Deirdre Johnson

u0806153@umail.utah.edu

Crystal Structures Graphical User Interface User Manual

University of Utah

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# Introduction

The purpose of this document is to provide instructions on how to use the Crystal Structures Graphical User Interface (GUI). A fundamental step to understanding material science is visualizing crystal structures in three dimensions. The GUI allows the user to plot 3-D crystal structures, including atoms, planes, and directions. This allows the user to graphically see where the atoms are located for simple, body-centered, face-centered, and other lattice types. Additional features of the GUI include plotting the reciprocal lattice, x-ray crystallography calculations, and creating pole figures. The equations and information necessary to construct the GUI are predominantly based on the Engineering Materials Science course lecture slides. Information pertaining to each feature of the GUI will be provided in various sections, broken up according to the tabs on the GUI. There are four tabs on the GUI named *Crystal Structure*, *Reciprocal Lattice*, *X-Ray Crystallography*, and *Pole Figures*.

# Opening the GUI

The Crystal Structures GUI was created in MATLAB R2018b. In order to use the GUI the operator will need access to MATLAB 2017 or 2018 (preferably 2018). There are two ways in which the user can open the GUI. The first option is to simply double click on the FinalProject.mlapp file (MATLAB App). The app will open without having to open MATLAB. The second option is to open MATLAB and type “appdesigner” in the Command Window. The App Designer interface will open, and the user must browse for the FinalProject.mlapp file. After opening FinalProject.mlapp the Design View of the GUI will display on the App Designer interface. This is the interface on which the app was created and edited. To run the app, press the green Run arrow, circled below in Figure 1. This is the preferable way to run the GUI while creating and debugging it. On the App Designer interface, the user has the option to switch from Design View to Code View in order to view and edit the code itself. The button to press in order to switch to Code View is circled in Figure 1 and the Code View is shown in Figure 2. All the code for the GUI is contained in the Code View. It is possible to call functions outside the GUI; however, for simplicity everything is self-contained. Depending on computer screen size, the user might want to adjust the size of the GUI, which can be done on the App Designer interface in the Component Browser. First select the UIFigure on the Design View and then uncheck the “Resize button” as shown in Figure 3.

A screenshot of a social media post

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Figure . Design View

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Figure . Code View

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First, select the UI Figure

Second, uncheck “Resize”

Figure . Resizing GUI

If the user wants to see the code that is written for each button on the GUI the simplest way is to open the Design View, right click on the desired button, go to Callbacks, and click “Go to XXXXcallback.” For example, on the *Crystal Structure* tab, if I wanted to see the code behind the first Plot pushbutton, I would right click the Plot pushbutton and navigate as shown in Figure 4. The Code View will automatically pop up at the desired Callback (in this case the “CellPlotPushed” Callback), as shown in Figure 5. Note that there is not a callback for every button on the GUI. Some of the buttons are only used to store data to be pulled in by other Callbacks. Another way to quickly navigate between Callbacks is to use the Code Browser located on the left-hand side of the Code View window (Figure 6). The following sections provide instructions on how to use each tab of the GUI.

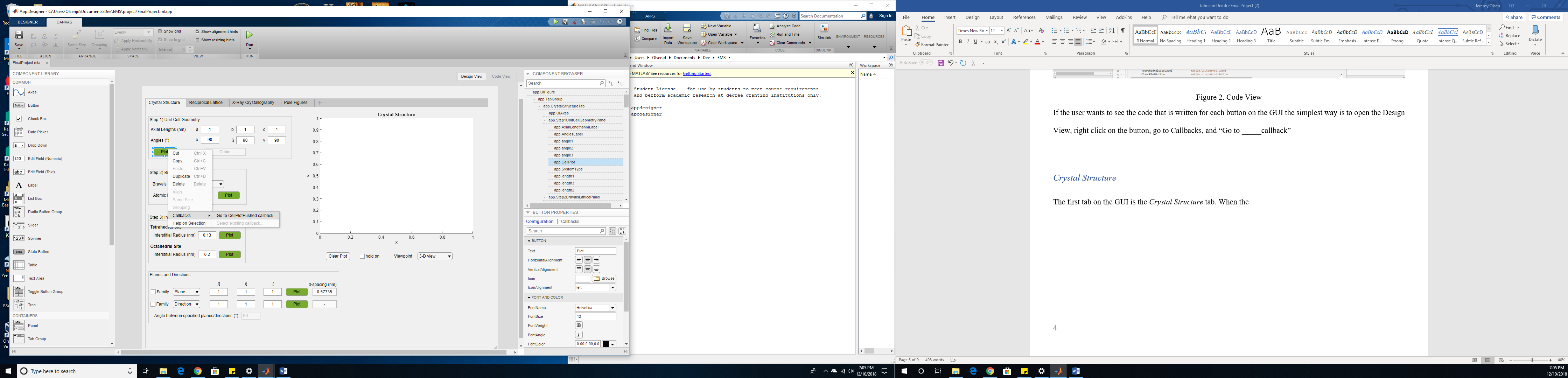


Figure . Navigate to Callback

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Figure . Callback

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Figure . Code Browser

# Crystal Structure Tab

The first tab on the GUI is the *Crystal Structure* tab which is displayed upon opening the GUI. There are predefined values in each text box, as shown in Figure 7. The user can adjust the axial lengths and angles that define the unit cell geometry. The system type will automatically display in the “System” textbox. For example, in Figure 7, axial lengths of 1 and angles of 90° correspond to a Cubic structure. If The inputs are invalid, the “System” textbox will say “Invalid inputs” and all the “Plot” pushbuttons will be disabled.

