Coefficient of Thermal Expansion Analysis Suite (CTEAS) - User Manual

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Thanks to Dr. Ryan P. Haggerty for the initial steps in the development of CTEAS and later bug-fixing. Special thanks to the Kriven Research Group at the University of Illinois at Urbana-Champaign for testing and feature suggestions.

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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.

It is strongly recommended that the user becomes familiar with this user manual and that the user has the understanding that the output of this program is consistent with the user input of this program. If there are further questions that this user manual does not address, please locate the contact information at the end of this manual. Supporting technical documentation can be found at `http://www.something.com/docs.docx`.

Installation and Setup

The installation of CTEAS is straightforward. The following support programs are required for it to fully function:

1. Windows XP SP3 or newer
2. Matlab (2007 and later) (`http://www.mathworks.com/products/matlab/index.html`)
3. Microsoft Office 2003, 2007, or 2010 (`http://office.microsoft.com/`)
4. Office Web Components 2003 with latest updates from Microsoft Update (`http://www.microsoft.com/download/en/details.aspx?displaylang=en&id=22276`)

The downloaded .zip file containing the CTEAS installer and support files should be unzipped in an accessible location on the computer. Running the setup.exe file will start the CTEAS installer. It will ask for a location (program files by default) and begin installing. The CTEAS installer should install the National Instruments RunTime 2010 libraries during installation. If any errors are encountered during installation, continue the installation (ignoring errors) and install these libraries manually. They can be found at:

`http://joule.ni.com/nidu/cds/view/p/lang/en/id/2087`

The CTEAS installer will install the CTEAS executable and a folder containing Matlab functions that are used during operation. These Matlab functions are also usable without the CTEAS graphical interface, using only Matlab for operation. It is recommended that the user becomes familiar with these files, if only to understand the background operation of CTEAS. They are read-only to protect program operation, but copyable to other directories. More advanced functionality can be obtained using the Matlab command line, however the difficulty of using these functions without the CTEAS interface is increased.

A folder in the Start menu will be created containing a link to the CTEAS executable. CTEAS can be uninstalled using the Control Panel Add/Remove Programs functionality in Windows. Subsequent updates of the CTEAS program will need to be installed by first uninstalling the old version and then installing the new version to eliminate file conflicts.

How to Use CTEAS

CTEAS is divided into a three-step tabbed interface. The content of each tab relates to the functions of the program that are applicable at that stage during operation. A green light in the bottom right corner of each tab will signal that the user is ready to proceed to the next step. The following sections describe the operation of the program during each step and a basic operation flow.

