miXAFS

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Chapter 1

Introduction

1.1 What is miXAFS

miXAFS is an analysis software for X-ray absorption Fine Structure. It has several features which is based on the concept that the same analysis is done similarly. The first one is to analyze a lot of data in bulk. The second one is to analyze from experimental raw data to obtain the structural parameters in sequence by one click. Third feature is the analysis of the data for multiple absorption edges simultaneously.

1.2 Surface map

In the EXAFS analysis we set a lot of parameters. If we assume two sites, it is a standard to set the atomic distance, the coordination number, the Debye-Waller factor, and the third cumulant for each site. In this case there are eight parameters, so the initial values are very important to obtain the reasonable results.

The structural parameters correlate with each other, and there is an especially strong correlation between the coordination number and Debye-Waller factor. We wrote the paper of the local structures of the amorphous tellurium (J. Synchrotron Rad. (2014). 21, 409–412). To check this correlation, we performed least-squares fitting with fixed the interchain coordination number and the interchain Debye-Waller factor for the crystalline tellurium. There are the three-dimensional shaded surface plots. The x-, y- and z-axis represent the interchain coordination number, the interchain Debye-Waller factor and R-factor, respectively. There is only one clear deep trough, which suggests that the values of the interchain coordination number and the interchain Debye-Waller factor at the trough are the reasonable values of them.

In the surface plot for amorphous tellurium the surface is mostly flat with a very shallow valley
Figure 1.1: The window of miXAFS as compared with crystalline tellurium. The instability of the least-squares fitting suggests that the contribution from the interchain is probably small. This implies also that it is difficult to obtain the reliable interchain coordination. Hence, we decided not to discuss the interchain, and we focused on the intra-chain structural parameters.

This function is done with two modes. One is that the values of two parameters are fixed while the least-squared fitting, the other is that the values are just initial values and they are optimized while the fitting.

This function is useful to judge whether the optimized parameters are valid or not. It is also useful to teach the beginners the importance of the selection of the initial values.

1.3 Analysis of multiple files

This surface plot uses the feature of the operation of multiple files. Other application is the analysis by using file list like this. miXAFS reads this kinds of file list and analyze them in sequence. This file
list contains the file name, experimental conditions, and the initial values of fitting parameters. You can set arbitrary experimental condition, such as temperature, pressure, concentration and so on. If you measure XAFS with several temperatures and pressures, you can investigate the temperature and pressure dependence of the structural parameters.

1.4 One click analysis

miXAFS continuously analyzes from the experimental raw data to obtain the structural parameters. We can obtaine the structural parameters from the experimental raw data only with one click of this Run button. The figures contain the absorption coefficients, XAFS function, Fourier transform, Fourier filtered XAFS function, and optimized XAFS function and Fourier transform. You can look over the whole process of the XAFS analysis on a window.

In the tab for the fitting parameters we set the initial parameters of the structure at this lower table. We can see the optimized parameters at this upper table. In the initial parameter table, you will set the initial value, the variation range, and FEFF files and so on. There are no limitations of number of sites. Target file name is changed in this main part, so you can do the least-squared fitting analysis with changing the initial parameter easily. It is same in other tabs.

The continuous analysis is the important feature of MiXAFS, but you can use it like other analysis softwares. It is possible to stop the analysis at getting the XAFS function, Fourier transform, and Fourier filtered XAFS function. On the other hand, you can use the miXAFS to do the least-squared fitting to the XAFS function obtained by other softwares, that is, you can use the analysis software according to your needs.

1.5 Tab: Folder

The parameters for the analysis are gathered for each group. Conditions for the extraction of XAFS function, Fourier transform, Fourier filtered XAFS functions, and designation of folders.

This is very useful when you do the XAFS measurements at the synchrotron radiation facilities. We have to judge the quality of the XAFS data as soon as possible. Most of the software requires us to several steps to obtain the XAFS function, or the structural parameters. However, our MiXAFS provides the XAFS function, Fourier transform, and also the optimized structural parameters with only few steps.

If the Matlab runtime routine is installed in the control computer, you can obtain the structural parameters by designating the folder of the raw data. Otherwise, you copy the experimental raw data to
the storage on the cloud, for example, iCloud, Dropbox, OneDrive and so on. At second, you change
the experimental file name. Last, you just click this Run button. Only few steps give you all what you
want to know.

1.6 Setting File

Don’t you think that it is troublesome to set the parameters every time you analyze them? Don’t worry about it. Once you designate the configuration file, you can use it every time. When you analyze
the similar types of data, it will load the configuration file and set up MiXAFS automatically. You can
specify the file on the directory box or by using the dialog box. MiXAFS uses over 100 parameters for
the analysis, but if you make use of the functions you are free from the troublesome procedures. You
can set the configuration file by following the examples. Of course, you can have infinite numbers of
the configuration files, so you can use the right configuration file at the right time. Of course, after
loading the configuration file and setting the values, you can easily change them on this graphical user
interface.

When you use Multi(file) mode, the number of sites in sequence file must be same with the number
of sites defined on the table of initial parameters. The mode is limited to an analysis for one edge.

1.7 Multiple edge

Third feature is the analysis of the data for multiple absorption edges simultaneously. Sometimes the
XAFS measurements for multiple edges are done for the same materials. I guess that in the most case
they are analyzed individually. I think that it is reasonable to analyze them together in principle.

