

miXAFS: a program for X-ray absorption fine-structure data analysis

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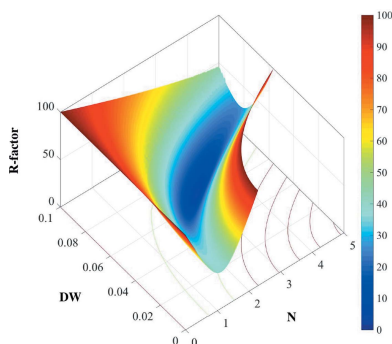
A new program called *miXAFS* for the analysis of X-ray absorption fine-structure (XAFS) data is presented. *miXAFS* can analyze the XAFS functions simultaneously for all measured X-ray absorption edges of the constituent elements in a sample under the constraints for the structural parameters over the edges. The program provides a surface plot of the *R*-factor as a function of two structural parameters, which is useful to validate the optimized structural parameters. The structural parameters can be obtained from the XAFS data in a few steps using the setting file and batch process. The program, which is coded in MATLAB and freely available, runs on Macintosh and Windows operating systems. It has a graphical user interface and loads experimental data and XAFS functions in a variety of ASCII data formats.

1. Introduction

X-ray absorption fine-structure (XAFS) analysis is a powerful tool for characterizing the local structure of materials (Lee *et al.*, 1981; Rehr & Albers, 2000; Bunker, 2010). XAFS analysis has notable advantages over more conventional X-ray diffraction methods. The first is its applicability to any form of matter regardless of whether it has long-range order or not. Therefore, XAFS is an extremely powerful tool to analyze the structure of amorphous materials, liquids and nanomaterials.

The second advantage of XAFS is element specificity. Each element has a set of unique X-ray absorption edges, so the local structure around the target element can be analyzed by XAFS measurements around its edge. For chemical compounds, it is usual to perform XAFS measurements for as many constituent elements as possible, so the atomic pair correlation around the X-ray-absorbing atoms is determined. It is ideal to simultaneously analyze the XAFS data for all the measured absorption edges considering the atomic correlations over the absorption edges (Di Cicco *et al.*, 2000). However, in most cases, the acquired XAFS data are not fully utilized because the XAFS functions $\chi(k)$ for each edge are analyzed independently not simultaneously.

Nonlinear least-squares curve fitting is typically used to determine the structural parameters in XAFS analysis. This method is popular and useful, but the results depend on the initial values of the structural parameters; that is, the results sometimes look odd from the viewpoint of physical considerations. It is therefore necessary to check the effect of the initial values of the structural parameters on the results. According to the standard XAFS equation, the main parameters that influence the phase of $\chi(k)$ are the atomic distance and third cumulant; the main parameters that determine the amplitude of $\chi(k)$ are the coordination number and Debye–