STEP 1: LOAD FILES

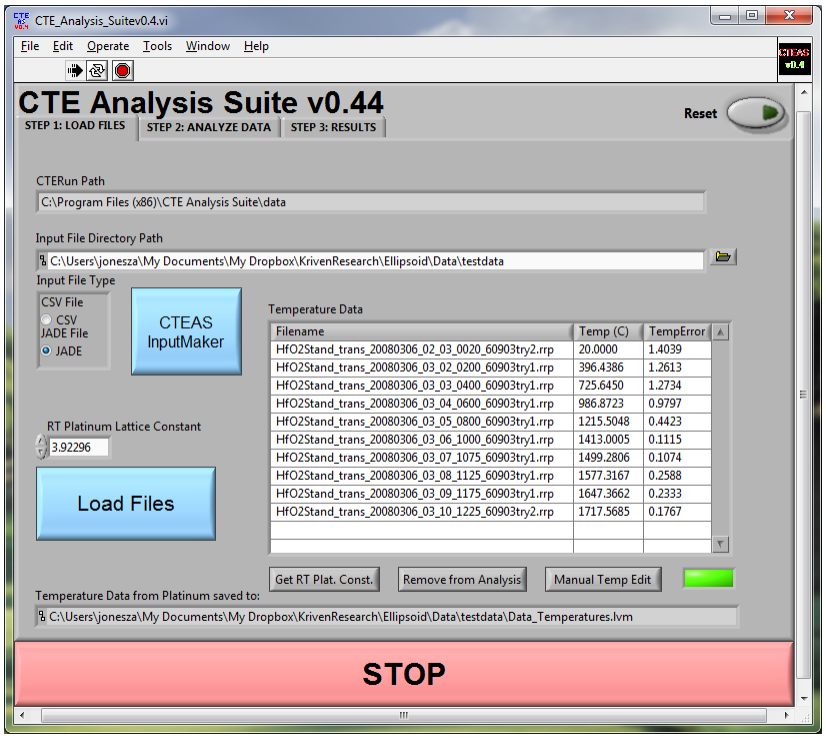

Figure 1: CTEAS GUI - Step 1: Loading Files

1.1 Specifying a Working Directory

CTEAS requires the user to specify a folder containing input files for it to load and analyze. The following steps must be taken to ensure the correct operation of the program:

1. Click on the file icon beside the text box under "Input File Directory Path."
2. Navigate to the folder containing the files to be analyzed, navigate inside the directory, then click the "Current Folder" button in the bottom right of the selection window.
3. Specify a room temperature Platinum lattice constant in the box below "RT Platinum Lattice Constant" if applicable. This is optional and only used if Platinum peaks have been used to determine temperature for analysis. Note that this can be any value for loading files and the temperatures can be manually changed if incorrect. If Platinum peaks will not be used to correct temperatures, set this value to zero. A second method of temperature correction will be described later.

1.2 File Support and Formatting Custom Files

CTEAS is configured to read output from its own CTEAS InputMaker. A button has been included on the front panel of the graphical interface to load CTEAS InputMaker during operation. Since CTEAS InputMaker is a separate interface from the main program, it will be described later. Refer to Appendix B for CTEAS InputMaker operation.

NOTE: CTEAS will NOT function until the Stop button has been clicked on the CTEAS InputMaker panel.

1.3 Loading Files Into CTEAS

If files exist in the "File Directory Path" location, the "Load Files" button can be clicked. CTEAS will then locate all .csv data files and list them in the "Temperature Data" area. The files will be listed in order of increasing temperature. A green light will turn on in the bottom right of the interface, signaling the user that data have been loaded and values have been saved. It is then up to the user to decide whether the displayed temperature values are correct before proceeding to Step 2: Run Setup.

1.4 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 contained in the input files. Adjustment of this value can also be performed using the input box on the left of the screen, titled "RT Platinum Lattice Constant." After changing the value in the "RT Platinum Lattice Constant" box, the user should click the "Load Files" button again to update the values in the file list window. The user can also manually edit values by double-clicking on incorrect values in the "Temperature Data" window and assigning new values. During this editing period, the green light will turn off, signaling the user that the program is not ready to proceed to Step 2 anymore. Once all desired new values are set manually, click the "Manual Temp Edit" button and the CTEAS backend will update with the new values. The green light will then appear lit again. The user is now able to proceed to Step 2: Run Setup.