1.8 Citation

To cite miXAFS in a publication, use

H. Ikemoto

miXAFS: a program for X-ray absorption fine-structure data analysis
https://doi.org/10.1107/S1600577518001765
Journal of Synchrotron Radiation, 2018, Volume 25, pages 618-624
Chapter 2

How to install and run miXAFS

2.1 How to obtain miXAFS

Please send e-mail to ikemoto@sci.u-toyama.ac.jp (change #&? to @) with title ”getting miXAFS program”. I am afraid that I will not receive e-mails that are not titled ”getting miXAFS program”, because I receive a lot of spam e-mails.

2.2 System requirement

miXAFS runs on Macintosh and Windows. miXAFS is coded by MatLab, so it will be delivered with Linux in the near feature.

2.3 MatLab Runtime Routine

Install the designated MATLAB Runtime routine. It is necessary that the version of the runtime is same with that of MatLab compiler. For miXAFS_yymmdd_20xx_OS, 20xx means the version of the Matlab compiler. (2016b: v91; 2018a:v94)

2.3.1 Install the MatLab runtime

Matlab requires the matching between the release of Matlab compiler and the version of Matlab runtime.

1. Get the runtime from the Mathwork’s site.
2. Boot the installer, and follow the wizard. In the macOS, the runtime is installed in ”/Application/MATLAB” folder by default.

---

2https://www.mathworks.com/products/compiler/mcr.html
2.4 Install of miXAFS

2.4.1 Minimum setting

To use miXAFS, following files and folders are necessary at the same folder.

- Executive file.
  - macOS
    - miXAFS.app (Automator application)
    - miXAFS_yymmdd_20xx_mac (executive file)
    - run_miXAFS_yymmdd_20xx_mac.sh
  - Windows
    - miXAFS_yymmdd_20xx_win

- 'Setting' folders and contained files.
  - File_spell.txt
  - miXAFS_setting.txt
  - Database_yymmdd.txt

- 'miXAFS_log.fig' folder
- 'Temporary' folder
- default_icon.icns
- splash.png

There are no other restrictions for the location for files and folders. If a folder is synchronized with a cloud system, miXAFS can load and save the data on the cloud. It is very convenient to analyze the XAFS data while measuring the XAFS data in the synchrotron facilities.

2.4.2 Initial installation

The easiest way to install the miXAFS is shown here at first.

1. Decompress the distributed ZIP file on your computer. If the full path contains two bytes code, the Matlab applications do not run.
2. macOS: Move the decompressed folder under " /Application/MATLAB".
   Windows: Move the decompressed folder to your favorite folder.
3. Change the name of the decompressed folder name from "miXAFS_yymmdd_20xx_distribution" to "miXAFS".
4. Change all " /⋯⋯/Data/" in the setting file (ex. Setting_CsBr_Br_yymmdd.txt), that is located in "Data" folder, to adequate folder name. If OS is Windows, change the character "/" to backslash.
5. Change "File_initial.txt" that designates the setting file in "Setting" folder.

In the case of macOS, the folder may be like follows. < .... > indicate folder.
File_initial.txt: This file designates two files. The first one is stated at the first line and names as miXAFS_Setting_yymmdd.txt in the distributed files. This file designated GUI and data formats. The first one must locates in “Setting” folder. The second one is designated at the second line, and named as Setting_CsBr_yymmdd.txt in the distributed files. This file designates the condition for XAFS analysis. The location of the files is arbitrary, but must be stated by absolute position. The lines below the third line are neglected, so they may be used as memo for other analysis conditions.

miXAFS_Setting_yymmdd.txt: This file define the GUI and the data formats, and so on. The first line designates the version of the file. The second line designates the location the GUI window with four numbers. First and second ones are x and y coordinates of the left top corner, where the origin is a corner of top-left on your computer.

Database_yymmdd.dat: miXAFS loads Data automatically. This file is not allowed user to change it. Setting_CsBr_yymmdd.txt: This file designates the condition of the analysis.

Init_CsBr_yymmdd.txt: This file designates the file names, identical information, and the parameters of the least squared fitting to obtain the structural parameters.
2.4.3 Upgrade of miXAFS

When you upgrade miXAFS, copy following files to "miXAFS" folder. If the version of the runtime corresponded to the installed miXAFS is not installed in your computer, you have to install the runtime. cf §2.3

macOS

- miXAFS (for macOS; Automator application)
- miXAFS_yymmdd_20xx_mac (for macOS; executable file)
- run_miXAFS_yymmdd_20xx_mac.sh (for macOS; shell command)

Windows

- miXAFS_yymmdd_20xx_win.exe (for Windows; executable file)

2.4.4 Modification of Automator

In macOS Automator app (miXAFS.app) boots miXAFS. The procedure is as follows;

1. The current directory moves to the folder where run_miXAFS_yymmdd_mac.sh locates. The default is /Applications/MATLAB/miXAFS.
2. ./run_miXAFS_yymmdd_20xx_mac.sh is executed with the runtime which locates at /Applications/MATLAB/MATLAB_Runtime/vNM in default, where vNM means the runtime version which is assigned in Mathwork HP.