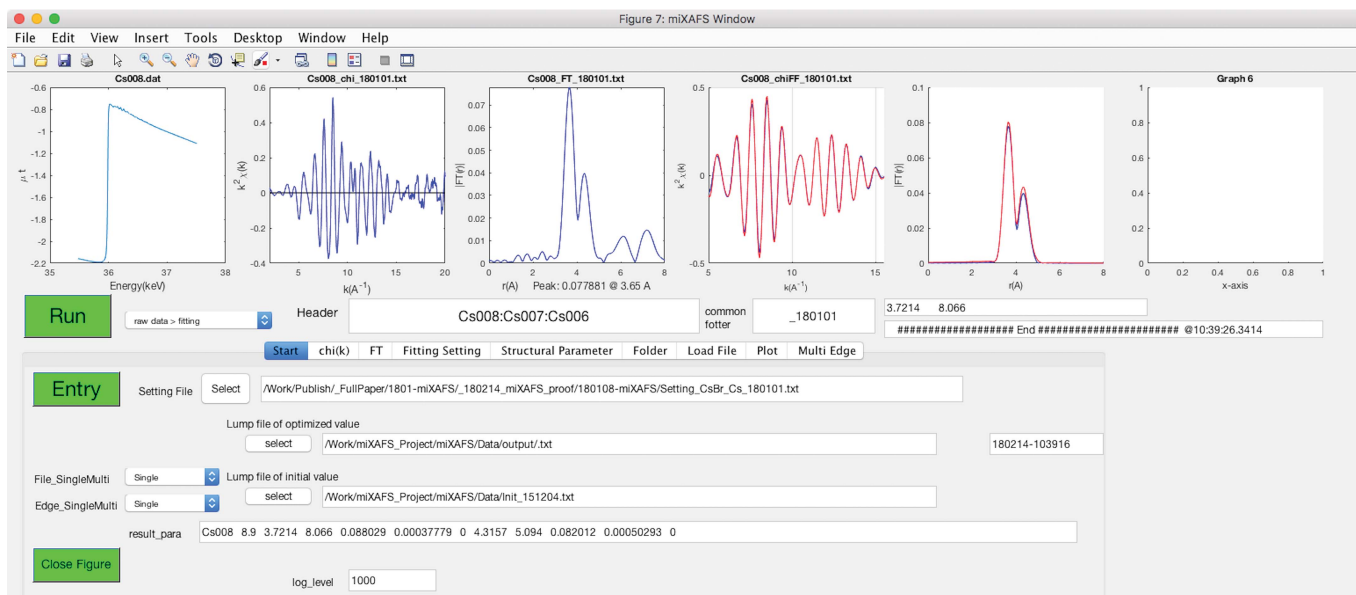


Figure 1

Screenshot of *miXAFS* analyzing experimental raw data to obtain the optimized structural parameters through a sequence of conventional XAFS analysis procedures. When the 'Entry' button is clicked, the parameters defined in the settings file are loaded to the edit windows. Clicking the 'Run' button starts all the procedures following the analysis mode. In the upper area of the window, the absorption coefficients, $\chi(k)$, the Fourier transform of $\chi(k)$ and Fourier-filtered $\chi(k)$ are shown. The optimized structural parameters are shown in the Structural Parameter tab. The analytic parameters for each procedure are described in each tab. The blue and red lines in the graphs represent the experimental and optimized values, respectively.

Waller factor. These interdependent parameters influence each other in terms of the phase or amplitude in the fitting process. Surface plots of the R -factor against the interdependent structural parameters are useful to validate the optimized structural parameters (Di Cicco, 1996; Ikemoto & Miyanaga, 2014).

A large number of parameters are required to extract structural parameters from experimental data. Many XAFS analysis packages are available, the majority of which have a graphical user interface (GUI) (Ressler, 1998; Klementev, 2001; Ravel & Newville, 2005; Hatada *et al.*, 2016). However, these packages require many steps to analyze the XAFS data. It would be convenient to obtain the structural parameters from experimental raw data with fewer procedures, especially when the XAFS spectra must be measured within a limited beam time at synchrotron radiation facilities.

This paper presents a new XAFS data analysis tool called *miXAFS*. *miXAFS* can analyze the XAFS functions simultaneously for all the obtained X-ray absorption edges under the constraints of the structural parameters. This program can construct the surface plot for the R -factor as functions of two structural parameters, which is helpful to obtain the structural parameters that are not located at the local minimum. The fitting procedures to obtain structural parameters are performed in both the k -space and r -space. *miXAFS* is freely available through the website http://www.sci.u-toyama.ac.jp/phys/3ken/children/miXAFS/_index-miXAFS.htm.

2. System requirements and data format

The program *miXAFS* is coded in MATLAB and the executable application is freely available for Macintosh and

Windows operating systems.¹ Running *miXAFS* requires the runtime routine of MATLAB, which can be downloaded from the MathWorks website (<https://www.mathworks.com/products/compiler/mcr.html>), so users do not need an expensive MATLAB system.

miXAFS can load various ASCII file types of experimental raw data and $\chi(k)$ data obtained by other XAFS programs. The loading procedure is designed to have flexibility, such that the user can define the loading rules according to their requirements. The *miXAFS* program stores several types of data, including $\chi(k)$, the Fourier transform of $\chi(k)$, the optimized structural parameters, the uncertainties of the optimized structural parameters, and the correlation coefficients in ASCII format. This allows the user to easily plot and analyze the results with familiar tools. A log of *miXAFS* is saved with several levels that can be defined by the user.

