CTE Analysis Suite 0.2.7 Alpha - Overview

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1 Introduction

The CTE Analysis Suite (CTEAS) is a utility for determining the thermal expansion characteristics of a material that has been analyzed via in-situ x-ray diffraction during a heating and/or cooling cycle. Its main function is to output three-dimensional plots of thermal expansion ellipsoids and animate them according to heating and cooling. A thermal expansion ellipsoid is the rate at which a material expands in all directions at a specific temperature. By analyzing these ellipsoids at a range of temperatures, the expansion characteristics of a material can be determined. CTEAS can also output a multitude of other analysis options such as the eigenvalues of the thermal expansion ellipsoid, lattice parameters, polar diagrams of the ellipsoid, and excel-readable file output. Currently, CTEAS uses a specific filetype produced by MDI JADE as an input. Future revisions of CTEAS will incorporate other formats.

1.1 Program Operation

CTEAS is designed to operate using a tabbed interface that dictate what the user should start with and proceed to. The tabs are labeled as Step 1, 2, and 3 respectively. When CTEAS has enough information for the step to be complete, a green indicator becomes lit on the current step. This is a signal to the user that CTEAS can move forward with analysis. In some cases, the user may require other configurations and changes that CTEAS does not recognize as important, such as modifying temperatures, removing files from analysis, or overriding crystal symmetry details. This is left to the knowledge of the user as, at the point the user is operating CTEAS, they will know the intricate details of their analysis setup better than the program can. The following sections detail the operation of CTEAS from Step 1 to 3.

1.1.1 Step 1 - Loading Files and Setting up Analysis

A diffraction pattern is obtained from an in-situ x-ray diffraction experiment and analyzed with the use of software such as MDI JADE. MDI JADE will output a series of crystal plane orientations, d-spacings, present phases at temperature, and lattice parameters which are saved to data files having a '.rrp' extension.

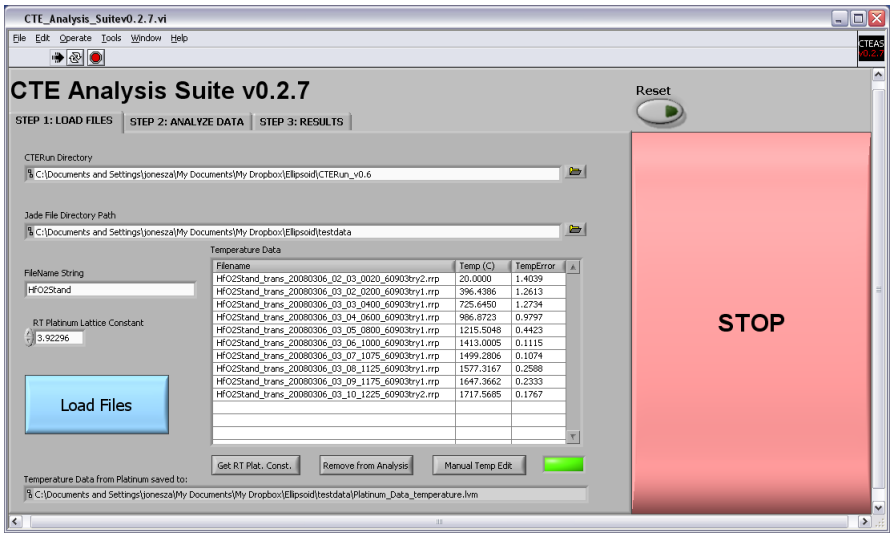

Figure 1: CTE Analysis Suite Interface - Step 1

These data files are the working inputs for the CTE Analysis Suite. The user can specify a directory containing a set of data files from a JADE analysis and load them into the CTEAS workspace. Figure 1 displays the current "Step 1" tab of the CTEAS user interface.

When the "Load Files" button is pressed, CTEAS runs a function that gathers the data from the JADE files and stores them in a container variable. Currently, CTEAS is equipped to determine data file temperatures using a room temperature platinum lattice constant. This constant can be manually input or obtained by selecting a file in the main listbox and pressing the "Get RT Plat. Const." button. Temperatures can also be manually entered in the listbox and saved for analysis by pressing the "Manual Temp Edit" button. The user also has the option of removing a JADE file from analysis by selecting it in the listbox and pressing the "Remove from Analysis" button. This will instruct the CTEAS program to ignore that specific JADE file and continue with its analysis. At the end of the "Step 1" tab, the user has loaded a set of JADE files, adjusted the corresponding temperatures, and removed any outlier data from the analysis. A green light will be lit when data is ready to be passed to the next step in CTEAS.

1.1.2 Step 2 - Running Analysis

Once CTEAS and the user have decided that "Step 1" is complete, the user may choose to proceed to "Step 2" by clicking the corresponding tab on the interface. Figure 2 shows the layout of the "Step 2 - Analyze Data" tab.

From the previous step, the user has loaded necessary data for program operation into CTEAS. A series of dropdown menus and options are displayed in

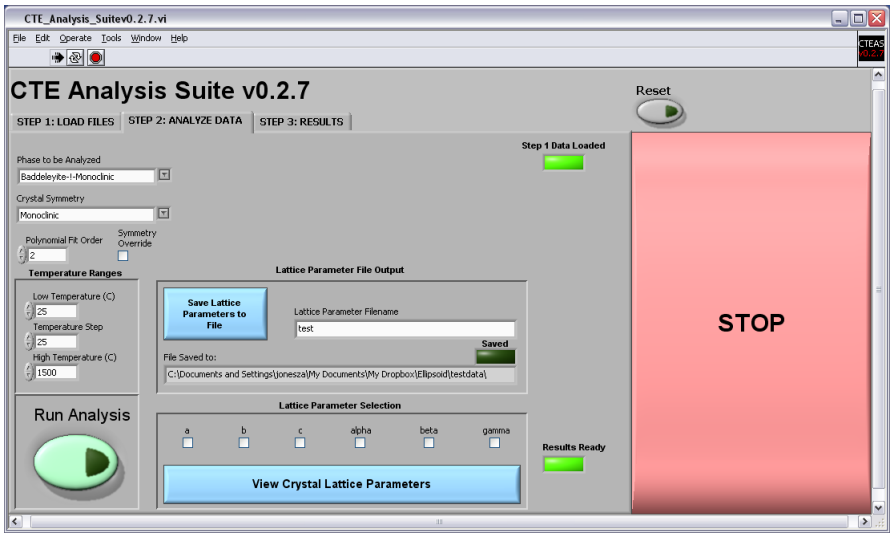

Figure 2: CTE Analysis Suite Interface - Step 2

"Step 2" that will allow the user to specify which phase to analyze, at what temperatures to simulate analysis, view crystal lattice parameters, and export these lattice parameters to a file. The user must select the phase from the corresponding dropdown menu before any other functions on the step will cooperate. These phases have been read directly from the JADE files. Once the user has selected a phase, the symmetry is automatically selected as well. If the user should decide to override the symmetry, a check box is available to "free" the dropdown menu for symmetry selection.

Polynomial fit order is left to the knowledge of the user. This polynomial order is the order of a least-squares curve fit to a, b, and c lattice parameters for use in determining functions for the coefficients of thermal expansion of the material in those axial directions. A second- or third-order polynomial has been most commonly used to fit these data. As per the temperature range from the data shown in "Step 1," the user can set a similar temperature range in boxes that require a low temperature, high temperature, and temperature step size between the extremes. If the user wished to analyze every 25 degrees (C) between a range of temperature, this configuration can accomodate.

At any time after the phase has been selected, the user can view lattice parameter values or export the lattice parameters to a spreadsheet-readable file. By checking which lattice parameters to view, one or two graphs (corresponding to a,b, and c and alpha, beta, and gamma respectively) will display showing the chosen lattice parameters. The user can visually assess whether the lattice parameter error from an input file is too large to include in the analysis. Following any further user-desired modification, the "Run Analysis" button can be pressed. A short time later, the "Results Ready" indicator will light. This is the