Contents of Automator.app are as follows,

```
cd /Applications/MATLAB/miXAFS
./run_miXAFS_yymmdd_20xx_mac.sh /Applications/MATLAB/MATLAB_Runtime/vNN
```
where ”NN” means the version of the runtime routine. If you want to modify the Automator file, change as follows.

1. Boot Automator and open the Automator file.
2. Edit execution of shell script.
   - To change the runtime routine; Change blue parts.
   - To change the executive file; Change green parts.
3. Save.

When miXAFS.app does not work, please check the contents of the app.
2.5 How to boot miXAFS

Booting miXAFS takes a bit time.\(^3\)

2.5.1 macOS

Double click the icon of "miXAFS.app". "miXAFS.app" is Automator application, which execute shell commands.

2.5.2 Windows

Double click miXAFS_yymmdd_20xx_win.exe

2.6 Run miXAFS

If the setting file designates all analysis condition, you can analyze with the following three steps.

1. Designate the setting file name with full path at 'Setting File' edit window.
2. Click "Entry" button on Start tag to load parameters from the setting file.
3. Click "Run" button on Start tag.

2.7 Example of execution

This section shows the example of execution. One of the features of miXAFS is the continuous procedures from experimental raw data to obtaining structural parameters through obtaining XAFS functions, Fourier transform, Fourier filters with few steps. In this section, manipulations of miXAFS are explained on the base that obtaining the structural parameters with least squared curve fitting from the experimental raw data.

2.7.1 Obtaining the structural parameters directly from the experimental data; Fitting in k-space

This sample shows how to obtain the structural parameters from experimental raw data through fitting \(\chi(k)\) in k-space.

1. Load "Setting_CsBr_yymmdd.txt" by selecting it in "Setting File" window with "Select" button on "Start" tab.

\(^3\)https://jp.mathworks.com/help/compiler/create-and-install-a-standalone-application-from-matlab-code.html
2.7. EXAMPLE OF EXECUTION

2. HOW TO INSTALL AND RUN MIXAFS

2. Click "Entry" button.
3. Push "Run" button.

The obtained parameters are shown in "Structural Parameter" tab, and are recorded in the result file designated in "Result file" edit window in "Start" tab.

2.7.2 Obtaining the structural parameters directly from the experimental data; Fitting in r space

1. Do the first process of §2.7.1
2. Change as follows.
   • "Fitting space" popupmenu in "Fitting Setting" tab: r space fitting
3. Push "Run" button.

2.7.3 Obtaining the structural parameters directly from the experimental data; Sequence analysis

This sample shows the sequence analysis following to the file list.

1. Do the first process of §2.7.1
2. Change as follows.
   • "File_SingleMulti" popupmenu in "Start" tab: Multi(table)
   • "header" edit window in Main window: Br
3. File list is Init_CsBr_Br_yymmd.txt.
4. Push "Run" button.

2.7.4 E0

1. Do the first process of §2.7.1
2. Change as follows.
   • "Fitting_type" popupmenu in "Fitting Setting" tab: E0
   • Change the values of "E0 Shift range".
3. Push "Run" button.

2.7.5 Lin_fix

1. Do the first process of §2.7.1
2. Change as follows.
2.7. EXAMPLE OF EXECUTION

- "Fitting_type" popupmenu in "Fitting Setting" tab: Lin_fix
- Change the values of "Mesh_fix".

3. Push "Run" button.

2.7.6 Mesh

This sample shows how to obtain a figure like the Figure 3 in J. Synchrotron Radiation 25(2018)618.

1. Do the first process of §2.7.1
2. Change as follows
   - "Fitting_type" popupmenu in "Fitting Setting" tab: Mesh_fix
3. Push "Run" button.

To change the analysis condition, change the following condition.

Number of mesh division:
Change x-axis:
Change y-axis:

2.7.7 Multi edge analysis

1. Do the first process of §2.7.1
2. Change as follows.
   - "Edge_SingleMulti" popupmenu in "Start" tab: Multi
   - "run_type" popupmenu in Main window: fitting
   - Empty "header" edit window in Main window:
3. Push "Run" button.

The definition of the multi edge are designated in "Multi Edge" tab.

2.7.8 Output file name

Table 2.1: Output file name

<table>
<thead>
<tr>
<th>file name</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
</tr>
<tr>
<td>header+'$_\mu$'+mu_fotter1+common_footer+mu_footer2</td>
</tr>
<tr>
<td>$\chi, FT$</td>
</tr>
<tr>
<td>header+fotter1+common_footer+footer2</td>
</tr>
</tbody>
</table>
2.7.9 Version history of miXAFS

miXAFS is under developing. In order to introduce new functions, the format of the setting files, the definitions of the format, GUI layout, and so on are modified. An application which help users to modify the setting files will be released in near feature. Comparison table between the format version is attached in the distribution files.

First release
Second release
Third release
Chapter 3

How to analyze the XAFS data in miXAFS

Identification data (ID) in the setting file are shown in ".....". Most of initial parameters are defined in the setting file which is identified on the first line of "File_initial.txt". The parameters which are not defined in the file are specified.

