CTEAS User Manual - Outline

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* Acknowledgements
* Introduction

The Coefficient of Thermal Expansion Analysis Suite (CTEAS) is an aid for determining the thermal expansion of a material. A series of heating and cooling X-ray diffraction patterns can be analyzed using Rietveld refinement in a program such as JADE or GSAS and the resulting hkl values and spacings can be used as an input for CTEAS.

CTEAS takes this input and fits a quadratic curve to the lattice parameters contained in the input. It then forms a rank two thermal expansion tensor, based on crystal symmetry for a range of temperatures. Using these tensors, thermal expansion is characterized in three dimensions of crystallographic space. CTEAS allows the user to specify various output options including spreadsheet data, two- or three-dimensional plots of thermal expansion, and movies of the expansion over a range of temperatures.

* Installation and Setup

The installation of CTEAS is straightforward. Two supporting programs are needed:

* + 2009 NI Run-Time Libraries
  + Matlab (2007 and later)

With Matlab and the NI Run-Time Libraries installed, the CTEAS executable file can run. A set of Matlab function files is included with the executable that must be kept in an easily-located area of the computer filesystem. These Matlab function files form the backbone of the CTEAS program. They can also be used independently from the CTEAS graphical user interface (GUI) to perform analyses in Matlab without the use of LabView Run-Time Libraries. It is much more difficult and time-consuming to perform an analysis this way, but other specialized options can be thought of and implemented between analysis steps in Matlab.

* How to Use CTEAS
  + Step 1: Loading Files
    - Pre-Run Path Configuration

CTEAS requires the location of the supporting Matlab function files to be specified. It also requires a folder containing the input files to be specified. To specify either of these locations, click the file icon to the right of the text box and navigate to the desired folder. Navigate inside the folder, then click the “Choose Folder” option. This will set the file paths.

* + - File Support and Formatting Custom Files

CTEAS is configured to read output from MDI JADE 9. If analyses were not performed in MDI JADE 9, a custom input file can be created. Refer to the example input file included in the Matlab function file titled <TITLE HERE> as a guide.

* + - Temperature Options

CTEAS can only output thermal expansion correctly if temperature is input correctly. There are three methods for determining or inputting temperatures in CTEAS once files are read. If Platinum peaks are being used to determine temperature, the Get RT Plat. Const. button will automatically adjust the temperatures using the Room Temperature Platinum Lattice Constant located in the input files. Adjustment of this value can also be performed using the input box on the left of the screen, titled <TITLE HERE>. The user can also manually edit values by clicking on them in the file list window and changing the values. Once all values are set manually, click the <MANUAL BUTTON> and the green light should appear lit. This signifies being able to proceed to Step 2.

* + Step 2: Run Setup
    - Choosing a Detected Material
    - Viewing Lattice Parameters
      * Saving Lattice Parameters
    - Run Options
      * Temperature Ranges
  + Step 3: Results
    - Viewing/Saving Figures
      * Polar Diagrams
      * Temperature Figures
      * Thermal Expansion Plots
      * Expansions Along a Vector
    - Creating a Movie of Thermal Expansion
    - Data Outputs
      * CSV File Outputs
  + Troubleshooting
  + Quick Start
  + Contact Information
  + List of Matlab Functions