833.4000	40000.2000
6961.99597	40790.4000	40064.2000
6966.99978	40742.4000	40135.2000
6972.01110	40563.4000	40062.2000
6977.00420	40481.4000	40096.2000
6982.00476	40311.4000	40025.2000
6987.01281	40110.4000	39929.2000
6992.00249	40043.4000	39964.2000
6996.99961	39948.4000	39975.2000
7002.00419	39859.4000	39976.2000

The plot window shows the 'fe.060 in energy' plot with Energy (eV) on the x-axis (7000 to 8500) and intensity on the y-axis (-0.5 to 3.5). The plot shows a sharp peak at approximately 7112 eV, followed by a decay. The legend indicates the data series is 'fe.060'.

<https://bruceravel.github.io/demeter/documents/Athena/examples/index.html>

DATA: <http://bruceravel.github.io/XAS-Education/>

4. Extracting the signal for fe.060

0. Import data

The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group as 'fe.060' with the element set to 'Iron' and the edge to 'K'. The interface is divided into several sections for parameter configuration:

- Normalization and background removal parameters:** Includes fields for E0 (7105.50673), normalization order (3), pre-edge range (-150.000 to -30.000), normalization range (150.000 to 1757.437), and edge step (2.8319775).
- Forward Fourier transform parameters:** Includes k-range (3.000 to 20.080), dk (1), window (Hanning), and arbitrary k-weight (0.5).
- Backward Fourier transform parameters:** Includes R-range (1 to 3), dR (0.0), and window (Hanning).
- Plotting parameters:** Includes plot multiplier (1) and y-axis offset (0).

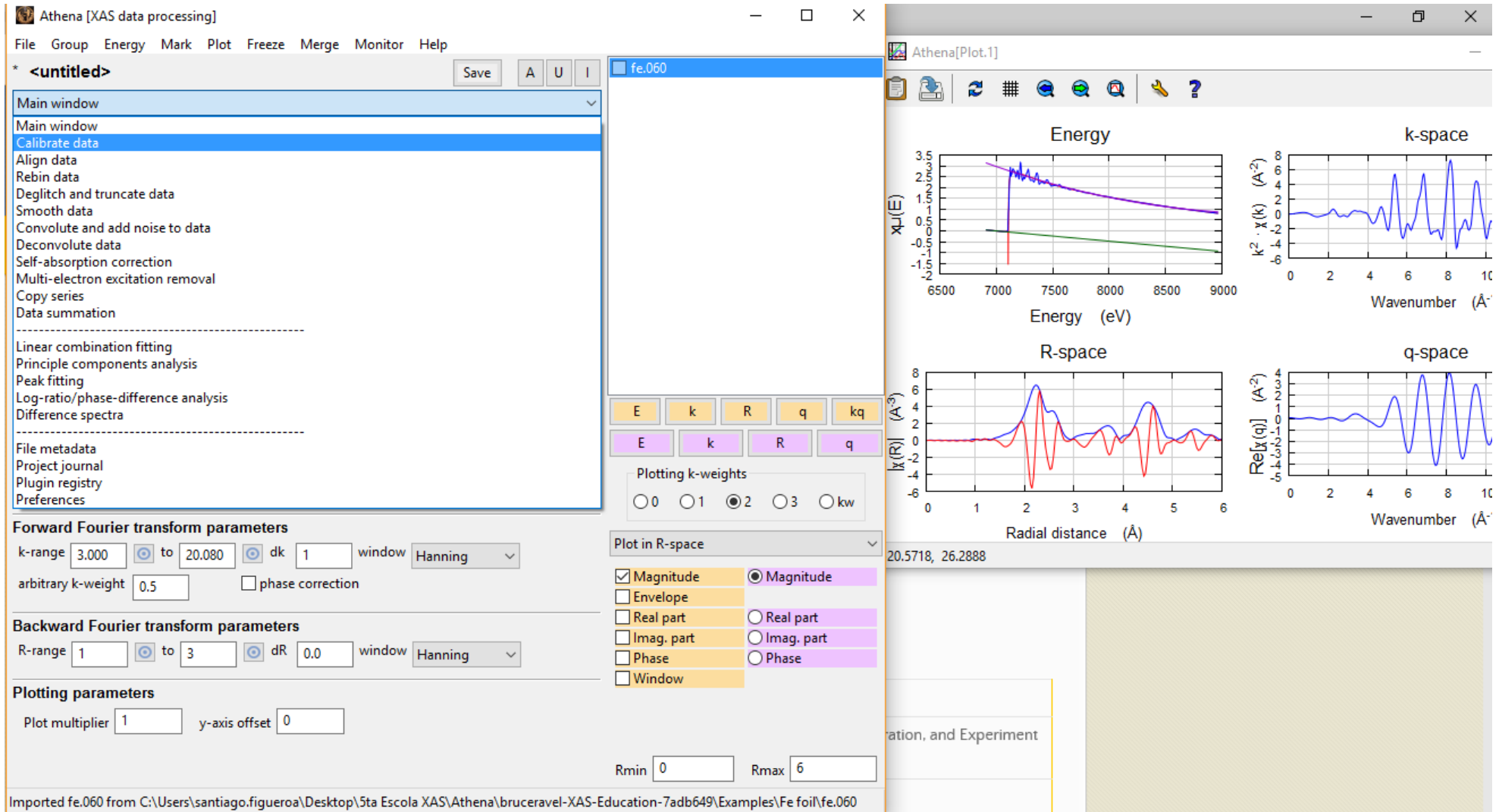
On the right, the 'Athena[Plot.1]' window displays four plots:

- Energy:** A plot of $\chi(E)$ versus Energy (eV), showing a sharp peak at approximately 7100 eV.
- k-space:** A plot of $k^2 \cdot \chi(k)$ (\AA^{-2}) versus Wavenumber (\AA^{-1}), showing oscillatory behavior.
- R-space:** A plot of $k(R)$ (\AA^{-3}) versus Radial distance (\AA), showing oscillatory behavior.
- q-space:** A plot of $\text{Re}[\chi(q)]$ (\AA^{-2}) versus Wavenumber (\AA^{-1}), showing oscillatory behavior.

At the bottom, there are checkboxes for 'Plot in R-space' and 'Plotting k-weights' (0, 1, 2, 3, kw), with 'Magnitude' selected for both.

4. Extracting the signal for fe.060

1. Calibration



Athena [XAS data processing]

File Group Energy Mark Plot Freeze Merge Monitor Help

* <untitled> Save A U I fe.060

Main window

- Main window
- Calibrate data
- Align data
- Rebin data
- Deglitch and truncate data
- Smooth data
- Convolute and add noise to data
- Deconvolute data
- Self-absorption correction
- Multi-electron excitation removal
- Copy series
- Data summation

- Linear combination fitting
- Principle components analysis
- Peak fitting
- Log-ratio/phase-difference analysis
- Difference spectra

- File metadata
- Project journal
- Plugin registry
- Preferences

Forward Fourier transform parameters

k-range 3.000 to 20.080 dk 1 window Hanning

arbitrary k-weight 0.5 phase correction

Backward Fourier transform parameters

R-range 1 to 3 dR 0.0 window Hanning

Plotting parameters

Plot multiplier 1 y-axis offset 0

Plot in R-space

- Magnitude Magnitude
- Envelope
- Real part Real part
- Imag. part Imag. part
- Phase Phase
- Window

Rmin 0 Rmax 6

Imported fe.060 from C:\Users\santiago.figueroa\Desktop\5ta Escola XAS\Athena\bruceravel-XAS-Education-7adb649\Examples\Fe foil\fe.060

Athena[Plot.1]

Energy

$X\mu(E)$ vs Energy (eV)

k-space

$k^2 \cdot \chi(k)$ (Å⁻²) vs Wavenumber (Å⁻¹)