3.1 Setting File

Setting file defines the parameters as follows. Each row consists the keyword and the parameter. The characters between the top and just before the semicolon mark indicate the identifier of the parameters. The characters between just after the semicolon and just before the percent mark indicates the parameter. For example, "Vic_pre_min;13.1%abcde" means that ID is "Vic_pre_min" and the value for "Vic_pre_min" is 13.1. Following characters "abcde" is a comment.

The parameters are grouped in the setting file in order of the tab of the GUI of the miXAFS, but they are freely located in it without some exception. The exception is the initial valued of the fitting parameters and the format for the data files.

3.2 miXAFS window

Fig. 3.1 is booted window. The window is separated to two regions. In the upper area graphs of $\chi(k)$, Fourier transform, and so on. There are also "Run" button and the edit windows which set up the header of the file name of the XAFS data. In the lower area the data processing parameters for all procedures are displayed along with the obtained structural parameters. They are grouped under each tab.
3.2. MIXAFS WINDOW TO ANALYZE THE XAFS DATA IN MIXAFS

3.2.1 The upper area

When the inevitable parameters are fullfilled, miXAFS runs with only your click the pushbutton "Run". After while you can get what you want parameters and the graphs.

run_type: selectin of run mode

- raw data > fitting: miXAFS loads the raw experimental data and get the experimental and Fourier filtered $\chi(k)$, Fourier transform of $\chi(k)$, and the structural parameters.
- raw data > Fourier Filter chi: miXAFS loads the raw experimental data and get the experimental and Fourier filtered $\chi(k)$, Fourier transform of $\chi(k)$
- fitting: miXAFS loads the experimental and Fourier Filtered $\chi(k)$ and get the structural parameters.

header: file header

common_footer: common footer

--- Filename ---

Filenames are created for $\chi(k)$, $FT(r)$ and so on as follows;

Header + footer1 + common footer + footer2

where footer1 and footer2 are defined in the "Folder" tab.

In the description of "header", character "#" has special meaning. If the header is described as "AB###ab<9 12>", miXAFS analyzes for AB009ab, AB010ab, AB011ab, AB012ab

as the header.
3.3.2 The lower area

3.3 tab: Start

Fig. 3.1 shows the tab "Start". When you click "Entry" button, miXAFS loads the parameters from the setting file which is assigned by the "File_initial.txt" in the miXAFS folder(/Setting). You can change the file name with two ways; the first is to edit the file name directory, and the second is to click the "select" button left of the edit window and to choose the folder and write the filename.

File_SingleMulti: Number of analyzed file.

Single: The analyzed file name is assigned with "header"

Multi(table): The user can analyze the data sequently. The data names are defined as the file name designated at 'Initial file' are inserted between "Header" and footer part. In the fitting process to get the structural parameters the initial parameters are set following the 'Initial' table at 'Structural parameter' tab.

Multi(file): The initial parameters are set following as Initial file’. Others are same with 'Multi(table)'

Edge_SingleMulti: Number of edge for fitting to get the structural parameters.

Single: The fitting for only one edge.

Multi: The fitting for some edges. There are no limitation for the number of the edges. In this mode "Run" type must be set as "Fitting".

Result_file: File name of output file

Results are outputted to the file designated as 'Result_file'. If the name is defined only with extension, the output file name is automatically named as 'yymmdd-hhmmsss-Result.txt'.

File_list: File for sequence procedure. It contains part of file name, identified information (for example, temperature, pressure), and the initial values of the structural parameters for fitting process.

Theory:

FT_method:

invFT_method:

log_level: Level of output of log file. This initial value is defined at "miXAFS_setting.txt"

The user control the level of output message at 'Progress' window and the log file. The larger number, the lower level output. Therefore, it is better to set it large number, for example, 1000, 10000 when the user analyze unfamiliar data. After the setting file is well, it is recommended to set the number small, for example, 10, 100 because MATLAB takes time to write on edit window and file.
3.4 Extraction of $\chi(k)$

The absorbance is

$$
\mu_{\text{raw}}(E) = \begin{cases} 
-\ln\left(\frac{I}{I_0}\right) & \text{transmittance} \\
\frac{I}{I_0} & \text{fluorescence} \\
\mu & \text{for the experimental raw data where } \mu \text{ is recorded}
\end{cases}
$$

(3.1)

In the equation it is right to describe as $\mu d$, where $\mu$ is the absorption coefficient and $d$ is the sample thickness. It is no problem thinking about following procedures.

---

**Figure 3.2**: The window of the tab "$\chi(k)$"

$\mu_{\text{raw}}(E)$ is fitted with the following Victoreen equation in the preedge and the postedge regions to obtain the background of $\mu_{\text{raw}}(E)$.

$$
\mu_{\text{BG}}(E) = \begin{cases} 
A \cdot E^{-3} - B \cdot E^{-4} + c & E < E_0 \text{ ("Vict\_pre\_min" \sim "Vict\_pre\_max")} \\
(C_{\text{high}} - C_{\text{low}})E^{-3} - (D_{\text{high}} - D_{\text{low}})E^{-4} & E > E_0 \text{ ("Vict\_post\_min" \sim "Vict\_post\_max")}
\end{cases}
$$

(3.2)

where $A$ and $B$ are the free parameters, $C_{\text{high}}, C_{\text{low}}, D_{\text{high}}, D_{\text{low}}$ are the literal values\(^1\).