3. Graphical user interface

Fig. 1 shows the GUI window of *miXAFS*, which exhibits all the parameters used to run *miXAFS* and the obtained results. The window is separated into two areas. In the upper area of the window, the user can observe the absorption coefficients, $\chi(k)$, the Fourier transform of $\chi(k)$ and Fourier-filtered $\chi(k)$ at a glance. This area also includes edit windows that set up the file name of the XAFS data, and the Run button. The lower area of the window displays the data-processing parameters for all procedures along with the obtained structural parameters. The windows in the lower area are switched by clicking the tabs. When *miXAFS* is booted up, the identification data

¹ *miXAFS* for Linux will be provided in the near future.

(ID) defined in the settings file are shown in the edit windows of the GUI, such that the user can easily know where the values of the parameters in the setting file are loaded. The parameters on the edit window are overwritten with the values of the parameters in the settings file by clicking the Entry button, and the user can also change the parameters directly through the edit windows. Several *miXAFS* GUI windows can be activated, allowing the user to compare the results between different data or different analytical conditions.

miXAFS contains all necessary processes for conventional XAFS data analysis to obtain the structural parameters from experimental data. *miXAFS* can be run in several modes; for example, to obtain the structural parameters from experimental raw data, to obtain $\chi(k)$ from experimental data, and to determine structural parameters from $\chi(k)$ obtained using other programs.

4. Analysis method

4.1. Extraction of $\chi(k)$

$\chi(k)$ is defined as

$$\chi(k) = \frac{\mu(k) - \mu_0(k) - \mu_b(k)}{\mu_0(k)}, \quad (1)$$

$$k = \left[\frac{2m}{\hbar^2} (E - E_0) \right]^{1/2}, \quad (2)$$

where k is the photoelectron wavenumber, m is the mass of an electron, E is the energy of the incident X-ray and E_0 is the threshold energy. $\mu(k)$, $\mu_0(k)$ and $\mu_b(k)$ are the experimental absorption coefficient, the absorption for virtual isolated atoms and the background contribution to $\mu(k)$ from the other shells, respectively.

$\mu_b(k)$ is estimated by a least-squares fitting calculation in the pre-edge and post-edge regions using the Victoreen formula (Victoreen, 1947; Sakane *et al.*, 1993). $\mu(E)d$ is fitted with following equations,

$$\begin{cases} \mu_b(E)d = (AE^{-3} - BE^{-4} + c)d, & E < E_0, \\ \mu_b(E)d + [(C_{\text{post}} - C_{\text{pre}})E^{-3} - (D_{\text{post}} - D_{\text{pre}})E^{-4}]d, & E > E_0, \end{cases} \quad (3)$$

where d is the sample thickness; A , B and c are the free parameters; and C_{post} , C_{pre} , D_{post} and D_{pre} are the literal values (MacGillavry & Rieck, 1983). $\mu_0(k)$ is obtained following the method proposed by Matsubayashi *et al.* (Sakane *et al.*, 1993; Ikemoto *et al.*, 2011).

4.2. Fourier transform and Fourier filtering

$\chi(k)$ is Fourier transformed as

$$\text{FT}(r) = \frac{1}{\sqrt{\pi}} \int_{k_{\text{min}}}^{k_{\text{max}}} W(k) \frac{k}{F(k)} \chi(k) \exp \left\{ i [2kr + \varphi(k)] \right\} dk \quad (4)$$

and $\text{FT}(r)$ is inverse Fourier transformed as

$$\chi(k) = \frac{F(k)}{W(k)k} \frac{2}{\sqrt{\pi}} \int_{r_{\text{min}}}^{r_{\text{max}}} W(r) \text{FT}(r) \exp \left\{ -i [2kr + \varphi(k)] \right\} dk, \quad (5)$$

where $W(k)$ and $W(r)$ are the window functions, which are selected from the Hamming and Hanning windows. $F(k)$ and $\varphi(k)$ are the backscattering amplitude and phase shift functions, respectively, which are calculated using theoretical codes; for example, *FEFF* (Ankudinov *et al.*, 1998), *GNXAS* (Di Cicco, 2009) and *Excurve* (Tomic *et al.*, 2004).