R-space

$\chi(R)$ (Å⁻³) vs Radial distance (Å)

q-space

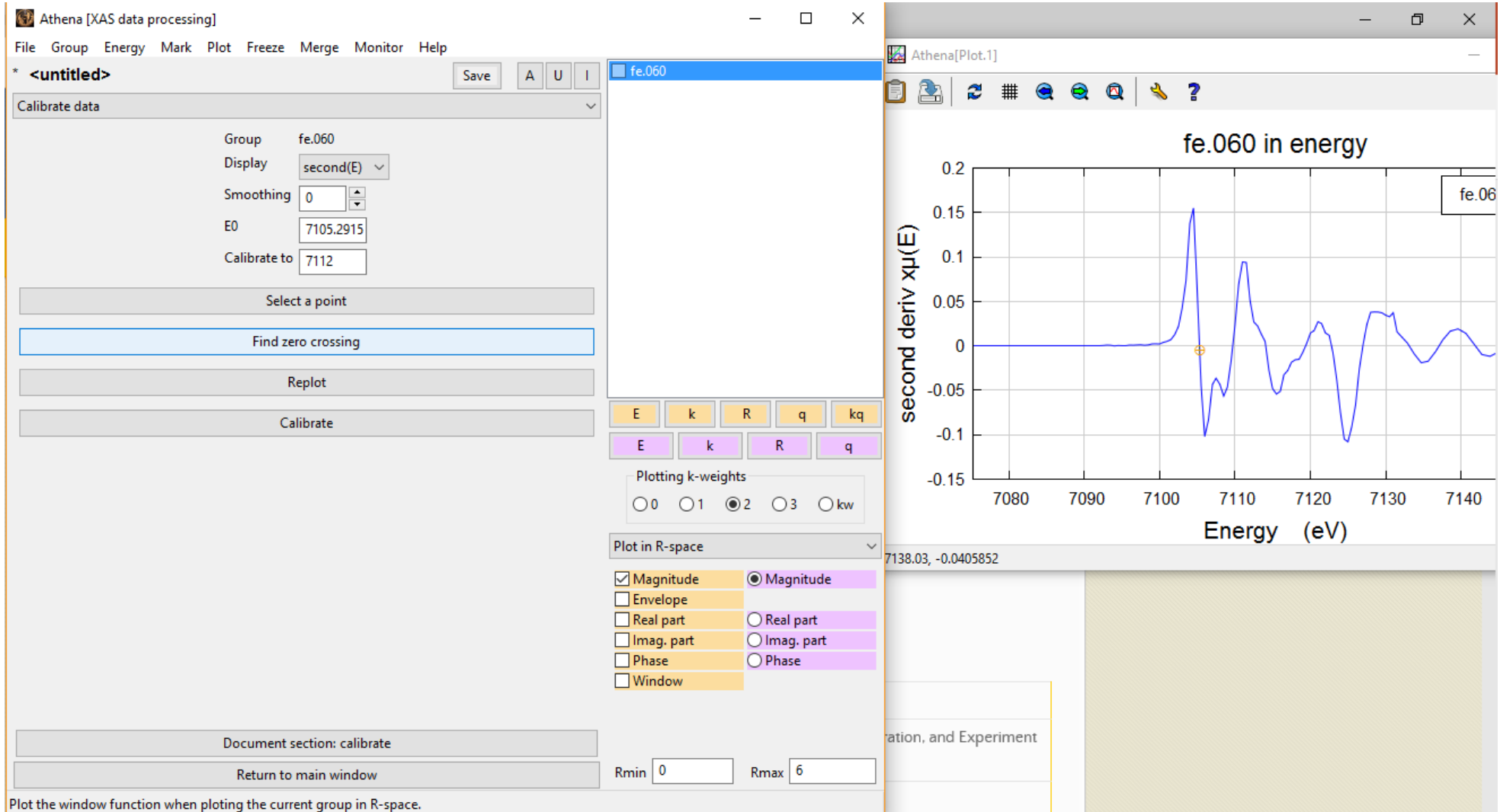
Re[$\chi(q)$] (Å⁻²) vs Wavenumber (Å⁻¹)

20.5718, 26.2888

ation, and Experiment

4. Extracting the signal for fe.060

1. Calibration



The screenshot displays the Athena [XAS data processing] interface. The main window is titled "Athena [XAS data processing]" and contains a menu bar (File, Group, Energy, Mark, Plot, Freeze, Merge, Monitor, Help) and a toolbar. The "Calibrate data" panel is active, showing the following settings:

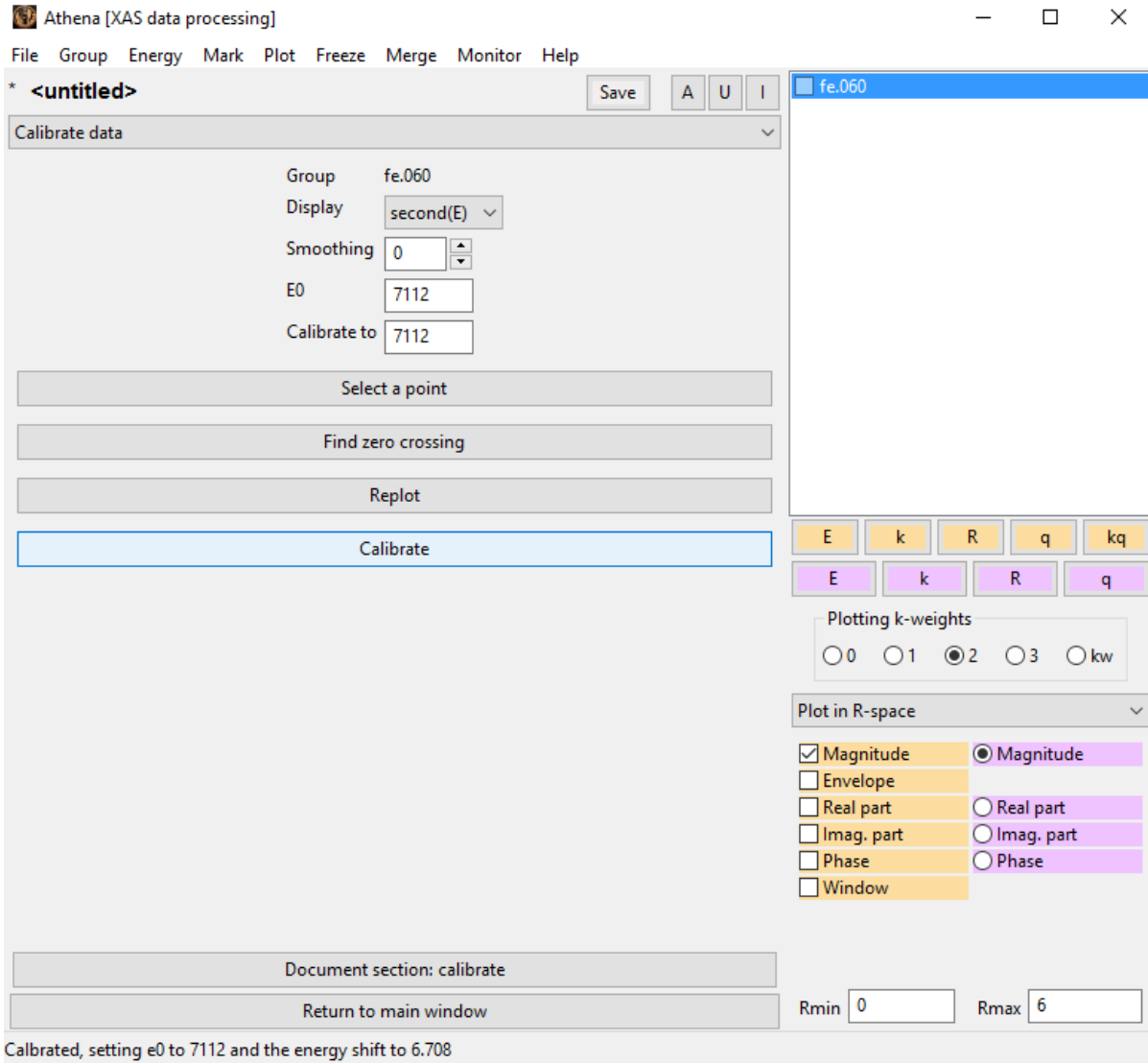
- Group: fe.060
- Display: second(E)
- Smoothing: 0
- E0: 7105.2915
- Calibrate to: 7112

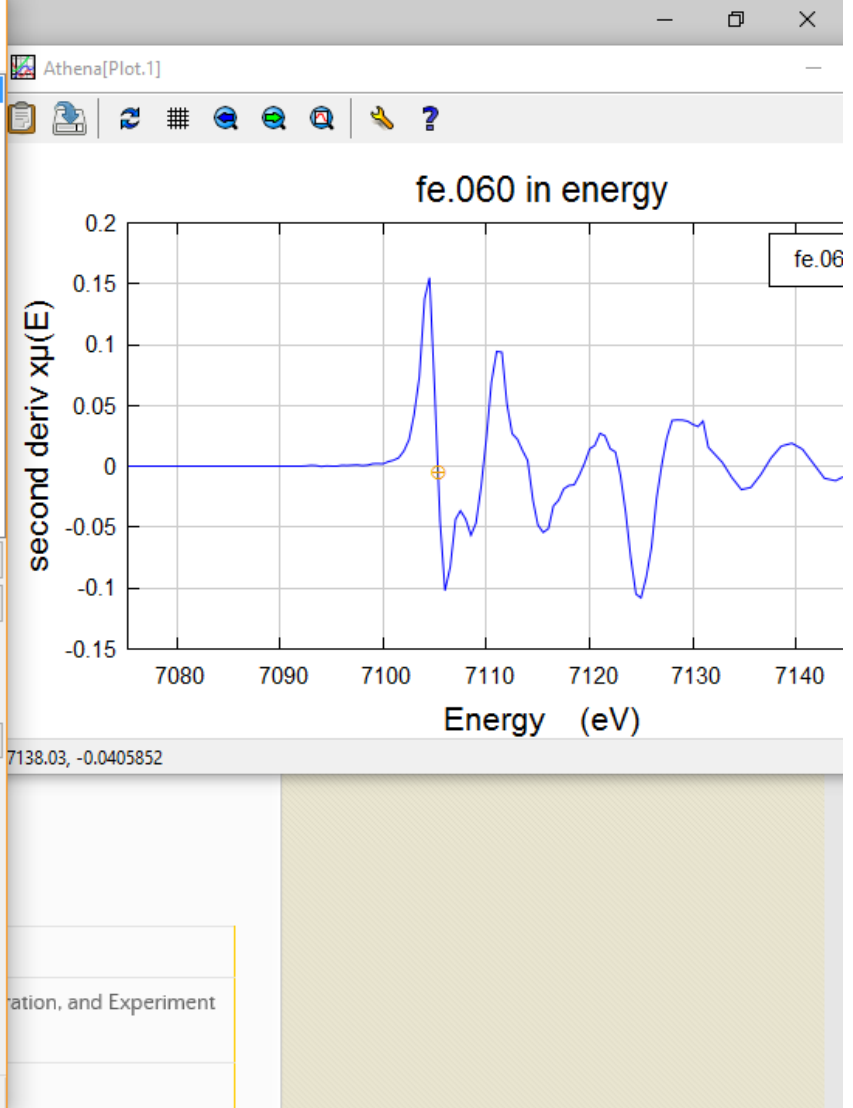
Buttons for "Select a point", "Find zero crossing", "Replot", and "Calibrate" are visible. Below the calibration panel, there are buttons for "E", "k", "R", "q", and "kq", and a "Plotting k-weights" section with radio buttons for 0, 1, 2 (selected), 3, and kw. The "Plot in R-space" section includes checkboxes for Magnitude (checked), Envelope, Real part, Imag. part, Phase, and Window. At the bottom, there are input fields for "Rmin" (0) and "Rmax" (6).

On the right, a plot window titled "Athena[Plot.1]" shows the "second deriv xp(E)" versus "Energy (eV)" for the "fe.060" signal. The plot displays a blue line with a prominent peak at approximately 7112 eV. A cursor is positioned at the peak, showing coordinates: 7138.03, -0.0405852. The x-axis ranges from 7080 to 7140 eV, and the y-axis ranges from -0.15 to 0.2.

4. Extracting the signal for fe.060

1. Calibration

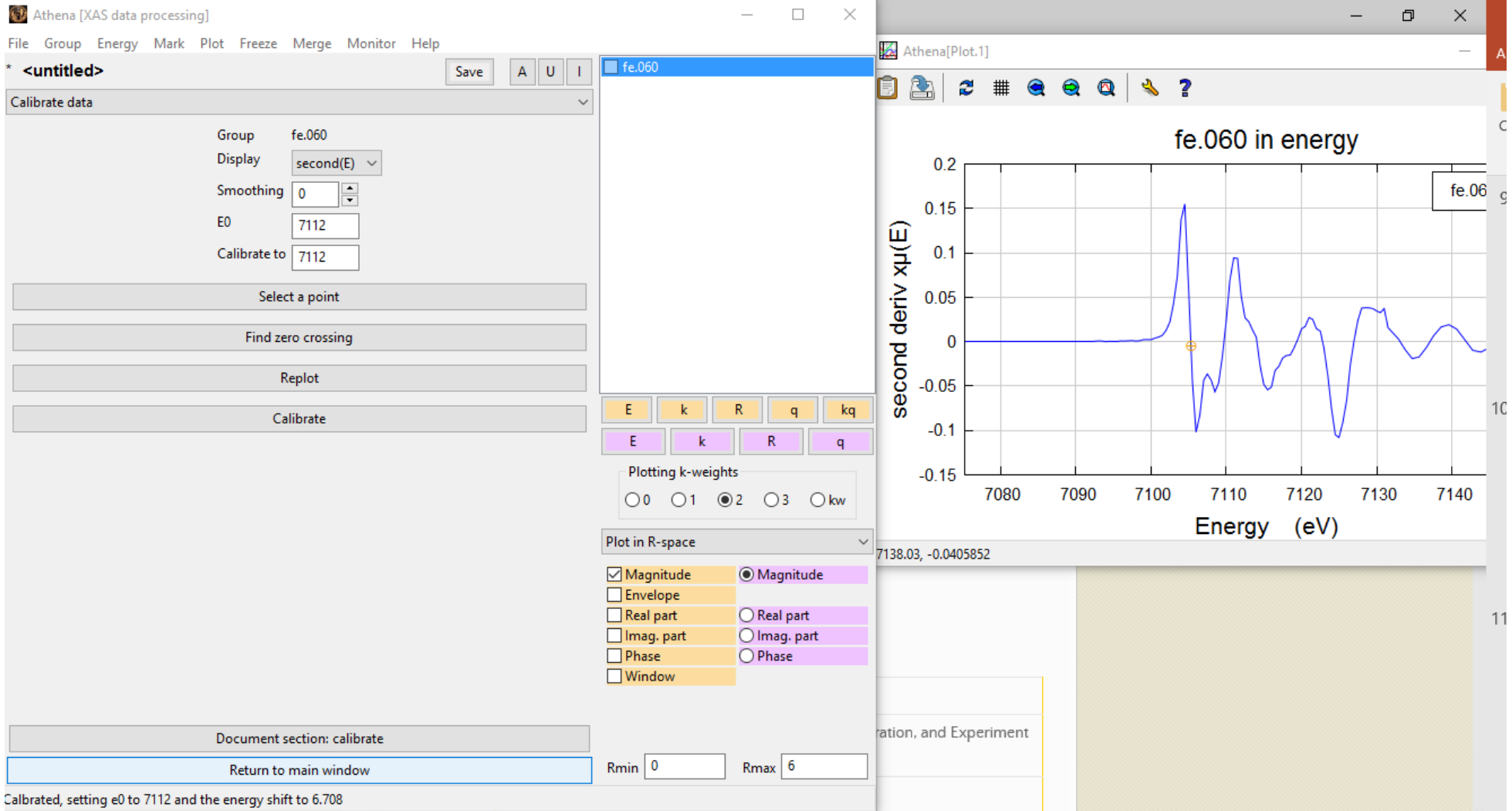




Calibrated, setting e0 to 7112 and the energy shift to 6.708

4. Extracting the signal for fe.060

1. Calibration



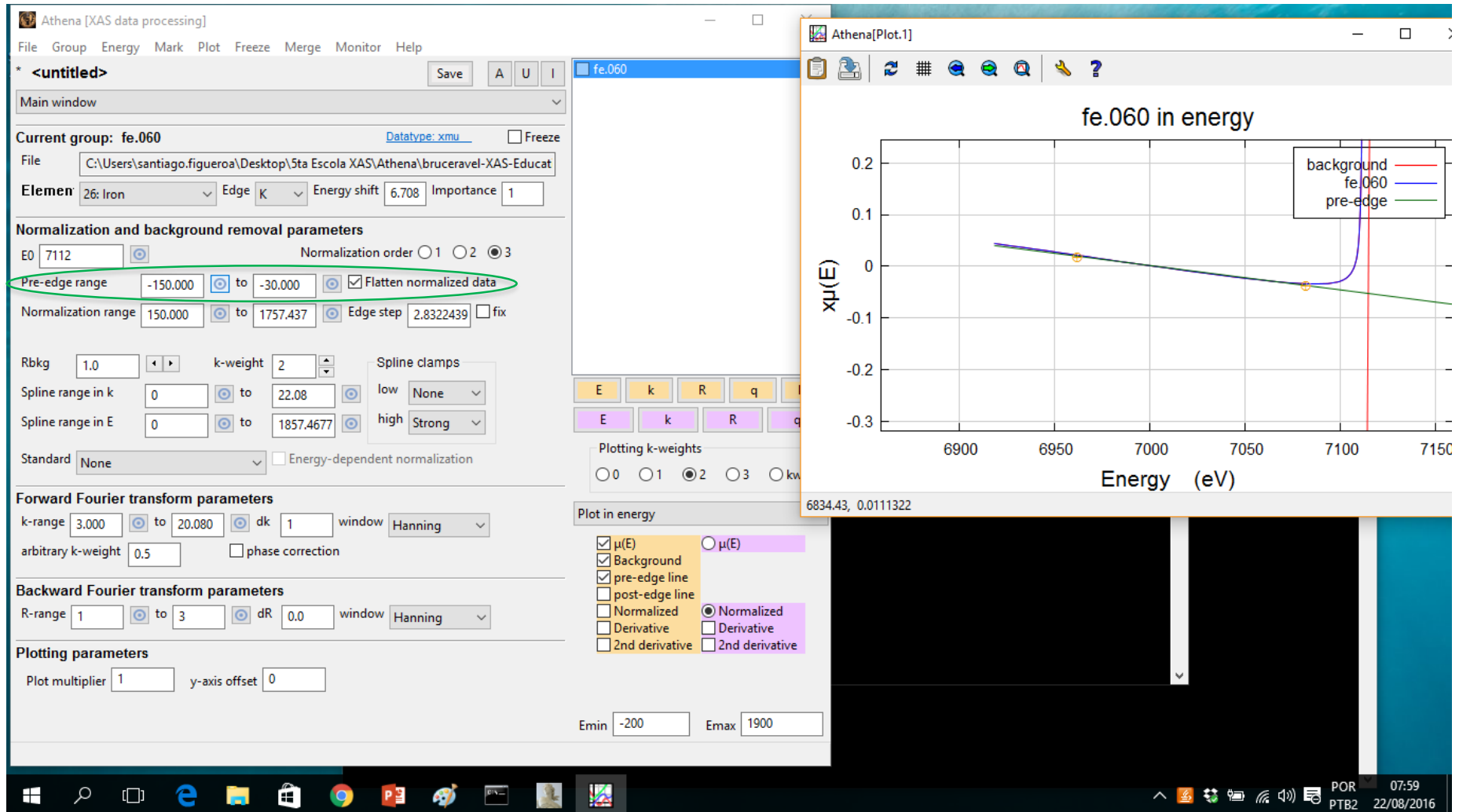
The screenshot displays the Athena software interface for XAS data processing. The main window is titled "Athena [XAS data processing]" and shows a "Calibrate data" panel on the left. The "Group" is set to "fe.060", the "Display" is "second(E)", and the "E0" is set to 7112. The "Calibrate to" value is also 7112. Below these settings are buttons for "Select a point", "Find zero crossing", "Replot", and "Calibrate".

The right panel shows a plot titled "fe.060 in energy". The y-axis is labeled "second deriv $\chi\mu(E)$ " and ranges from -0.15 to 0.2. The x-axis is labeled "Energy (eV)" and ranges from 7080 to 7140. The plot shows a blue line representing the second derivative of the signal, with a prominent peak at approximately 7108 eV. A yellow crosshair is positioned at the peak, with coordinates (7138.03, -0.0405852) displayed below it.

At the bottom of the interface, there is a status bar that reads "Calibrated, setting e0 to 7112 and the energy shift to 6.708".

4. Extracting the signal for fe.060

2. Pre-edge fitting

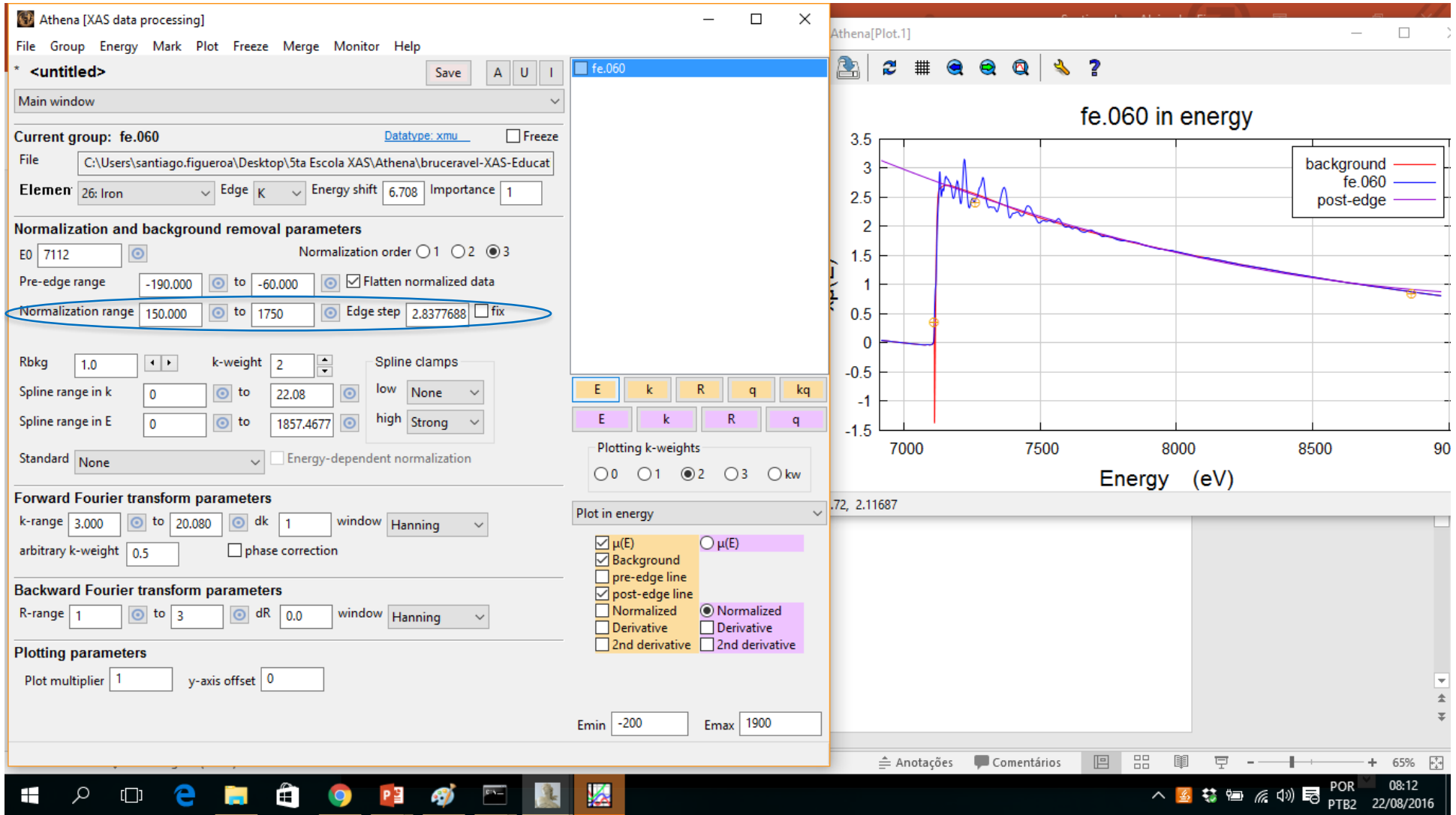


The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group as 'fe.060' and the element as '26: Iron'. The 'Normalization and background removal parameters' section is highlighted, showing the 'Pre-edge range' set to -150.000 to -30.000, with the 'Flatten normalized data' checkbox checked. The 'Forward Fourier transform parameters' section shows a k-range from 3.000 to 20.080. The 'Plotting parameters' section shows a plot multiplier of 1 and a y-axis offset of 0.

The plot window, titled 'Athena[Plot.1]', shows the 'fe.060 in energy' plot. The x-axis is 'Energy (eV)' ranging from 6900 to 7150. The y-axis is $x\mu(E)$ ranging from -0.3 to 0.2. The plot displays the experimental data (blue line), the background (red line), and the pre-edge fit (green line). A vertical red line is drawn at approximately 7112 eV, indicating the edge position. The plot also shows the 'Plotting k-weights' set to 2 and the 'Plot in energy' section with 'Normalized' selected.

4. Extracting the signal for fe.060

3. Post-edge normalization

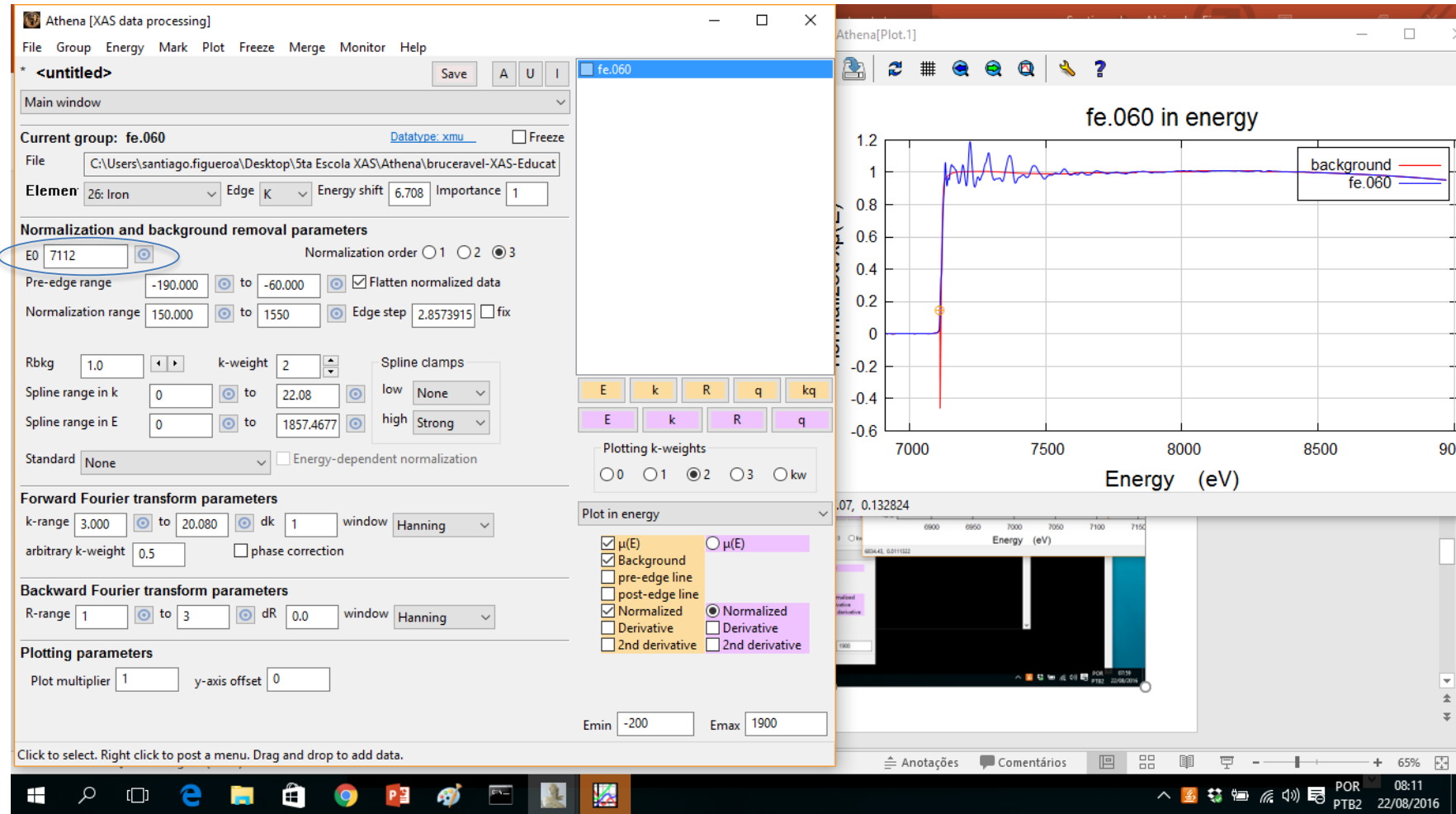


The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group as 'fe.060' and the element as '26: Iron'. The 'Normalization and background removal parameters' section is highlighted, showing the 'Normalization range' set to 150,000 to 1750, with an 'Edge step' of 2,837,7688. The 'Plotting parameters' section shows the 'Plot multiplier' set to 1 and the 'y-axis offset' set to 0. The 'Plot in energy' section is checked, and the 'Normalized' option is selected.

The plot window, titled 'Athena[Plot.1]', shows the 'fe.060 in energy' plot. The x-axis is 'Energy (eV)' ranging from 7000 to 9000, and the y-axis is $\mu(E)$ ranging from -1.5 to 3.5. The plot displays three curves: 'background' (red), 'fe.060' (blue), and 'post-edge' (purple). The 'post-edge' curve shows the signal after normalization, which is a smooth, decaying curve. The 'fe.060' curve shows the raw data with a sharp peak at approximately 7112 eV. The 'background' curve is a smooth, decaying curve that follows the general trend of the data.

4. Extracting the signal for fe.060

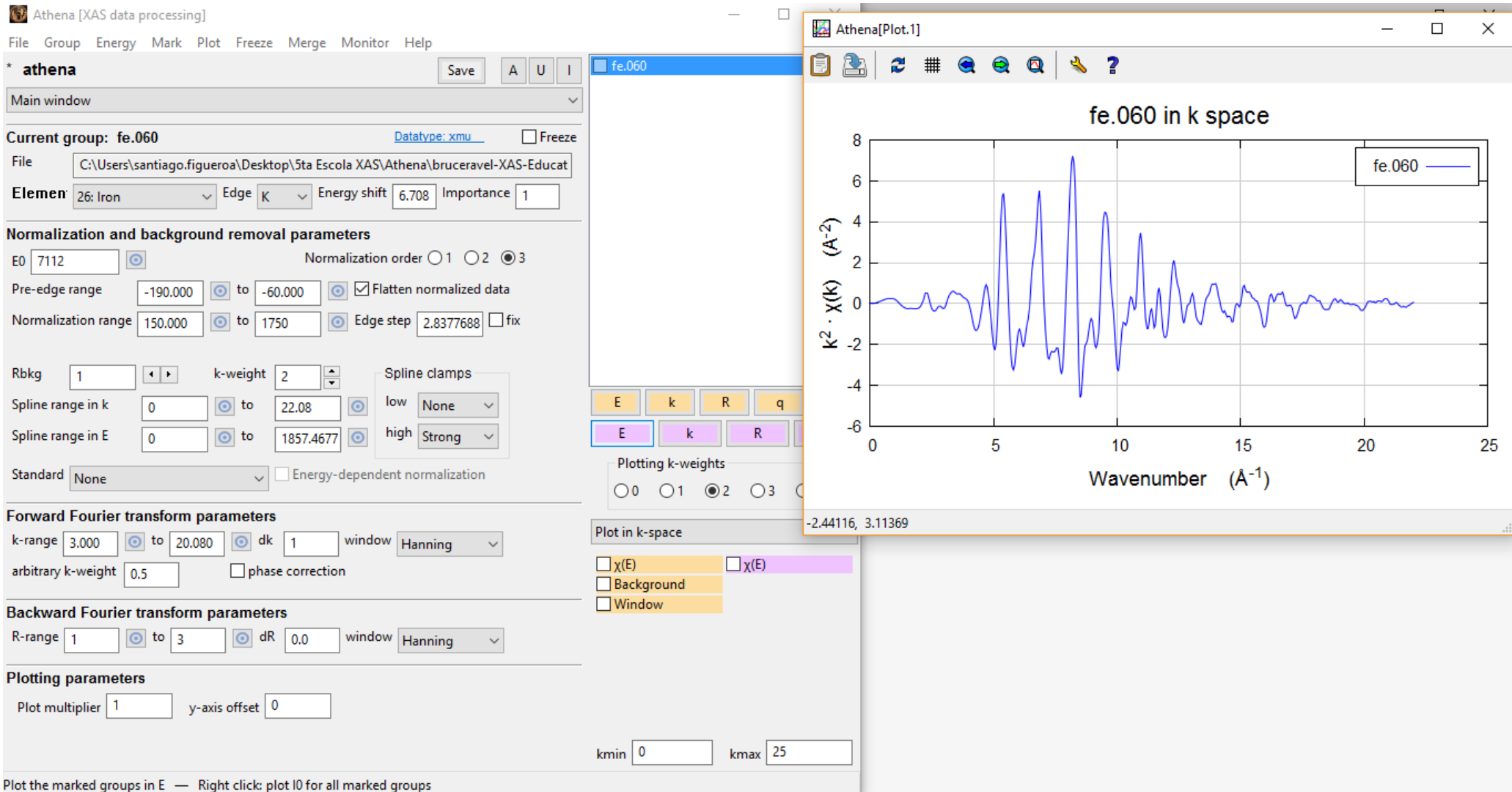
4. E0



The screenshot displays the Athena [XAS data processing] application window. The main window shows the current group as 'fe.060'. The 'Normalization and background removal parameters' section is highlighted, with the 'E0' parameter set to 7112. The 'Forward Fourier transform parameters' section shows a k-range from 3.000 to 20.080. The 'Backward Fourier transform parameters' section shows an R-range from 1 to 3. The 'Plotting parameters' section shows a plot multiplier of 1 and a y-axis offset of 0. The 'Plot in energy' section is checked, and the 'Normalized' option is selected. The 'Athena[Plot.1]' window shows a plot titled 'fe.060 in energy' with 'Normalized k(E)' on the y-axis and 'Energy (eV)' on the x-axis. The plot shows a sharp peak at approximately 7112 eV, with a red line representing the background and a blue line representing the signal. The 'Plotting k-weights' section shows the 'Normalized' option selected. The 'Plot in energy' section shows the 'Normalized' option selected. The 'Athena[Plot.1]' window shows a plot titled 'fe.060 in energy' with 'Normalized k(E)' on the y-axis and 'Energy (eV)' on the x-axis. The plot shows a sharp peak at approximately 7112 eV, with a red line representing the background and a blue line representing the signal. The 'Plotting k-weights' section shows the 'Normalized' option selected. The 'Plot in energy' section shows the 'Normalized' option selected.

4. Extracting the signal for fe.060

5. Extraction of the signal



The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group as 'fe.060' and the element as '26: Iron'. The normalization and background removal parameters are set as follows:

- File: C:\Users\santiago.figueroa\Desktop\5ta Escola XAS\Athena\bruceravel-XAS-Educat
- Element: 26: Iron, Edge: K, Energy shift: 6.708, Importance: 1
- Normalization order: 3
- Pre-edge range: -190.000 to -60.000, Flatten normalized data: checked
- Normalization range: 150.000 to 1750, Edge step: 2.8377688
- Rbkg: 1, k-weight: 2, Spline clamps: low (None), high (Strong)
- Spline range in k: 0 to 22.08, Spline range in E: 0 to 1857.4677
- Standard: None, Energy-dependent normalization: unchecked

The Forward Fourier transform parameters are:

- k-range: 3.000 to 20.080, dk: 1, window: Hanning
- arbitrary k-weight: 0.5, phase correction: unchecked

The Backward Fourier transform parameters are:

- R-range: 1 to 3, dR: 0.0, window: Hanning

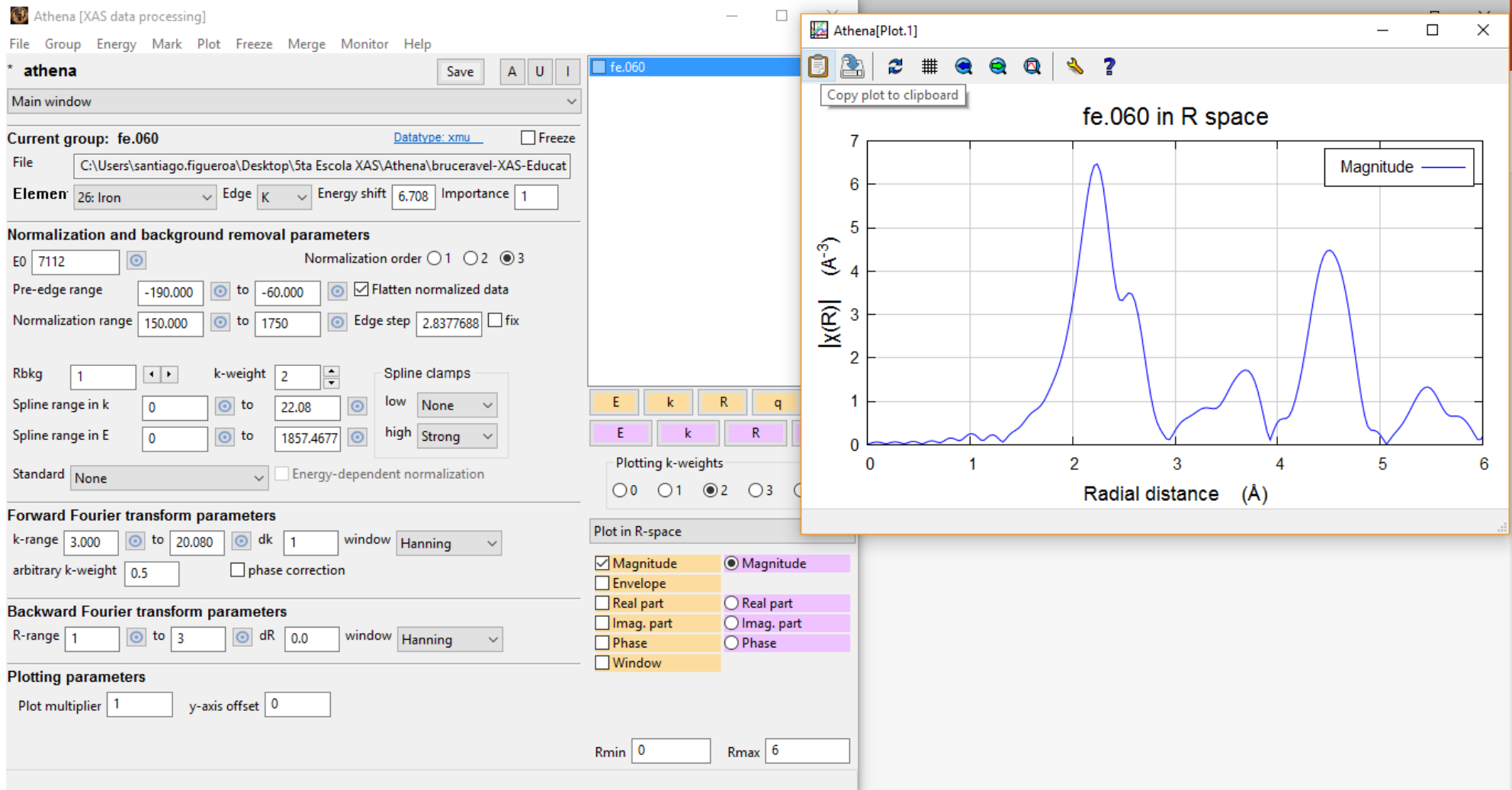
The Plotting parameters are:

- Plot multiplier: 1, y-axis offset: 0

The plot window, titled 'Athena[Plot.1]', shows the extracted signal for 'fe.060 in k space'. The y-axis is labeled $k^2 \cdot \chi(k) \text{ (}\text{\AA}^{-2}\text{)}$ and ranges from -6 to 8. The x-axis is labeled 'Wavenumber (\AA^{-1})' and ranges from 0 to 25. The plot shows a blue line representing the signal, with a legend indicating 'fe.060'.

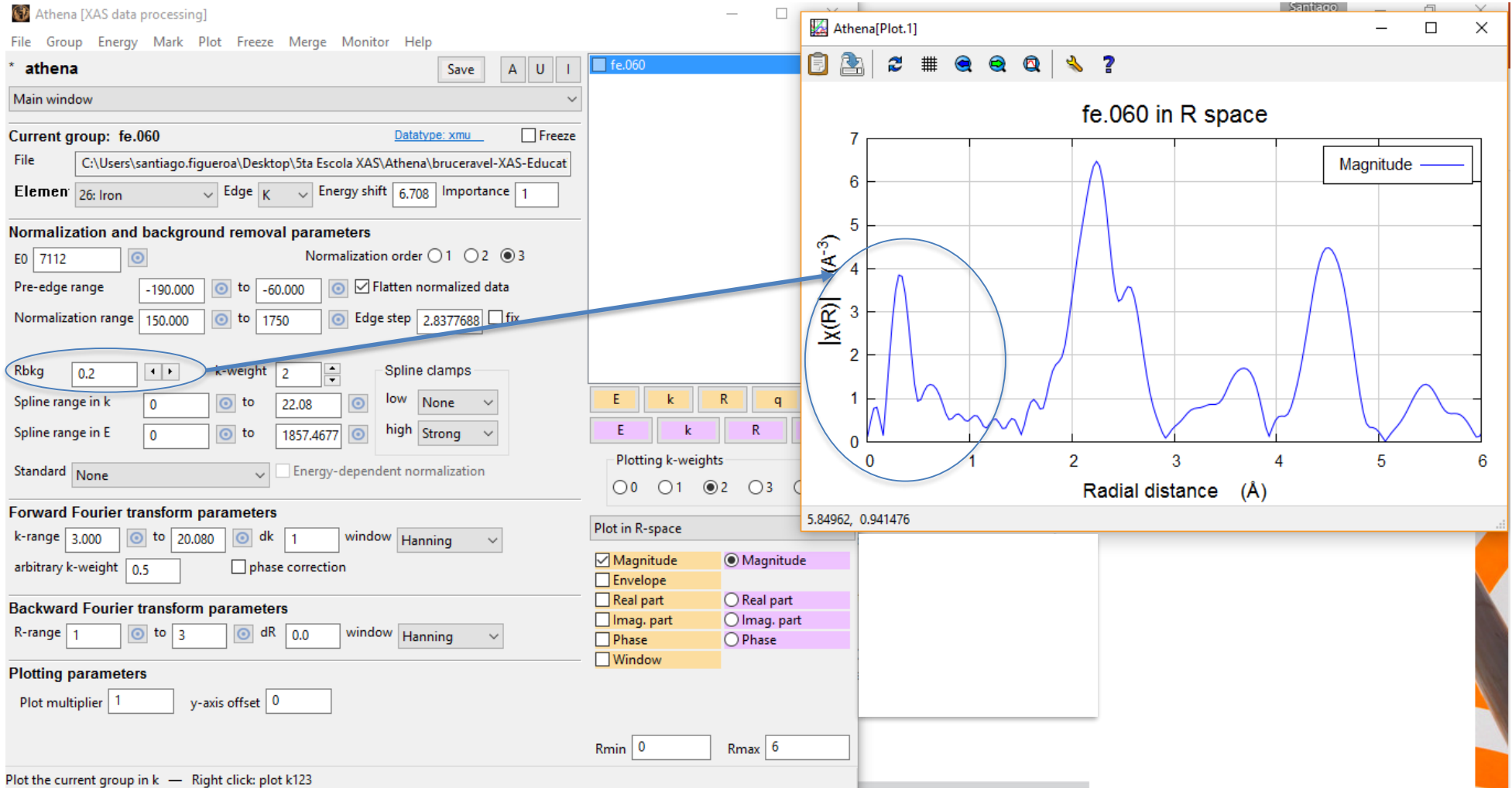
4. Extracting the signal for fe.060

6. Fourier Transform



4. Extracting the signal for fe.060

7. Rbkg

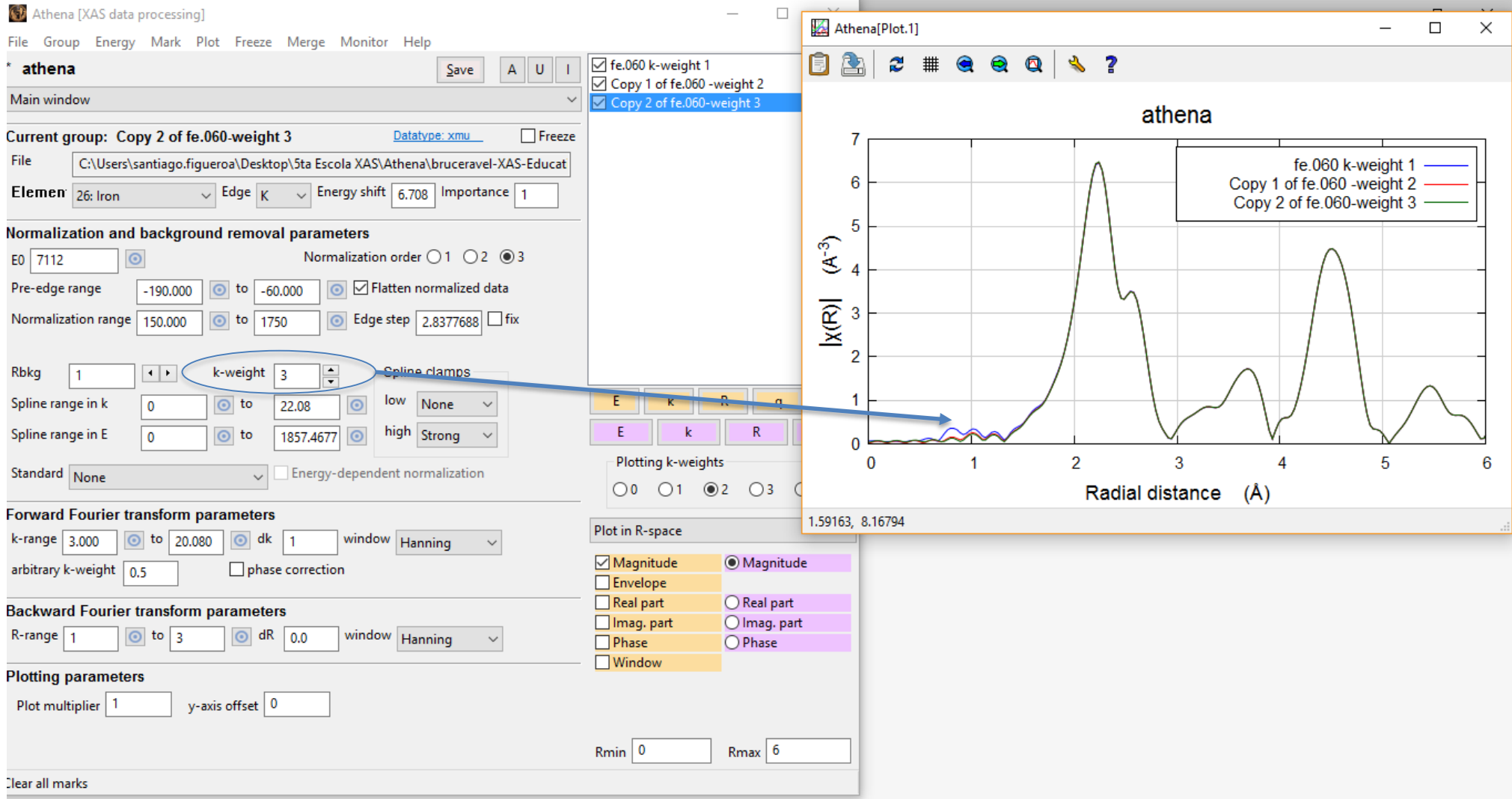


The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group as 'fe.060' with the element set to '26: Iron' and the edge to 'K'. The 'Normalization and background removal parameters' section is active, with the 'Rbkg' parameter set to 0.2. A blue circle highlights the 'Rbkg' input field, and a blue arrow points from it to a corresponding peak in the plot.

The plot, titled 'fe.060 in R space', shows the magnitude of the signal $|X(R)|$ in \AA^{-3} versus the radial distance R in \AA . The x-axis ranges from 0 to 6 \AA , and the y-axis ranges from 0 to 7 \AA^{-3} . The plot shows several peaks, with the most prominent one at approximately 2.2 \AA . A blue circle highlights a peak at approximately 0.5 \AA , which is the background level. The plot is titled 'fe.060 in R space' and the y-axis is labeled $|X(R)|$ (\AA^{-3}) and the x-axis is labeled 'Radial distance (\AA)'. The legend indicates 'Magnitude' is plotted as a blue line. The plot is titled 'fe.060 in R space' and the y-axis is labeled $|X(R)|$ (\AA^{-3}) and the x-axis is labeled 'Radial distance (\AA)'. The legend indicates 'Magnitude' is plotted as a blue line. The plot is titled 'fe.060 in R space' and the y-axis is labeled $|X(R)|$ (\AA^{-3}) and the x-axis is labeled 'Radial distance (\AA)'. The legend indicates 'Magnitude' is plotted as a blue line.

4. Extracting the signal for fe.060

8. K-weight



Athena [XAS data processing]

File Group Energy Mark Plot Freeze Merge Monitor Help

* **athena** Save A U I

Main window

Current group: Copy 2 of fe.060-weight 3 Datatype: xmu Freeze

File C:\Users\santiago.figueroa\Desktop\5ta Escola XAS\Athena\bruceravel-XAS-Educat

Elemen 26: Iron Edge K Energy shift 6,708 Importance 1

Normalization and background removal parameters

E0 7112 Normalization order 1 2 3

Pre-edge range -190,000 to -60,000 Flatten normalized data

Normalization range 150,000 to 1750 Edge step 2,8377688 fix

Rbkg 1 **k-weight 3** Spline clamps

Spline range in k 0 to 22,08 low None

Spline range in E 0 to 1857,4677 high Strong

Standard None Energy-dependent normalization

Forward Fourier transform parameters

k-range 3,000 to 20,080 dk 1 window Hanning

arbitrary k-weight 0,5 phase correction

Backward Fourier transform parameters

R-range 1 to 3 dR 0,0 window Hanning

Plotting parameters

Plot multiplier 1 y-axis offset 0

Plot in R-space

Magnitude Magnitude

Envelope Real part

Real part Imag. part

Imag. part Phase

Phase Phase

Window

Rmin 0 Rmax 6

Athena[Plot.1]

athena

Legend: fe.060 k-weight 1 (blue), Copy 1 of fe.060 -weight 2 (red), Copy 2 of fe.060-weight 3 (green)