$\mu(k)$ is defined as follows,

$$
\mu(k) = \mu_{\text{raw}}(k) - \mu_{\text{BG}}(k)
$$

(3.3)

$$
k = \sqrt{\frac{2m}{\hbar^2}(E - E_0)}
$$

(3.4)

3.4. **EXTRACTION OF** XAFS DATA IN MIXAFS

$k$ is obtained in the range(“$k_{\min}$” ~ “$k_{\max}$”) with equal interval(“$k_{\text{interval}}$”). $m$ is the mass of the electron, and $E_0$ is the threshold energy, which is determined to be the midpoint of the edge jump.

The EXAFS functions, $\chi(k)$, are extracted from the experimental X-ray absorption spectra. $\chi(k)$ is defined as

$$\chi(k) = \frac{\mu(k) - \mu_0(k)}{\mu_0(k)}$$  \hspace{1cm} (3.5)

where $\mu_0(k)$ is the absorption for virtual isolated atoms. However, it is difficult to determine $\mu_0(k)$ by the measurements or the theory. Therefore, $\mu_0(k)$ is obtained by the following two methods.

### 3.4.1 Setting values

**Element:** ex. S, Te  
**Edge:** ex. K, L3  
**SSD_weight:**  
**BG_method:**  
**exp_file_type:** Input tag name which is defined in ”Load File” tab.  
**E0_method:** Three modes  
- lineicr : half_1  
- fixed $E_0$: ex. @E0_fix@<E0=25.5> unit is keV  
- initial $E_0$: ex. @E0_init@<E0=25.5> unit is keV  
**Vict_pre_min, Vict_pre_min:** The area of the pre-edge Victoreen fitting.  
**Vict_post_min, Vict_post_min:** The area of the post-edge Victoreen fitting.  
**exp_cut:** Remove several experimental data areas. At this stage, the unit is keV. When remove data areas, the value of $k_{\text{interval}}$ may be recommended zero.  
- ex. @keV@<12.3 12.5>@<13.5 14.2>  
**exp_NR:** examples  
- @medF1@<medF1_ord=5>  
- @medF1+isol_movmed@<medF1_ord=5>@isol_mmd_win=2>@isol_mmd_thF=3>@end_tmnr=5>  
**Victoreen_NR, mu_NR, chi_NR:**  
**chi_file_type:**  
**chi_file_appd:**  
**chi_k_min:**  
**chi_k_max:**  
**k_interval:** Three modes. The unit is $\text{Å}^{-1}$  
- positive value: even intervals.  
- zero: The energy of experimental data points are changed to the wavelength.  
**chi_ext_method:** Two options.  
- Modified Matsubayashi:
3.4. **EXTRACTION OF**

**CHAPTER 3. HOW TO ANALYZE THE XAFS DATA IN MIXAFS**

@xanadu@<cut_degree=11><smt_k_power=2><smt_repeat=3><ext_degree=5>

**AUTOBK:**

@AUTOBK@<clamp_high=off><clamp_high_num=5><clamp_high_weight=10>
<br/>&lt;k_power=1&gt;&lt;init=spline&gt;&lt;k_width=6&gt;&lt;delta_R=0&gt;&lt;k_window=Hanning&gt;

autobk_Rbkg :
chi_error_method :
FT_error_method :

3.4.2 **Algorithm of the extraction of** $\chi(k)$

**AUTOBK’s method**

An algorithm of AUTOBK ² is used. In the algorithm of AUTOBK, $\mu_0(k)$ is obtained with minimizing $FT(r)$ below ”autobk_Rbkg”. If ”clamp_high” is on, points of $\mu_0(k)$ are clamped on the experimental $\mu(k)$ for the number of ”clamp_high_num” in the high k region.

autobk_Rbkg : A value of below which $FT(r)$ is minimized.
clamp_high : Options are ”on” or ”off”
clamp_high_num :
clamp_high_weight :
k_power : $k^{k\text{power}}\chi(k)$ is Fourier transformed.
k_width : The window width of Fourier transform
delta_R :
k_window : The window function type of Fourier transform

**Xanadu’s method**

An algorithm of Xanadu ³ is used.

1. $\mu(k)$ is fitted with the polynomial equations (the polynomial order is ”cnt_degree”), and $\mu_0^0$ is its optimized value. $\Delta\mu(k)$ is defined as,

$$\Delta\mu(k) = \mu(k) - \mu_0^0(k)$$ (3.6)

2. $k^{n_{\text{ext}}}\Delta\mu(k)$ ($n_{\text{ext}}$ is ”sm_k_power”) is smoothed with smoothing of 11 points (reputation is ”sm_repeat”), and the smoothed values are $k^{n_{\text{ext}}}\Delta\mu_{\text{smooth}}(k)$.

3. $k^{n_{\text{ext}}}\Delta\mu_{\text{smooth}}(k)$ is fitted with the polynomial equations (the polynomial order is ”ext_degree”), and $k^{n_{\text{ext}}}\Delta\mu_{\text{smooth} – center}(k)$ is its optimized value. After that, the values of k for maximum and minimum, respectively, of $k^{n_{\text{ext}}}\Delta\mu_{\text{smooth} – center}(k)$ are searched. They are $k_{\text{maximum}}$ and $k_{\text{minimum}}$.