STEP 2: ANALYZE DATA

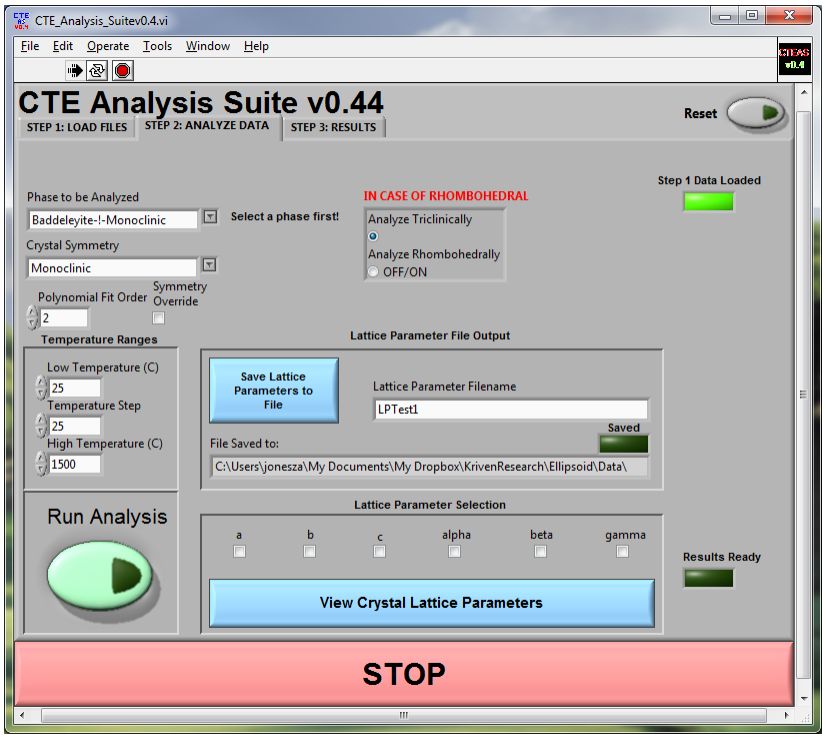

Figure 2: CTEAS GUI - Step 2: Run Setup

Step 2 centers around setting up an analysis and choosing a phase contained within the input files. An input file can contain multiple phases and materials, leaving the user to decide which phase and material to analyze. The following steps should be followed for desired operation of CTEAS:

2.1 Choosing a Detected Phase

Click on the drop-down arrow beside the box under "Phase to be Analyzed" and select a material and phase for analysis. Note that platinum may be listed in the drop-down menu if it was used to gauge temperature. This should never be selected as it will cause errors to occur. The Crystal Symmetry box will be automatically set for the corresponding symmetry. If this symmetry is undesirable (instantaneous strain calculations, etc), check the "Symmetry Override" box and select a new symmetry. This override is for advanced use of the CTEAS program and not wholly described in this user manual.

2.2 Decide on Polynomial Fit Order

Specify a "Polynomial Fit Order." The polynomial fit order (usually 2) specifies the order of the polynomial used to fit the lattice parameters for calculation of thermal expansion coefficients.

NOTE: In order to use a polynomial fit order of 2, there must be at least 4 temperature files at which the phase exists. In order to use a polynomial fit order of 3, there must be at least 5 temperature files at which the phase exists. This is to ensure that a curve can be fit to the data. **If the end results show linear expansions using a second-order polynomial fit, it may be useful to re-run the analysis using a third-order polynomial fit.**

2.3 Optional - Rhombohedral Symmetry and Alternative View Options

If a specified phase is considered to be in rhombohedral symmetry, a special case can be triggered using the "IN CASE OF RHOMBOHEDRAL" box. This special case will analyze a phase as a true rhombohedral symmetry rather than triclinic. Limited functionality is available in Step 3 for this case because of the orientation correction applied to the thermal expansion tensor that is generated for this case. The current standard for a true rhombohedral symmetry is to set the orthonormal Z-axis parallel to the crystallographic (111) hkl. In all other symmetries, the standard is to set the orthonormal Z-axis parallel to the crystallographic c axis. It is therefore recommended to analyze a rhombohedral symmetry triclinically for comparison with any other phases contained in a material, but left to the user's expertise for this special case.

2.4 Set Temperature Ranges for Analysis

1. Temperature ranges must be specified for analysis. The "Low Temperature" may not be more than 50°C lower than the minimum temperature specified in the input files. For example, if room temperature data (20°C) was taken, the lowest temperature that could be entered in the "Low Temperature" box would be -30. Any temperature entered beyond this bound will result in a coefficient of thermal expansion matrix of zeroes. An upper bound of 50°C is placed on the "High Temperature" as well to ensure that the analysis does not extrapolate too far beyond collected data. It is recommended that $(HighT - LowT)/\Delta T$ is a positive integer for later analysis.

   (a) A quick method of determining at what temperatures a phase exists is to look at the lattice parameter data using the "View Crystal Lattice Parameters" functionality described later.

   (b) The resolution of the temperature ranges can be specified down to 0.01°C. Therefore, setting LowT to 20 and HighT to 20.01 with a Temperature Step of 0.01 will produce two temperature analyses. This is the preferred workaround method for extracting all thermal expansion data CTEAS can produce for a single temperature. The output files written in Step 3 will be limited to two temperatures, leaving the user an uncluttered workspace in other analysis programs such as Microsoft Excel.

2. The "Temperature Step" box determines the ΔT for analysis. A temperature step of 25 will calculate a coefficient of thermal expansion matrix for every 25°C within the low and high temperature range. It is recommended that $100/\Delta T$ is equal to a positive integer for later analysis.