4.3. Obtaining structural parameters

$\chi(k)$ is calculated using the following theoretical function,

$$\begin{aligned} \chi_{\text{cal}}(k) &= \sum_j \frac{PS_{0,j}^2(k_0) N_j}{k_0 r_j^2} f_j(k_0, r_j) \\ &\times \exp \left(-2\sigma_j^2 k_0^2 + \frac{2}{3} C_{4,j} k_0^4 \right) \exp \left[-\frac{2r_j}{\lambda_j(k_0)} \right] \\ &\times \sin \left[2k_0 r_j + \varphi_j(k_0) - \frac{4}{3} C_{3,j} k_0^3 \right], \end{aligned} \quad (6)$$

$$k_0 = \left(k^2 - \frac{2m}{\hbar^2} \Delta E_0 \right)^{1/2}, \quad (7)$$

where P is the scaling factor and ΔE_0 is the energy shift. $S_{0,j}^2(k)$, $f_j(k, r_j)$, $\varphi_j(k)$ and $\lambda_j(k)$ are the k -dependent reduction factor resulting from the many-body effect, the backscattering amplitude, the total phase shift functions and the electron mean free path length for an atom in the j th shell, respectively, which are calculated using the theoretical codes mentioned above. 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. σ_j is the Debye–Waller factor, and $C_{3,j}$ and $C_{4,j}$ are the third and fourth cumulants, respectively.

To obtain the structural parameters, least-squares curve fitting is conducted to minimize the following function using the *nlinfit* or *lsqcurvefit* functions of MATLAB,

$$\sum_{i=1}^N \frac{|\text{Data}_i - \text{Model}_i|^2}{\varepsilon_i^2}, \quad (8)$$

where N is the number of data points in the fitting range and ε_i is the measurement uncertainty for the i th data point. This equation is applied to $k^n \chi(k)$ or $\text{FT}(r)$.

The IXS Standards and Criteria Committee recommends that the results obtained by XAFS must be accompanied by estimation of the uncertainty (IXS, 2000). The uncertainty δP_j of the j th independent structural parameter P_j is calculated using *nlinfit* and *nlparci* functions (MATLAB *nlparci*, <https://www.mathworks.com/help/stats/nlparci.html>). The correlation coefficient between the i th and j th independent parameters is calculated as

$$r_{ij} = \frac{C_{ij}}{(C_{ii} C_{jj})^{1/2}}, \quad (9)$$

where the C terms are the respective elements of the fit covariance matrix.

ε_i can be defined in the following ways. The first method is to estimate ε_i from independent scans by the equation

$$\varepsilon_i^2 = \frac{1}{M(M-1)} \sum_{j=1}^M |\text{Data}_j - \langle \text{Data}_j \rangle|^2, \quad (10)$$

where M is the number of independent scans. The second method is to use the values of ε_i defined in the file of $\chi(k)$ or $\text{FT}(r)$. The third approach is to give ε_i as a constant value in the GUI window.

The index of fit is the R -factor calculated by

$$R = \left(\frac{\sum_{i=1}^N |\text{Data}_i - \text{Model}_i|^2}{\sum_{i=1}^N |\text{Data}_i|^2} \right)^{1/2} \times 100, \quad (11)$$

where the summation is of all the data points used for fitting.

5. Features of *miXAFS*

5.1. Multiple edge fittings

XAFS is an element-specific spectroscopy technique that provides reliable and useful information about the local structure around the specified elements of materials. When the XAFS data for each element of a compound are measured, in most cases they are analyzed individually for each absorption edge. This sometimes gives contradictory results; for example, the atomic distance between two elements obtained from the individual XAFS analysis of each X-ray absorption edge may be different. In contrast, *miXAFS* can simultaneously analyze the XAFS functions for all the obtained X-ray absorption

edges under the constraints of the structural parameters. In principle, there is no limit to the number of edges and sites that can be simultaneously analyzed.