²Phys. Rev. B, 47, p14126
3.5. FOURIER TRANSFORM

4. $\Delta \mu_{\text{center}}$ is the average of spline curves of maxima and minima, that are calculated by spline functions of $\Delta \mu_{\text{smooth}}(k_{\text{maximum}})$ and $\Delta \mu_{\text{smooth}}(k_{\text{minimum}})$.

5. At last, the $\mu_0(k)$ is obtained by the following equation

$$\mu_0(k) = \mu_1^0(k) + \Delta \mu_{\text{center}}$$ (3.7)

3.4.3 Noise reduction

MATLAB functions, medfilt1$^4$ and isoutlier$^5$, are used to remove noise.

medF1 : medfilt1
medF1_ord : nth-order one-dimensional median filter of medfilt1
medF1+isol_movmed : medfilt1 & ’movmedian’ mode of isoutlier
isol_mmd_win : window of ’movmedian’ in isoutlier
isol_mmd_thF : ThresholdFactor of ’movmedian’ in isoutlier
end_tmn : last points for number of ”end_tmn” are fixed with zero

3.5 Fourier transform

![Figure 3.3: The window of the tab ”Fourier transform”](https://jp.mathworks.com/help/signal/ref/medfilt1.html?lang=en)

![Figure 3.3: The window of the tab ”Fourier transform”](https://jp.mathworks.com/help/matlab/ref/isoutlier.html?lang=en)
3.5. **Fourier Transform**

### 3.5.1 Window function

The Hamming and Hanning functions for the window function are installed at this stage.

**Hamming window**

\[
W(x) = \begin{cases} 
0.54 - 0.46 \cdot \cos\left(\frac{x - x_{1\text{min}}}{x_{1\text{min}} - x_{1\text{max}}} \pi\right) & x_{1\text{min}} < x < x_{1\text{max}} \\
1 & \\
0.54 - 0.46 \cdot \cos\left(\frac{x - x_{1\text{max}}}{x_{1\text{max}} - x_{1\text{min}}} \pi\right) & x_{1\text{max}} < x < x_{1\text{max}} 
\end{cases} \tag{3.8}
\]

**Hanning window**

\[
W(x) = \begin{cases} 
0.5 - 0.5 \cdot \cos\left(\frac{x - x_{1\text{min}}}{x_{1\text{min}} - x_{1\text{max}}} \pi\right) & x_{1\text{min}} < x < x_{1\text{max}} \\
1 & \\
0.5 - 0.5 \cdot \cos\left(\frac{x - x_{1\text{max}}}{x_{1\text{max}} - x_{1\text{min}}} \pi\right) & x_{1\text{max}} < x < x_{1\text{max}} 
\end{cases} \tag{3.9}
\]

### 3.5.2 Fourier transform

\(\chi(k)\) is Fourier transformed,

\[
FT(r) = \frac{1}{\sqrt{\pi}} \int_{k_{\text{min}}}^{k_{\text{max}}} W(k) \frac{k}{F(k)} \chi(k) \exp[-i(2kr + \phi(k))] dk \tag{3.10}
\]

where \(W(k), F(k)\) and \(\phi(k)\) are the window function, the backword scattering function and the phase shift. \(W(k)\) is defined in §3.5.1 and set with "FF_FT_k_window". \(F(k)\) and \(\phi(k)\) are the theoretical values (the file is "FF_Theory"). \(k_{\text{min}}\) and \(k_{\text{max}}\) is "FF_FT_k_min" and "FF_FT_k_max", respectively. The values of \(x_{1\text{min}} - x_{1\text{min}}\) and \(x_{1\text{max}} - x_{1\text{max}}\) are equal to "FF_FT_k_width". Fourier transformed range of \(r\) is between "FF_FT_r_min" and "FF_FT_r_max", and the interval is "FF_FT_r_interval".

### 3.5.3 inverse Fourier transform

\(FT(r)\) is inverse Fourier transformed,

\[
\chi(k) = \frac{F(k)}{W(k)k \sqrt{\pi}} \int_{r_{\text{min}}}^{r_{\text{max}}} W(r)FT(r) \exp[i(2kr + \phi(k))] dr \tag{3.11}
\]

where \(W(k), F(k)\) and \(\phi(k)\) are the window function, the backword scattering function and the phase shift. \(F(k)\) and \(\phi(k)\) are the theoretical values (the file is "FF_Theory"). \(W(k)\) is defined in §3.5.1 and set with "FF_invFT_r_window". \(x_{0\text{min}}, x_{0\text{min}}, x_{0\text{max}},\) and \(x_{1\text{max}}\) are "FF_invFT_r_min_0", "FF_invFT_r_min_1", "FF_invFT_r_max_1", and "F_invFT_r_max_0", respectively. Inversed Fourier transformed range of \(k\) is between "FF_FT_k_min" and "FF_FT_k_max", and the interval is "FF_invFT_k_interval".
3.6 EXAFS fitting

The EXAFS function is fitted to the following theoretical function by the nonlinear least squared curve fitting method:

\[
\chi_{\text{cal}}(k) = \sum_j \frac{P N_j}{k_0 r_j^2} f_j(k_0) \exp\left(-2\sigma_j^2 k_0^2\right) \exp\left(-\frac{2r_j}{\lambda_j(k_0)}\right) \sin\left[2k_0 r_j + \phi_j(k_0) - \frac{4}{3} C_{3j} k_0^3\right] \quad \text{(3.12)}
\]

\[
k_0 = \sqrt{k^2 - \frac{2m}{\hbar^2} \Delta E_0} \quad \text{(3.13)}
\]

