STRONTIUM IN PLAGIOCLASE FELDSPAR – DIFFUSION AND FFT ANALYSIS

Setup:

First, make sure you are using an up-to-date interface. This project was completed using the Spyder interface through Anaconda. An included environment (the yaml file included) should be loaded through Anaconda to ensure the scripts run without problems.

Step 1: Initializing your dataset

Included alongside the code is an xslx workbook. Consider this workbook a template to follow in constructing the input for the *Diffusion\_Script\_v1.0* model. Each sample profile must have 1) distance information in microns, 2) anorthite number for that distance step, and 3) strontium concentration for the same step. Each sheet in the book constitutes a separate sample profile, and the name of the sheet should be altered to that of the sample profile number/ID. The last sheet in the book provides temperature data (given in Celsius) used during modelling. Make sure at least 1 temperature is given for every sample sheet. Delete any unused sample sheets. Lastly, when saving the input data, rename the file to a proper identifier, such as “Sample\_A.xlsx” or “U1440B.xlsx”. This name will be referenced within the *Diffusion\_Script\_v1.0* code.

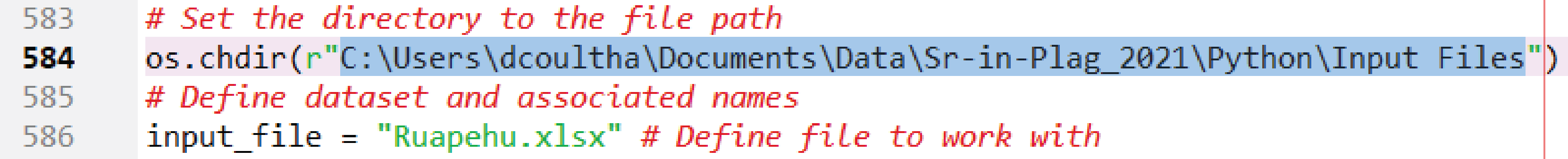
Step 2: Prepare for diffusion modelling

Open Spyder and ensure the environment provided in the repository is used. This is easily done through Anaconda. Open the *Diffusion\_Script\_v1.0* script. Navigate to the folder containing your input data using the File Explorer and copy the address as text.

Graphical user interface, application

Description automatically generated

Then navigate to line 584 in *Diffusion\_Script\_v1.0* and replace everything inside of the quotes with your copied text.



You may notice that line 586 similarly sets the name of the file to work with. Go ahead and replace everything in quotes with your input file name. Line 595 similarly sets the output path. You may use the same folder for output as you use for input; simply change the quoted text.

Step 3: Run the diffusion model

Now that your data and paths are properly set, go ahead and press f5 (or run file, the “play” button). Diffusion modelling should begin with text appearing in the console.

Graphical user interface, text, application, email

Description automatically generated

The first sample name, which in this case is “*96-11*”, is written followed by an initial time stamp. Then the diffusion iterations follow. End steps for these model runs are listed alongside the total number of iterations needed for the first model run. As explained in the main text of this project, diffusion is first modelled until a system-scale equilibrium condition is achieved and a second run is conducted along a logarithmic time vector that approaches the first set of linearly timed data. Once the second diffusion step has ended, the script moves on to the next sheet in the input workbook. The output workbook is created once all diffusion steps are complete.

Step 4: FFT analysis

Open *Profile\_v1.1* and press f5. This will open the user interface for FFT analysis of the diffusion output. Navigate to the open window, and you will see the first a button that reads “Open Profile”. Press this and select the output file created from the diffusion modelling. After a brief wait, the open window should rearrange to 6 tiles with various buttons, switches, and sliders. The switches on top (labelled as “Derivative”, “An”, or “Sr*Obs*”, etc.) simply alter the appearance of the first two panels in the top row to what is selected.

The bottom three panels are used in FFT analysis. Press the “Calculate FT” button at the bottom. This calculates a power spectral density (psd) plot for each time step taken during diffusion and stacks it along a logarithmic time vector to form a heat map (1st panel, bottom row). This panel illustrates the decay of certain frequencies contributing to the ρ' profile (see main text) over time. The second panel is a psd plot for the selected time. See the slider above the heatmap. By sliding the grey bar across the heatmap, the psd shown will change (solid line). The initial psd remains for reference (dashed line).

Graphical user interface

Description automatically generated

Finally, the third panel in the bottom row illustrates the inverted FT at the selected time. At the moment, this is a carbon copy of the first panel in the top row saving for the line of the inverted FT data is blue in the final panel.

Graphical user interface, diagram

Description automatically generated

However, using the frequency and/or the magnitude threshold switches above the psd plot, one can alter which frequencies are inverted back into concentration information. This changes the blue line relative to the solid black line in the first panel. Here, I have selected very low frequencies for IFT using a frequency filter (red slider below the psd plot).

This stage of analysis is very forgiving, and many steps could be taken which can immediately be undone or redone to preference. Selecting frequencies for filtering is not a straightforward process though and care should be taken to ensure that all relevant frequencies are included in the next step. Play around with the data at this point to familiarize yourself with the interface. It should be mentioned that FT analysis can only be performed on the ρ' profile. Frequency filtering should be performed at the initial time step for IFT analysis.

Step 5: Inverse FT modelling and stepping backwards in time

Press the “IFT regression” button. This opens a second panel. Here, are illustrated the regressed amplitude decay rates for each selected frequency. Ensure the “Correct to initial” switch in the bottom right corner is enabled.

Graphical user interface, chart, histogram

Description automatically generated

The data on these panels will change as backwards time steps are taken. Switch back to the original interface and notice that a second time slider has appeared above the heatmap.

Graphical user interface

Description automatically generated

This slider denoted “-T”, will perform backwards time steps and calculate Sr concentration profiles (bottom right panel in the second interface) for states prior to those observed for the initial condition. Time steps should be taken until one of the points along the Sr profile approaches 0, which is a limiting condition for concentration information. Notice that the total amount of time stepped backward is listed in the top right panel in red.

Again, this step should be taken numerous times. Preferably with different frequency input in order to understand your dataset. The save icon in the top of the interface will create a png image of the panel at the time you pressed save, so you can always save your steps in this way.

Congratulations, you have now learned how to model backwards diffusion using a FT method. Please use this script responsibly.

Chart

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