CCFIT

User Manual

Contents

License

1. Introduction

The *CC-FIT* program is a simple and robust tool for the fitting of experimental AC magnetic data, in the Cole-Cole (or Argand) format. This manual does not contain a comprehensive overview of the theory of relaxation dynamics; consultation of the following publication and references therein is recommended:

Y.-N. Guo, G.-F. Xu, Y. Guo and J. Tang, *Dalton Trans.*, 2011, **40**, 9953.

The program fit both the in-phase and out-of-phase data simultaneously directly in the Cole-Cole regime. The fitting starts with an initial guess for the lowest temperature data provided by the user and then proceeds to fit all temperatures one after the other, using the best fit for the previous (lower) temperature as the initial guess. This process is usually successful, however can fail when the user's initial guess is poor or the low temperature data is featureless and therefore the fitted parameters are meaningless. The user is therefore encouraged to plot the fits of all isotherms for comparison with experiment as well as examining the residual value produced by the fitting algorithm, to make sure the results are meaningful.

2. User Guide

2.1 Input files and syntax

Input files are simple text files and can be prepared in any text editor and have any extension, however Windows users should use 'WordPad' and ***not*** 'Notepad' to prepare their input files. For Macintosh users, DOS or UNIX formatting should be used and files can be converted using the free utility flip, found here: https://ccrma.stanford.edu/~craig/utility/flip/.

The first line of the input file specifies the number of relaxation processes to be modelled (1 or 2), the number of experimental temperatures and the number of experimental frequencies.

The second line provides a starting guess for the fitting parameters, based on the low temperature data. For a single processes, these are: χ_S, χ_T, τ and α. For two processes, these are: $\chi_{S,tot}$, $\Delta\chi_1$, τ_1, α_1, $\Delta\chi_2$, τ_2 and α_2, following the notation of Tang *et. al.*, *Dalton Trans.*, 2011, **40**, 9953.

The subsequent lines list the frequencies as well as the $\chi^{'}$ and $\chi^{''}$ values for each temperature. The columns should be ordered such that the lowest temperature is first (following the frequency column) and such that temperature increases across the columns. Note that all isotherms must have the same set of frequencies. Frequencies should be given as linear frequencies (i.e. ***not*** converted to angular frequencies, ω), ν, in Hz. Susceptibilities can be given in any units, providing the starting guesses for the values are in the same units.

A representative layout of an input file is given below:

```
processes temperatures frequencies
χS χT τ α      OR      χS,tot Δχ1 τ1 α1 Δχ2 τ2 α2
ν1 χ'F1,T1 χ''F1,T1 χ'F1,T2 χ''F1,T2 χ'F1,T3 χ''F1,T3 .   .   .
ν2 χ'F2,T1 χ''F2,T1 χ'F2,T2 χ''F2,T2 χ'F2,T3 χ''F2,T3 .       .   .
.    .      .      .      .      .      .      .    .  . .
.    .      .      .      .      .      .      .    .  . .
.    .      .      .      .      .      .      .    .  . .
```

2.2 Initial guess

A good estimate for the starting guess can be obtained from examining the Cole-Cole plot for the lowest isotherm. Figure 2.2.1 shows how the experimental data can be interpreted to provide estimates for χ_S, χ_T or $\chi_{S,tot}$, $\Delta\chi_1$ and $\Delta\chi_2$. τ can be estimated as $\tau \approx 1/2\pi\nu$ for the frequency where χ'' has a maximum. In general, α can be assumed to be around $\alpha \approx 0.1$.
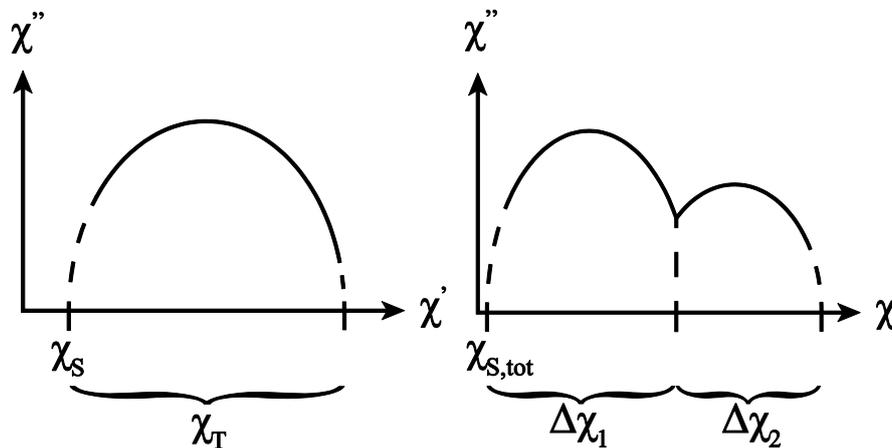

Figure 2.2.1 – Estimating initial parameters for a single relaxation process (left) or two relaxation processes (right)

2.3 Program execution

The program can be run on Linux, Windows or MaxOS and is executed *via* the command line as: 'cc-fit <input-file>', where '<input-file>' is the name of the input file. Alternatively, the program can be run in a 'drag-and-drop' style, by dropping the input file onto the executable.

Linux and MacOS users may have to run 'chmod +x cc-fit' and/or 'chown *user* cc-fit' before running the program, if permission errors are obtained.

2.4 Output files and interpretation

CC-FIT produces two output files. The first output file, named '<input-file>_cc-fit.out' contains the fitted parameters for each temperature, in rows corresponding to the column order in the input file. The second output file, named '<input-file>_cc-fit.res' contains the calculated data for the optimal fit parameters, in a similar format to the input file – the only difference being the omission of the frequency column.

3. Bugs and Feedback

The author is keen to hear from users who have bug reports, feature requests, comments, suggestions or queries about the code. Please address correspondence to nfchilton@gmail.com.