P is the scaling factor, and \(\Delta E_0\) is the energy shift. \(f_j(k)\) and \(\phi_j(k)\) are the backscattering amplitude and the total phase shift functions, and \(\lambda_j(k)\) is the electron mean free path length for an atom in the \(j\)-th shell, which are calculated by the theoretical calculation. \(r_j\) is the interatomic distance between X-ray absorbing and photoelectron scattering atoms, and \(N_j\) is the coordination number in the \(j\)-th shell. \(\sigma_j^2\) is the mean square relative displacement, and \(C_{3j}\) and \(C_{4j}\) are the third and fourth cumulants, respectively.

The index of fit is the residual, \(R\)-factor, calculated by

\[
R = \sqrt{\frac{\sum (k^{\text{fit}} \chi - k^{\text{fit}} \chi_{\text{cal}})^2}{\sum k^{2\text{fit}} \chi^2}} \times 100 \quad \text{(3.14)}
\]

where \(\chi\) is the EXAFS signal, and the summation is taken over all the data points in the \(k\)-range used for fitting. \(n_{\text{fit}}\) is defined with "Fit_k_power".

3.6.1 Fitting Setting

---

Fit_space: Define the fitting space (k-space or r-space)

- k space fitting:
- r space fitting:

Fit_LSQ_code:

- nlinit: use of nlinit\(^6\) code of MATLAB
- lsqcurvefit: use of lsqcurvefit\(^7\) code of MATLAB
- lsqcurvefit>nlinit: use of lsqcurvefit and nlinit code of MATLAB

Fitting_control:

- Table: The initial values of the table "Initial" in the "Structural Parameter" tab.

---

\(^7\)https://jp.mathworks.com/help/optim/ug/lsqcurvefit.html?lang=en
Figure 3.4: The window of the tab "Fitting Setting"

E0: For linear plot of R-factor, the x-axis is the structural parameters.

Lin_fix: For linear plot of R-factor, the x-axis is the structural parameters. Their initial values are defined by "Fit_mesh_set1", and is fixed. The initial values of other structural parameters are defined at "Initial" table. Control and the range are defined at "Initial" table.

Lin_free: For linear plot of R-factor, the x-axis is the structural parameters. Their initial values are defined by "Fit_mesh_set1", and is fixed. The initial values of other structural parameters are defined at "Initial" table. Control and the range are defined at "Initial" table.

Mesh_fix: For mapping of R-factor, the x- and y-axis are the structural parameters. Their initial values are defined by "Fit_mesh_set1" and "Fit_mesh_set2", respectively, and they are fixed. The initial values of other structural parameters are defined at "Initial" table. Control and the range are defined at "Initial" table.

Mesh_free: For mapping of R-factor, the x- and y-axis are the structural parameters. Their initial values are defined by "Fit_mesh_set1" and "Fit_mesh_set2", respectively, and they are free. The initial values of other structural parameters are defined at "Initial" table. Control and the range are defined at "Initial" table.

DW_format:
Fit_exp_error:
Fitexp_error_constant:
Fit_error_Report:
Fit_mesh_division: How many points to set for one axis for mapping or linear plot.
Fit_mesh_set1: The definition of x-axis of mapping or linear plot.
Fit_mesh_set2: The definition of y-axis of mapping.
3.6. **HOW TO ANALYZE THE XAFS DATA IN MIXAFS**

--- **Fitting condition** ---

Fit_file: for multi edges fitting  
Fit_weight: for multi edges fitting  
Fit_E0_control: Set whether the value of the energy shift $E_0$.  
- $0$: $E_0$ is fixed.  
- $1$: $E_0$ is free parameter.  
Fit_E0_init: the initial value of the energy shift  
Fit_E0_range: The energy range of $E_0$ when $E_0$ is free parameter.  
Fit_E0_str_para: The y-axis of linear plot

--- **In the case of k-space fitting** ---

Fit_k_power: $k^{\text{Fit}_k\text{.power}} \chi(k)$ is fitted.  
Fit_k_min: The minimum of the fitting area.  
Fit_k_max: The maximum of the fitting area.

--- **In the case of r-space fitting** ---

When the fitting area is set to the area where the interested sites locate, the least squared curve fitting code gives the parameter set that have peaks outside of the fitting area. To avoid such case, Fit_r_min and Fit_r_max are set wider than the interested area, and the interested area defined by Fit_r_win_min_0 and so on of the window function.

Fit_r_FT_Theory: define the theoretical file for the Fourier transform.  
Fit_r_FT_k_window: select the window function on $\chi(k)$ for the Fourier transform  
Fit_r_FT_k_min: the minimum of the k-range for the Fourier transform.  
Fit_r_FT_k_max: the maximum of the k-range for the Fourier transform.  
Fit_r_min: the minimum of the fitting area.  
Fit_r_max: the maximum of the fitting area.  
Fit_r_interval: The interval of r.  
Fit_r_window: Type of the window function.  
Fit_r_win_min_0: $x_0^{\text{min}}$ for the window function.  
Fit_r_win_min_1: $x_1^{\text{min}}$ for the window function.  
Fit_r_win_max_1: $x_1^{\text{max}}$ for the window function.  
Fit_r_win_max_0: $x_0^{\text{max}}$ for the window function.