   (a) Note that if $100/\Delta T$ is not met, the final calculation (HighT) may not be performed because the step size would cause the temperature range to be outside the bounds of the analysis. This may be changed in later versions of CTEAS.

   (b) The movie creation function displays updated temperatures as the title every 100°C. If the temperature step does not match this, the title will not match the actual temperature. Later versions of CTEAS may fix this.

2.5 Running the Analysis

Once the above steps have been completed, the "Run Analysis" button can be pressed. This may take some time for the analysis to run, but once it has completed, the "Results Ready" light will turn on. This signifies that Step 2: Analyze Data has been completed and that the user can proceed to the final operations tab. Details of the background operations can be found in Appendix A. It may be worthwhile to have familiarity with these operations.

2.6 Optional - Viewing Lattice Parameters

At any time after selecting a phase to be analyzed, the user can view and save lattice parameters. Lattice parameters themselves tell many details about the phase to be analyzed such as the temperature range over which the phase is present and whether the axes of the crystal are converging for a phase transformation.

The lattice parameters will be saved to the same folder containing the input files as a comma separated variable (.csv) file. There is no need to include the file extension while specifying a filename.

The lattice parameters can also be plotted directly from the interface by checking the boxes corresponding to which parameters the user wishes to view and clicking the "View Crystal Lattice Parameters" button. Note that two separate graphs may appear that contain the a,b, and c and alpha, beta, and gamma parameters respectively. The example in Figure 2 shows just the "b" parameter checked. This will produce a single graph with the "b" lattice parameter plotted. Note that these parameters are the actual lattice parameters parsed from the input files. Later versions of CTEAS may include support for viewing the polynomial fits alongside the lattice parameters, but this is not implemented as of this publication.

STEP 3: RESULTS

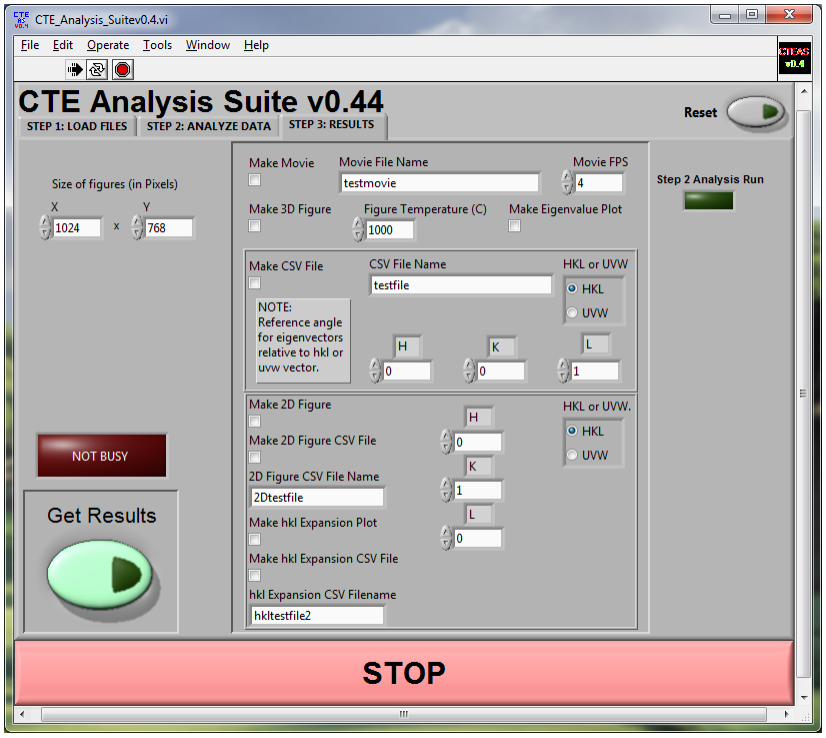

Figure 3: CTEAS GUI - Step 3: Results

3.1 Viewing and Saving Output

The function of Step 3: Results is to allow the user to view and save a variety of methods for displaying the thermal expansion of a chosen material and phase. The following list will detail what each option means:

Make Movie: A movie of a thermal expansion ellipsoid can be created and saved. This movie shows the change of the thermal expansion ellipsoid over the range of temperatures from Step 2: Analyze Data. Note that there is a 5-second "freeze" at the end of the temperature range to allow a still frame for description during a presentation (some older movie softwares go to a black screen when the movie is complete, thus a 5 second "pause" allows the presenter to have a picture for a few seconds longer). The movie file name can be user-specified (once again, the extension is not needed) and the movie will be saved in the same directory as the input files. Creating a movie will output an uncompressed .avi file. The size of the file can be very large depending on the size (in pixels) that is chosen for the movie/figure output. It is recommended that a 640x480 movie be generated, but larger movies may be generated and transcoded with editing software should they be necessary.