Fig. 2 shows an example of the simultaneous analysis of the Fourier-filtered $\chi(k)$ for the caesium and bromine K -edges of caesium bromide by least-squares curve fitting. For this analysis, the atomic distance r_{CsBr} (from the X-ray-absorbing Cs atoms to the nearest X-ray-scattering Br atoms), r_{CsCs} , the coordination numbers N_{CsBr} and N_{CsCs} are equal to r_{BrCs} , r_{BrBr} , N_{BrCs} and N_{BrBr} , respectively, in view of the CsBr structure. The constrained conditions are defined at the column of $r(\text{control})$ and $N(\text{control})$ in the table of the initial parameters. The ways to express the constraints are stated in §5.4. The upper area of the *miXAFS* window shows the Fourier-filtered $\chi(k)$ and its Fourier transform for the Cs and Br K -edges; both the experimental and optimized values are displayed. $\chi(k)$ and its Fourier transform for both edges are well reproduced. The initial and optimized structural parameters with their uncertainties are shown in the Structural Parameter tab of the GUI window. Following the constraint conditions, the optimized values of r_{CsBr} , r_{CsCs} , N_{CsBr} and N_{CsCs} are equal to those of r_{BrCs} , r_{BrBr} , N_{BrCs} and N_{BrBr} , respectively.

5.2. Surface plot of the R -factor

In the standard XAFS equation, the structural parameters can be classified into two groups: those that contribute to the phase of $\chi(k)$ and those that contribute to its amplitude. For example, the coordination number and Debye–Waller factors are the main determinants of the amplitude, and are strongly correlated in the least-squares curve-fitting process. Thus, it is important to check the effect of the Debye–Waller factor on

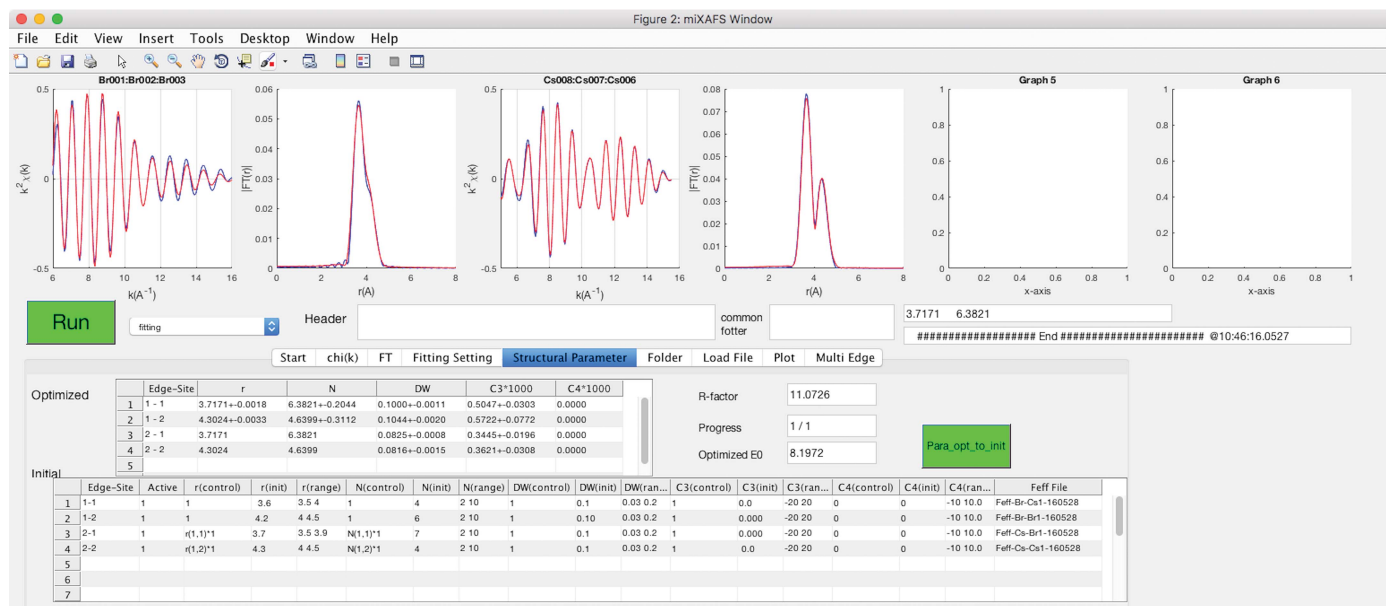


Figure 2

The simultaneous analysis of the caesium and bromine K -edges of caesium bromide by least-squares curve fitting against $\chi(k)$. The Structural Parameter tab shows the initial and optimized structural parameters. The 'Initial' table contains the initial values and constraints for the structural parameters. The optimized parameters are shown in the 'Optimized' table. The graphs display the Fourier-filtered XAFS function and Fourier transform for the bromine and caesium edges, respectively. The blue and red lines in the graphs represent the experimental and optimized values, respectively.

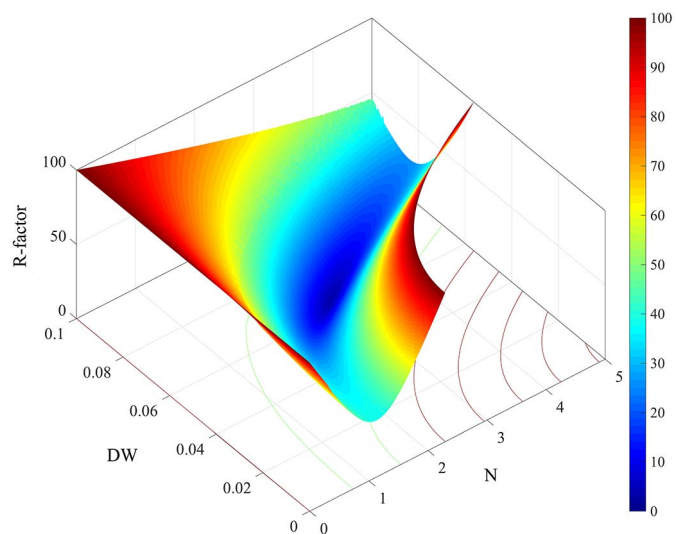


Figure 3
Three-dimensional shaded surface plot of the R -factor as functions of the coordination number and the Debye–Waller factor for isolated selenium chains in carbon nanotubes. The R -factor is indicated by the color and height.

the coordination number to correctly interpret the obtained coordination number.

Contour maps indicating the R -factor or the correlation statistical error on some parameters are useful to check the correlation between the parameters (Di Cicco, 1996). *miXAFS* provides a surface plot of the R -factor as a function of any two structural parameters without the restriction of the number of data points. Fig. 3 provides an example of a surface plot of the R -factor as a function of the coordination number and Debye–Waller factor of isolated selenium chains in carbon nanotubes. There is only one minimum, indicating that the obtained parameters are not located at local minima and are reliable. The surface plot can be obtained in two ways: one with fixed values on the x - and y -axes of the surface plot during least-squares fitting throughout the fitting process, and the other one in which these values are initially defined and free parameters in the fitting process. Such plots are useful to determine the reliability of the optimized parameters and to check whether the obtained structural parameters are located at local minima or not. Furthermore, this teaches beginners the importance of the initial values of parameters in least-squares curve-fitting analysis.

5.3. Batch process

It is usual to measure XAFS spectra while varying experimental conditions like temperature and pressure and to analyze them under the same analysis conditions. The repeated analysis is a boring procedure, and prevents analysts from trying many kinds of analysis. *miXAFS* can analyze large sets of experimental data and $\chi(k)$ data in sequence following a list that defines the file names, experimental conditions and initial values of the structural parameters for the least-squares curve fitting. This function encourages users to analyze their data

under many kinds of analytical conditions, and frees them from tedious work.

The value of ΔE_0 , which is set in the Fitting Setting tab of the GUI window, is important in XAFS fitting procedures. In most cases, the value is defined for the smallest R -factor or for reproducing the literature values; for example, the atomic distance of the most important atomic correlation. Therefore, the analyst performs the least-squares curve fitting by setting ΔE_0 as the free parameter or by changing the value of ΔE_0 incrementally, and then checks the R -factor and focused structural parameters. *miXAFS* can perform the least-squares curve fitting with a varying value of ΔE_0 and display the R -factor and a structural parameter as a function of ΔE_0 . Therefore, the user can define ΔE_0 easily with an understanding of its dependence on the R -factor and the structural parameter in question.

5.4. Settings file

The parameters for *miXAFS* are initially set by loading the settings file through clicking the Entry button on the Start tab. The parameters can be changed manually in the GUI at any time, even after loading them. The settings file is very convenient for routine analysis and especially for XAFS measurements in synchrotron radiation facilities where beam time is limited. If a settings file for each absorption edge is prepared, the structural parameters can be quickly and easily obtained from the experimental raw data or $\chi(k)$ in just three steps; that is, loading the settings file, changing the file name and clicking the Run button.

An example of a settings file is shown in Fig. 4. Because the number of data-processing parameters greatly exceeds 100, the parameters are sampled in the figure. The characters between the top line and semicolon are the ID of the parameters for running *miXAFS*. The characters between the semicolon and percent sign are the values of the parameters. The characters following the percent sign are annotations.

In the fitting process, the constraints for the structural parameters are defined in the control column in the table of the initial parameters in the Structural Parameter tab of the *miXAFS* window. In the control column, the characters 0 and 1 refer to fixed and free parameters during least-squares fitting, respectively. The constraints for the structural parameters are also expressed with four arithmetic operations or their sum. For example, `r_control;r(1,2)*1` means that the focused atomic distance is constrained on one times the atomic distance for the second shell of the first absorption edge, which is also shown in Fig. 2. The first and second numbers in the brackets designate the edge number and the site number of the edge, respectively, which are numbered following the order listed in the settings file. Another example is `N_control;N(1,2)=4.0`, which is a useful constraint when the total coordination number seems to be constant but the XAFS oscillation dumps due to a large value of the Debye–Waller factor (Tamura *et al.*, 1991), which means that the sum of the focused coordination number and that of the second site of the first absorption edge is 4.0.

```

miXAFS_Format;180101
%=====
% Main
%=====
run_type;raw data > fitting%fitting%raw data > chi%raw data > chi%
header;Cs008:Cs007:Cs006%
.....
%=====
% Start
%=====
File_SingleMulti;Single%Multi(table)%Single%Multi(file)%Multi(table)%
Edge_SingleMulti;Single%Multi%
Result_file;/Work/miXAFS_Project/miXAFS/Data/output/.txt%
File_list;/Work/miXAFS_Project/miXAFS/Data/Init_151204.txt%
.....
%=====
% Fitting
%=====
Fit_space;k space fitting%r space fitting%
Fit_LSQ_code;nlinfit%
Fit_control;Table%Mesh_fix%Lin%Lump%
Exp_Error_type;multi_data%constant%File_w_error%
Exp_Error_value;0.0009%
Error_Report;On%Off%
Fit_mesh_division;2%
Fit_mesh_set1;r(1,1)%
Fit_mesh_set2;N(1,1)
%=====
% Fitting Parameter Cs
%=====
==== Parameter_Edge_Head ====;%
Fit_file;Cs008_chiFF_170901.txt%
Fit_weight;1%
Fit_E0_control;0%
Fit_E0_init;8.1972%
Fit_E0_range;2 -10 20%
Fit_E0_str_para;r(1,1)%
%-----
Fit_k_power;2%
Fit_k_min;5%
Fit_k_max;15.5%
%-----
Fit_r_FT_Theory;Feff-Cs-Br1-160528%
Fit_r_FT_k_window;Hamming%Hanning%
Fit_r_FT_k_min;4%
Fit_r_FT_k_max;16%
Fit_r_FT_k_width;6%
Fit_r_min;0%
.....
==== Parameter_Site_Head ====;%
Active;1%
r_control;r(1,2)*1%
r_init;3.7%3.6%
r_range;3.5 3.9%2.7 4.7%
.....
N_control;N(1,2)=4.0%
.....
%=====
% Folder and footer
%=====
Exp_footer;.dat%
Exp_folder;/Work/miXAFS_Project/miXAFS/Data/raw-data%
.....
%=====
% Load file setting
%=====
File_exp_tag;PF9809-Trans%
File_exp_format;PF9809%
File_exp_exp_type;Transmission%
File_exp_energy;2%
File_exp_dwell;0%
File_exp_I0;4%
.....
SettingFileEnd;

```

Figure 4

Part of a settings file. The data-processing parameters are set when the 'Entry' button is clicked.

6. Conclusions

A new program for XAFS analysis, called *miXAFS*, has been developed. This program is coded in MATLAB and runs on Macintosh and Windows operating systems. In contrast to existing XAFS analysis software, *miXAFS* can simultaneously analyze the XAFS functions for all the absorption edges of the constituent elements under the constraints of the structural parameters. *miXAFS* provides a surface plot of the *R*-factor as a function of the two structural parameters, which is very useful for investigating their interdependence. The user can obtain structural parameters from experimental data in just a few steps, which is particularly useful for beam-time measurements at synchrotron facilities as well as for routine analysis.

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