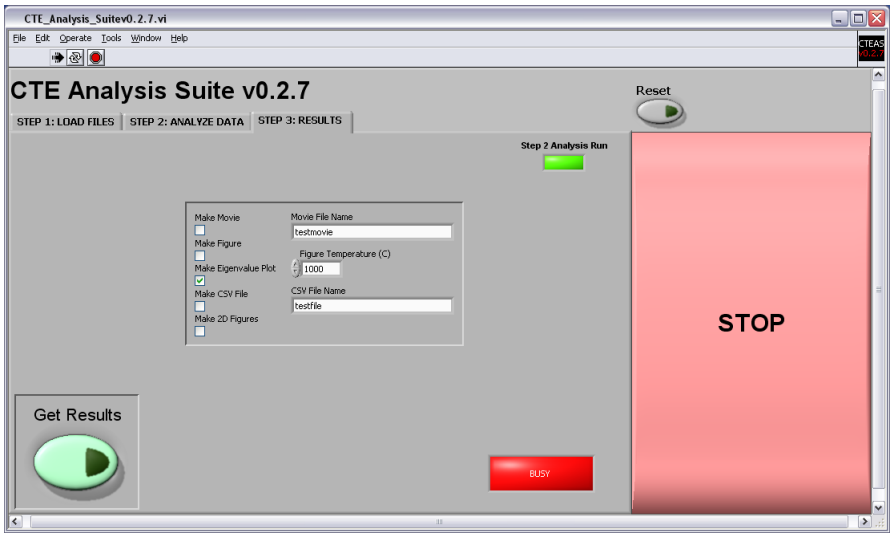

Figure 3: CTE Analysis Suite Interface - Step 3

indication that the user can proceed to the "Step 3 - Results" tab.

1.1.3 Step 3 - Viewing Results

After the user has completed "Step 2," the results of the analysis can be configured and viewed through the "Step 3 - Results" tab, shown in Figure 3. The options currently include the ability to create a thermal expansion movie, a figure at a desired temperature, plot and view eigenvalues of the thermal expansion tensors, create cutaway figures (2-dimensional) along crystallographic axes of the thermal expansion ellipsoid, and output tensors and eigenvalues to a file. The thermal expansion movie option will plot the thermal expansion ellipsoid of the analyzed data at the range of temperatures set in "Step 2," encoding them as they are plotted into an '.avi' file. This can be used to show how the rate of thermal expansion of a material changes as temperature increases. A single frame, or figure can be plotted using the "Make Figure" option and specifying a temperature in the corresponding temperature box.

The "Plot Eigenvalues" option will generate a plot of the eigenvalues of the thermal expansion tensors across the range of temperatures set in "Step 2." Generally, sharp changes in the eigenvalue slopes can indicate a radical change in the thermal expansion behavior of the material. These eigenvalues and the thermal expansion tensor values can be output to a '.csv' file using the "Make CSV File" option and assigning a filename in the corresponding text box.

The "Make 2D Figures" option will generate figures of a cross-section of the thermal expansion ellipsoid. An example figure is shown in Figure 4. These cross-sections correspond to the 010 and 001 planes of the thermal expansion ellipsoid and are configured to show how temperature has changed the orientation

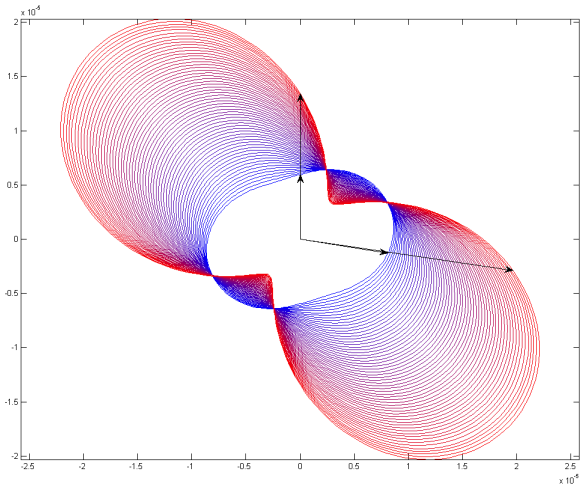

Figure 4: CTE Analysis Suite - 2D Figure

and shape of the ellipsoid. The blue rings correspond to the lowest temperature and the red rings correspond to the highest temperature.

Any or all of these options can be checked before the "Get Results" button is pressed. Once the "Get Results" button is pressed, the "Busy" indicator will light. Depending on the options selected, it may remain on for a period of time. When it has gone off, the results will display shortly after and the '.csv' file, if requested, will have been saved to the directory containing the original input files.