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Figure . Crystal Structure Tab

When a valid system type is specified, the user can press the first “Plot” button and the crystal structure will be displayed in 3-D as shown in Figure 8. The user can plot cubic, tetragonal, orthorhombic, hexagonal, rhombohedral, monoclinic, or triclinic systems. The next step is to plot the atoms on the unit cell. In order to do this, the user must select the bravais lattice (e.g. Simple, Face-Centered, Body-Centered, etc.). The GUI will automatically update the Bravais Lattice dropdown box to only allow the configurations that are applicable to the system type (i.e. for tetragonal the only options are simple or body-centered). Once the lattice type is specified, enter the desired atomic radius and press the Plot button (Figure 9).

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Figure . Cubic Crystal Structure

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Figure . Cubic Structure with Atoms

The next option is to plot interstitials, either tetrahedral or octahedral interstitials. The user must specify the desired radius and press the “Plot” buttons. The interstitial atoms will be plotted on the unit cell in the tetrahedral or octahedral sites (Figure 10). If the user would like to view multiple options at a time, he or she can check the “hold on” checkbox (circled in Figure 10). If the user would like to clear the plot, he or she can press the “Clear Plot” pushbutton (circled in Figure 10). Additionally, the user can specify different viewpoints (e.g. X-Y plane, Y-Z plane, etc.) using the “Viewpoint” dropdown (circled in Figure 10).

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Figure . Cubic Structure with Interstitials

The final panel on the *Crystal Structure* tab is the “Planes and Directions” panel. The user can specify up to two planes or directions (or one plane and one direction) at a time. For planes, the spacing between adjacent planes (labeled as d-spacing) will automatically be calculated and displayed on the GUI. Also, the angle between the specified planes/directions will automatically be calculated and displayed on the GUI. Finally, the user can plot the planes/directions using the “Plot” pushbuttons, as well as the family of planes/directions. Each of these features are shown in Figure 11 and Figure 12. Note that planes cannot be plotted for some system types (e.g. rhombohedral and triclinic). When the feature is not available, the “Plot” button will be disabled.

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Figure Planes and Directions

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Figure . <111> Family

# Reciprocal Lattice Tab

The second tab is the *Reciprocal Lattice* Tab, shown below in Figure 13. Values are pre-defined when the GUI opens but can be modified by the user if desired. On the “Unit Cell Geometry” panel, the user specifies the axial lengths of the unit cell as well as the viewing direction and can then press the “Plot” button. Like the *Crystal Structure* tab, a 3-D plot of the crystal structure will display on the bottom left figure window of the GUI. Next, on the “Planes” panel, the user can plot up to 4 planes at a time. When each “Plot” button is pressed, the plane will be plotted on the Crystal Structures figure (bottom left) and the diffraction pattern will be plotted on the Diffraction Pattern figure (bottom right) as shown in Figure 13. Having these two figures side by side helps with visualization. The d-spacing is automatically calculated and displayed on the GUI for each plane. If a wavelength is specified, the d\* value is also automatically calculated and displayed on the GUI. The Clear Plots pushbutton, hold on checkbox, and Viewpoint dropdown are also available on this tab.

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Figure . Reciprocal Lattice Plots

# X-Ray Crystallography Tab

The third tab is the *X-Ray Crystallography* Tab (Figure 14). This tab calculates any parameter of Bragg’s Law. The user can specify the Bravais Lattice using the dropdown and then select which parameter to calculate. The text boxes will automatically update to be highlighted yellow if the parameter needs to be input. For example, in Figure 14, the user wants to calculate the wavelength, so the “n,” “theta,” “hkl,” and “a” text boxes are all highlighted (note: for primitive hexagonal the “c” text box would also be highlighted). The “d” text box is automatically populated depending on the specified plane and lattice parameters. Additionally, the GUI will notify the user if it is an allowed reflection or not (circled below in yellow). If it is a forbidden reflection, the text will display “Warning: forbidden reflection” in red text. The allowed reflection rules are based on the course lecture notes.

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Figure . X-Ray Crystallography: Bragg's Law

# Pole Figures Tab

The final tab is the *Pole Figures* Tab (Figure 15). This tab is based off Homework #4. The user can specify a family of directions and set of Euler Angles and plot the Pole Figures using both Stereographic Projection (bottom left figure) and Equal Area Projection (bottom right figure). Alternatively, the user can load a file containing multiple Euler Angles and plot the corresponding pole figures. The file needs to be in the same format as the “texran.ang” file provided with Homework #4 and be saved in the current working directory. If the user wishes to use a file, he or she must check the “Use File” checkbox and specify the name of the file (Figure 16).

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Figure . Pole Figures Tab

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Figure . Pole Figures with File

# Future Improvements

As is the case with most coding projects, there is always room for improvement. It is hard to ever say that an app is officially complete. There are a lot of things that I would have liked to incorporate on this version of the App. Below is a list of some of the main things I would have liked to incorporate (and might still try to do after the class is over). One last note, it is possible that you find bugs in the GUI. Sometimes it is hard to find bugs as the creator because I know how the GUI “should” work. If you come across any feel free to let me know.

*Crystal Structure* Tab:

1. Automatically calculate the maximum atomic radius
2. Automatically calculate the maximum interstitial radius
3. Enable plotting of planes and directions for every system type (attempting triclinic was a bit of a headache)

*Reciprocal Lattice* Tab:

1. Perform the same thing in reverse
2. Allow for more than 4 planes at a time
3. Enable functionality for more system types (e.g. monoclinic)

*X-Ray Crystallography* Tab:

1. Add a figure to help visualize what the calculations mean

*Pole Figures* Tab:

1. Add a 3-D figure showing all the poles, not just the projection of the northern hemisphere

General:

1. Improve coding technique, particularly with coordinate transformations

http://duffy.princeton.edu/sites/default/files/pdfs/links/xtalgeometry.pdf