A "Movie FPS" box is located in the movie controls area that can be used to specify how many frames per second at which the movie plays. Each calculated temperature step is considered to be a "frame" of the movie, therefore a very small temperature range of analysis may require a lower FPS than a large range of analysis. A "Movie FPS" value of 4 has generally been used during the development of CTEAS with acceptable results.

Make Figure: This will plot a figure of the thermal expansion ellipsoid at a temperature specified. Any temperature within the high and low temperature bounds can be specified for generation. The plot can be saved as a multitude of different filetypes. For users familiar with saving plots in Matlab, this is a

Matlab plot. Users of the command-line (Matlab-only, user-unfriendly) version can plot multiple figures and temperatures at once. This is a limitation of the GUI.

Make Eigenvalue Plot: This will plot a figure of the eigenvalues of the second-rank thermal expansion tensors from lowest temperature to highest temperature. The plot is a Matlab plot similar to the Make Figure plot.

Make CSV File: A comma-separated variable file can be written containing lines formatted as the following:

Temperature, CTE Tensor (1,1)-(3,3), Eigenvalues, Eigenvectors(x,y,z), Eigenvector Angles

The Make CSV File option requires a reference hkl (or uvw) to be set for calculation of the Eigenvector Angles. This is by default, the c-axis (parallel to the z-axis in orthonormal space).

Make 2D Figure: A two-dimensional "cut" of the thermal expansion ellipsoid can be created using this option. The surface of the "cut" ellipsoid is displayed as a Matlab plot and able to be manipulated and saved as any other Matlab plot. The H, K, and L values in the boxes to the right of the Make 2D Figures checkbox compose a reference hkl (or uvw if the option is selected) that is perpendicular to the "cut" plane. For example, in a cubic system an hkl of (010), the b-axis, will display a "cut" plane that is in the a-c plane.

Make 2D Figure CSV File: Outputs the x and y data of the "Make 2D Figures" option to a file specified by "2D Figure CSV Filename." NOTE that a filename extension is not needed.

Make hkl Expansion Plot: A thermal expansion plot is created corresponding to the chosen hkl (using the same H,K, and L boxes from the Make 2D Figures option) that details the thermal expansion along a specific hkl (or uvw if the option is selected).

Make hkl Expansion CSV File: Outputs the CTE and Temperature data of the "Make hkl Expansion Plot" option to a file specified by "hkl Expansion CSV Filename." NOTE that a filename extension is not needed.

Troubleshooting

While problems are not expected to occur during the operation of CTEAS, the most likely cause of software malfunction deals with the formatting of input files. The CTEAS InputMaker creates a file that will always be able to be read by CTEAS.

Other problems that may occur during operation are arranged by program tab and listed as follows:

Error	Reason(s)	Suggested Solution
• Error 7 occurred at Open File+.vi:Open File	• No input files located in folder. • No files contain Platinum (Get RT Plat. Const. function)	• Check Input File Directory Path • Check if any files exist. • Manually Correct RT Plat. Const. or load files with Platinum in them.
• Error 43 occurred at Open File+.vi:File Dialog	• Remove from Analysis clicked with no loaded files	• Load input files.
• Freeze After Run Analysis Clicked	• Platinum selected as Phase	• Terminate Program, re-open. Select different phase for analysis.
• No movie output	• Plot window closed during movie frame creation	• Re-run Get Results for movie, do NOT close any popups.
• File outputs have two ending extensions (eg: file.csv.csv)	• Extension added automatically, one isn't necessary	• Rename the file. Do not add an extension to filenames in CTEAS. It is done automatically for you.

Table 1: Common Errors During CTEAS Operation

If a problem occurs that isn't formally addressed in this documentation, please contact the Kriven Research Group using the contact information below and address the problem with them.

Contact Information


```
Waltraud M. Kriven, Ph.D.
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Tel: +1 217 333 5258
Fax: +1 217 333 2736
e-mail: kriven@illinois.edu
```

APPENDIX A: List of Matlab Functions

This is a list of the included Matlab functions with CTEAS and a short explanation of their purpose and use. Further details and operation information can and should be gained by reading the documentation within each function and analyzing the contained Matlab code. Any suggestions for improvement, better description, and bug-fixes should be forwarded to the Kriven Research Group using the above contact information and are greatly appreciated. There are 36 Matlab files associated with CTEAS in its current release state. These files are constantly being updated and improved, therefore a detailed description of their mathematical functionality can be found in the CTERun Technical Documentation document included in the CTEAS installation directory.

addArrow4.m Adds an arrow to a two-dimensional thermal expansion plot. Returns true or false, depending on the arrow being in the plane of expansion.

angToorth.m Converts a set of θ and ϕ angles to orthonormal x,y, and z coordinates with unit-length.

antirotateVect.m Rotates a vector by θ and ϕ about crystallographyic axes in the opposite way of rotateVect.m.

CTERun.m Wrapper script to run CTEAS using only Matlab. All options are set within the CTERun.m file itself and some examples have been left commented out to show how syntax MUST be followed. There are many options, all of which are internally documented to aid the user.

eigenshuffle.m Function created by John D'Errico (contact information within file) that outputs an unsorted list of eigenvectors and eigenvalues. This is useful for overlapping plots of eigenvalues getting sorted incorrectly. This function also utilizes code written by Yi Cao called munkres.m. eigenshuffle.m has been included with permission from the author.

EllipseWrap.m Creates a plot of two-dimensional expansion perpendicular to a vector in hkl or uvw space. This is a complicated function that will require reading to understand fully.

EVAngles.m Calculates the angles between the eigenvectors of the thermal expansion ellipsoid and the c-axis (parallel to the Z-axis) by default, or any other specified vector in hkl or uvw space.

evplotcut.m Plots and labels the eigenvectors of a two-dimensional thermal expansion plane.

getcsvdata.m Function to read .csv files created by CTEAS InputMaker and save as Matlab variables.

getCTEeigVecAngle.m Function to calculate the angles between a specified hkl or uvw and the eigenvectors of the thermal expansion ellipsoid.

getCTEPlane.m Function to get the average thermal expansion in a plane where T1 is the angle between the plane normal and the z axis and T2 is the angle between the projection of the plane normal on the x-y plane and the x axis.

getCTEVect.m Function to calculate the thermal expansion along a vector at a given temperature.

getPtTemp.m Function to look through saved data and adjust temperatures based on platinum lattice constants.

getRotationMat.m Function to calculate a rotation matrix between two systems of coordinates.

getrrpdata.m Function to read JADE .rrp files and save as Matlab variables (Not used in public CTEAS version due to formatting options).

HKLExpansion.m Creates a plot of the thermal expansion along a vector in hkl or uvw space.

hklToAng.m Converts an hkl to ϕ and θ angles (deg) with unit length.

hklToorth.m Converts a vector specified by an hkl coordinate into orthonormal X,Y, and Z components.

HKLtoUVW.m Converts an hkl into a uvw, taking temperature into account.

HKLtoUVWnotemp.m Converts an hkl into a uvw, NOT taking temperature into account. This is not used in CTEAS but is included as a tool.

MakeMovieFrames.m Creates a series of frames for the thermal expansion movie. These frames are compiled using the movie2avi function included in Matlab. No compression is used because the GNU/Linux version of Matlab does not include video compression options.

namevects.m Function to output a name for vectors plotted in two-dimensional diagrams.

orthToAng.m Converts a vector specified by X, Y, and Z coordinates in orthonormal space to ϕ and θ angles with unit length.

orthTohkl.m Converts an orthonormal vector to an hkl vector.

PlotEigenvalues.m Creates a plot of the eigenvalues of the thermal expansion ellipsoid from lowest to highest analyzed temperature. The eigenvalues are sorted using the eigenshuffle.m function to preserve continuity.

plotEllipse.m Function to plot a slice of a thermal expansion ellipsoid.

plotEllipsoid.m Outputs coordinates for a mesh of points to be used for plotting a thermal expansion ellipsoid.

PlotTempFigure.m Creates a plot of three-dimensional thermal expansion at a specified temperature. In the CTERun.m script, a range of temperatures can be used as input, creating a new plot for each specified temperature.

RhomtoHex.m Converts Rhombohedral to Hexagonal.

rotateVect.m Rotates a vector by ϕ and θ.

tdfread.m Matlab library to read tab delimited files. Typically included with Matlab.

UVWtoHKL.m Converts a uvw to an hkl.

xtalCTE.m Function to calculate thermal expansion tensors and conversion matrices between crystallographic axes and orthonormal axes.

xtalCTEprep.m Function to prepare and sort data for calculating thermal expansion tensors.

APPENDIX B: CTEAS InputMaker Operation

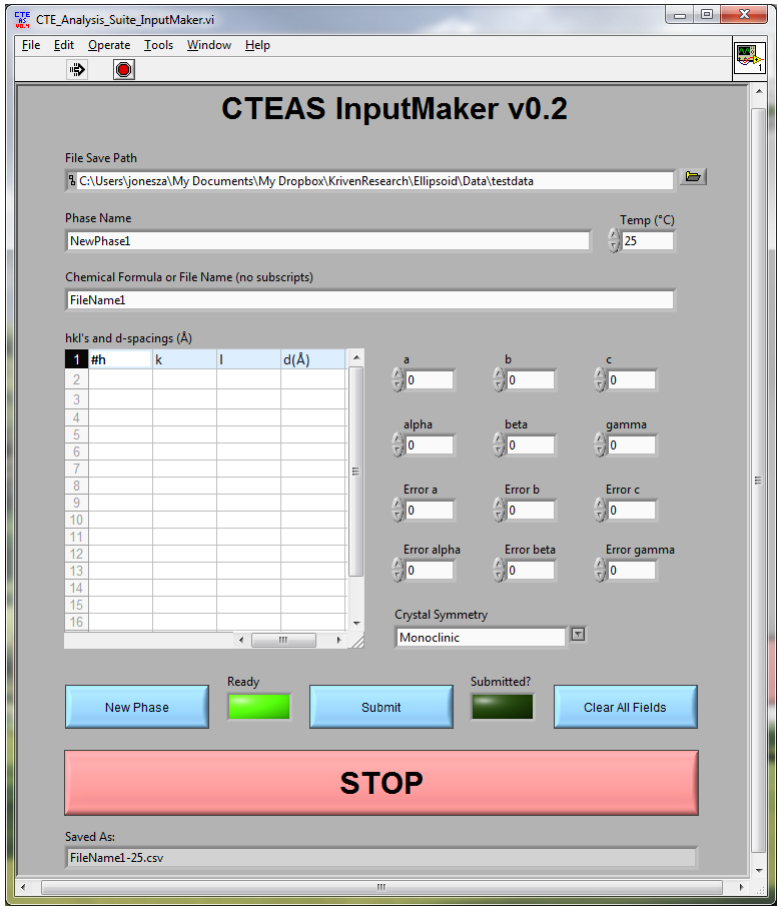

Figure 4: CTEAS InputMaker GUI

CTEAS InputMaker is an extension of CTEAS that allows the user to create input files for CTEAS based on data gathered and analyzed from a multitude of analysis programs. The number of softwares that can perform Reitveld analysis is ever-growing and rather than create algorithms that can parse the output files from every software, a form is presented to the user for inputting data. As of the current release of CTEAS, CTEAS InputMaker has very basic functionality. If an incorrect value is written to a file, the user must locate that file, open it in a text editor, and change it there manually without disturbing the syntax and layout of the file. It is recommended that an advanced text editor (Notepad++, Geany) be used to show hidden file characters in the text file.

The following sections describe the operation of CTEAS InputMaker and how it saves files. Later versions of the InputMaker will include the option of editing and deleting input data.

NOTE: CTEAS will NOT function again until the "Stop" button on the CTEAS InputMaker GUI has been clicked and the window has closed. This is a GUI limitation.

1 Using CTEAS InputMaker to Create Input Files

CTEAS InputMaker is designed to be as simple to use as possible. The following steps should be followed, per phase, to create input files for CTEAS:

1. The "File Save Path" should already be populated with the same directory that CTEAS will be using

to load files from. Should the user desire to save the files elsewhere, change the path to the desired directory.

2. Specify a name for the phase in the "Phase Name" box. This should be the same for all created input files of the same phase that will be included in the CTEAS analysis.

3. Enter the Temperature at which the input file will contain phase data for in the "Temp (°C)" box.

4. Enter the chemical formula (no subscripts) or a filename in the "Chemical Formula or Filename" box (eg: Filename1_1_2011). No file extensions are necessary.

5. In the "hkls and d-spacings" spreadsheet, enter all h, k, l, and d-spacing data in the respective columns. Note that the top row of the spreadsheet contains which column corresponds to which value. The first column contains a #h in the spreadsheet. This # sign is a communication to CTEAS that the line is considered as a comment.

   (a) The spreadsheet data will be treated as a list of comma-separated variables in the backend of the InputMaker program.

6. Specify the a, b, c, α, β, and γ lattice parameter values in their corresponding boxes.

7. Specify the errors in the lattice parameters in their corresponding boxes.

8. Choose a symmetry that describes the phase.

9. Click the "Submit" button. All fields will then be cleared except for the "Phase Name," "Chemical Formula or Filename," and "hkls and d-spacings" areas of the entry form.

   (a) The "hkls and d-spacings" spreadsheet area of the entry form cannot be cleared by the GUI as this is a limitation of the ActiveX implementation of Microsoft Excel using Office Web Components. It is the great hope of this author that this will change someday. While the LabVIEW GUI libraries contain spreadsheet-like components, the Office Web Components utility offers the only spreadsheet component that supports both copy/paste multiple cells support and data output in a reasonable format.

10. Once all files have been written for a phase, the "New Phase" button can be clicked. This will clear all fields except for the "Chemical Formula or Filename" and "hkls and d-spacings" areas of the entry form.

11. The "Clear All Fields" button will clear all fields on the entry form except for the "hkls and d-spacings" area.

12. Once all data has been input for all phases and temperatures, the Stop button should be clicked to close the window. It can be re-opened from the CTEAS GUI at any time.

2 Example Input File Contents

The syntax contained within an input file is very basic. It contains comma-separated variables and a few hidden text components. The hidden components can be seen with an advanced text editor and the rest of the text is shown below for two example phases:

```
Random other information,,,
Random other information,,,
Random other information,,,
!TEMPERATURE,100,,
!PHASE,Phasename,,
!SYMMETRY,Symgroup,,
!LPA,30,1,
```

```
!LPB,20,2,
!LPC,10,3,
!LPALPHA,5,6,
!LPBETA,7,8,
!LPGAMMA,9,11,
!BEGINHKL,,,
#h,k,l,d(Å)
1,1,1,2.2807
!ENDHKL,,,
!ENDPHASE,,,
Random other information,,,
Random other information,,,
!PHASE,Phasename22,,
!SYMMETRY,Symgroup22,,
!LPA,30,1,
!LPB,20,2,
!LPC,10,3,
!LPALPHA,5,6,
!LPBETA,7,8,
!LPGAMMA,9,11,
!BEGINHKL,,,
#h,k,l,d(Å)
1,1,1,2.2807
!ENDHKL,,,
!ENDPHASE,,,
!EOF,,,
```

3 Troubleshooting

Most problems with input files will arise from incorrect formatting of the file. While the CTEAS InputMaker will create a correctly-formatted input file, user-edited files may not work. It is best to compare the edited file with an untouched file in an advanced text editor to ensure compatibility. Any further problems or concerns can be voiced by contacting the previously-provided contact information.

3.0.1 Blank Box where hkls and d-spacings spreadsheet should exist

A blank box will be present where the hkls and d-spacings spreadsheet should exist when the Office Web Components from Microsoft are not fully up-to-date. Even if they are installed, there are two (as of 09/26/2011) updates that must be applied with Windows Update that will allow the CTEAS InputMaker to function properly.