### 3.6.2 Structural Parameter
### Initial Parameter

Set the initial values of the structural parameters for the least squared fitting.

\[
\begin{align*}
\text{Parameter}_{\text{Edge Head}} & = \quad \text{Parameter}_{\text{Site Head}} = \quad \\
\text{Active}: & \text{ choose whether the site is active or nonactive} \\
\text{r\_control}: & \text{ set the control of r parameter. } 0 \text{ and } 1 \text{ mean the parameter fixed and free, respectively.}
\end{align*}
\]

When the parameter is constrained with other parameter, the constraint is defined by the four operation of arithmetice. For example, \(r(1,2)\times1\) means that the focused atomic distance is constrained on one times the atomic distance for the second shell of the first absorption edge.

\[
\begin{align*}
\text{r\_init}: & \text{ the initial value of the parameter for the least square curve fitting.} \\
\text{r\_range}: & \text{ the varying range of the value of the parameter in the fitting process.} \\
\text{N\_control}: & \text{ }N(1,2)=4.0 \text{ } \text{ means that the sum of the focused coordination number and that of the second site of the first absorption edge is 4.0.}
\end{align*}
\]

\[
\begin{align*}
\text{N\_init}: \\
\text{N\_range}: \\
\text{DW\_control}: \\
\text{DW\_init}: \\
\text{DW\_range}: \\
\text{C3\_control}: \\
\text{C3\_init}: \\
\text{C3\_range}: \\
\text{C4\_control}: 
\end{align*}
\]
C4 init:
C4 range:
Fit_Theory: The theoretical file for the fitting, which must include the values of amplitude and the
phase shift.

In the setting file, following character string must be set at the top for each definitions.

====== Parameter_Edge_Head ======: The head of absorbing element for fitting.
====== Parameter_Site_Head ======: The head of absorbing site for fitting

--- Optimized Parameter ---

The optimized structural parameters are shown at the ”Optimized” table at the ”Structural Parameter”
tab. μ, χ(k), Fourier filtered χ(k), FT(r), and their optimized values are saved at designated folders
with designated footers. The file names are described at §2.7.8

3.7 Folder

Components of the file names, footer1 and footer2, are defined, and storge folders are designated in this
tab.

3.8 Load File

Parameters for experimental raw data are defined in ”miXAFS_Setting_yymmd.txt” in ”Setting” folder.
3.8. HOW TO ANALYZE THE XAFS DATA IN MIXAFS

3.8.1 Experimental raw data format

File_exp_tag: text
File_exp_exp_type: text
    Transmission;
    Fluorescence;
    \mu; \mu
File_exp_E_unit: text
    angle;
    eV;
    keV;
File_exp_header_sign: miXAFS recognizes the line which contains the characters of “File_exp_header_sign” as the header of data set of the experimental raw data. miXAFS loads the lines between the header line and the footer line as the data of experimental raw.
File_exp_footer_sign: miXAFS recognizes the line which contains the characters of ”File_FF_chi_footer_sign” as the footer of data set of the experimental raw data.
File_exp_energy: Column number of energy
File_exp_I0: Column number of \( I_0 \)
File_exp_I_start: Start column number of \( I \)
File_exp_I_end: End column number of \( I \). When the values of \( I \) are recorded at one column, set ‘File_exp_I_end’ the same number of ‘File_exp_I_end’
File_exp_appd:
3.8.2 Format of Fourier filtered $\chi(k)$

File_FF_chi_format: The name of format. Some formats are named, and following definitions are defined. Except "Free" you do not need to define the format.

   Free: The format is defined in miXAFS already, so you don’t need to define the following definitions.
   miXAFS: The format is defined in miXAFS already for miXAFS.
   label: text
   label: text
   label: text
   label: text

File_FF_chi_header_sign: miXAFS recognizes the line which contains the characters of ”File_FF_chi_header_sign” as the header of data set of the Fourier filtered $\chi(k)$ data. miXAFS loads the lines between the header line and the footer line as the data of $\chi(k)$.

File_FF_chi_footer_sign: miXAFS recognizes the line which contains the characters of ”File_FF_chi_footer_sign” as the footer of data set of the Fourier filtered $\chi(k)$ data.

File_FF_chi_num_column: The number of columns of the data of $\chi(k)$

File_FF_chi_k: The column of $k$

File_FF_chi_chi: The column of $\chi(k)$

File_FF_chi_error: The column of error of $\chi(k)$

File_FF_chi_k_weight_cancel: In some $\chi(k)$ files the data are recorded as $k^{n}\chi(k)$. The number of n is defined as File_FF_chi_k_weight_cancel.

3.9 Multi Edges

At this stage the operation of the multi edges fitting is limited in the k-space and under only fitting process.

3.10 Sub Window

The formats for the various values are loaded from ‘...’ in ’Setting’ folder.

3.10.1 Experimental raw data format

File_exp_tag: text
3.10. SUB WINDOW

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Figure 3.8:

Figure 3.9: