

Introduction to the analysis of EXAFS data

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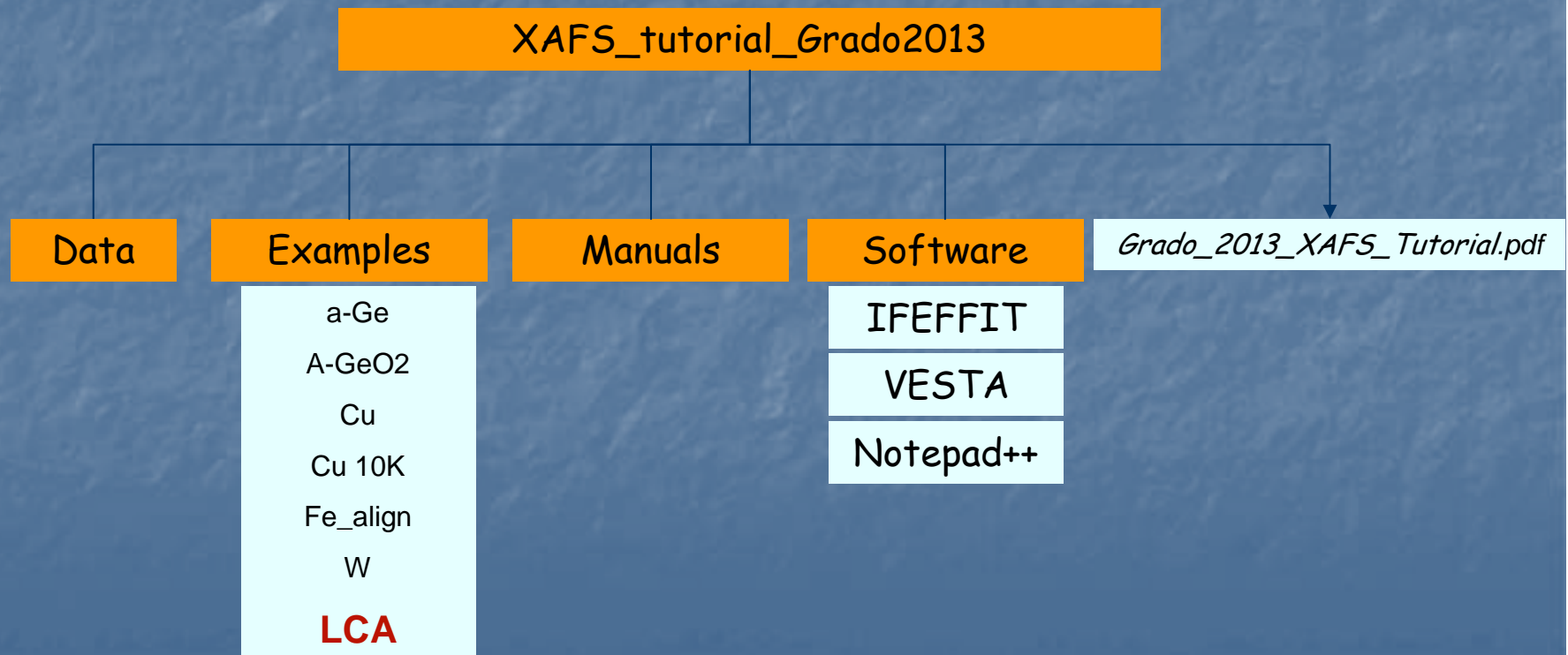
Grado2013_XAFS_TUTORIAL

http://dl.dropbox.com/u/20746560/Meneghini_EXAFS-Tutorial-DUINO-2011.zip

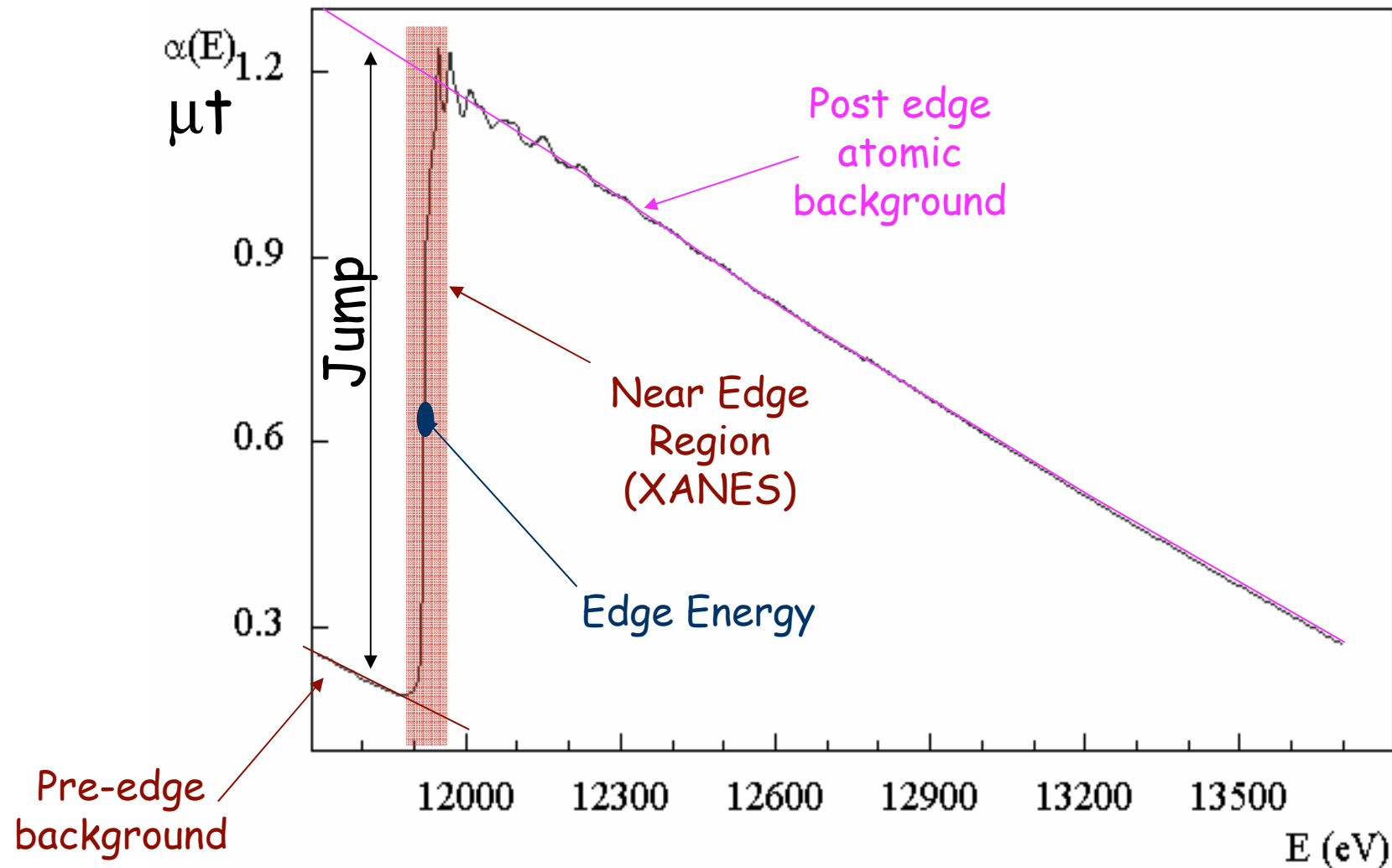
PDF slides:

<https://db.tt/UmF9HOc2>

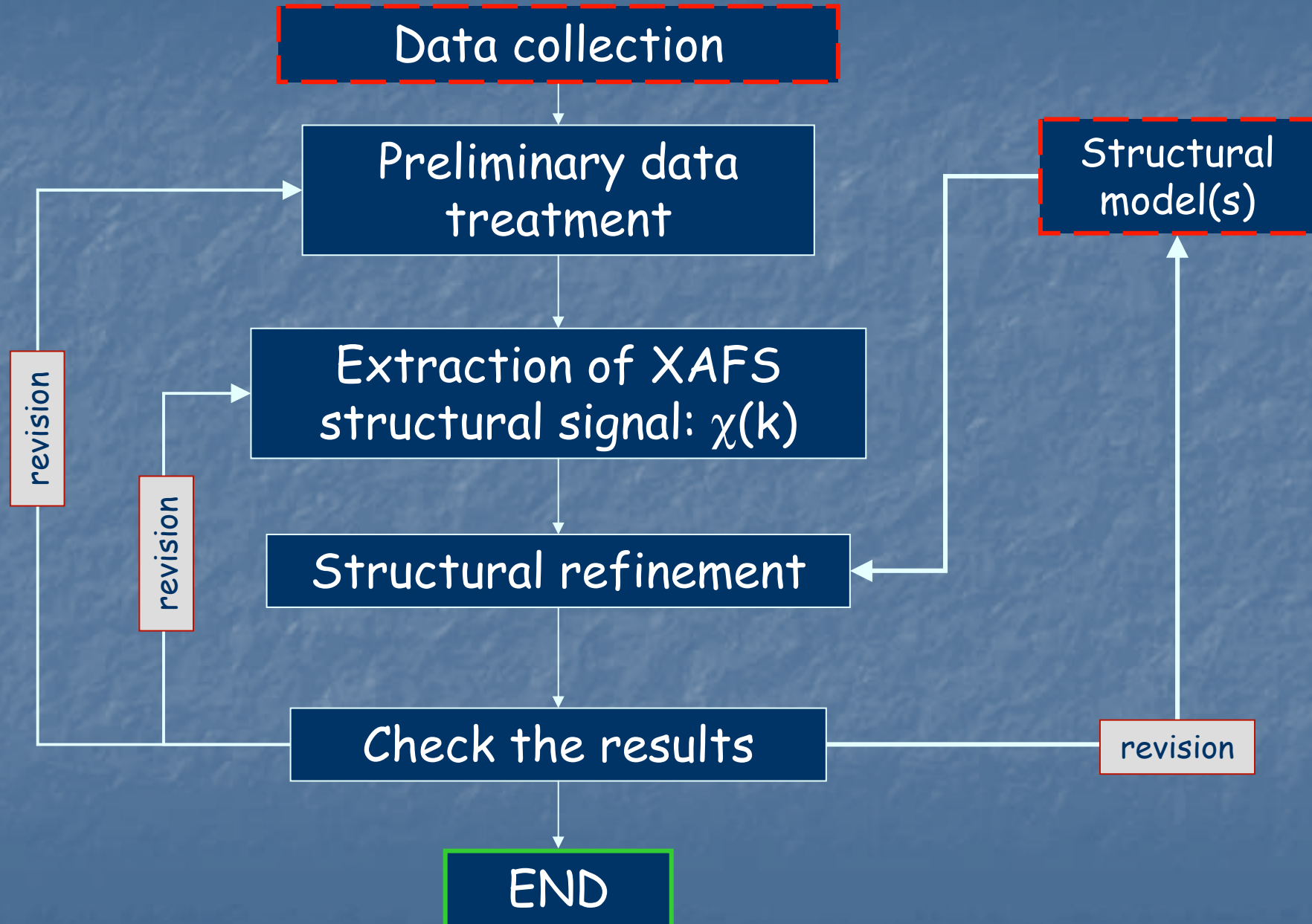
Complete directory

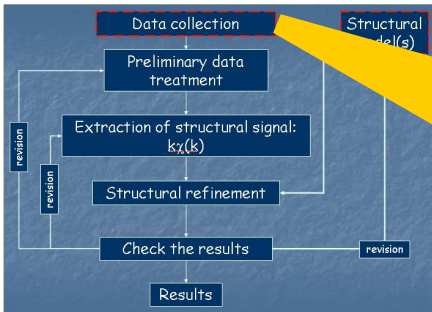


Characteristics of a XAS spectrum



XAFS ANALYSIS: from the experimental data to results





Data collection

Proposal submission + proposal evaluation + beamtime scheduling = 6 to 12 months!

It is difficult to obtain new beamtime for the same proposal in case of failure!!!!

XANES/EXAFS
Fluo/TEY/transmission
....

Choose properly the experimental set-up & sample preparation

Optimize your beamtime!

Choose properly data collection strategy

Check the data quality during the experiment

Quality is better than quantity

Always measure reference data

XAFS rarely gives absolute quantitative details

- Check the proposal submission deadlines,
- discuss your experiment with local contacts,
- check your data during the experiment

ELETTRA: 15-09 + 15-03
ESRF: 01-09 + 01-03

Data collection

Errors in XAFS data analysis are dominated by systematic errors:

- spurious structures
- background subtraction
- wrong models
- inaccurate theory

a

Experimental set-up & sample preparation

Transmission: massive concentrated samples

$$0.5 \leq \Delta\mu t \leq 1.5 \quad \mu t \leq 2.$$

inhomogeneities, holes, not parallel surfaces, etc...

Fluorescence: thin concentrated
thick diluted samples

Self absorption, detector linearity, Bragg reflections

TEY: thick concentrated

Surface sensitivity, sample charge, Bragg reflections

IXS Standards and Criteria Subcommittee Reports

d

Measure reference samples

1-energy calibration

2-data analysis procedures calibration

The power of XAFS technique consists in highlighting the smallest structural differences

c

Data quality

S/N ratio

glitches

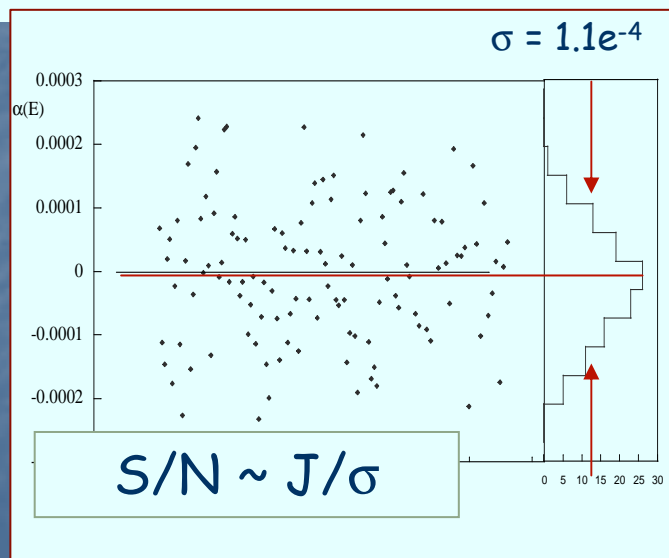
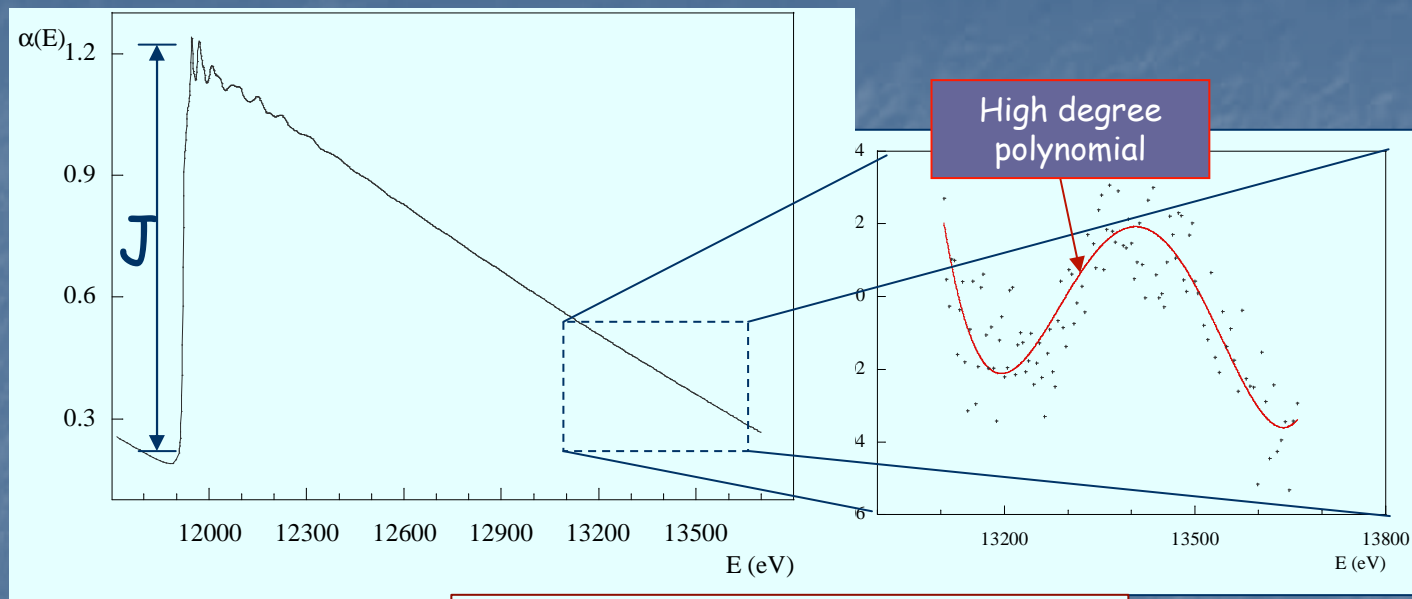
discontinuities

b

Collection strategy

- step scan / quick EXAFS
- Fixed Energy or K steps
- single scan/repeated scans
- temperature points
- ...

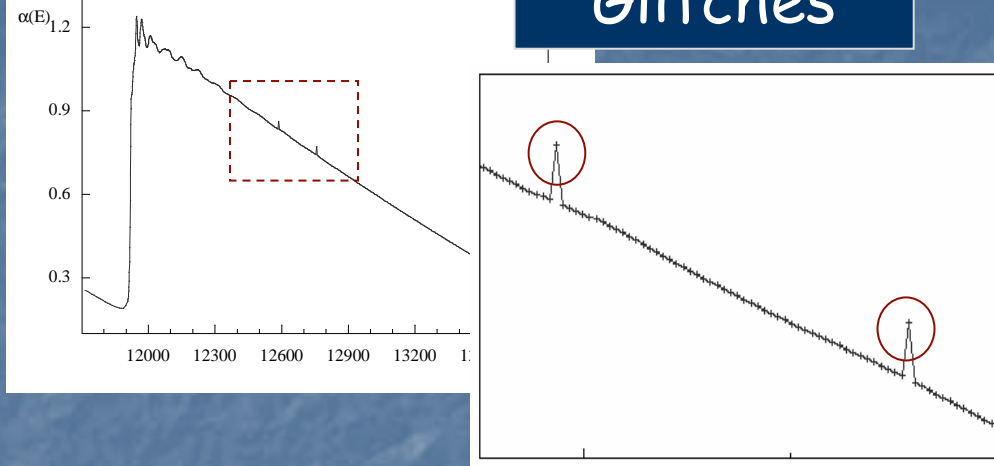
Evaluate S/N ratio



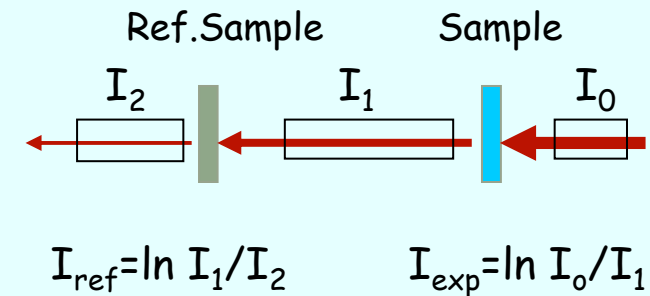
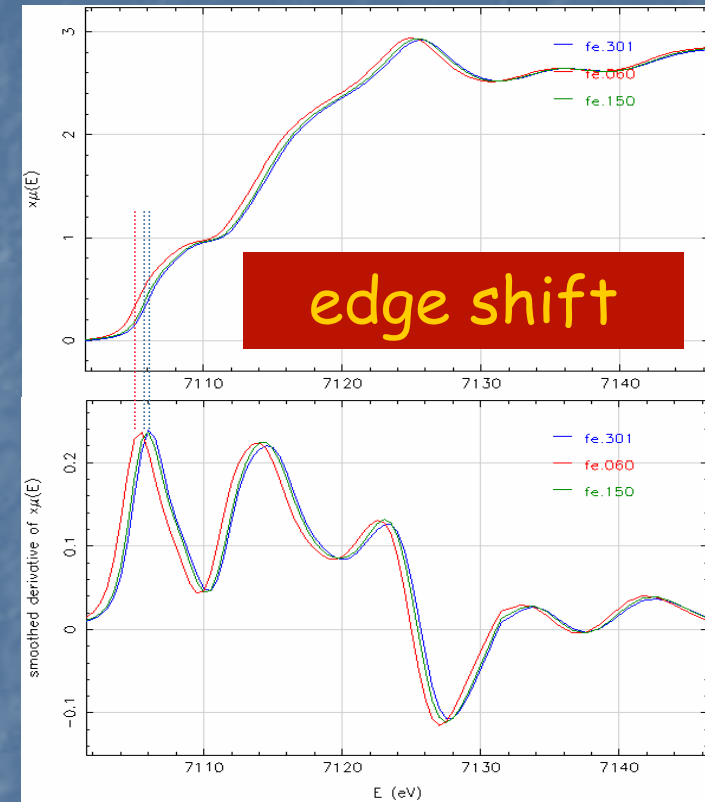
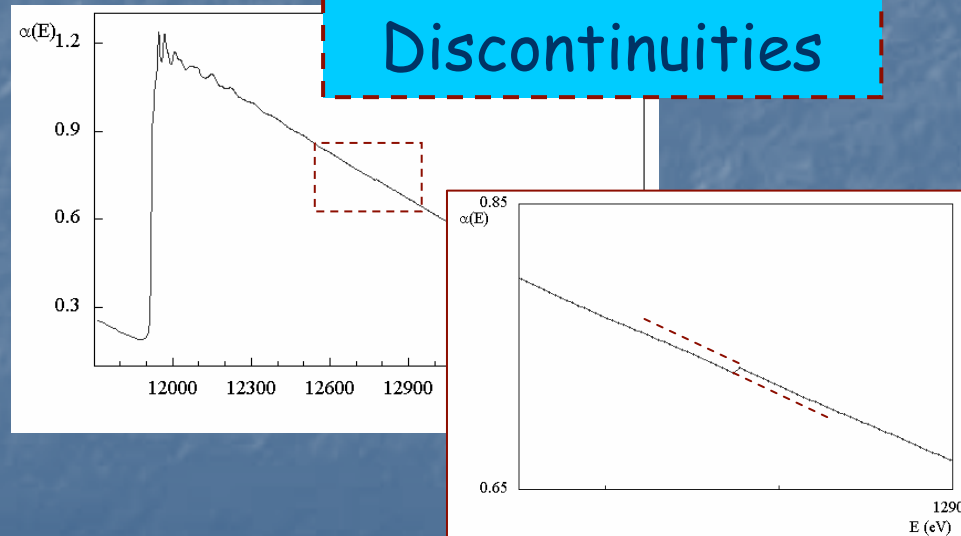
Check regularly during the experiment

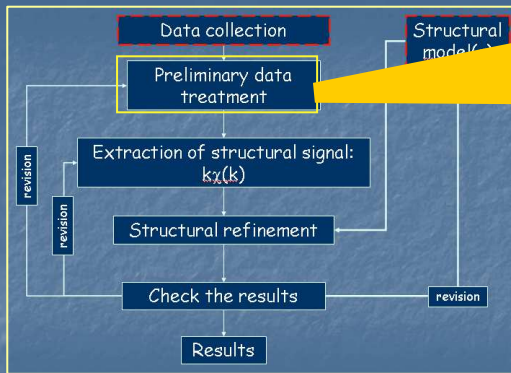
Check systematically during the experiment

Glitches



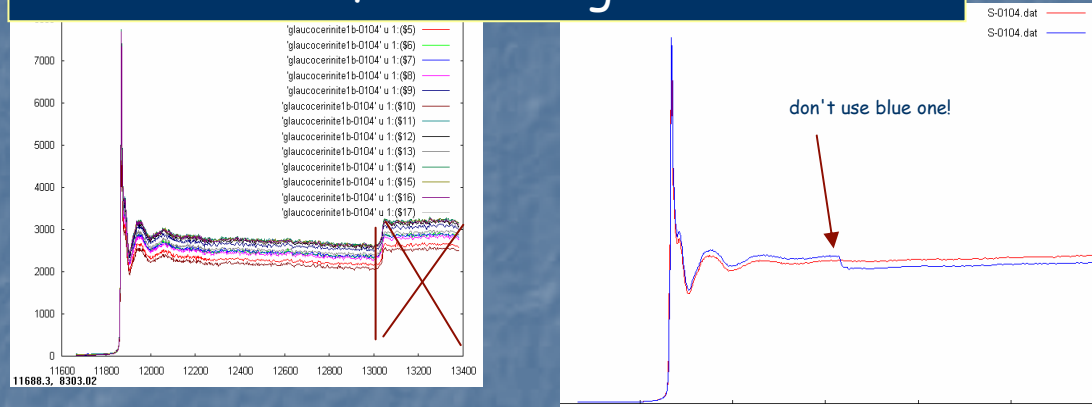
Discontinuities





Preliminary data treatment

a Select properly the best spectra and useful data regions



Absorption signal

Transmission $\alpha(E) = \log_e \frac{I_o}{I_t}$

Fluorescence & TEY $\mu x \ll 1$ $\alpha(E) = \frac{I_f}{I_o}$

Check carefully the data quality during the experiment

Experimental set-up generally provide macros for automatic data collection over several days: supervise your macros!

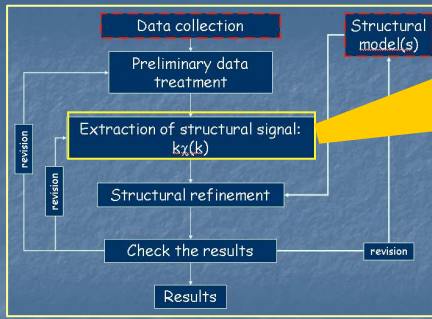
b Preliminary data treatment

- Self absorption corrections
- deglitching
- data interpolation
- data alignment

c Sum together the best spectra

Weighting by S/N

Extract $\chi(k)$ structural signal



Absorption signal

Transmission

$$\alpha(E) = \log_e \frac{I_o}{I_t}$$

Fluorescence & TEY

$$\alpha(E) = \frac{I_f}{I_o}$$

$$\alpha = \alpha_o + \alpha_{pre}$$

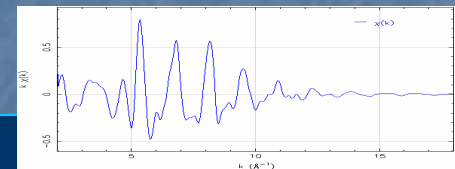
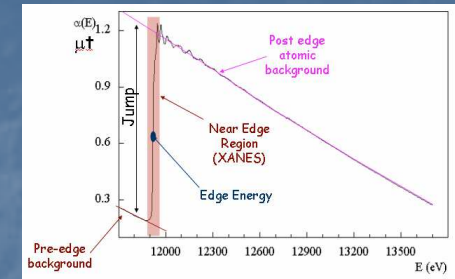
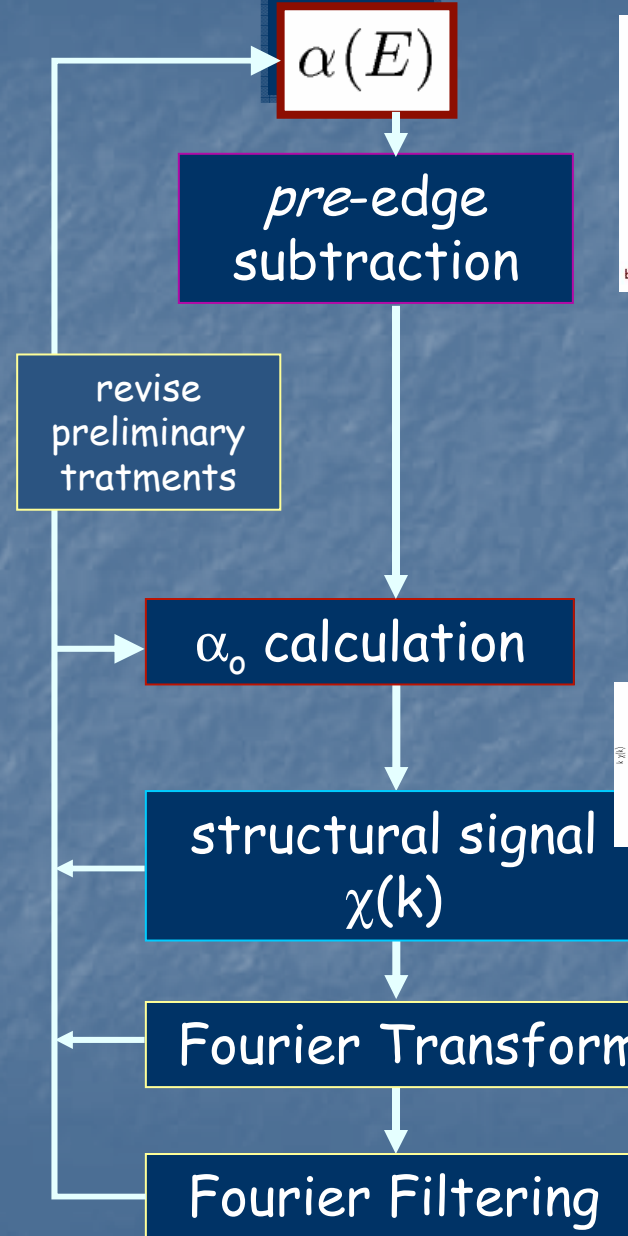
$$\alpha_o = (\mu_o + \mu)t$$

μ_o = free atom absorption
 μ = embedded atom absorption
 pre = all but the absorber

$$\alpha'(E) = \alpha(E) - \alpha_{pre}(E)$$

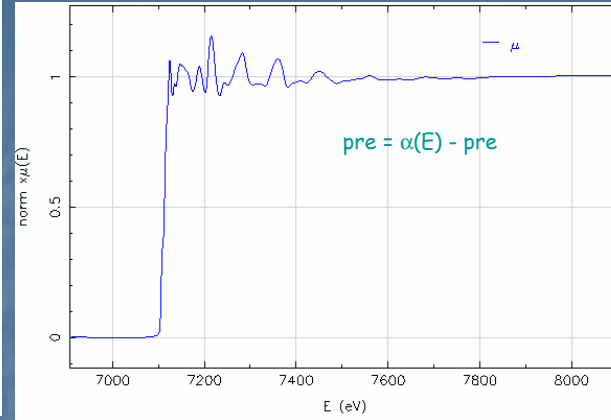
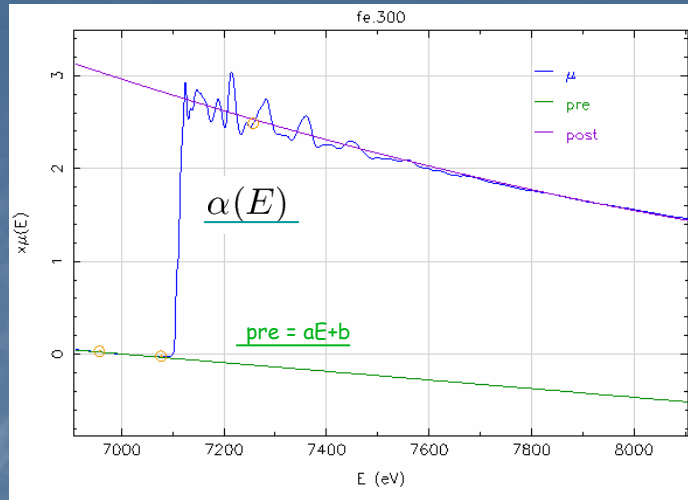
XAFS structural signal

$$\chi^{exp}(k) = \frac{\alpha'(k) - \alpha_o(k)}{\alpha_o(k)} J$$

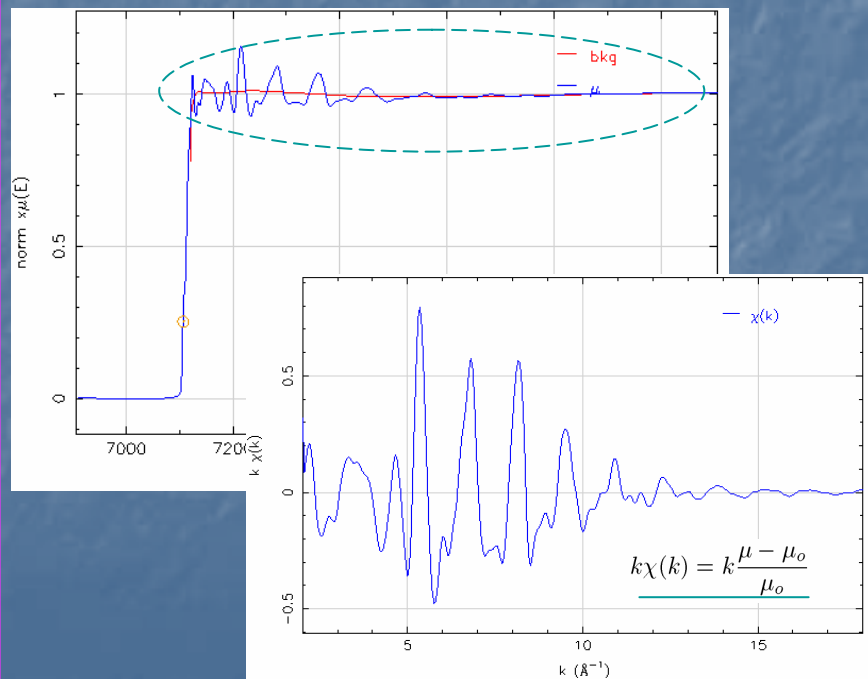


Structural refinement

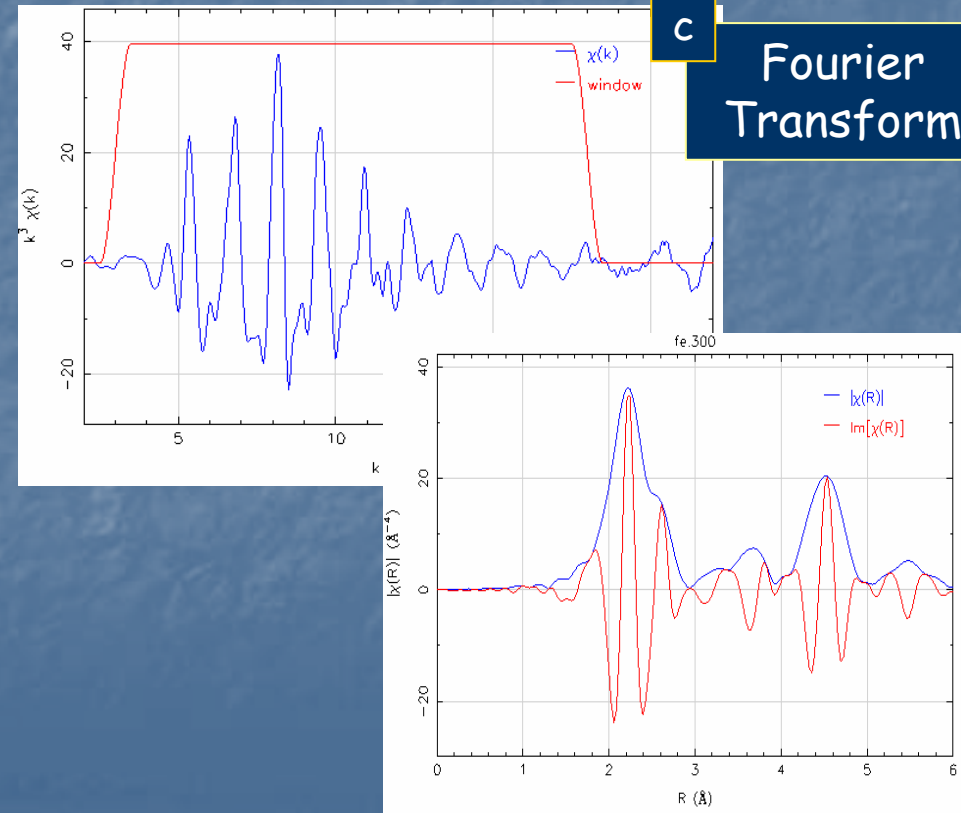
a Background subtraction



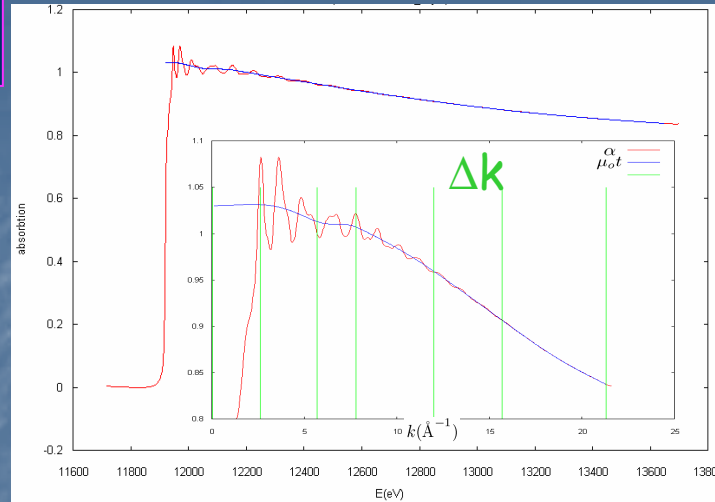
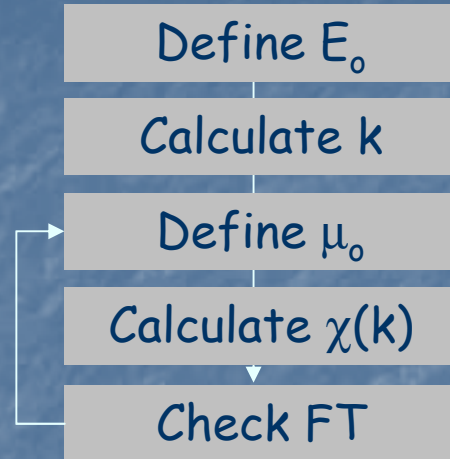
b calculate μ_0 and $\chi(k)$



c Fourier Transform



Structural signal



μ_0 = represents the bare atom absorption.

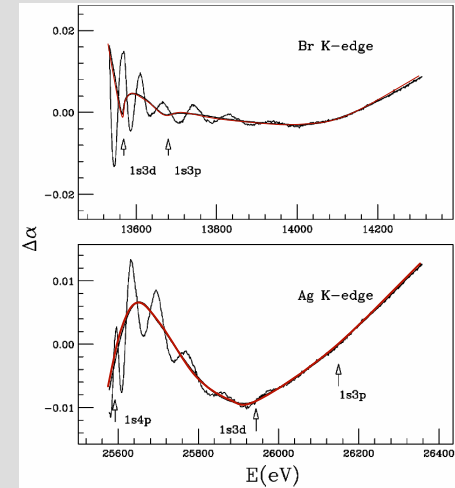
It is calculated empirically as a smooth curve across the data.

Different XAFS data analysis software apply different (generally equivalent) methods

Requirements for μ_0 :

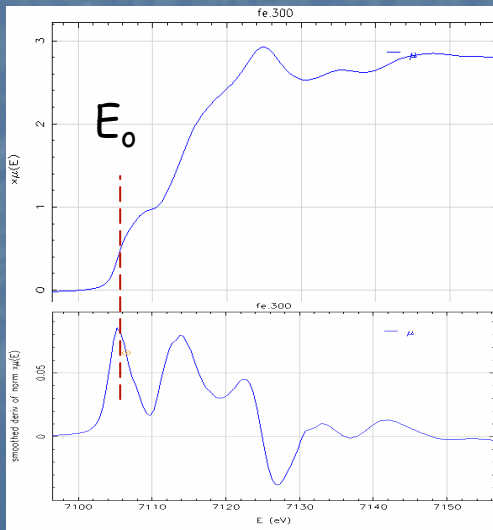
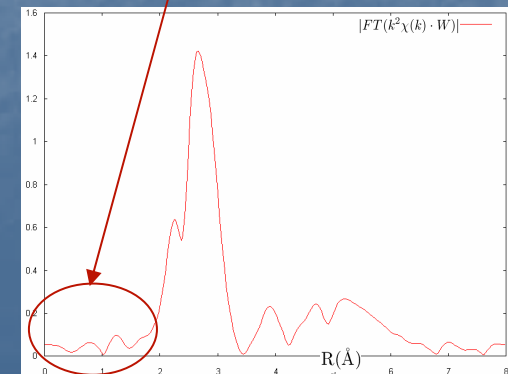
- 1) Smooth enough to not remove true structural features
- 2) Structured enough to remove background structures

Note: Multiple excitations may affect the background with (small) discontinuities



A. Di Cicco et al. Phys. Rev. B 62, 12001 (2000)

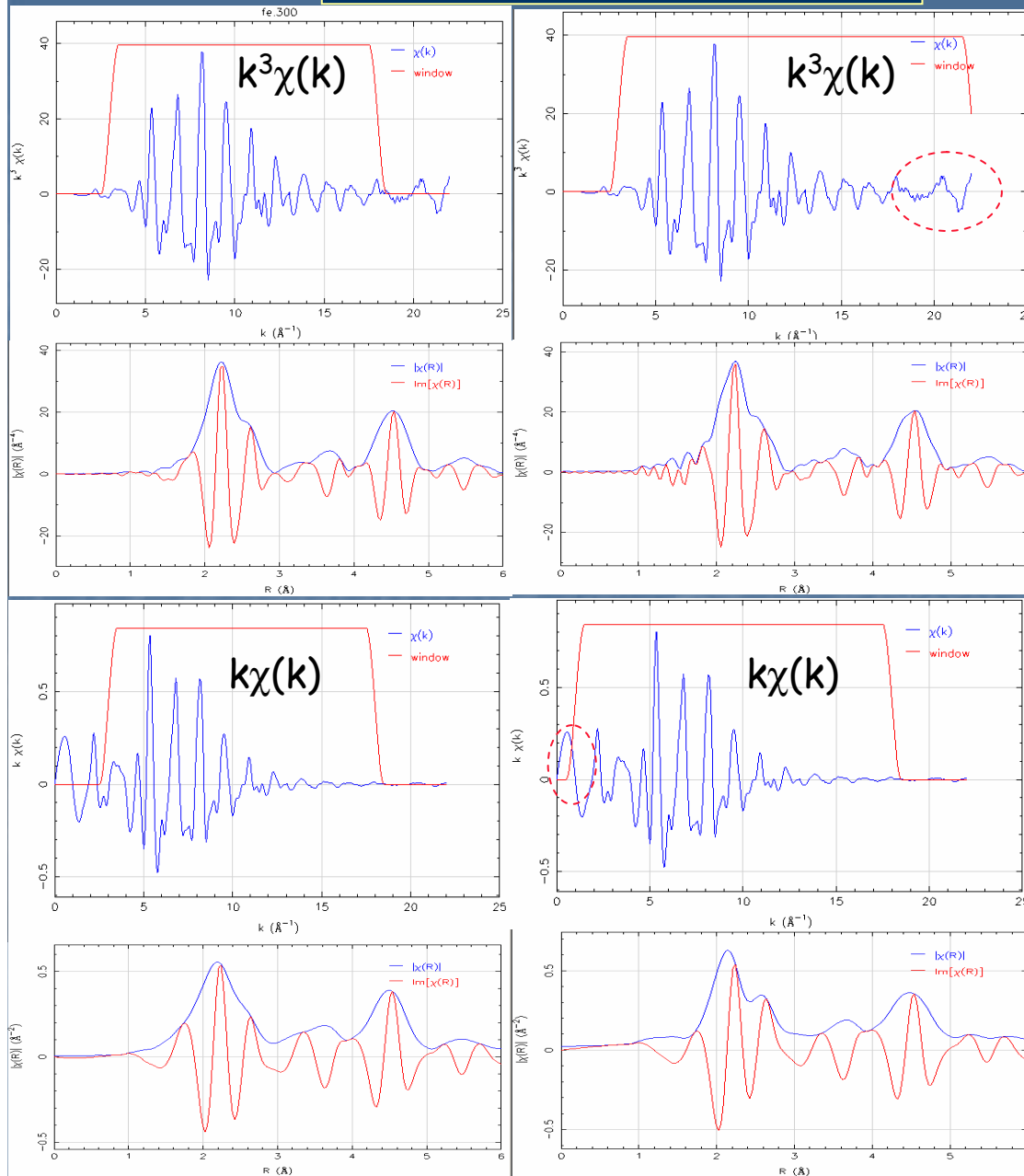
Large |FT| contributions at low (unphysical) distances may signify "wrong μ_0 "



Fourier Transform

Shape of FT widely changes as a function of:

- FT window
- k^w weight
- data range



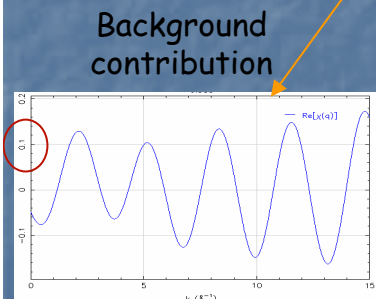
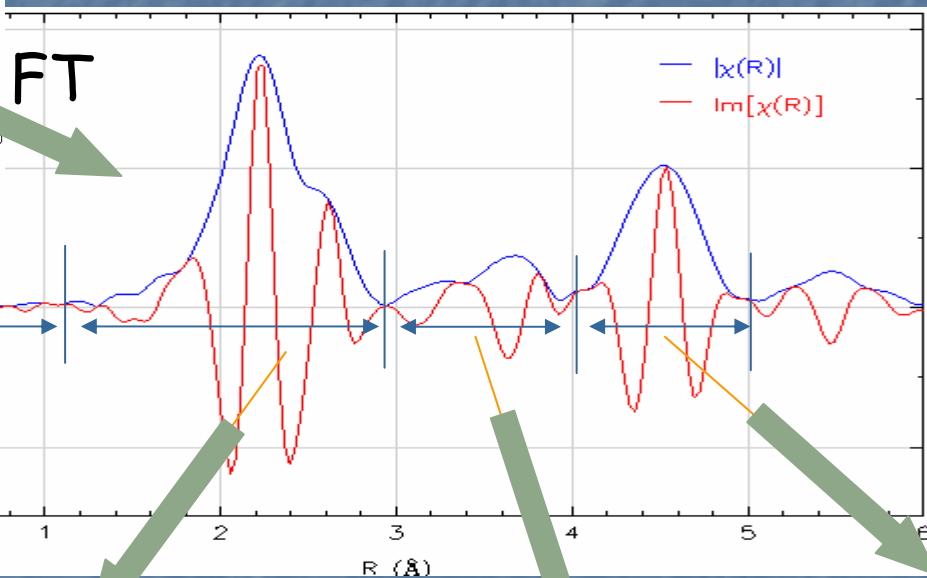
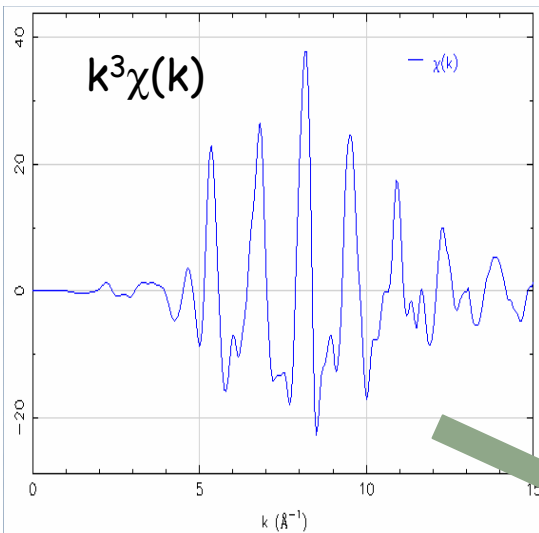
FT shows more intuitively the main structural features in the real space: the FT modulus represent a pseudo-radial distribution function modified by the effect of amplitude, phase and mean free path parameters:

$|FT|$ peaks point out interatomic correlations

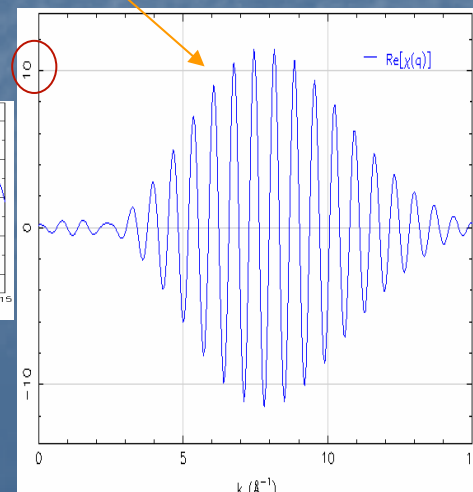
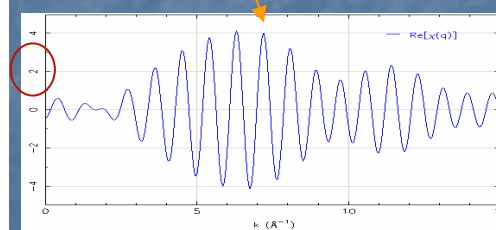
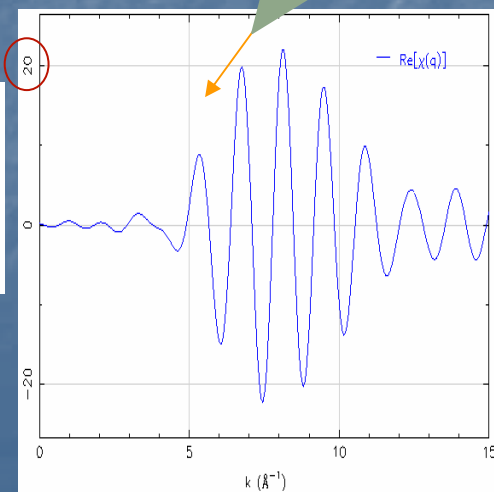
Peak positions are not the true distances due to the photoelectron phase shift

Fourier Filtering

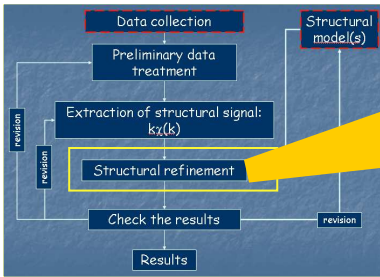
Fourier filtering allows isolating contributions of selected regions of the FT



Back Fourier transform (BFT)



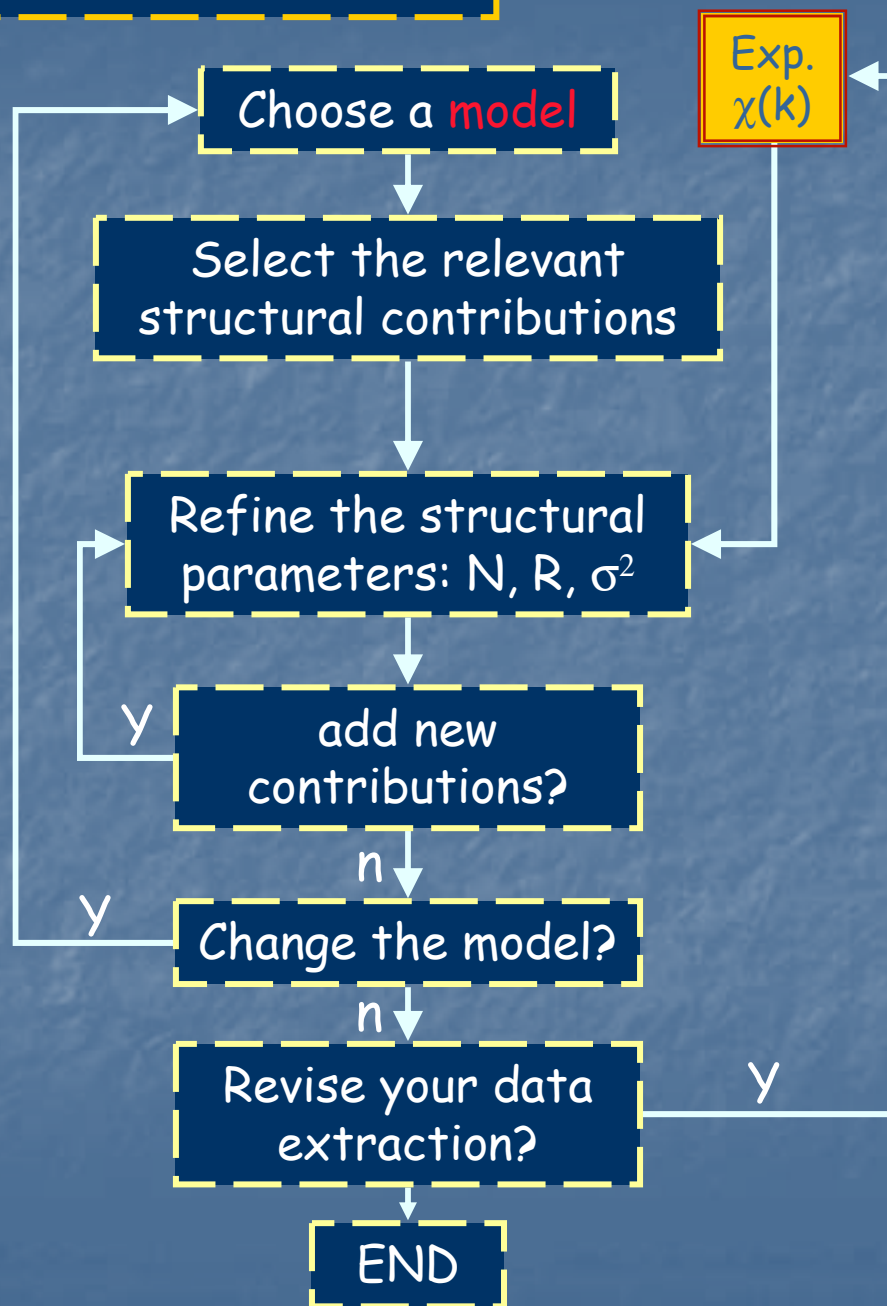
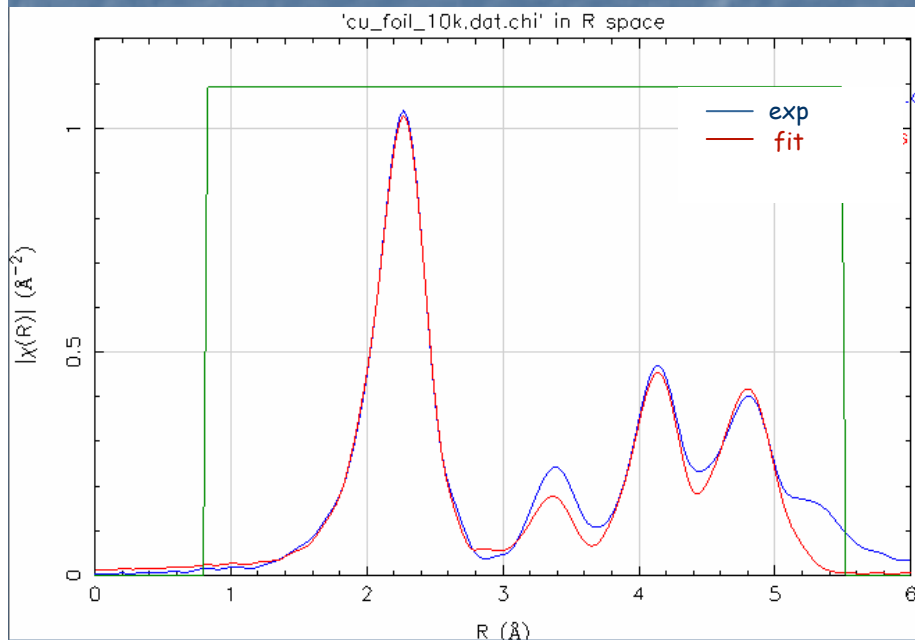
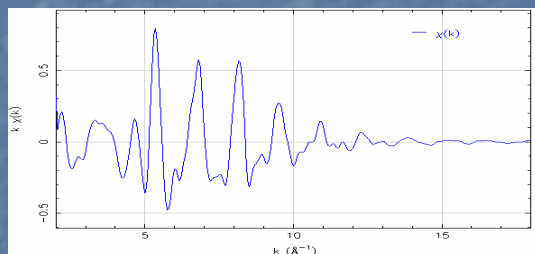
data refinement



Theoretical $\chi(k)$

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

Experimental $\chi(k)$



Exp. $\chi(k)$

Choose a structural model

How to find a model structure

How to visualize the structure

How to calculate distances and geometries



Barns.ill.fr



<http://database.iem.ac.ru/mincryst/>

Full inorganic structure database (ICSD) (registration fees)

Protein Data Base (Free)

PowderCell for Windows
Version 2.4
8.03.2000

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Bernd Müller (Uni Jena) bernd.mueller@uni-jena.de Size and Strain
U. Müller (Uni Kassel) u.mueller@uni-kassel.de subgroup data

VESTA
Visualization for Electronic and Structural Analysis

Site	(x)	(y)	(z)	Occupancy
1	1.00	0.00	0.00	1.00
2	0.50	0.50	0.50	1.00
3	0.00	0.50	0.00	1.00
4	0.00	0.00	0.50	1.00
5	0.50	0.00	0.50	1.00
6	1.00	0.50	0.00	1.00
7	1.00	0.00	0.50	1.00
8	0.50	0.00	0.00	1.00
9	0.00	0.00	0.00	1.00
10	0.00	0.50	0.50	1.00
11	0.50	0.50	0.00	1.00
12	0.50	0.00	0.50	1.00
13	1.00	0.00	0.00	1.00
14	1.00	0.50	0.00	1.00
15	1.00	0.00	0.50	1.00
16	0.50	0.50	0.50	1.00
17	0.00	0.50	0.00	1.00
18	0.00	0.00	0.50	1.00
19	0.50	0.00	0.00	1.00
20	0.50	0.00	0.50	1.00
21	0.00	0.00	0.00	1.00
22	0.00	0.50	0.50	1.00
23	0.50	0.50	0.00	1.00
24	0.50	0.00	0.50	1.00
25	1.00	0.50	0.00	1.00
26	1.00	0.00	0.50	1.00
27	0.50	0.50	0.50	1.00

total number of polyhedra and unique vertices on slices:
(0 2 0): 0 1 0
(0 2 1): 0 1 0
(0 2 2): 0 1 0
(0 2 3): 0 1 0
(0 2 4): 0 1 0
(0 2 5): 0 1 0
(0 2 6): 0 1 0
(0 2 7): 0 1 0
(0 2 8): 0 1 0
(0 2 9): 0 1 0
(0 2 10): 0 1 0
(0 2 11): 0 1 0
(0 2 12): 0 1 0
(0 2 13): 0 1 0
(0 2 14): 0 1 0
(0 2 15): 0 1 0
(0 2 16): 0 1 0
(0 2 17): 0 1 0
(0 2 18): 0 1 0
(0 2 19): 0 1 0
(0 2 20): 0 1 0
(0 2 21): 0 1 0
(0 2 22): 0 1 0
(0 2 23): 0 1 0
(0 2 24): 0 1 0
(0 2 25): 0 1 0
(0 2 26): 0 1 0
(0 2 27): 0 1 0
(0 2 28): 0 1 0
(0 2 29): 0 1 0
(0 2 30): 0 1 0
(0 2 31): 0 1 0
(0 2 32): 0 1 0
(0 2 33): 0 1 0
(0 2 34): 0 1 0
(0 2 35): 0 1 0
(0 2 36): 0 1 0
(0 2 37): 0 1 0
(0 2 38): 0 1 0
(0 2 39): 0 1 0
(0 2 40): 0 1 0
(0 2 41): 0 1 0
(0 2 42): 0 1 0
(0 2 43): 0 1 0
(0 2 44): 0 1 0
(0 2 45): 0 1 0
(0 2 46): 0 1 0
(0 2 47): 0 1 0
(0 2 48): 0 1 0
(0 2 49): 0 1 0
(0 2 50): 0 1 0
(0 2 51): 0 1 0
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(0 2 55): 0 1 0
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(0 2 64): 0 1 0
(0 2 65): 0 1 0
(0 2 66): 0 1 0
(0 2 67): 0 1 0
(0 2 68): 0 1 0
(0 2 69): 0 1 0
(0 2 70): 0 1 0
(0 2 71): 0 1 0
(0 2 72): 0 1 0
(0 2 73): 0 1 0
(0 2 74): 0 1 0
(0 2 75): 0 1 0
(0 2 76): 0 1 0
(0 2 77): 0 1 0
(0 2 78): 0 1 0
(0 2 79): 0 1 0
(0 2 80): 0 1 0
(0 2 81): 0 1 0
(0 2 82): 0 1 0
(0 2 83): 0 1 0
(0 2 84): 0 1 0
(0 2 85): 0 1 0
(0 2 86): 0 1 0
(0 2 87): 0 1 0
(0 2 88): 0 1 0
(0 2 89): 0 1 0
(0 2 90): 0 1 0
(0 2 91): 0 1 0
(0 2 92): 0 1 0
(0 2 93): 0 1 0
(0 2 94): 0 1 0
(0 2 95): 0 1 0
(0 2 96): 0 1 0
(0 2 97): 0 1 0
(0 2 98): 0 1 0
(0 2 99): 0 1 0
(0 2 100): 0 1 0

ATOMS on the Web

<http://millenia.cars.aps.anl.gov/cgi-bin/atoms/atoms.cgi>

Run ATOMS Clear Reset

Gold

Titles

Operational Parameters

Space Group: Fm-3m Rmax: 6 Edge: [dropdown]

Output Type: feff6.inp Shift: [input] [input] [input]

Lattice Constants and Angles

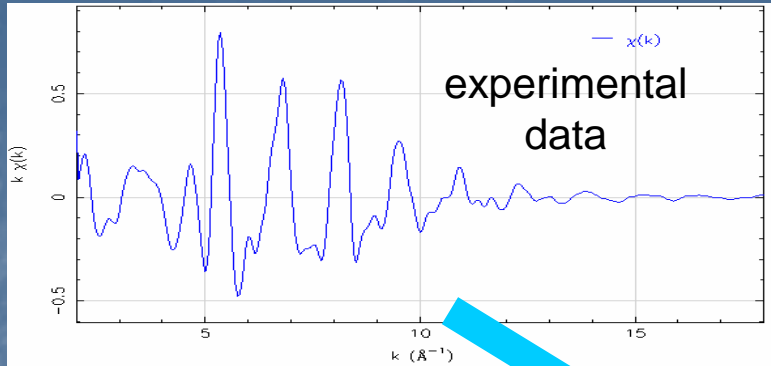
A: 4.08 B: 4.08 C: 4.08
Alpha: 90 Beta: 90 Gamma: 90

Run ATOMS Clear Reset

Table of Crystallographic Sites

Cent.	Element	X	Y	Z	Tag
1	Au	0	0	0	Au

Search on the web !

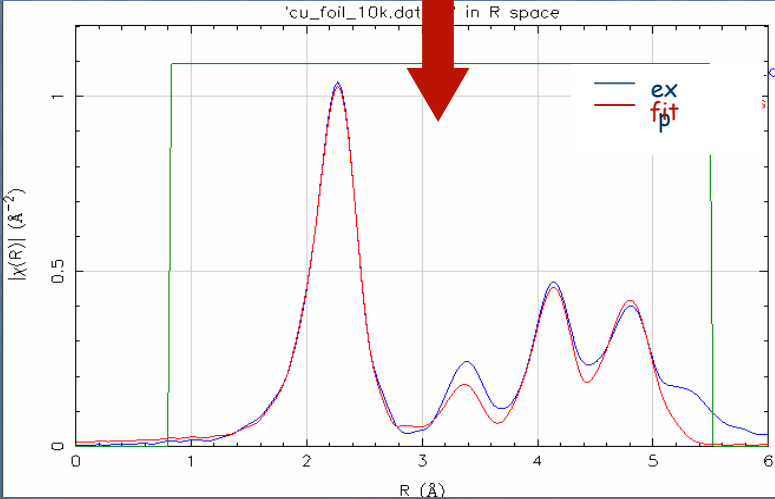


Theoretical formula

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2 \sigma_j^2}}{k R_j^2} \sin[2k R_j + \delta_j(k)]$$

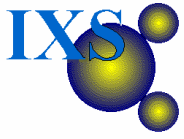
Amplitude and phase functions from atomic cluster models

How a data refinement program works



XAFS data analysis software

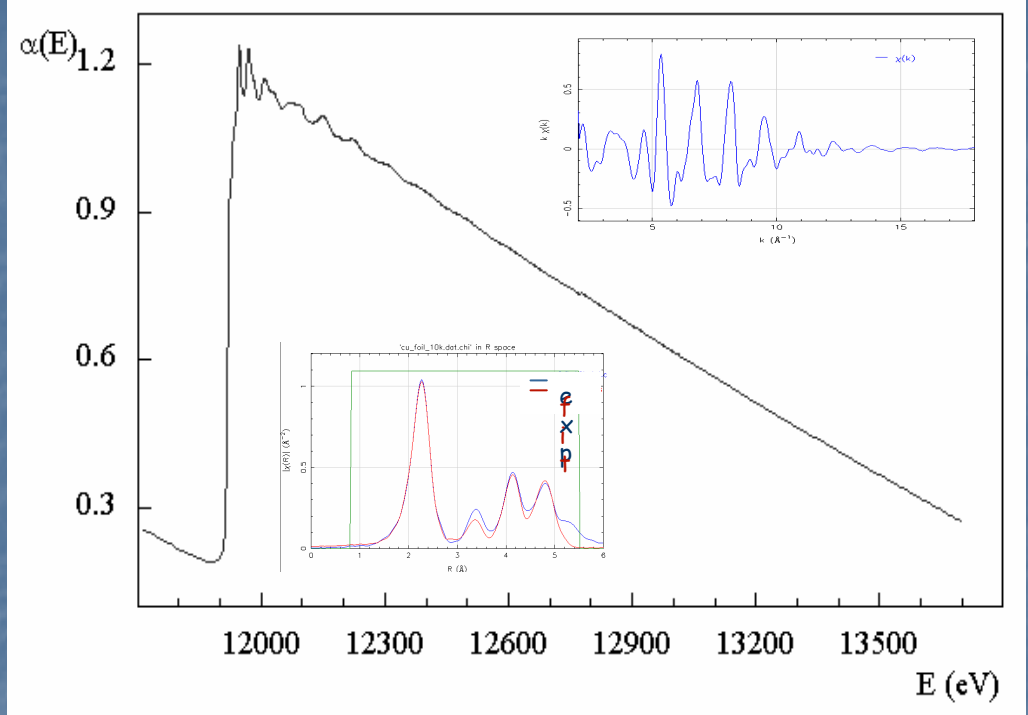
XAFS organizations



Welcome to the International XAFS Society Home Page www.i-x-s.org

xafs.org

- XAFS
- Recent News
- Applications
- Theory/Analysis
- Experiment
- Related Techniques
- Community
- Resources
- Software
- Help



GNXAS home-page



XAS LAB
X-ray Absorption Spectroscopy Laboratory - University of Cambridge

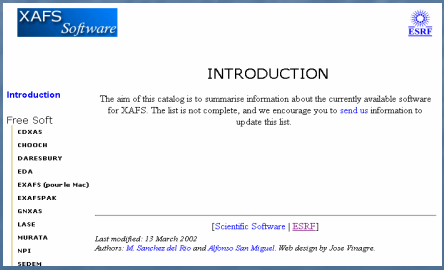
GNXAS
Current version: 12.2006

HOME
GNXAS
Info and News
Introduction
Description
Documentation

Amorphous & disordered systems

<http://gnxas.unicam.it>

XAFS data analysis



XAFS Software (ESRF logo)

INTRODUCTION

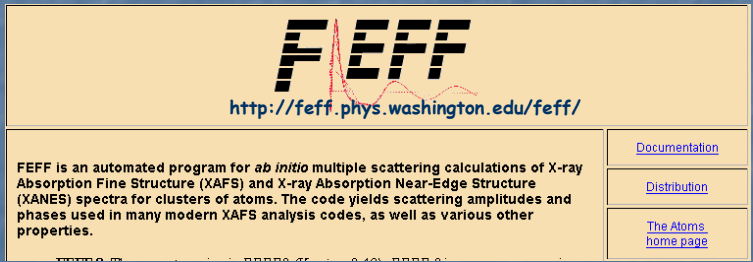
The aim of this catalog is to summarize information about the currently available software for XAFS. This list is not complete, and we encourage you to send us information to update this list.

Free Soft
EDXAS
CROUCH
DARESBU
EDA
EXAFS (Gourla Har)
EXAFSPAK
GNXAS
LASE
MURATA
NFI
STON

[Scientific Software] [ESRF]

Last modified: 13 March 2002
Authors: M. Sanchez del Rio and Alfonso San Miguel. Web design by Jose Pinague.

<http://www.esrf.eu/computing/scientific/exafs/>



FEFF
<http://feff.phys.washington.edu/feff/>

FEFF is an automated program for *ab initio* multiple scattering calculations of X-ray Absorption Fine Structure (XAFS) and X-ray Absorption Near-Edge Structure (XANES) spectra for clusters of atoms. The code yields scattering amplitudes and phases used in many modern XAFS analysis codes, as well as various other properties.

Documentation
Distribution
The Atoms home page

FEFF home-page



IFEFFIT

- Ifeffit
- Downloads
- Documentation
- Mailing List
- FAQ
- XAFS
- Help

<http://cars9.uchicago.edu/ifeffit/>

advantages:

- Freeware, multiplatform (Win, Mac, Linux)
- easy to handle,
- semi-automatic procedures



Ifeffit.exe



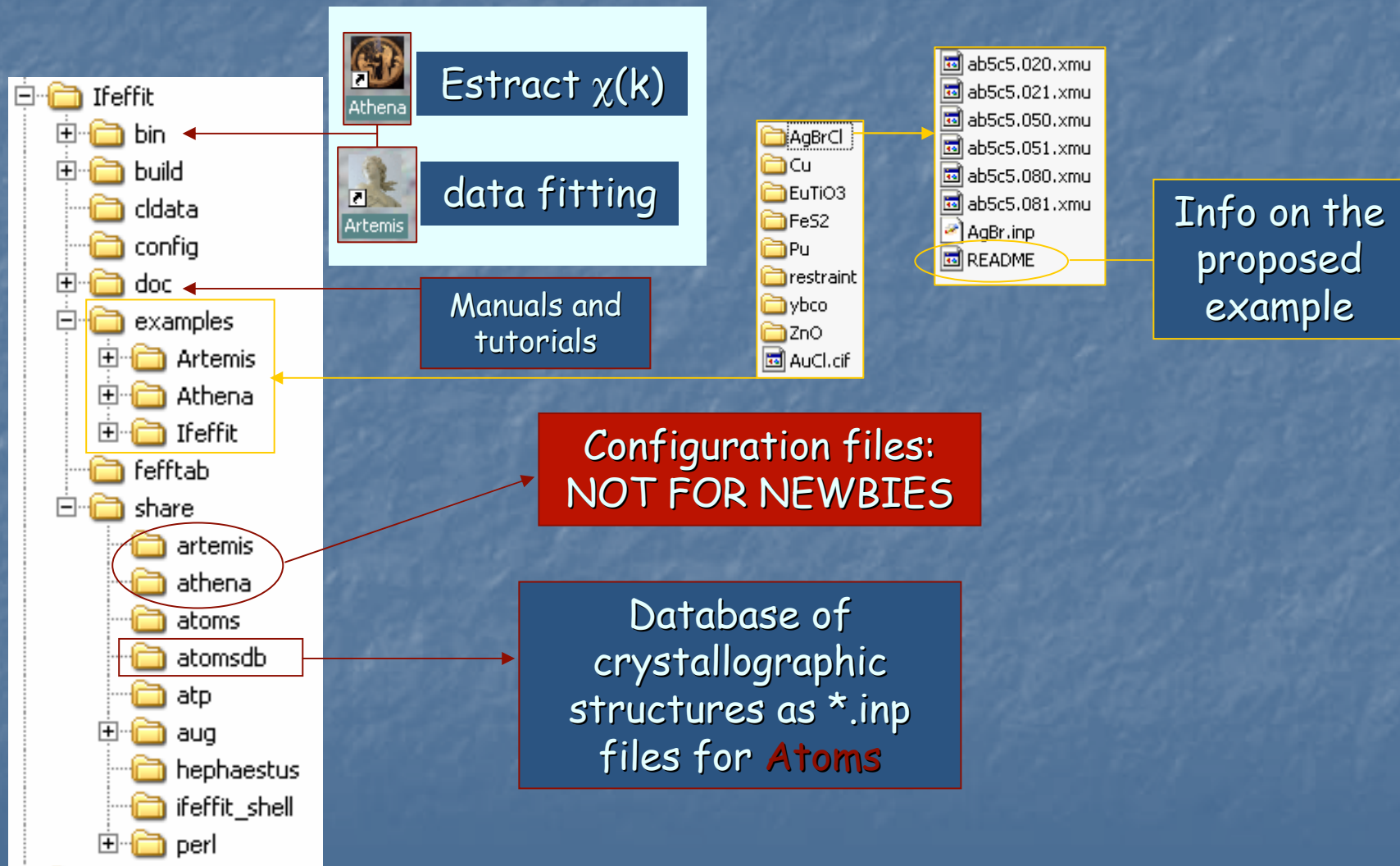
drawbacks:

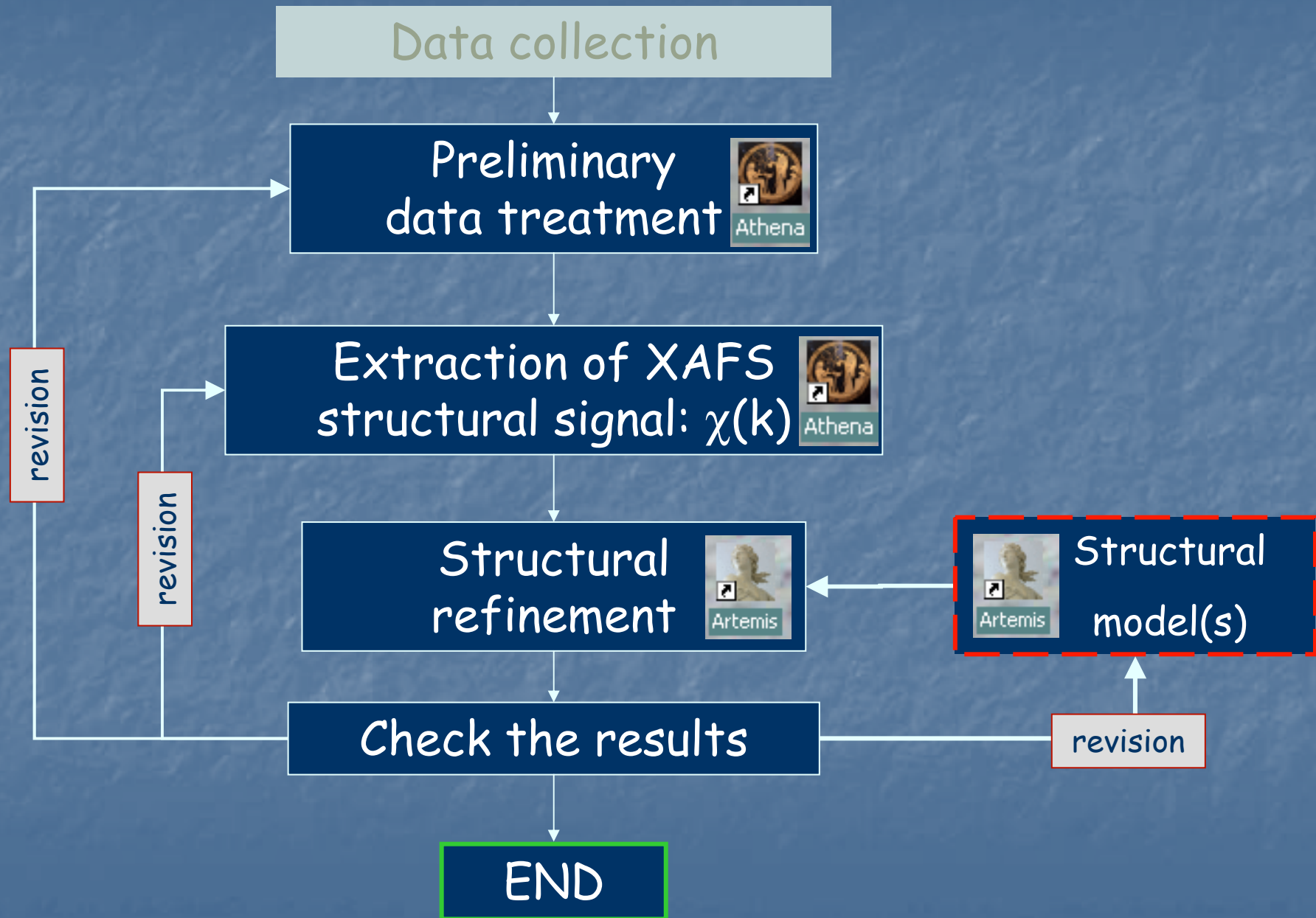
- easy to handle,
- semi-automatic procedures

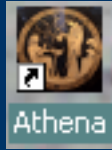
Install Ifeffit.exe

1. **athena** GUI for Data Processing with Ifeffit 
2. **artemis** GUI for XAFS Fitting with Ifeffit 
3. **hephaestus** GUI for general x-ray properties of the elements
4. **sixpack** GUI for XAFS Processing and Fitting with Ifeffit
5. **feff6L** Stand-alone program for ab inito EXAFS calculations
6. **atoms** Stand-alone, command line crystallography->feff.inp
7. **autobk** Stand-alone background removal program
8. **feffit** Stand-alone FEFF fitting program
9. **ifeffit** command-line version of Ifeffit

Inside the Ifeffit directory







Preliminary data treatment & Extraction of XAFS structural signal: $\chi(k)$

The screenshot shows the Athena software interface with several key sections:

- Project:** Current group is `cu_foil_10k.dat`. File path: `E:/Duino_ago09/Examples/Cu_10K/cu_foil_10k.dat`. Z: `Cu`, Edge: `K`, E shift: `0`, Importance: `1`.
- Background removal:** E_0 : `8977.58`, Rbkg: `1.0`, k-weight: `2`, Edge step: `2.32667` (fix step checked). Pre-edge range: `-150` to `-30`. Normalization range: `150` to `2284.89`. Spline range: k: `0.0` to `25.019`, E: `0.000` to `2384.861`.
- Forward Fourier transform:** k-range: `2` to `23.019`, dk: `1`, window type: `hanning`, Phase correction: `no`, arbitrary k-weight: `0.5`.
- Backward Fourier transform:** R-range: `1` to `3`, dr: `0.0`, window type: `hanning`.
- File List:** A list of files with `cu_foil_10k.dat` selected.
- Plotting options:** Buttons for `E`, `k`, `R`, `q`, `kq`. Radio buttons for `0`, `1`, `2`, `3`, `kw`. Checkboxes for `mu(E)`, `background`, `pre-edge line`, `post-edge line`, `Normalized`, `Derivative`.

List of files (group) opened into Athena

Plot highlighted files

Plot (several) marked files

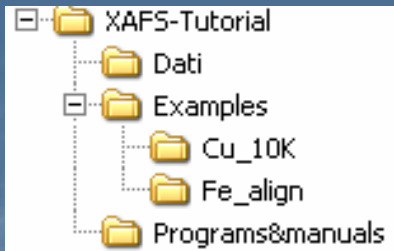
Options for plot

Warning: check if the full windows is visible on your PC, smal screens (i.e. e-pc) may cut the lower part

Warning: check the graphic windows and never close it leaving Athena/Artemis open... sometime the PC crashes

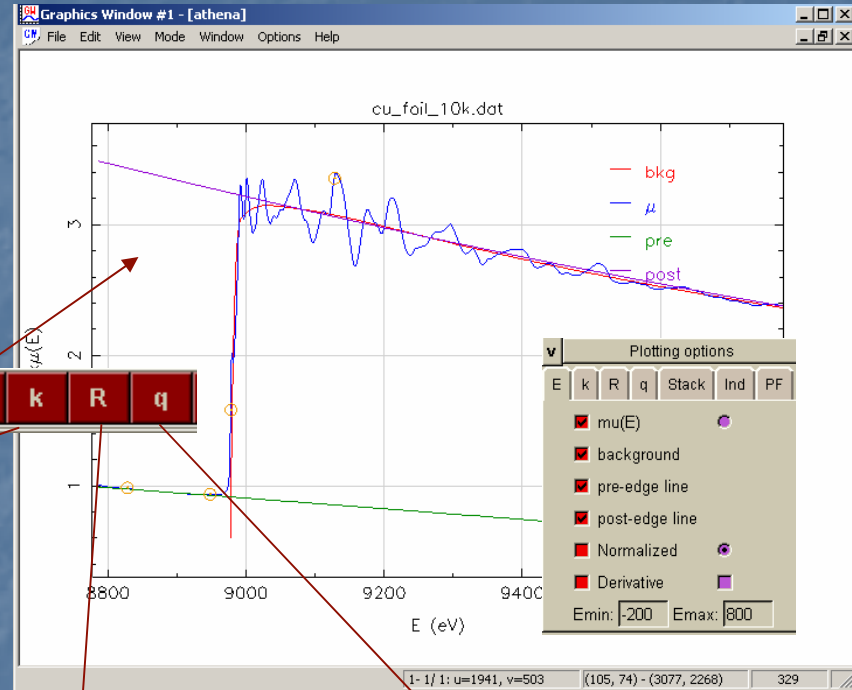
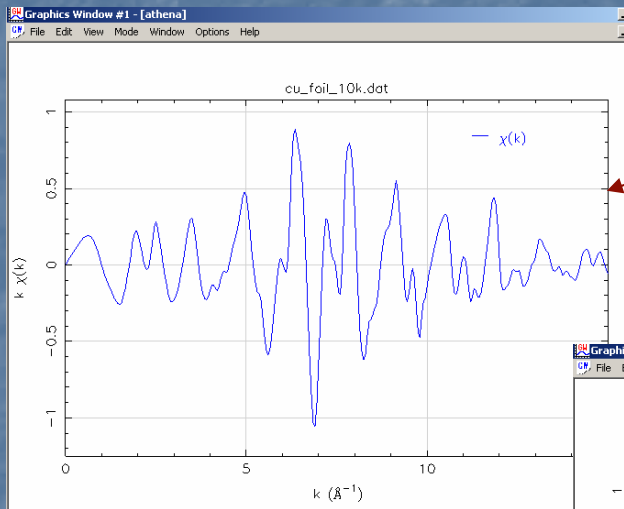
Example 1: Cu 10 K

Open cu foil 10k.dat into Athena

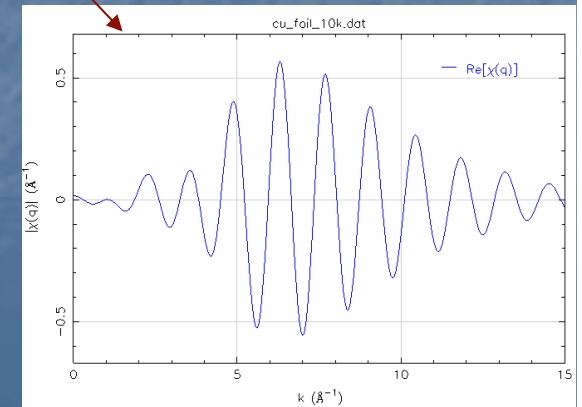
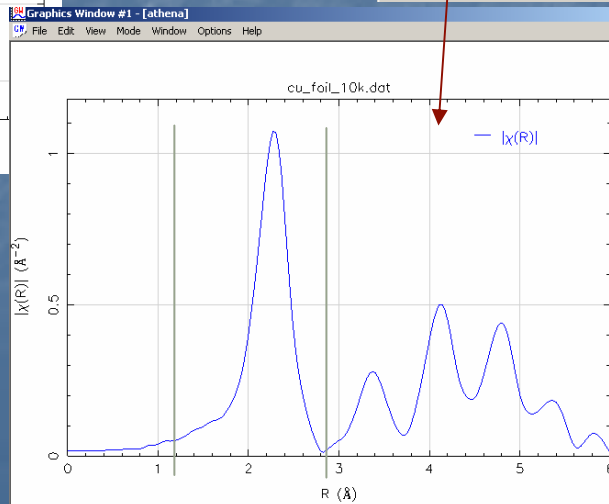


Exercise 1:

Look at the results obtained using the automatic extraction playing with plot options



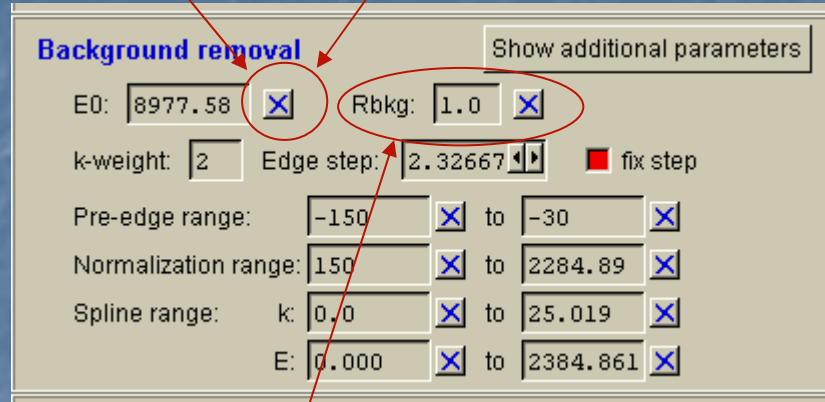
E k R q



Select E_0

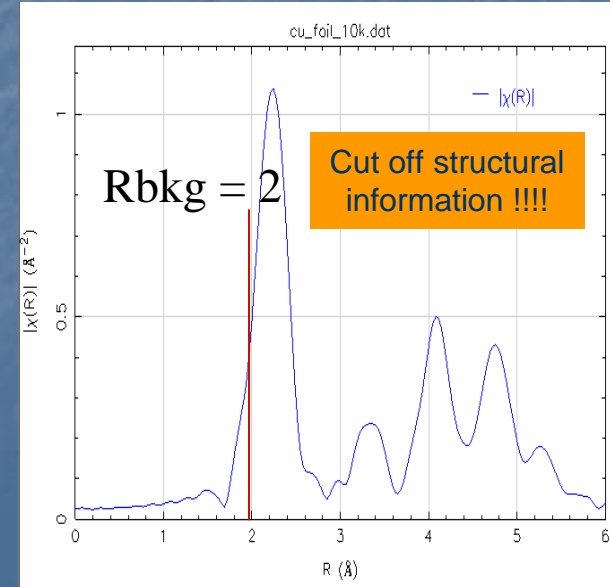
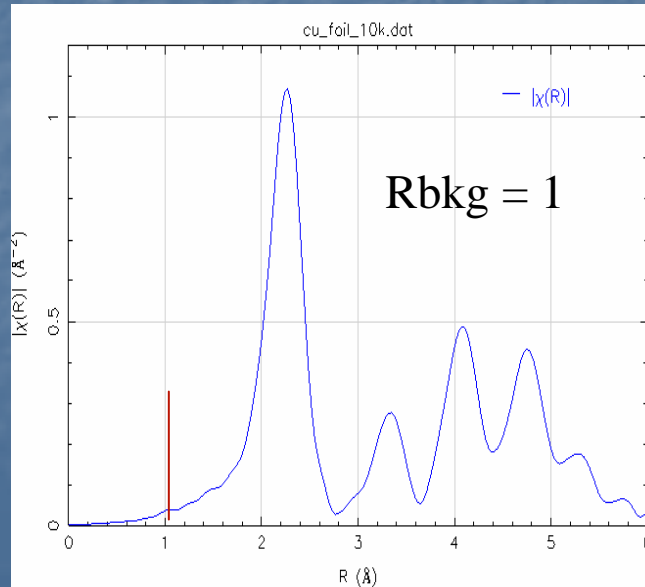
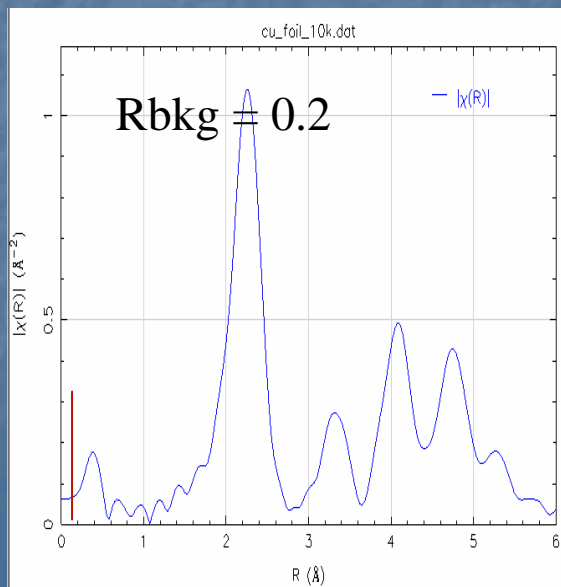
Takes the value from the cursor on the graph window

Exercise 2: Look at the effects of changing background subtraction parameters



- Change E_0
- Change R_{bkg}
-

R cut off for automatic background calculation



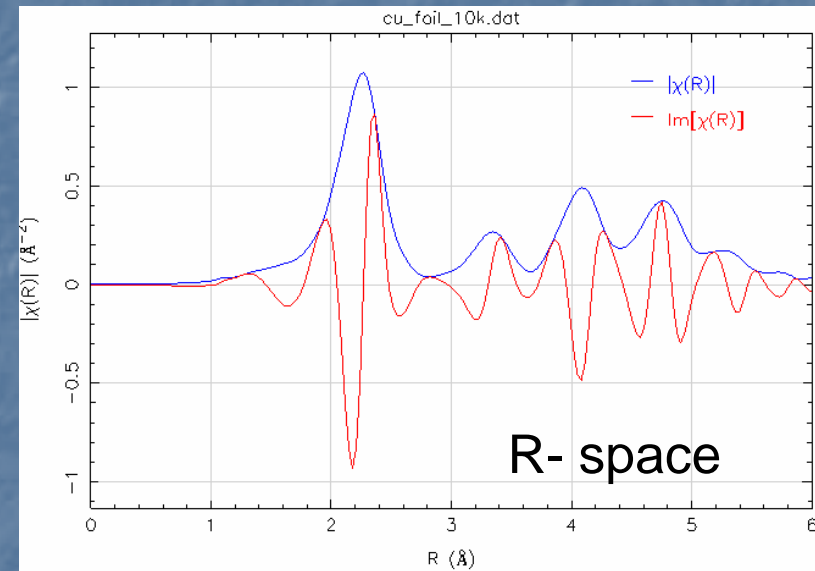
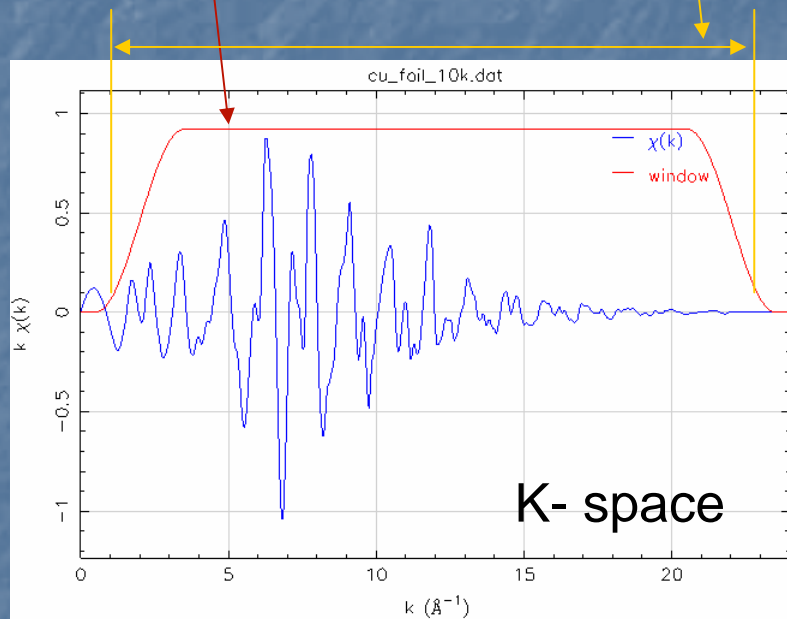
Exercise 3: in Real space look at the effects of changing extraction and FT parameters

Forward Fourier transform

k-range: to

dk: window type:

Phase correction: no arbitrary k-weight:



0 1 2 3 kw

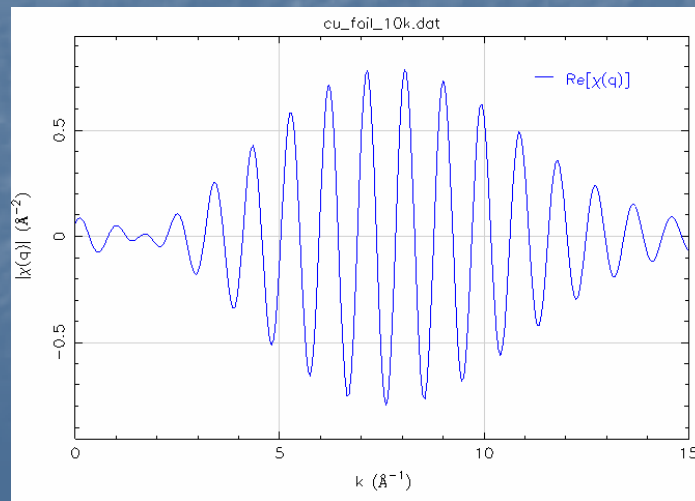
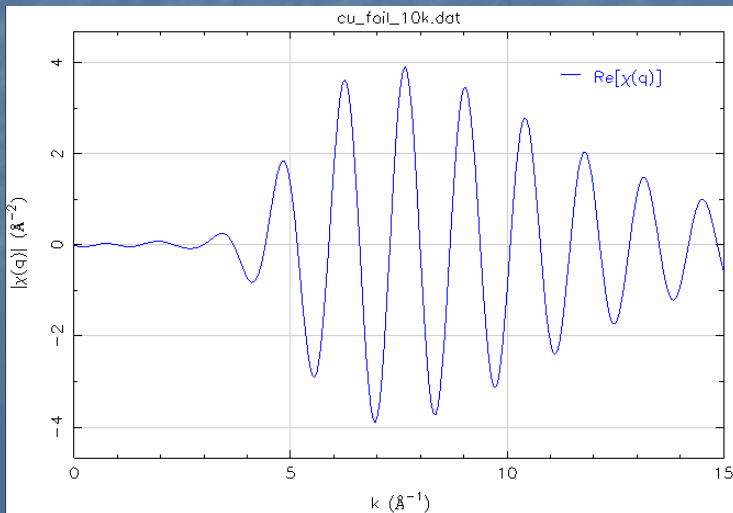
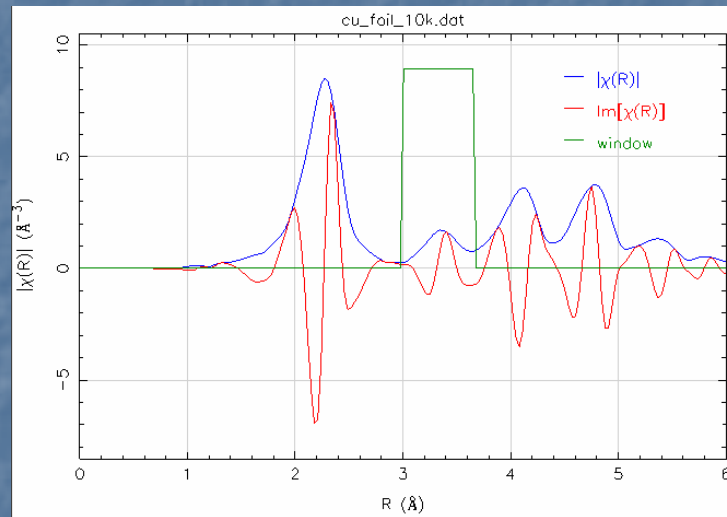
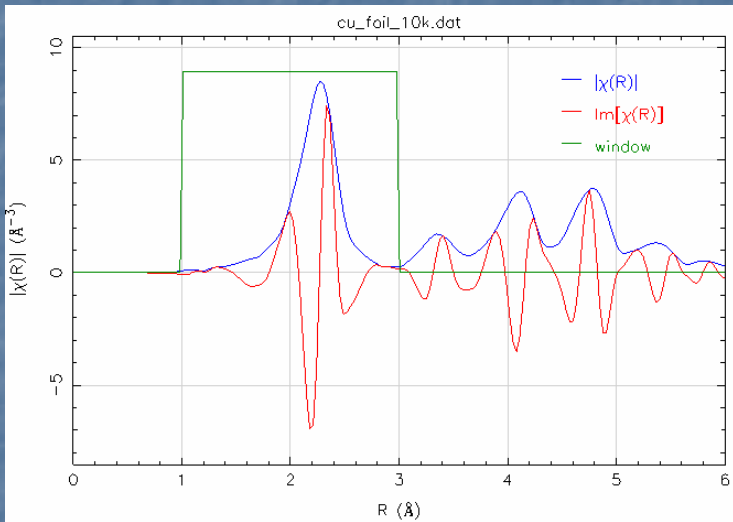
FT of: $k^{kw} \chi(k)$

Backward Fourier transform

R-range: to

dr: window type:

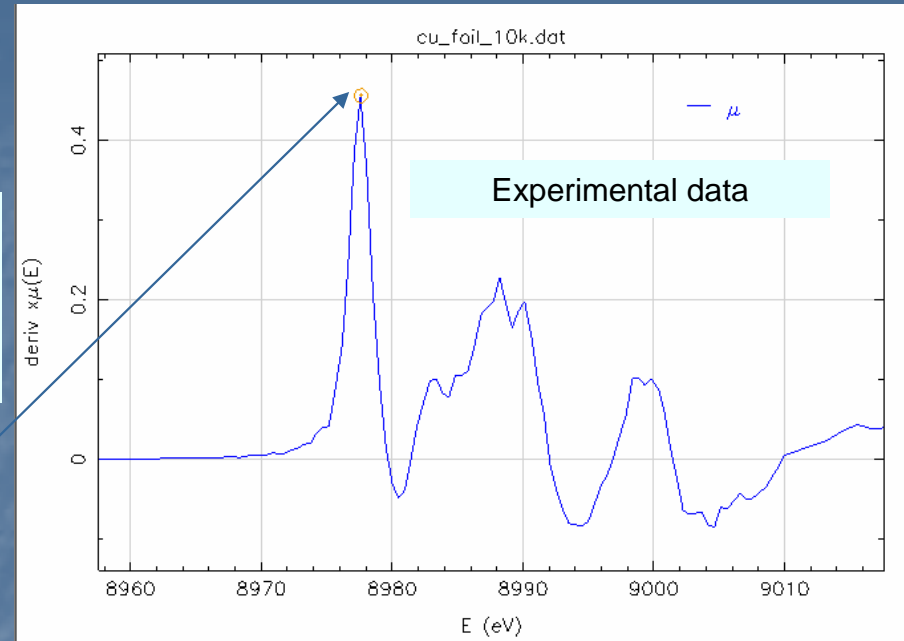
Exercise 4: in q (Back Fourier) space
look at the effects of changing BF
parameters and regions



Exercise 5: Data treatment

- Data Merge Analysis Settings
- Calibrate energies**
- Align scans
- Calibrate dispersive XAS
- Degitch
- Truncate
- Rebin $\mu(E)$
- Smooth $\mu(E)$
- Convolute $\mu(E)$
- Self Absorption
- MEE correction

Shifts the spectrum to have selected point (reference at) at the calibration energy (calibrate to)



Data calibration

Group: cu_foil_10k.dat

Display: deriv(E)

Smoothing: 0

Reference at: 8977.58

Calibrate to: 8979

Select a point

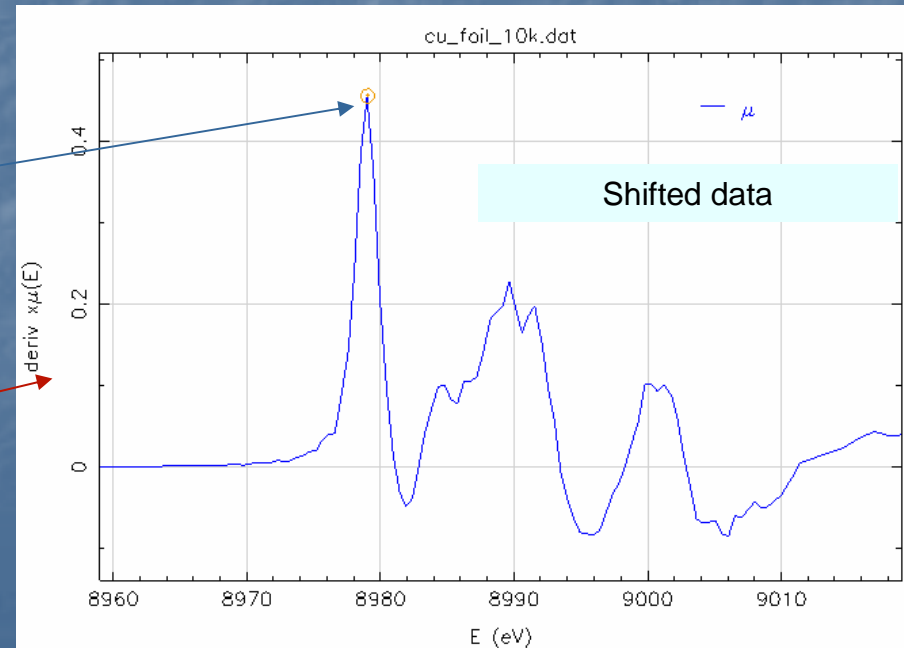
Find zero-crossing

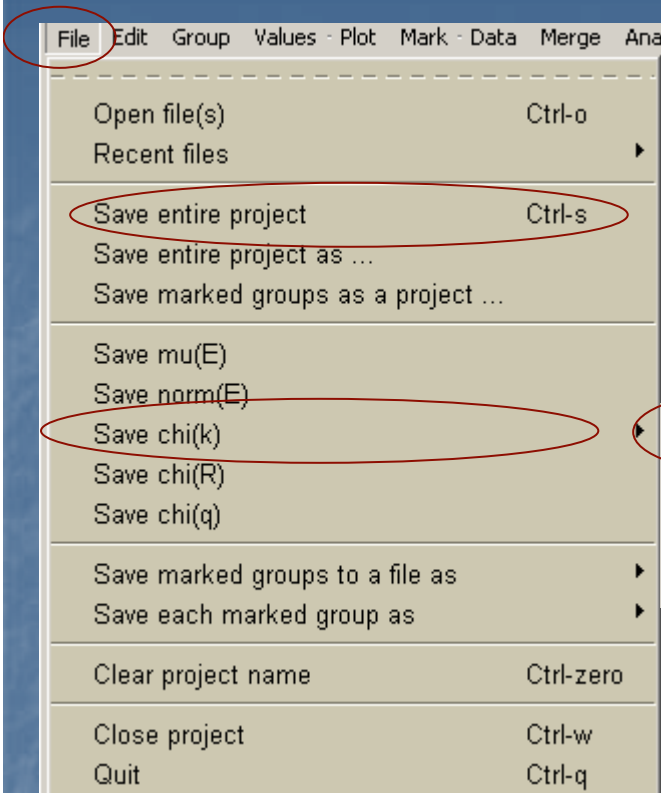
Replot

Calibrate

Document section: energy calibration

Return to the main window





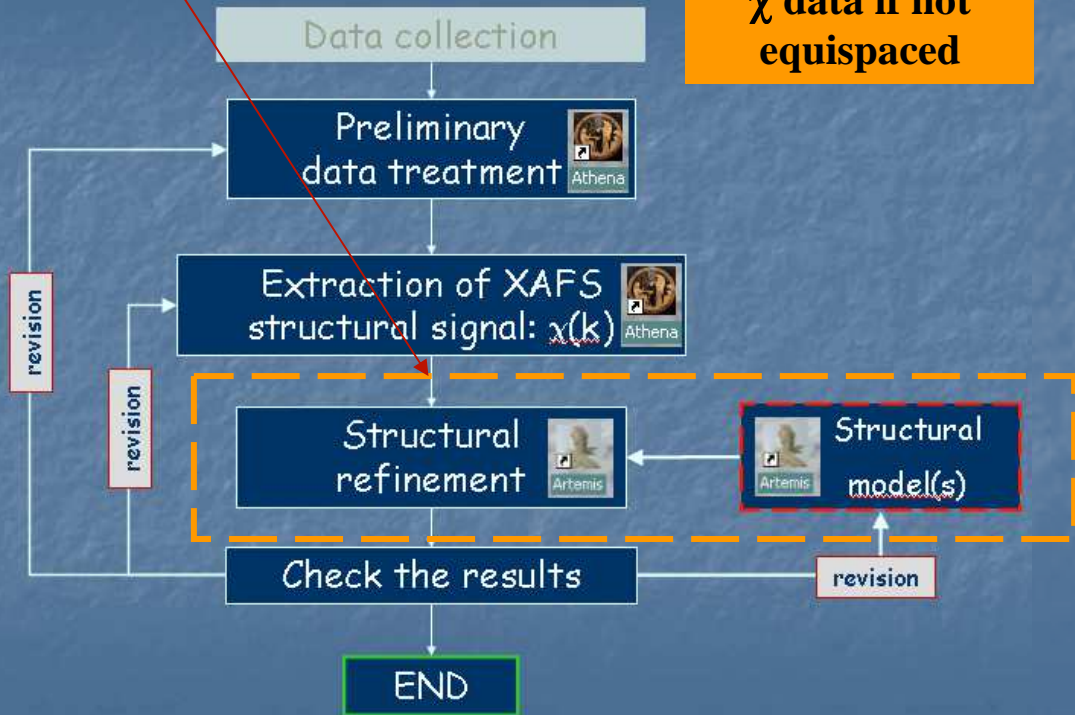
Save:

cu_foil_10k.dat.chi

$\chi(k)$ is required for ARTEMIS

Note: Artemis requires equispaced k data !!!
(i.e. $\delta k = 0.05$)

You cannot use χ data if not equispaced



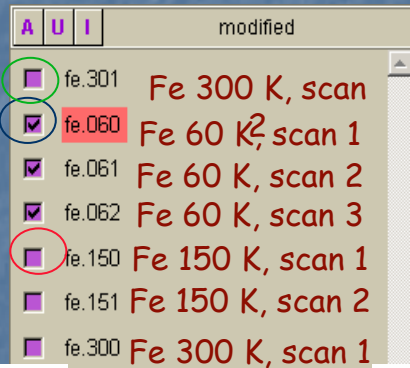
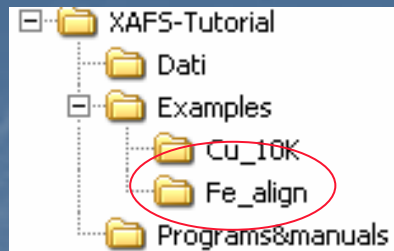
Working with several files

Go into the **Fe_Align** directory

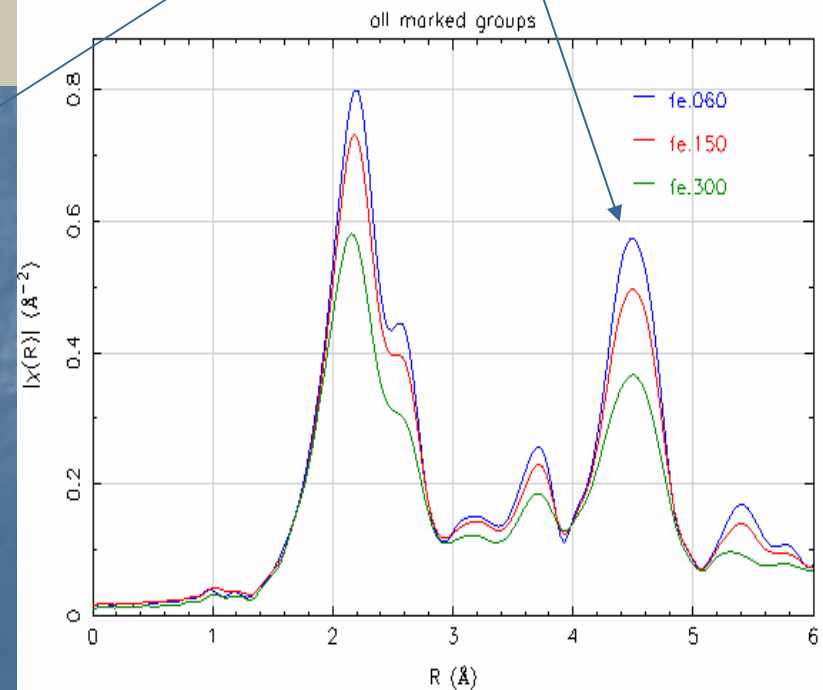
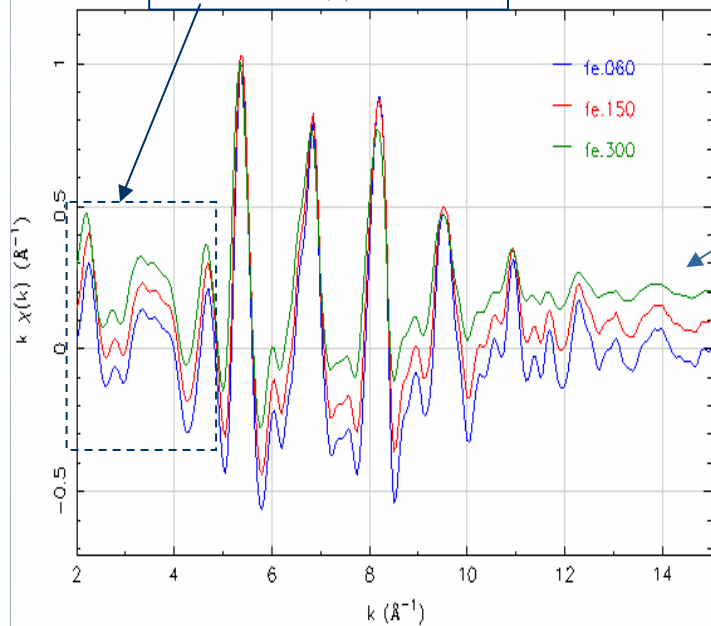
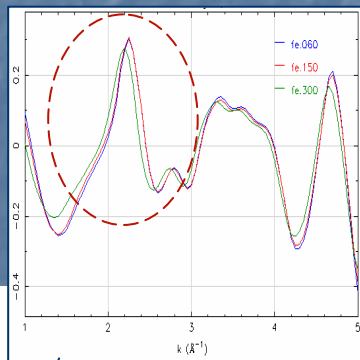
Open all **Fe files** into Athena

Data Merge Analysis Settings

Calibrate energies
Align scans
Calibrate dispersive XAS
Deglitch
Truncate
Rebin $\mu(E)$
Smooth $\mu(E)$
Convolute $\mu(E)$
Self Absorption
MEE correction

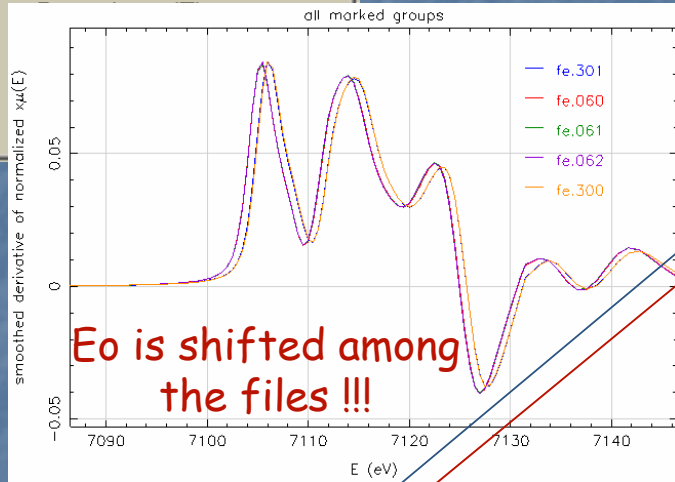
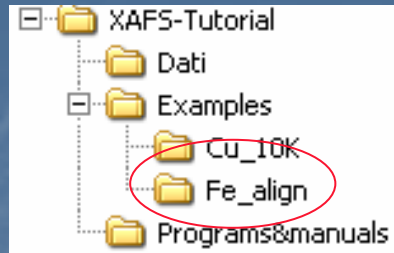
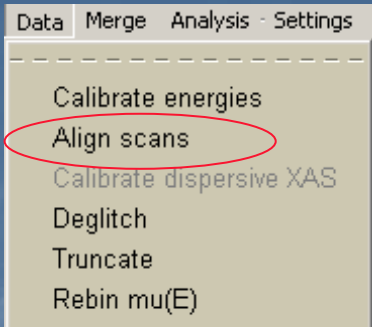


Temperature effect on EXAFS and FT data

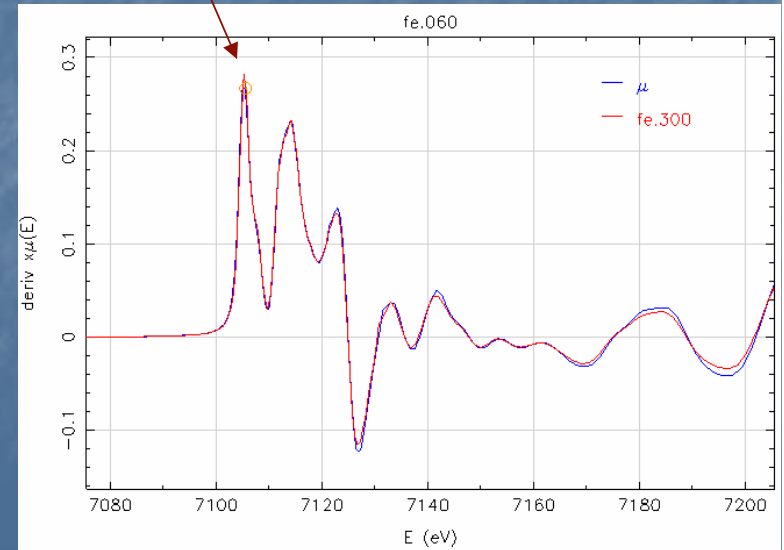
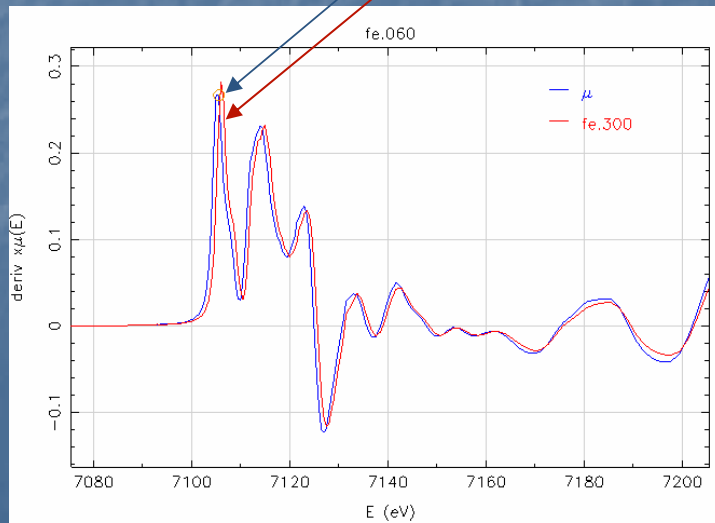
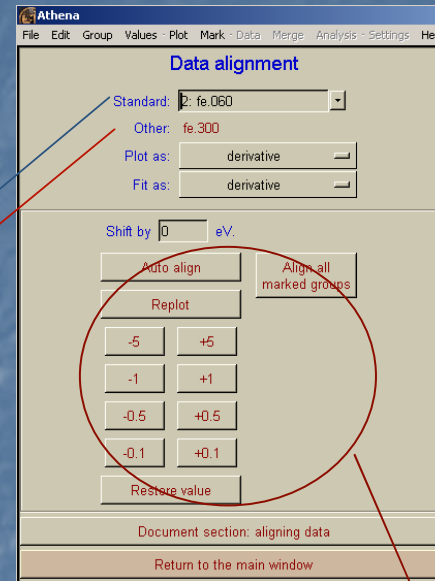


Exercise 6: align E₀

Open Fe files into Athena



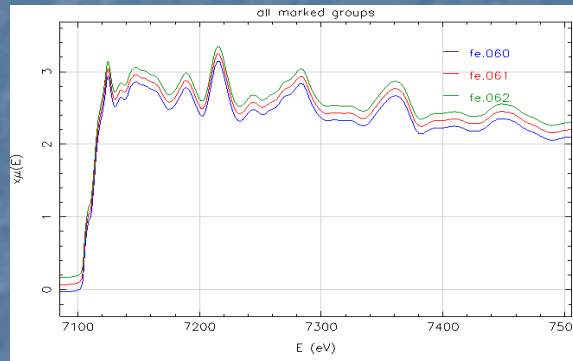
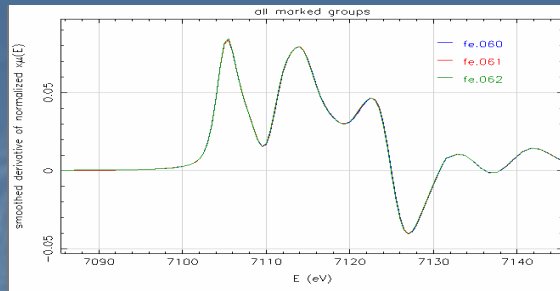
E₀ is shifted among the files !!!



Exercise 7: Merge several files

Merge Analysis - Settings Help

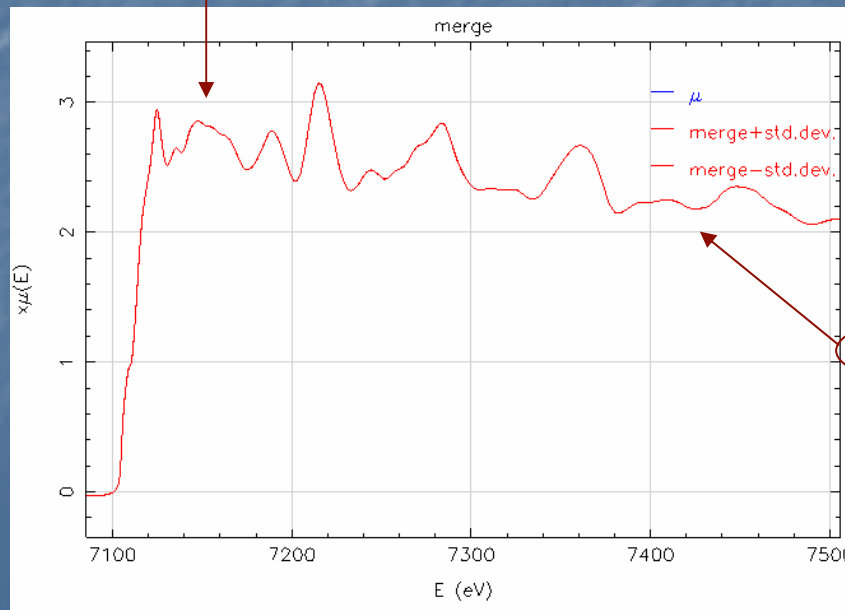
- Merge marked data in $\mu(E)$
- Merge marked data in $\text{norm}(E)$
- Merge marked data in $\chi(k)$
- Weight by importance
- Weight by chi_noise



A U I modified

- fe.301
- fe.060
- fe.061
- fe.062
- fe.150
- fe.151
- fe.300

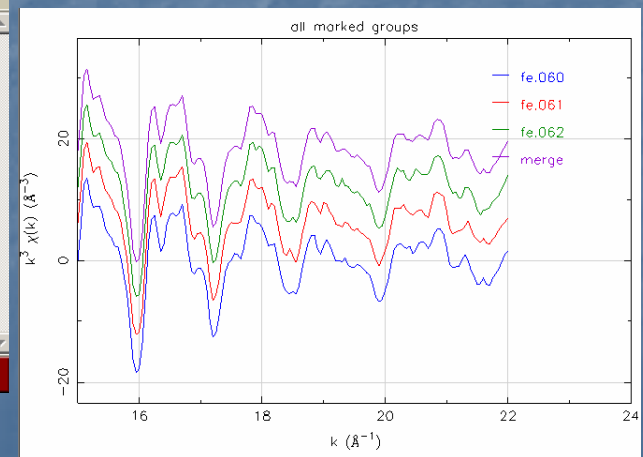
Fe 60 are now aligned



A U I modified

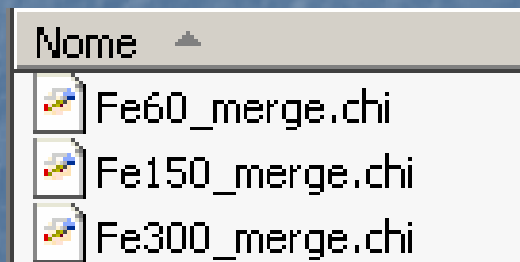
- fe.301
- fe.060
- fe.061
- fe.062
- fe.150
- fe.151
- fe.300
- merge

E k R q kq



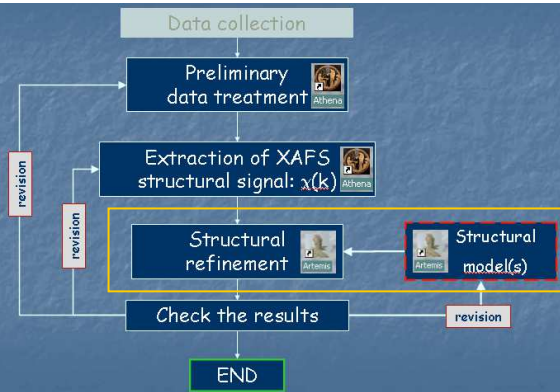
Full Exercise:

1. Read Fe Files
2. Align Fe files on order to have the same E_0
3. Merge files having the same T
4. Save $\chi(k)$ of merged files, to be used for the structural analysis



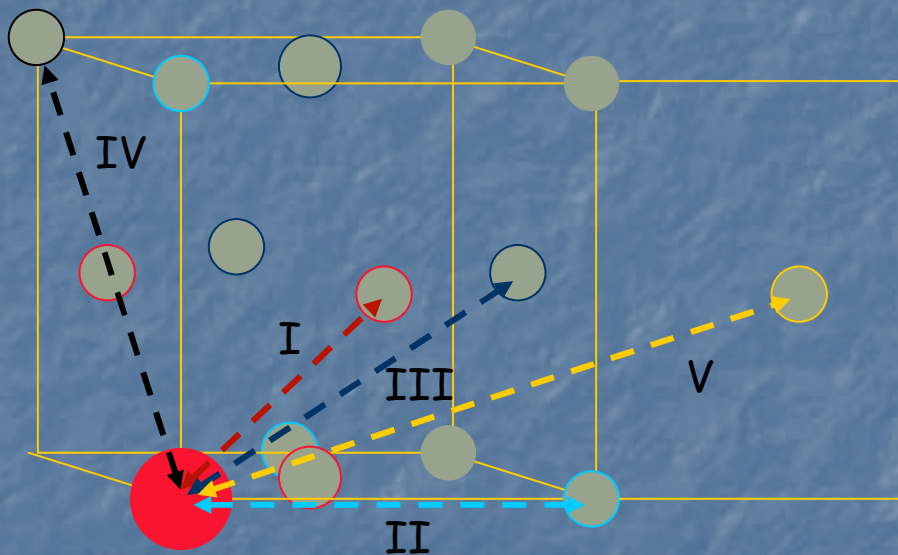


Structural model & Data refinement



Cu-fcc

metal
 SPG: fcc, f m 3 m (# 220)
 $a = 3.61 \text{ \AA}$
 Cu 0.0 0.0 0.0



Sh	R	N	$R_{Cu}(A)$
I:	$a/\sqrt{2}$	12	2.553
II:	a	6	3.610
III:	$a \cdot \sqrt{1.5}$	24	4.421
IV:	$a \cdot \sqrt{2}$	12	5.105
V:	$a \cdot \sqrt{2.5}$	24	5.708
....			

You can visualize the structure using VESTA program

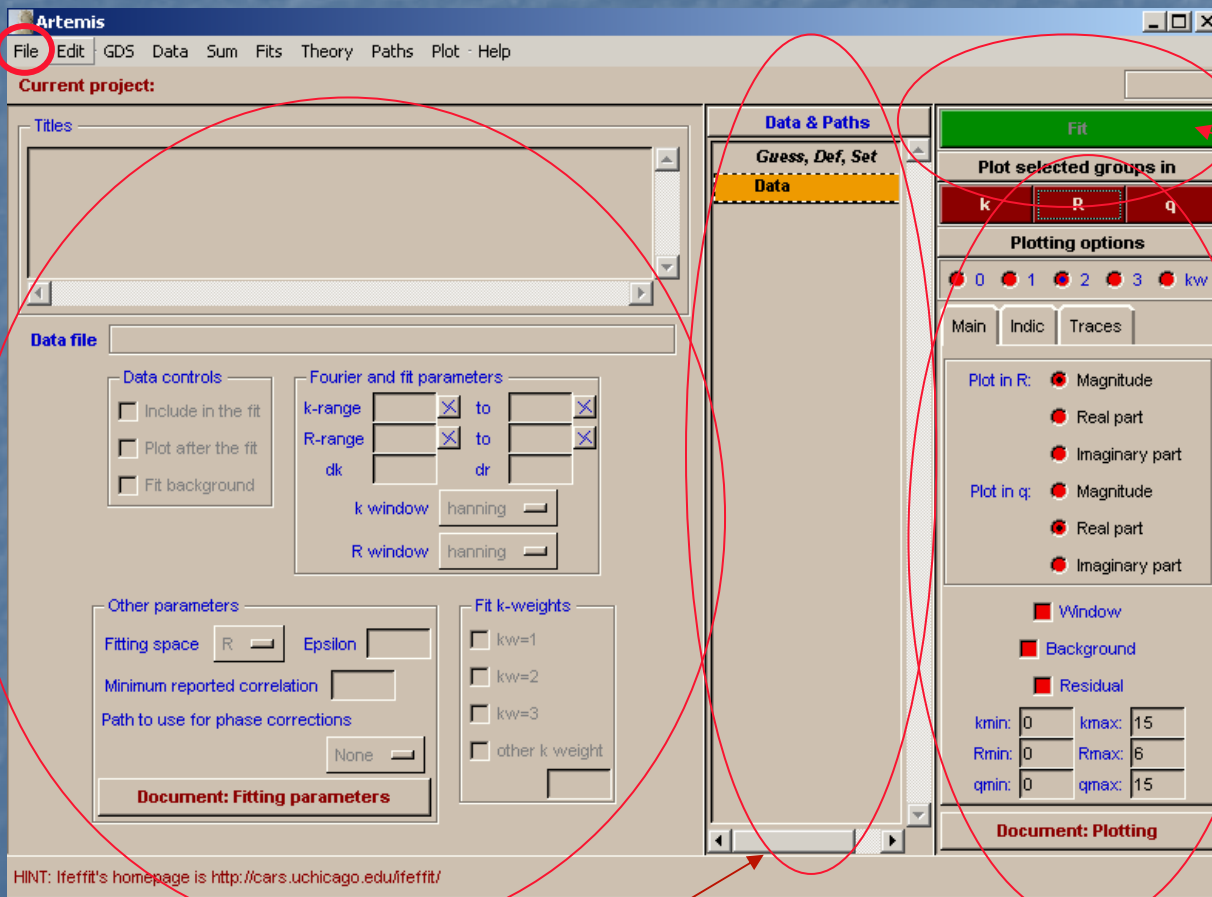
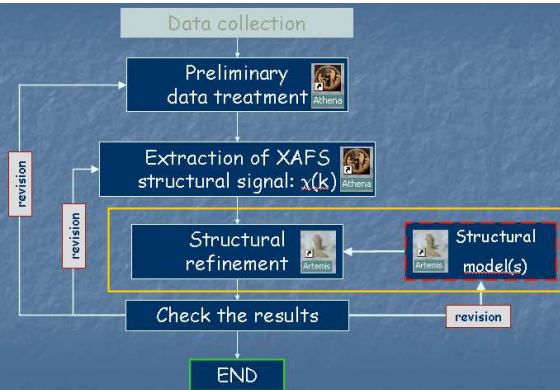
icsd_43493_Copper.cif



Structural model & Data refinement

Start the ARTEMIS program

The ARTEMIS panel



Start the refinement

Warning: check the full windows is visible on your PC, smaller screens may cut the lower part

Warning: check the graphic windows and never close it leaving Athena/Artemis open... sometime the PC crashes

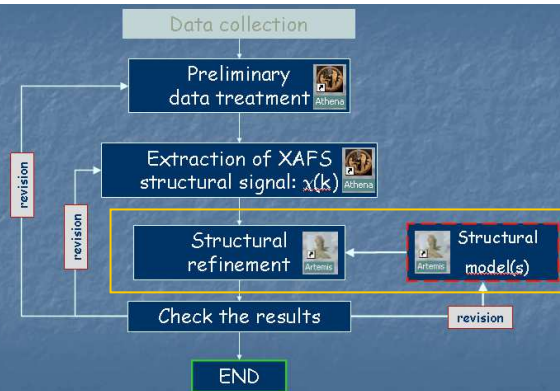
Depends on what is highlighted in the Data & Paths panel

Controls for plotting

HINT: Ifeffit's homepage is <http://cars.uchicago.edu/ifeffit/>



Structural model & Data refinement



Artemis
File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project:

Titles

Data file

Data controls

- Include in the fit
- Plot after the fit
- Fit background

Fourier and fit parameters

k-range [] to []
R-range [] to []
dk [] dr []

k window hanning
R window hanning

Other parameters

Fitting space R Epsilon []
Minimum reported correlation []
Path to use for phase corrections [None]

Fit k-weights

- kw=1
- kw=2
- kw=3
- other k weight []

Document: Fitting parameters

Main Indic Traces

Plot in R: Magnitude Real part Imaginary part

Plot in q: Magnitude Real part Imaginary part

- Window
- Background
- Residual

kmin: 0 kmax: 15
Rmin: 0 Rmax: 6
qmin: 0 qmax: 15

Document: Plotting

HINT: Ifeffit's homepage is <http://cars.uchicago.edu/ifeffit/>

Theory
→ new atoms page

- Import **Cu.inp** file from the **Cu_10k** directory
- Or
- Blank Atom page (you must type the crystallographic info)

Warning: check the full windows is visible on your PC, smaller screens may cut the lower part

Artemis

File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project:

Atoms feff.inp Interpretation

Titles

name: copper
formula: Cu
sites: Cu1

Space group f m 3 m

A 3.61000 1 Cu 0.00000 0.00000 0.00000

B

C

Alpha 90.00000

Beta

Gamma

Cluster size 6.00000

Edge K

Shift vector 0 0 0

Define the parameters describing the structure

Edit selected site

Comment: Tag: Define

New

Run Atoms Document: Atoms

Data & Paths

Guess, Def, Set

Data

FEFF0

Fit

Plot selected groups in

k R q

Plotting options

0 1 2 3 kw

Main Indic Traces

Plot in R: Magnitude Real part Imaginary part

Plot in q: Magnitude Real part Imaginary part

Window Background Residual

kmin: 0 kmax: 15
Rmin: 0 Rmax: 6
qmin: 0 qmax: 15

Document: Plotting

Artemis

File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project:

Atoms feff.inp Interpretation

Data & Paths

Guess, Def, Set

Data

FEFF0

```
* This feff6 input file was generated by Artemis 0.
* Atoms written by and copyright (c) Bruce Ravel, 1
*
* -- * -- * -- * -- * -- * -- * -- * -- * -- * -- *
* total mu*x=1: 4.06 microns, unit edge step
* specific gravity = 8.971
*
* Normalization correction: 0.00046 ang^2
*
* -----
* The following crystallographic data were used:
*
* title name: copper
* title formula: Cu
* title sites: Cu1
* title refer1: Kittel, ISSP
* title refer2:
* title schoen:
* title notes1: metal, fcc
* space = F m -3 m
* a = 3.610 b = 3.610 c = 3.610
* alpha = 90.0 beta = 90.0 gamma = 90.0
* edge = v
```

Run Feff Document: Feff and it's input file

Running atoms ... done!

Sh	R	N	$R_{Cu}(A)$
I:	$a/\sqrt{2}$	12	2.553
II:	a	6	3.610
III:	$a \cdot \sqrt{1.5}$	24	4.421
IV:	$a \cdot \sqrt{2}$	12	5.105
V:	$a \cdot \sqrt{2.5}$	24	5.708
....			

Check the distances and multiplicities are those you expect

Artemis

Atoms feff.inp Interpretation

```
* this list contains 79 atom
y z ipot tag dis
000 0.00000 0.00000 0 Cu1 0.00000
500 1.80500 0.00000 1 Cu1_1 2.55266
500 1.80500 0.00000 1 Cu1_1 2.55266
500 -1.80500 0.00000 1 Cu1_1 2.55266
500 -1.80500 0.00000 1 Cu1_1 2.55266
500 0.00000 1.80500 1 Cu1_1 2.55266
500 0.00000 1.80500 1 Cu1_1 2.55266
000 1.80500 1.80500 1 Cu1_1 2.55266
000 -1.80500 1.80500 1 Cu1_1 2.55266
000 -1.80500 1.80500 1 Cu1_1 2.55266
500 0.00000 -1.80500 1 Cu1_1 2.55266
500 0.00000 -1.80500 1 Cu1_1 2.55266
000 1.80500 -1.80500 1 Cu1_1 2.55266
000 -1.80500 -1.80500 1 Cu1_1 2.55266
000 0.00000 0.00000 1 Cu1_2 3.61000
000 0.00000 0.00000 1 Cu1_2 3.61000
000 3.61000 0.00000 1 Cu1_2 3.61000
000 -3.61000 0.00000 1 Cu1_2 3.61000
000 0.00000 3.61000 1 Cu1_2 3.61000
000 0.00000 -3.61000 1 Cu1_2 3.61000
000 1.80500 1.80500 1 Cu1_3 4.42133
000 1.80500 1.80500 1 Cu1_3 4.42133
500 3.61000 1.80500 1 Cu1_3 4.42133
500 3.61000 1.80500 1 Cu1_3 4.42133
```

How many feff paths do you want to import right now?

No paths Just the first The first 10 All paths

FEFF0

- Path 1: [Cu1_1]
- Path 2: [Cu1_2]
- Path 3: [Cu1_1 Cu1_1]
- Path 4: [Cu1_2 Cu1_1]
- Path 5: [Cu1_3]
- Path 6: [Cu1_1 Cu1_1]
- Path 7: [Cu1_3 Cu1_1]
- Path 8: [Cu1_4]
- Path 9: [Cu1_1 Cu1_1]
- Path 10: [Cu1_4 Cu1_1]
- Path 11: [Cu1_1 [*] Cu1_1]
- Path 12: [Cu1_1 [*] Cu1_1]
- Path 14: [Cu1_1 Cu1_4 Cu1_1]
- Path 15: [Cu1_1 Cu1_1 Cu1_1]
- Path 18: [Cu1_3 Cu1_1]

Artemis
File Edit GDS Data **Sum** Fits Theory Paths Plot Help

Current project:
FEFF0: Path 1: [Cu1_1]

All included paths for this data set
Selected & included paths for this data set
All selected paths for this data set

Plot after the fit
 Make this path the default after the fit

Artemis: Information about this summation

You are about to make a summation. This needs some information to help you organize your project.

Label:
Comment:
Figure of merit:

Make a new fit entry Reuse previous fit entry

Document: fit information dialog

Data & Paths

Guess, Def, Set

Data

- Sum
 - sum_ALL_Paths
 - FEFF0

Fit

Plot selected groups in

k R q

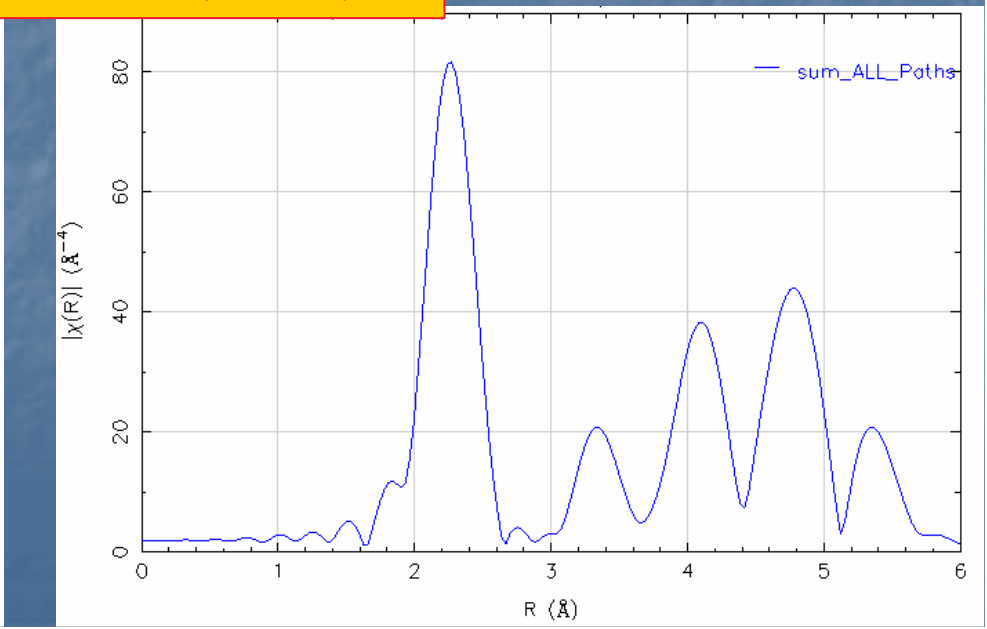
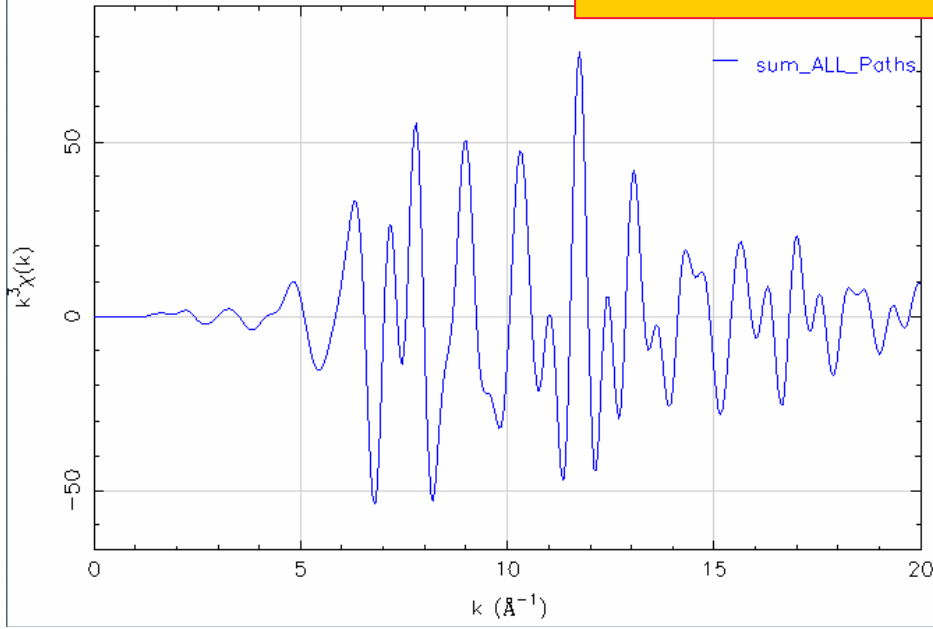
Plotting options

0 1 2 3 kw

Main Indic Traces

Plot in R: Magnitude Real part

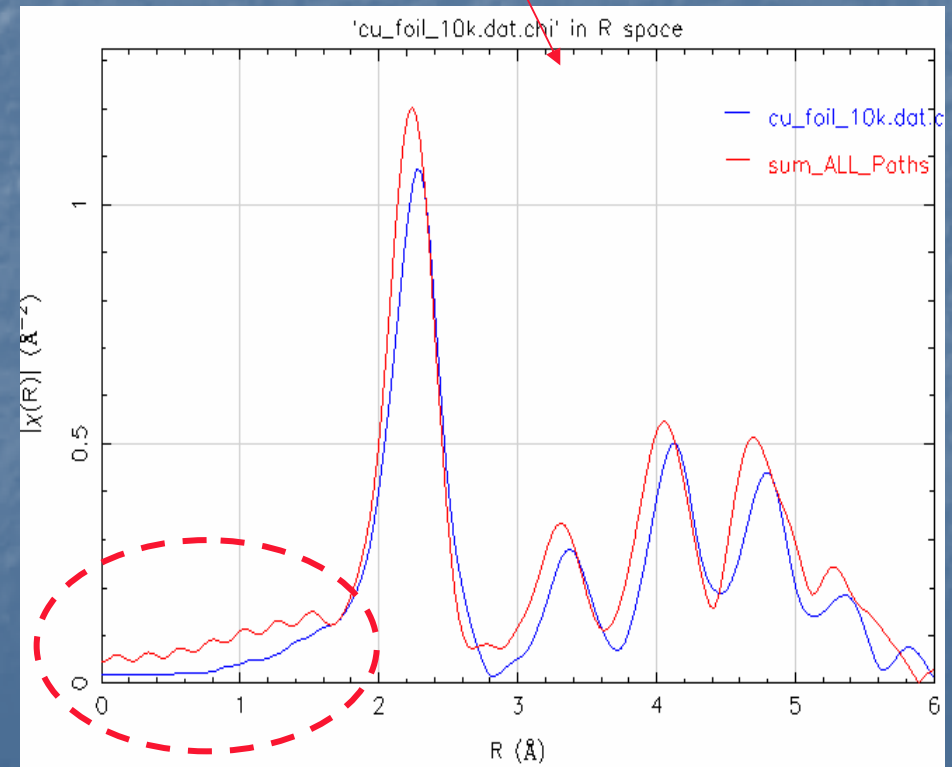
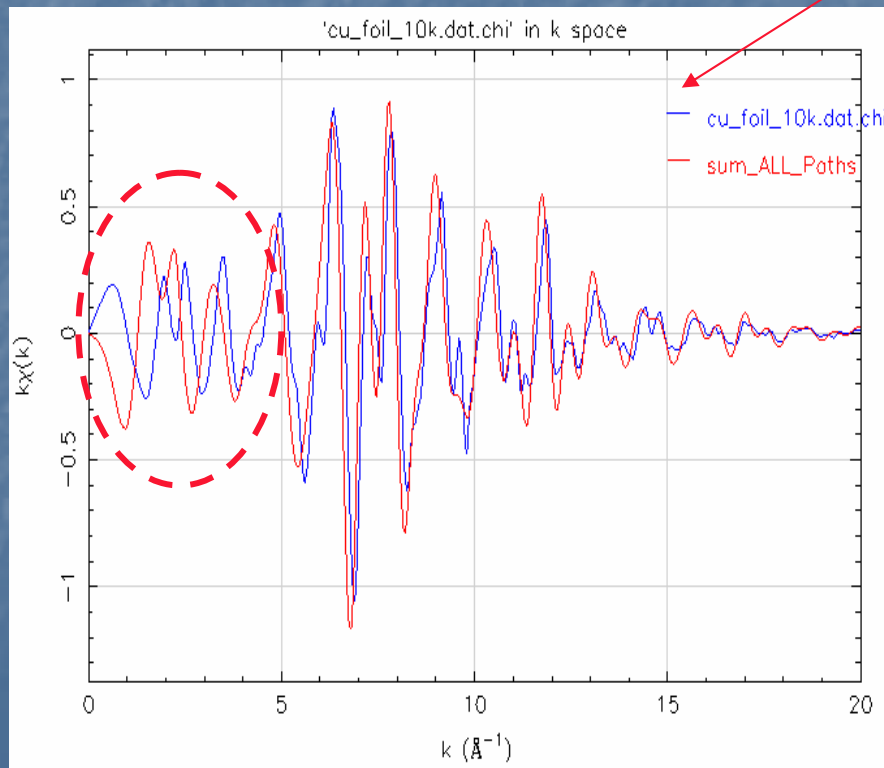
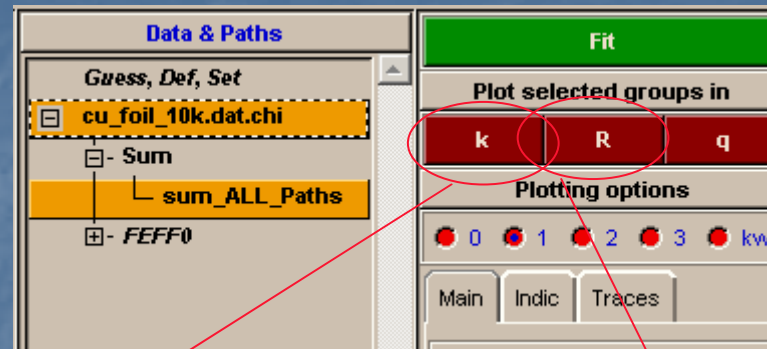
Theoretical XAFS and FT for Cu fcc



Compare model and experimental data

Open `Cu_foil_10k.inp`

Using CTRL key you can select groups for plot



1st shell analysis

remove all paths or
restart ARTEMIS

Right click

Discard paths

- Discard this path
- For this feff calculation ...
 - discard all paths**
 - discard all paths after current
 - discard all paths with more than N legs
 - discard all paths longer than R
 - discard all paths with amplitude smaller than A
- Discard selected paths

add 1st shell path to the list

select and Right click

#	Deg.	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00	[+]	Cu1_1 [+]
2	6	3.610	22.98	[+]	Cu1_2 [+]
3	48	3.829	10.59	[+]	Cu1_1 Cu1_1 [+]
4	48	4.358	8.65	[+]	Cu1_2 Cu1_1 [+]
5	24	4.421	5.41	[+]	Cu1_2 [+]

Add feff0001.dat to the path list
Add and jump to feff0001.dat
Show geometry for View

Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Sum
 - sum_ALL_Paths
 - FEFF0
 - Path 1: [Cu1_1]**

FEFF0: Path 1: [Cu1_1]

Plot after the fit Include in the fit

Make this path the default after the fit

[+] Cu1_1 [+]

2 legs Reff=2.5527 amp=100.000 degen=12

leg 1: 0.00000 -1.80500 1.80500 1 Cu
rleg=2.5527 beta=180.000

leg 2: 0.00000 0.00000 0.00000 0 Cu
rleg=2.5527 beta=180.000

Path parameter math expressions

label:

N: 12 S02: amp S_0^2 Path label

delE0: enot Energy shift

delR: delr Distance correction

sigma^2: ss Debye Waller factor

Ei:

3rd:

...

Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Sum
 - sum_ALL_Paths
 - FEFF0
 - Path 1: [Cu1_1]

#	Name	Math Expression
1	g: amp	1
2	g: enot	0
3	g: delr	0
4	g: ss	0.003

FEFF0: Path 1: [Cu1_1]

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Sum
 - sum_ALL_Paths
 - FEFF0
 - Path 1: [Cu1_1]

Edit selected parameter

amp =

Guess Def Set Skip Restrain After

Undo edit New Grab Discard Hide

Document: Guess, Def, Set

guess: optimized in the refinement

def: math expressions updated during the fit

set: numbers or expressions evaluated once at the fit beginning and not updated

Current project: E:\Duino_ago09\Examples\Cu_10K\artemis.apj

Titles

0

Data file: cu_foil_10k.dat.chi

Data controls

Include in the fit

Plot after the fit

Fit background

Fourier and fit parameters

k-range: 3 to 18

R-range: 1 to 3

dk: 1 dr: 0.0

k window: Hanning

R window: Hanning

Other parameters

Fitting space: R Epsilon: 0

Minimum reported correlation: 0.25

Path to use for phase corrections: None

Fit k-weights

kw=1

kw=2

kw=3

other k weight

Document: Fitting parameters

Data & Paths

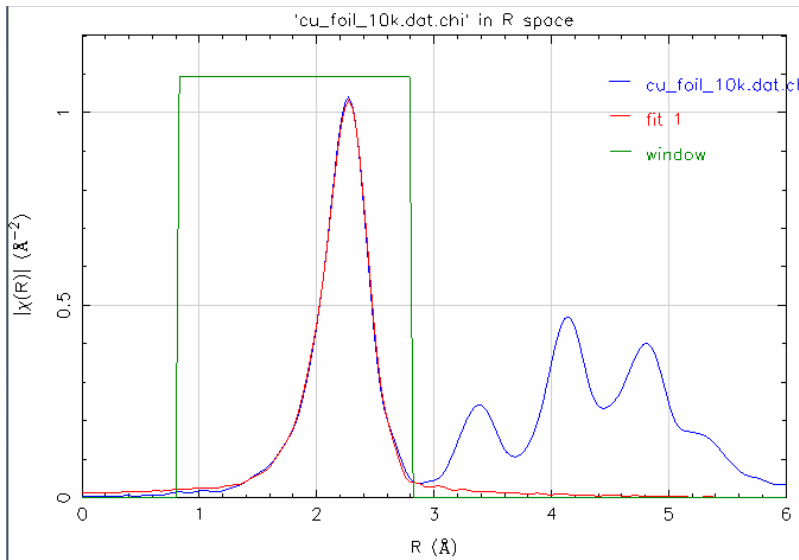
Guess, Def, Set

- cu_foil_10k.dat.chi
 - Sum
 - sum_ALL_Paths
 - FEFF0
 - Path 1: [Cu1_1]

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

The Data screen allow defining the fitting strategy and parameters





Examine log files

Current fit: fit 1

Choose a parameter: enot

Get parameters from Guess, Def, Set list

Parameter report

Calculations

- Compute the average value
- Fit Einstein temp. to sigma^2 values
- Absorber: Scatterer:
- Prefer R-factor
- Prefer reduced chi-square
- Show y=0 in plot

Quick summaries of selected fits

Select all

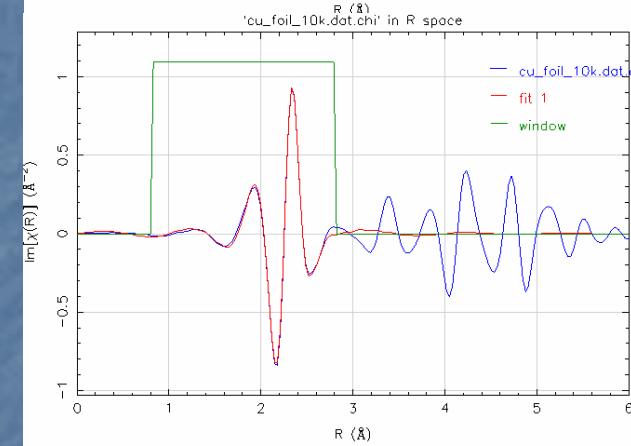
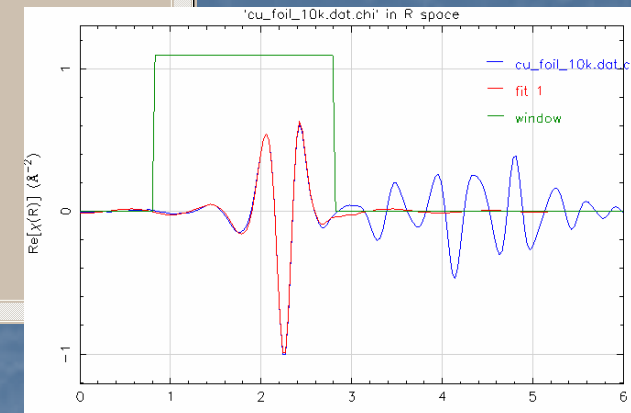
Clear selection

Document: Log viewer

Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Fit
 - fit 1
 - FEFF9
 - Path 1: [Cu1_1]



$$\chi^2 = \frac{N_{ind}}{\epsilon N_{pts}} \sum_{i=1}^{N_{pts}} \left((\Re(\tilde{\chi}^{exp}(r_i)) - \Re\tilde{\chi}^{th}(r_i))^2 + (\Im(\tilde{\chi}^{exp}(r_i)) - \Im\tilde{\chi}^{th}(r_i))^2 \right)$$

$$\chi^2_{\nu} = \frac{\chi^2}{\nu} \quad \nu = N_{ind} - N_{var}$$

The refinement is performed in Real space, on the Real and Imaginary parts of the FT

$$R^2 = \frac{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i)) - \Re\tilde{\chi}^{th}(r_i))^2 + (\Im(\tilde{\chi}^{exp}(r_i)) - \Im\tilde{\chi}^{th}(r_i))^2 \right]}{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i)))^2 \right]}$$

Absolute misfit between experimental data and theory

Structural results

Edit GDS Data Sum

- Write Iffffit script
- Display Iffffit buffer Ctrl-1
- Display fit results Ctrl-2
- View files Ctrl-3
- View messages Ctrl-4
- Display echo buffer Ctrl-5
- Write in journal Ctrl-6
- Edit project properties Ctrl-7
- Compact project
- Edit preferences

Artemis palettes

Iffffit Results Files Messages Echo Journal Properties

Results from the last fit Raw log file Save

```

Independent points = 18.687500000
Number of variables = 4.000000000
Chi-square = 92.986879023
Reduced Chi-square = 6.331021550
R-factor = 0.000735237
Measurement uncertainty (k) = 0.001028657
Measurement uncertainty (R) = 0.004036509
Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):
amp = 0.9199910 +/- 0.0211700 (1.0000)
enot = 5.4482800 +/- 0.2569030 (0.0000)
delr = -0.0046610 +/- 0.0015030 (0.0000)
ss = 0.0035760 +/- 0.0001700 (0.0030)

Correlations between variables:
amp and ss --> 0.8753
enot and delr --> 0.8699
All other correlations are below 0.25

==== Data set >>cu_foil_10k.dat.chi<< =====
    
```

#	Name	Math Expression
1	g: amp	1
2	g: enot	0
3	g: delr	0
4	g: ss	00.003

right click

- Make "amp" ...
- Move "amp" ...
- Insert separator ...
- Copy "amp"
- Build restraint from "amp"
- Annotate "amp"
- Grab best fit for "amp"
- Find where "amp" is used
- Change name of "amp" globally
- Discard "amp"

1	g: amp	0.919991 (0.021170)
2	g: enot	0
3	g: delr	0
4	g: ss	00.003

$$\chi^2 = \frac{N_{ind}}{\epsilon N_{pts}} \sum_{i=1}^{N_{pts}} \left((\Re(\tilde{\chi}^{exp}(r_i) - \Re\tilde{\chi}^{th}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i) - \Im\tilde{\chi}^{th}(r_i)))^2 \right)$$

$$R^2 = \frac{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i) - \Re\tilde{\chi}^{th}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i) - \Im\tilde{\chi}^{th}(r_i)))^2 \right]}{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i)))^2 \right]}$$

Effects of Fitting parameters

Data file: cu_foil_10k.dat.chi

Data controls

- Include in the fit
- Plot after the fit
- Fit background

Fourier and fit parameters

k-range: 3 to 18

R-range: 0.8 to 2.8

dk: 1 dr: 0.0

k window: Hanning

R window: Hanning

Other parameters

Fitting space: R Epsilon: 0

Minimum reported correlation: 0.25

Path to use for phase corrections: None

Document: Fitting parameters

Fit k-weights

- kw=1
- kw=2
- kw=3
- other k weight

Artemis palettes

Results from the last fit

Raw log file Save

Kwt = 1

Independent points	=	18.687500000
Number of variables	=	4.000000000
Chi-square	=	92.986879023
Reduced Chi-square	=	6.331021550
R-factor	=	0.000735237
Measurement uncertainty (k)	=	0.001028657
Measurement uncertainty (R)	=	0.004036509
Number of data sets	=	1.000000000

Guess parameters +/- uncertainties (initial guess):

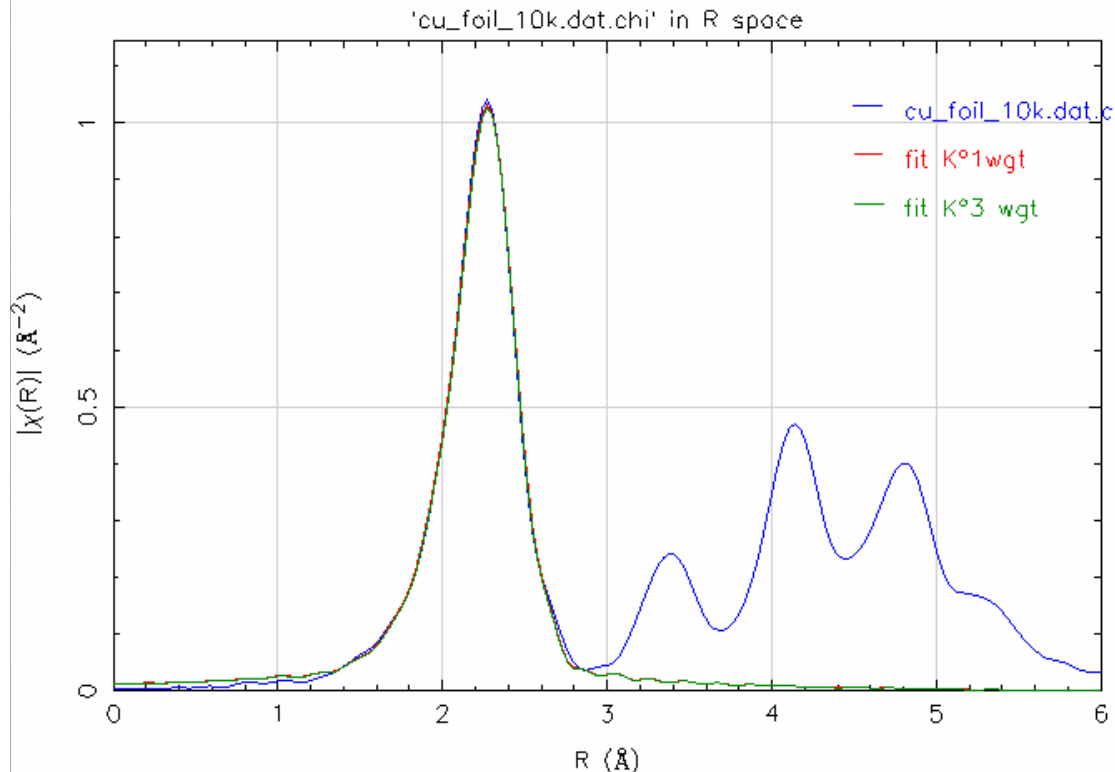
amp	=	0.9199910	+/-	0.0211700	(1.0000)
enot	=	5.4482800	+/-	0.2569030	(0.0000)
delr	=	-0.0046610	+/-	0.0015030	(0.0000)
ss	=	0.0035760	+/-	0.0001700	(0.0030)

Correlations between variables:

amp and ss	-->	0.8753
enot and delr	-->	0.8699

All other correlations are below 0.25

==== Data set >>cu_foil_10k.dat.chi<< =====



Independent points = 18.687500000

Number of variables = 4.000000000

Chi-square = 191.610462627

Reduced Chi-square = 13.045818732

R-factor = 0.118453126E-05

Measurement uncertainty (k) = 0.000533874

Measurement uncertainty (R) = 0.445387356

Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):

amp	=	0.8886660	+/-	0.0263100	(0.0000)
enot	=	5.4650780	+/-	0.4109850	(0.0000)
delr	=	-0.0043940	+/-	0.0012080	(0.0000)
ss	=	0.0033710	+/-	0.0001530	(0.0000)

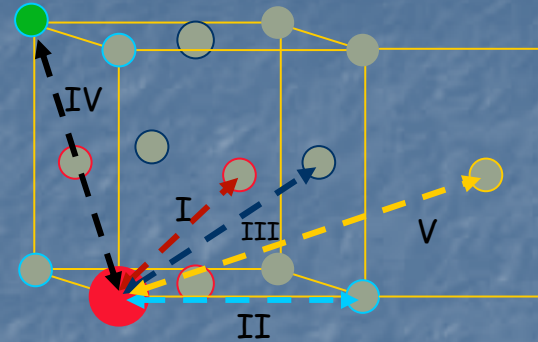
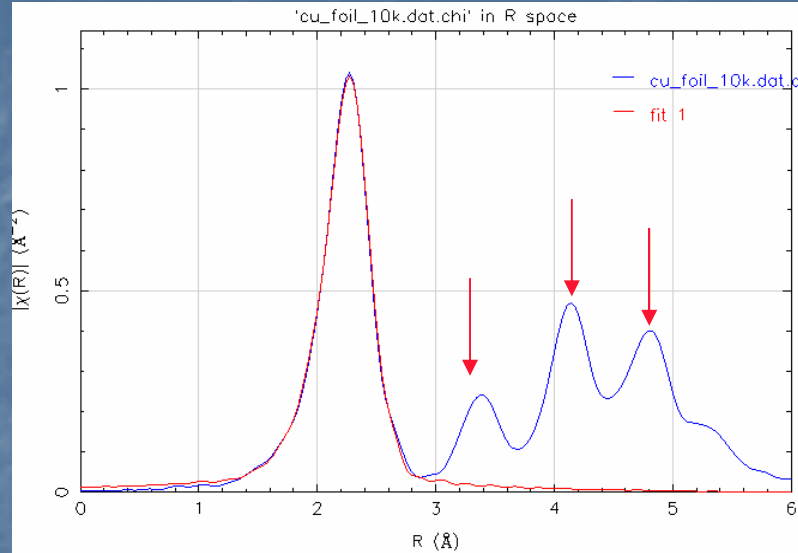
Correlations between variables:

amp and ss	-->	0.7805
enot and delr	-->	0.7766
amp and enot	-->	-0.2833

All other correlations are below 0.25

Kwt = 3

Add new contributions



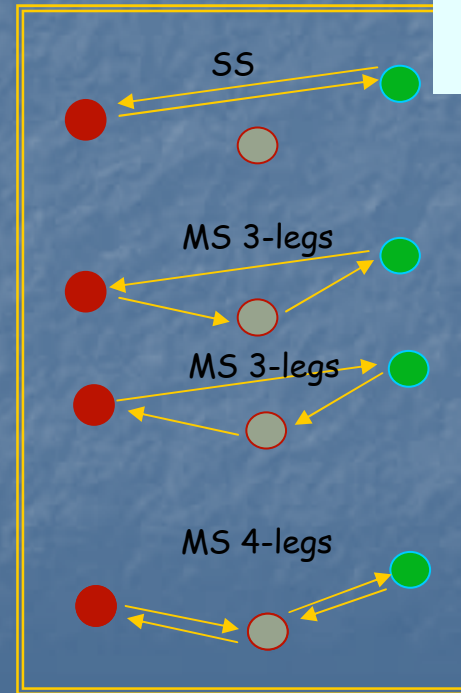
Visualize the structure and understand the neighbour shells!

Take care about multiple scattering contributions

#	Deg.	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00		[+] Cu1_1 [+]
2	6	3.610	22.98		[+] Cu1_2 [+]
3	48	3.829	10.59		[+] Cu1_1 Cu1_1 [+]
4	48	4.358	8.65		[+] Cu1_2 Cu1_1 [+]
5	24	4.421	55.41		[+] Cu1_3 [+]
6	48	4.763	10.63		[+] Cu1_1 Cu1_1 [+]
7	96	4.763	21.81		[+] Cu1_3 Cu1_1 [+]
8	12	5.105	18.94		[+] Cu1_4 [+]
9	12	5.105	8.46		[+] Cu1_1 Cu1_1 [+]
10	24	5.105	43.71	1	[+] Cu1_4 Cu1_1 [+]
11	12	5.105	8.21	1	[+] Cu1_1 [+] Cu1_1 [+]
12	12	5.105	3.57		[+] Cu1_1 [+] Cu1_1 [+]

Single Scattering

MS + Focusing



Understand the MS contributions!!!

Data & Paths

Guess, Def, Set

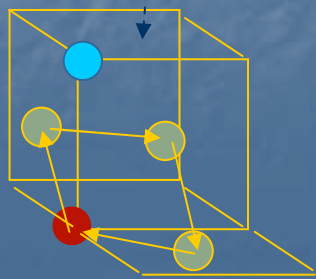
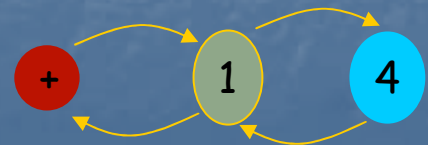
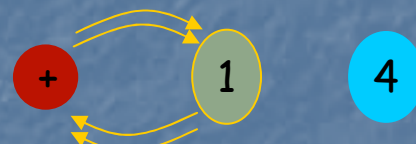
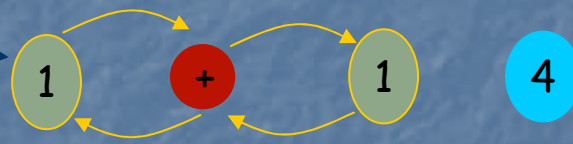
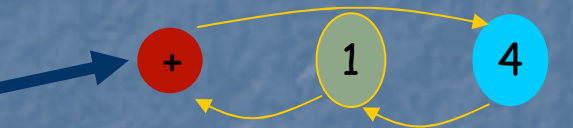
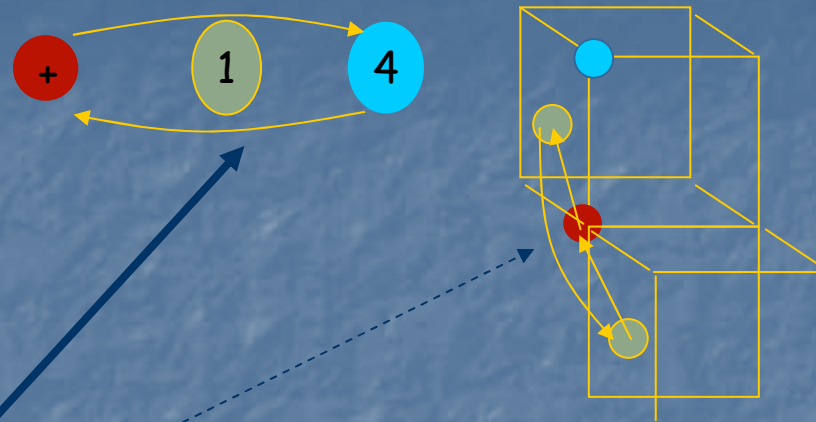
- cu_foil_10k.dat.chi
 - Fit
 - fit K^1wgt
 - fit K^3 wgt
 - fit K^3 wgt-multishel
 - FEFF0
 - Path 1: [Cu1_1]
 - Path 2: [Cu1_2]
 - Path 5: [Cu1_3]
 - Path 8: [Cu1_4]
 - Path 10: [Cu1_4 Cu1_1]
 - Path 11: [Cu1_1 [+] Cu1_1]
 - Path 14: [Cu1_1 Cu1_4 Cu1_1]

SS paths

MS paths

8	12	5.105	18.94		[+] Cu1_4 [+]
9	12	5.105	8.46		[+] Cu1_1 Cu1_1 [+]
10	24	5.105	43.71	1	[+] Cu1_4 Cu1_1 [+]
11	12	5.105	8.21	1	[+] Cu1_1 [+] Cu1_1 [+]
12	12	5.105	3.57		[+] Cu1_1 [+] Cu1_1 [+]
14	12	5.105	32.80	2	[+] Cu1_1 Cu1_4 Cu1_1 [+]
15	48	5.105	3.26		[+] Cu1_1 Cu1_1 Cu1_1 [+]

Focusing effect may raises some MS contributions well above the SS one



Artemis

File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project: E:\Duino_ago09\Examples\Cu_10K\artemis.apj

FEFF0: Path 2: [Cu1_2]

Plot after the fit Include in the fit

Make this path the default after the fit

[+] Cu1_2 [+]

```

2 legs Reff=3.6100 amp=22.980 degen=6

leg 1: -3.61000 0.00000 0.00000 1 Cu
      rleg=3.6100 beta=180.000
leg 2:  0.00000 0.00000 0.00000 0 Cu
      rleg=3.6100 beta=180.000
  
```

Path parameter math expressions

label:

N: 6 S02: amp

delE0: enot

delR: delr2

sigma^2: ss2

Ei:

3rd:

4th:

Document: Paths and path parameters

Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Fit
 - fit K^1wgt
 - fit K^3 wgt
 - FEFF0
 - Path 1: [Cu1_1]
 - Path 2: [Cu1_2]
 - Path 5: [Cu1_3]
 - Path 8: [Cu1_4]

#	Name	Math Expression
1	s: amp	0.919991 (0.021170)
2	g: enot	5.448280 (0.256903)
3	g: delr	-0.004661 (0.001503)
4	g: delr2	-0.004661
5	g: delr3	-0.004661
6	g: delr4	-0.004661
7	g: ss	0.003576 (0.000170)
8	g: ss2	0.004
9	g: ss3	0.004
10	g: ss4	0.004

Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Fit
 - fit K^1wgt
 - fit K^3 wgt
 - FEFF0
 - Path 1: [Cu1_1]
 - Path 2: [Cu1_2]
 - Path 5: [Cu1_3]
 - Path 8: [Cu1_4]

Fourier and fit parameters

k-range 3 to 18

R-range 0.8 to 2.8

dk 1 dr 0.0

k window Hanning

R window Hanning

In principle the same for each shell

In principle different for each shell

Warning:

The used path must be inside the fit range

#	Name	Math Expression
1	s: amp	0.919991
2	g: enot	5.448280
3	g: delr	-0.004
4	g: delr2	-0.004661
5	g: delr3	-0.004
6	g: delr4	-.004
7	g: ss	0.003596 (0.000283)
8	g: ss2	0.005123 (0.001735)
9	g: ss3	0.004593 (0.000671)
10	g: ss4	0.028058 (0.043714)
11	g: ss5	0.004597 (0.000968)
12	g: ss6	0.006

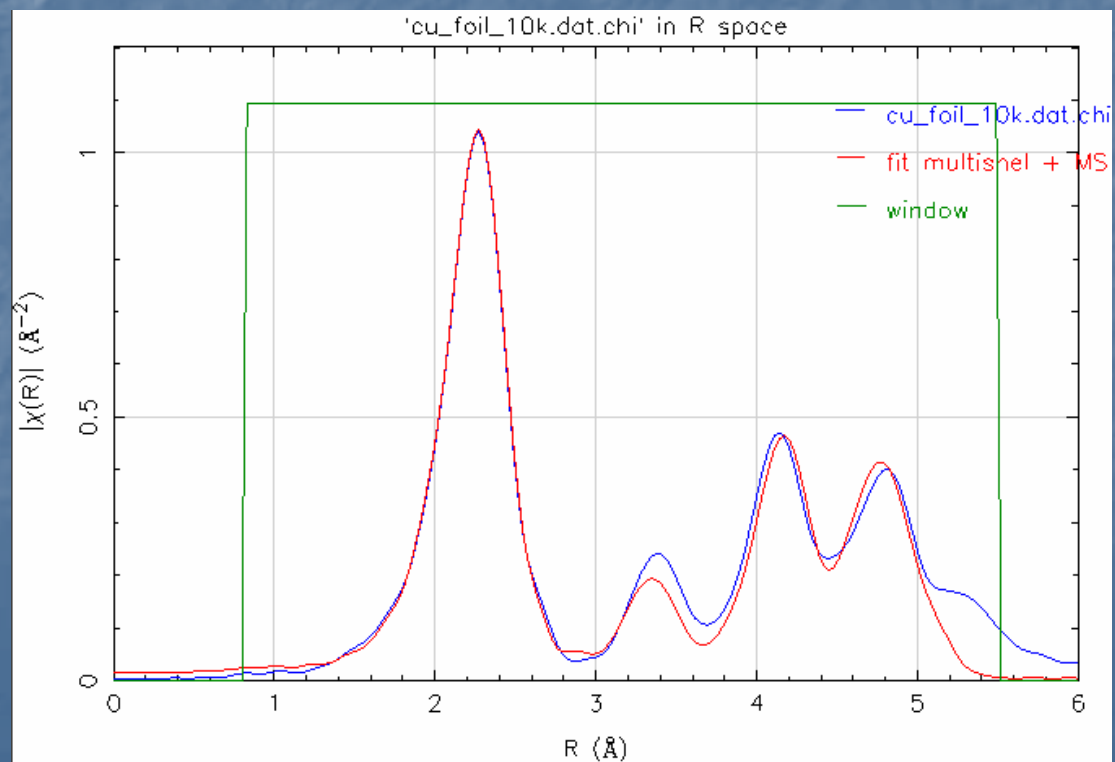
Independent points	=	44.382812500
Number of variables	=	12.000000000
Chi-square	=	1816.763460636
Reduced Chi-square	=	56.102707590
R-factor	=	0.011517825
Measurement uncertainty (k)	=	0.001028657
Measurement uncertainty (R)	=	0.004036509
Number of data sets	=	1.000000000

Guess parameters +/- uncertainties (initial guess):		
enot	=	5.1036410 +/- 0.6089100
delr	=	-0.0063660 +/- 0.0037480
delr2	=	-0.0235000 +/- 0.0122330
delr3	=	0.0189970 +/- 0.0075140
delr4	=	-0.0359130 +/- 0.0098410
ss	=	0.0035890 +/- 0.0002440
ss2	=	0.0044530 +/- 0.0013020
ss3	=	0.0045820 +/- 0.0005800
ss4	=	0.3097740 +/- 132.3316580
ss5	=	0.0151180 +/- 0.0062090
ss6	=	-0.0003130 +/- 0.0019450
ss7	=	0.0073710 +/- 0.0022950

Correlations between variables:

ss6 and ss7	-->	-0.8579
enot and delr	-->	0.8206
delr4 and ss5	-->	-0.6973
enot and delr3	-->	0.6923
delr and delr3	-->	0.5675
enot and ss5	-->	0.4211
enot and delr2	-->	0.3650
delr and ss5	-->	0.3464
delr3 and delr4	-->	0.3298
delr and delr2	-->	0.2970
delr4 and ss6	-->	-0.2649
enot and ss7	-->	0.2521

All other correlations are below 0.25



#	Name	Math Expression
1	s: amp	0.919991
2	g: enot	5.448280
3	d: delr delr2/sqrt(2)	
4	g: delr2	-0.004661
5	d: delr3 delr2*sqrt(1.5)	
6	d: delr4 delr2*sqrt(2)	
7	g: ss	0.003596 (0.000283)
8	g: ss2	0.005123 (0.001735)
9	g: ss3	0.004593 (0.000671)
10	g: ss4	0.028058 (0.043714)
11	g: ss5	0.004597 (0.000968)
12	g: ss6	0.006
13	g: ss7	0.006964 (0.006210)

```

Independent points      =      44.382812500
Number of variables    =      9.000000000
Chi-square             =     3499.926965502
Reduced Chi-square    =     98.916019339
R-factor              =      0.022188660
Measurement uncertainty (k) =    0.001028657
Measurement uncertainty (R) =    0.004036509
Number of data sets   =      1.000000000

Guess parameters +/- uncertainties (initial guess):
enot      =      4.5727030 +/-      0.7133360
delr2     =     -0.0051830 +/-      0.0061960
ss        =      0.0036500 +/-      0.0003280
ss2       =      0.0046410 +/-      0.0018030
ss3       =      0.0047920 +/-      0.0007880
ss4       =      0.0239730 +/-      0.0373920
ss5       =      0.0057660 +/-      0.0014520
ss6       =      0.0010460 +/-      0.0058090
ss7       =      0.0060830 +/-      0.0044900

```

```

Correlations between variables:
ss6 and ss7      --> -0.9544
enot and delr2   -->  0.8598
ss4 and ss5      -->  0.6684
ss5 and ss7      -->  0.6517
ss4 and ss7      -->  0.6019
ss5 and ss6      --> -0.5675
ss4 and ss6      --> -0.4966

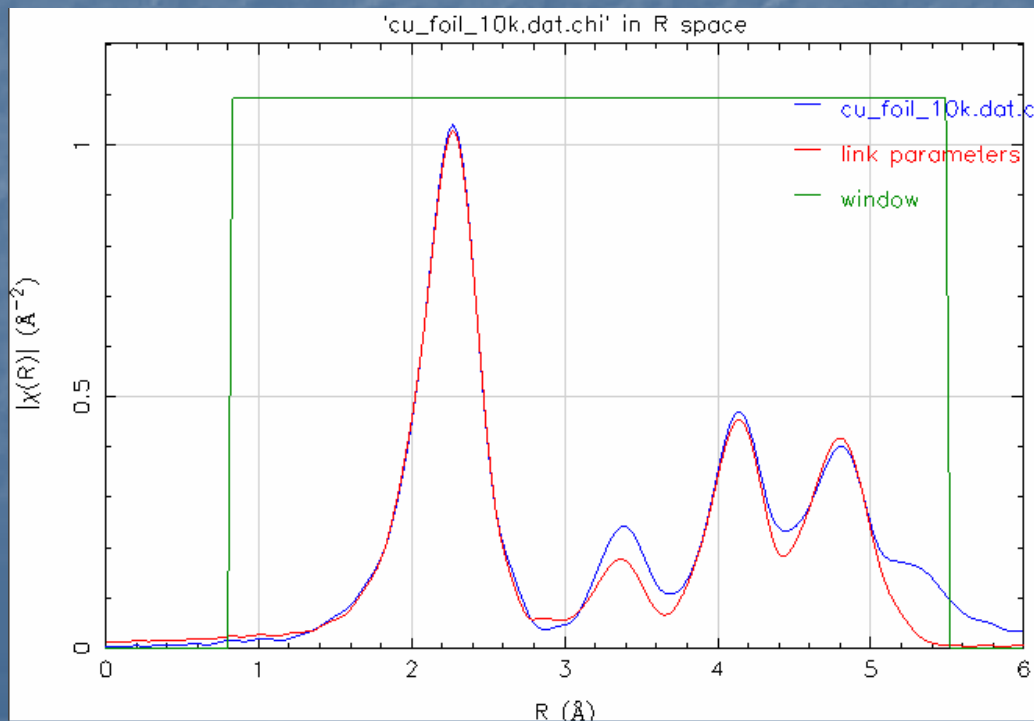
```

Edit selected parameter

delr3 = delr2*sqrt(1.5)

Guess
 Def
 Set
 Skip
 Restrain
 After

Document: Guess, Def, Set



Data & Paths Current project: E:\Duino_ago09\Examples\Cu_10k\Cu_10k

#	Name	Math Expression
1	g: amp	0.907810 (0.096404)
2	g: enot	5.448280
3	g: delr	0.0
4	g: delr2	-0.004661
5	d: delr3	delr2*sqrt(1.5)
6	d: delr4	delr2*sqrt(2)
7	d: delr5	delr2*sqrt(2.5)
8	g: ss	0.003596 (0.000283)
9	g: ss2	0.005123 (0.001735)
10	g: ss3	0.004593 (0.000671)
11	g: ss4	0.028058 (0.043714)
12	g: ss5	0.004597 (0.000968)
13	g: ss6	0.006
14	g: ss7	0.006964 (0.006210)
15	g: ss8	0.006964 (0.006210)

Independent points = 48.178710937
 Number of variables = 12.000000000
 Chi-square = 8110.229963402
 Reduced Chi-square = 224.171335939
 R-factor = 0.000045721
 Measurement uncertainty (k) = 0.000533874
 Measurement uncertainty (R) = 0.445387356
 Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):
 amp = 0.9054050 +/- 0.0941340
 enot = 3.7197170 +/- 0.3651800
 delr = -0.0094960 +/- 0.0028930
 delr2 = -0.0009550 +/- 0.0034220
 ss = 0.0034400 +/- 0.0004310
 ss2 = 0.0048280 +/- 0.0005880
 ss3 = 0.0048200 +/- 0.0004620
 ss4 = 0.0355080 +/- 0.1148830
 ss5 = 0.0047690 +/- 0.0009910
 ss6 = 0.0022460 +/- 0.0040870
 ss7 = 0.0078980 +/- 0.0043780
 ss8 = 0.0052190 +/- 0.0006400

Data file cu_foil_10k.dat.chi

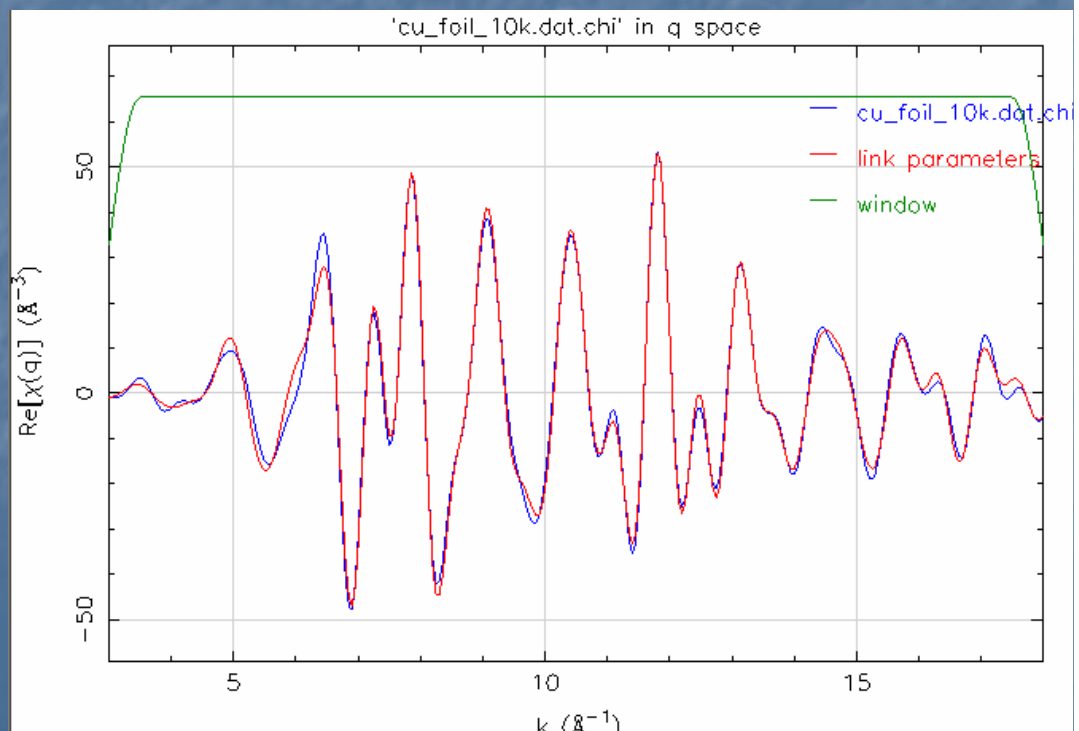
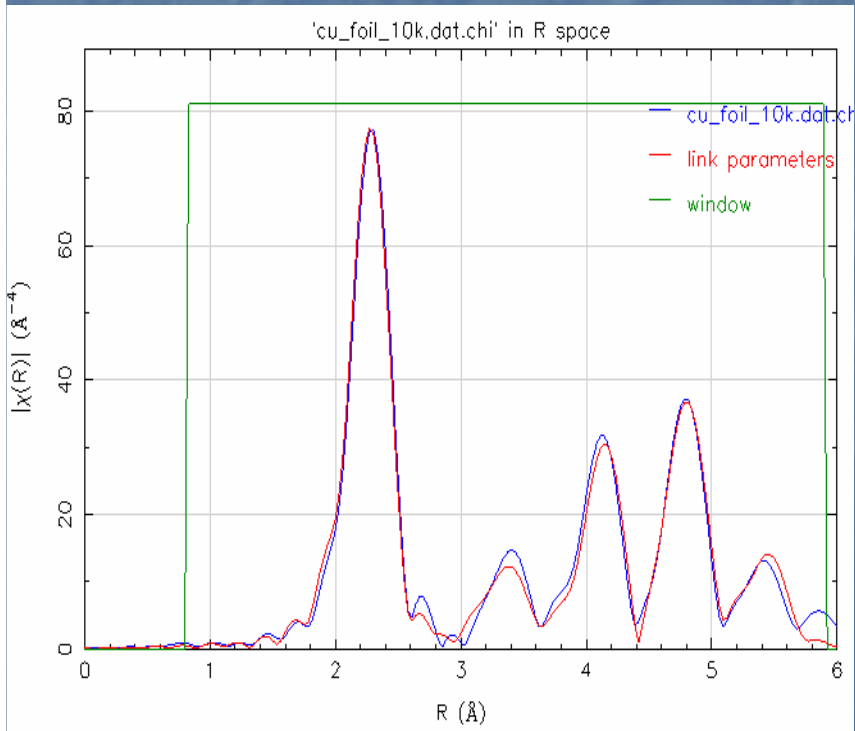
Data controls
 Include in the fit
 Plot after the fit
 Fit background

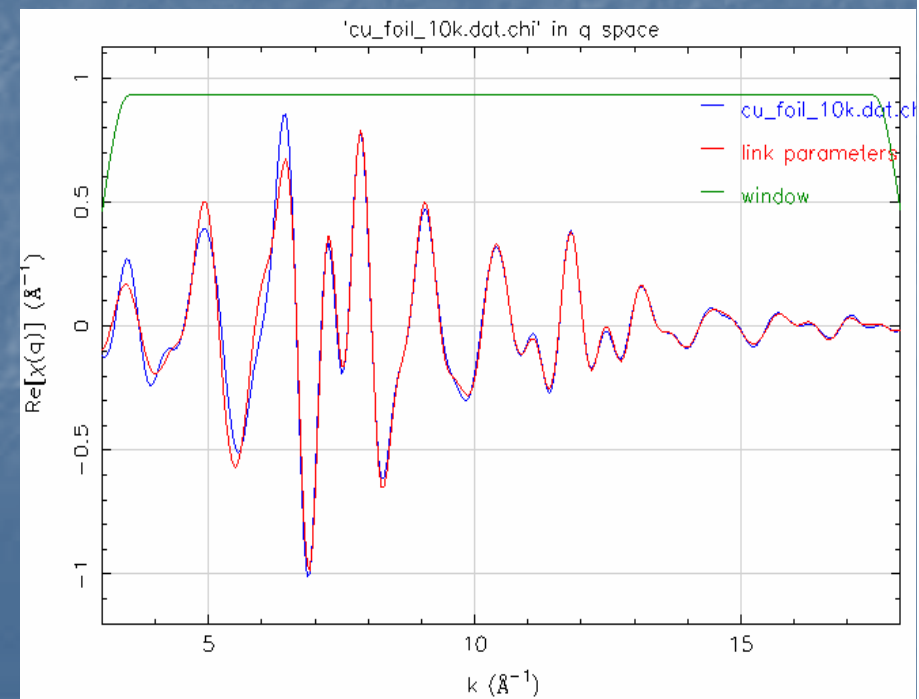
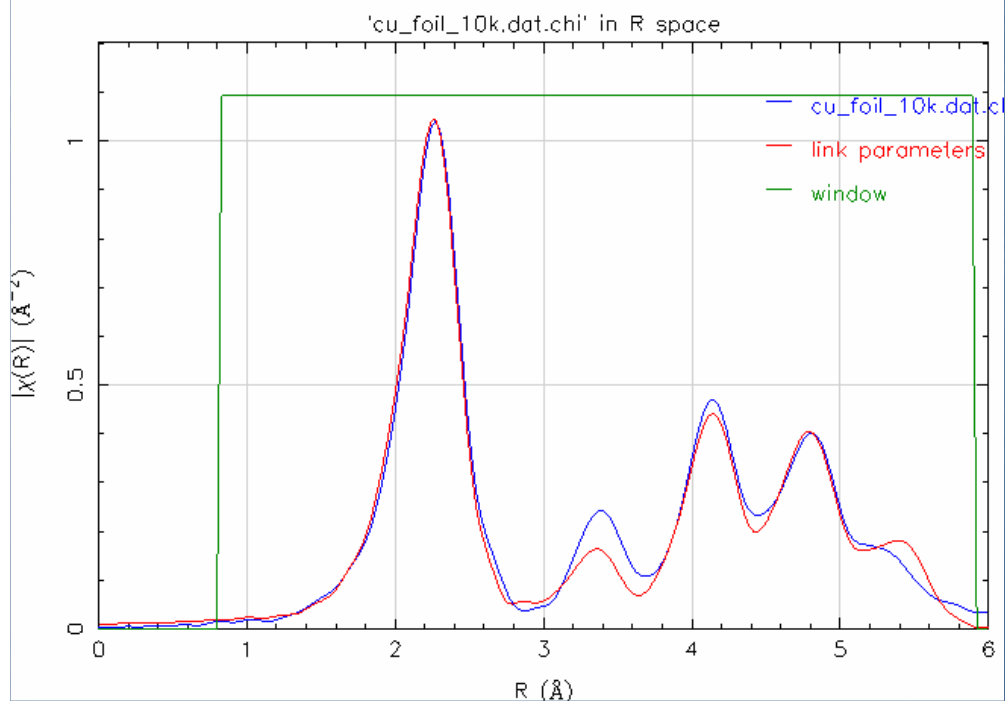
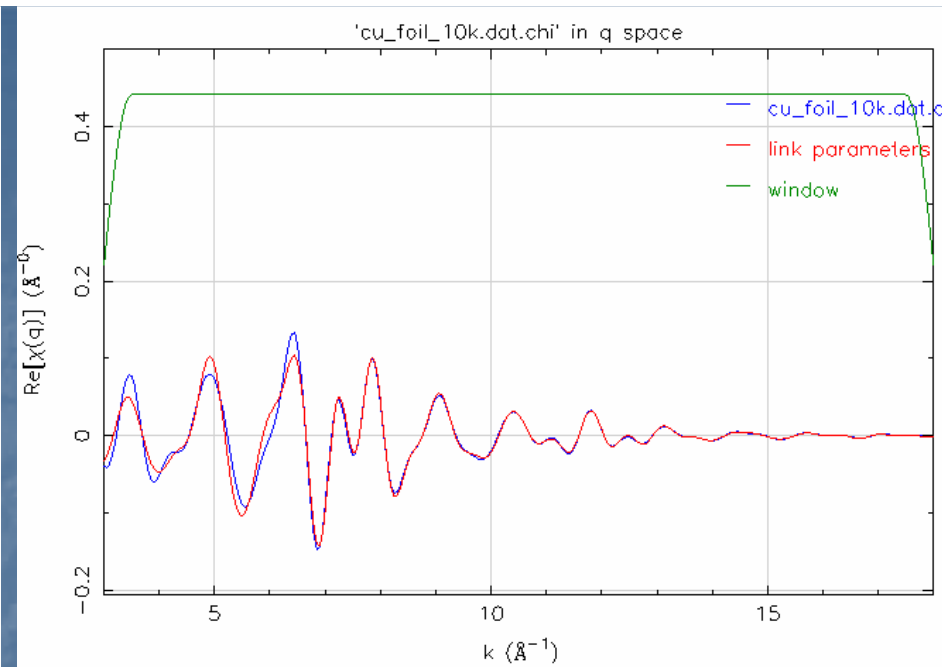
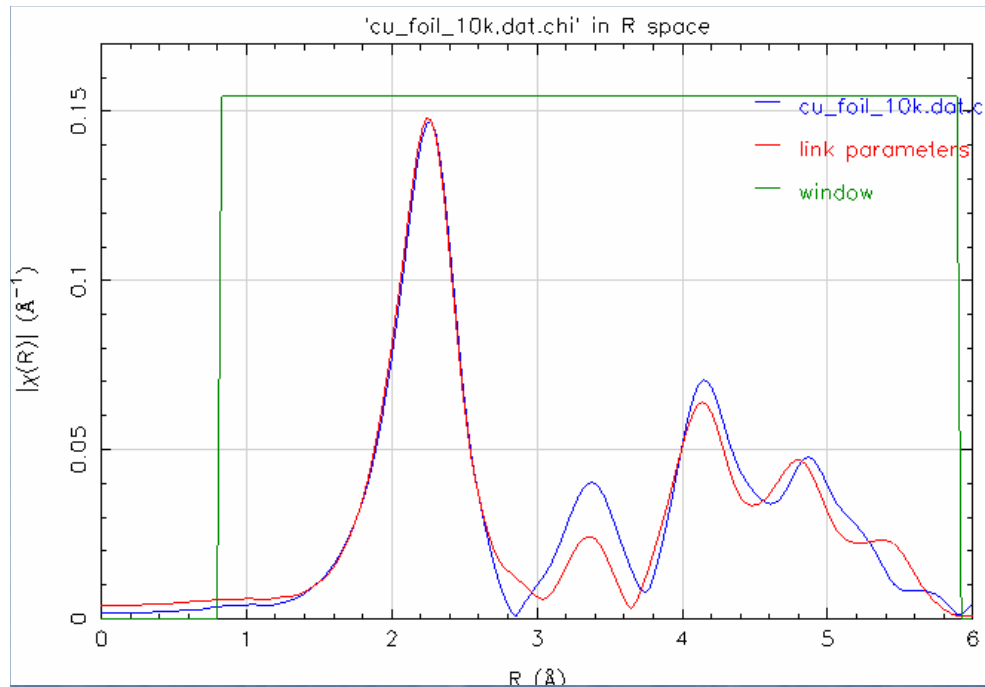
Fourier and fit parameters
 k-range: 3 to 18
 R-range: 0.8 to 5.9
 dk: 1 dr: 0.0
 k window: Hanning
 R window: Hanning

Other parameters
 Fitting space: R Epsilon: 0
 Minimum reported correlation: 0.25
 Path to use for phase corrections: None

Fit k-weights
 kw=1
 kw=2
 kw=3
 other k/weight

Document: Fitting parameters





it's your work now!

a. Fe bcc

b. GeO

c. ...