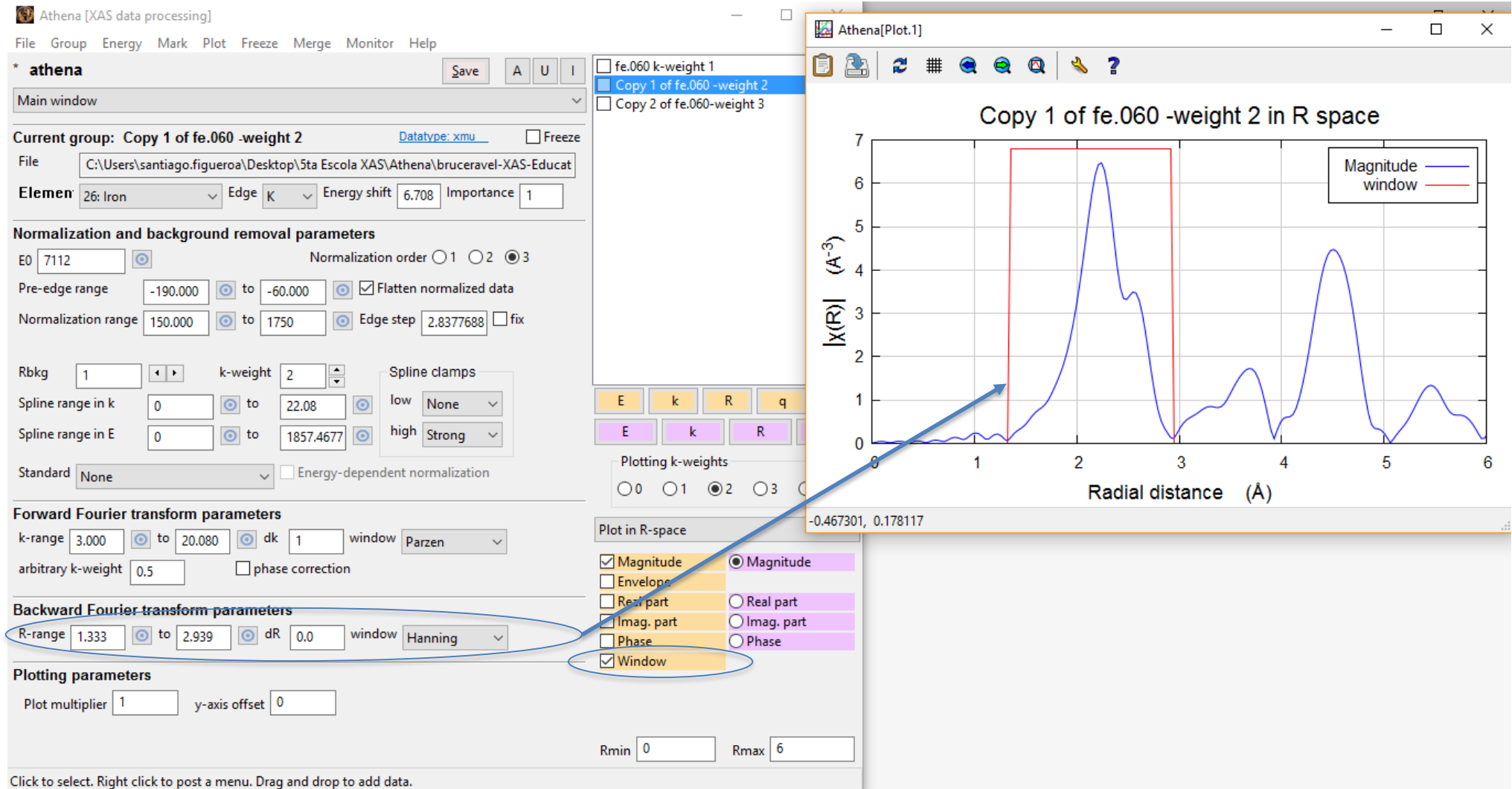
Y-axis: $|X(R)|$ (\AA^{-3})

X-axis: Radial distance (\AA)

Annotations: 1.59163, 8.16794

4. Extracting the signal for fe.060

9. Selection of the region of interest

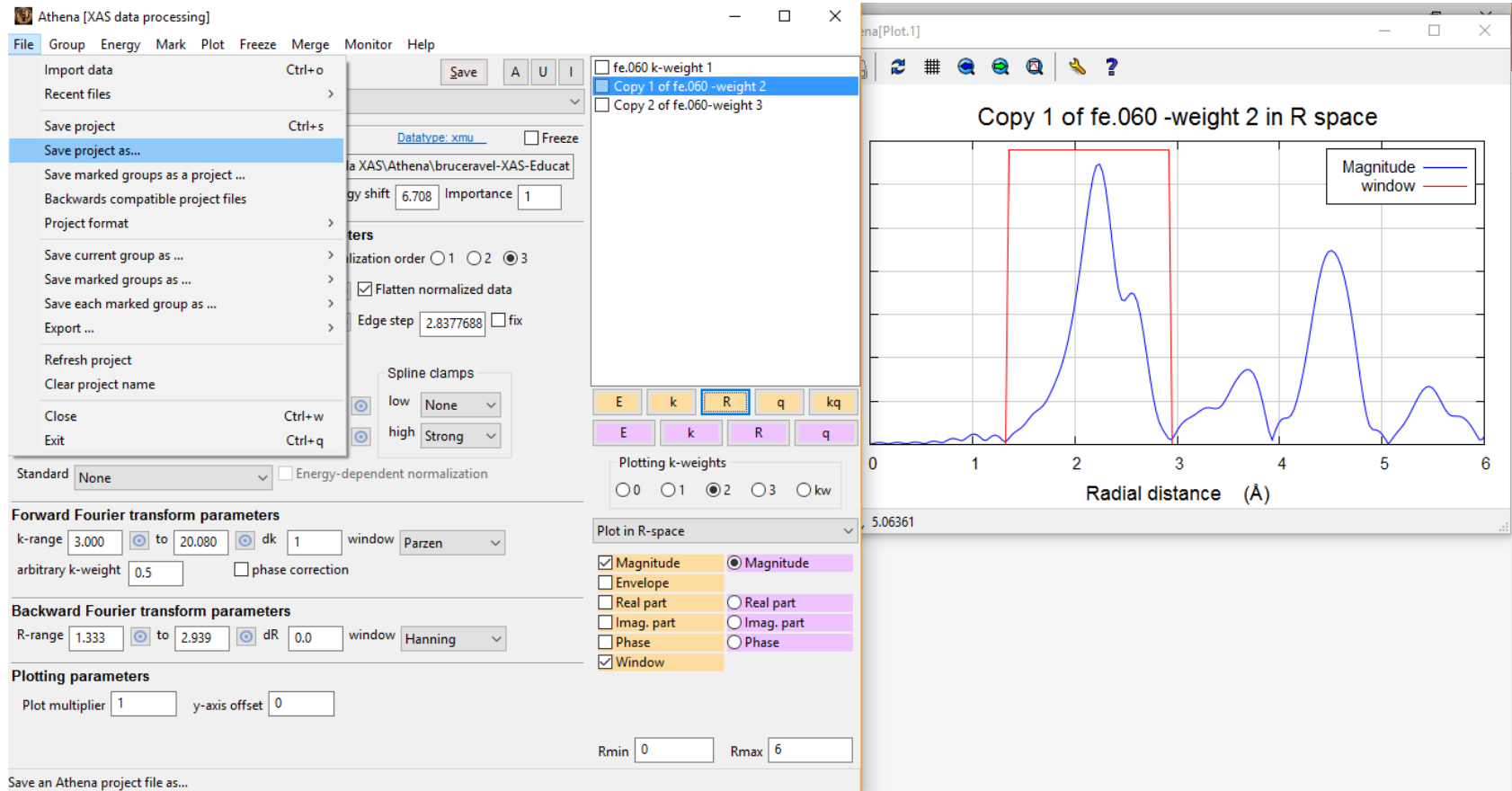


The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group as "Copy 1 of fe.060 -weight 2". The "Normalization and background removal parameters" section includes settings for E0 (7112), normalization order (3), and various ranges. The "Backward Fourier transform parameters" section shows an R-range from 1.333 to 2.939 with a Hanning window. The "Plotting parameters" section shows a plot multiplier of 1 and a y-axis offset of 0. The "Plot in R-space" section has checkboxes for Magnitude, Envelope, Residual part, Imaginary part, Phase, and Window, with Magnitude and Window selected. A plot window titled "Copy 1 of fe.060 -weight 2 in R space" shows the magnitude of the signal |X(R)| (A⁻³) versus radial distance (Å). A red window is drawn around the first peak, with a blue arrow pointing to it from the "Window" checkbox in the plotting parameters. The plot shows several peaks, with the first peak being the most prominent. The y-axis ranges from 0 to 7, and the x-axis ranges from 0 to 6. A legend in the plot indicates that the blue line represents "Magnitude" and the red line represents "window".

Click to select. Right click to post a menu. Drag and drop to add data.

4. Extracting the signal for fe.060

10. Save the file!!



This program is distributed in the hope that it will be useful, but **WITHOUT ANY WARRANTY**; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE

<http://bruceravel.github.io/demeter/pods/bugs.pod.html#OVERVIEW>

4. To do: following Bruce Ravel example on Iron

Please access this site and follow the part that we don't have done yet...

<https://bruceravel.github.io/demeter/documents/Athena/examples/data.html>

5. Linear Combination Fitting

Please access this site and follow the instructions:

<https://bruceravel.github.io/demeter/documents/Athena/examples/aucl.html>



It depends on you, but follow this can be an good option:

<https://speakerdeck.com/bruceravel>

<http://bruceravel.github.io/XAS-Education/>



Obrigado pela sua atenção!

Questions, please email me:

santiago.figueroa@lnls.br

More info about Iffeffit and XAFS:

<https://speakerdeck.com/bruceravel?page=2>

http://cars.uchicago.edu/iffefit/Mailing_List

<http://xafs.org/Tutorials>

<http://www.ixasportal.net/ixas/>

<http://cars.uchicago.edu/iffefit/Documentation>

Acknowledgments: Bruce Ravel, Matt Newville and all the people that help to develop Iffeffit and Feff.

