# Morphology Domain

## User Manual


6/26/2012

# User Manual

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# 1.0 General Information

## 1.0 GENERAL INFORMATION

### 1.1 Overview

MorphologyDomain application is intended to generate Morphology Graph and surface normals of the Morphology Domain from the crystal properties such as lattice parameters and Miller indices of F-faces. The F-faces can be obtained from other commercial software such as FACELIFT and Material Studio. The Miller indices of F-faces are supplied as an Excel file. The lattice parameters can be typed in the application.

There is another section in the MorphologyDomain for Accessible Region Analysis. This part of the software takes growth rate function from an Excel file and provide accessible domain in the Morphology Graph.

The software delivered in this form is fully functional and is capable of generating Morphology Graph and Morphology Domain, and showing accessible domains for a valid input data.

### 1.2 Authorized Use Permission

This is free software and hence anyone can use it. However, copying any part of the software is not allowed.

### 1.3 Contact Information

For additional information and any query please contact

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# 2.0 Getting Started

## 2.0 GETTING STARTED

*Extracting, Installing and Executing MorphologyDomain*

### 2.1 Extracting from the .ZIP archive

Once you have extracted the .ZIP archive, you should be able to find the following inside the folder:

- MorphologyDomain (an executable file)
- Read Me (notepad file)
- Video Tutorial
- User Manual
- Examples folder
    - Alum Folder
        - Miller Indices (excel file)
        - Growth Rate Function ALUM (excel file)
        - Document (pdf file)
    - Acetaminophen Folder
        - Miller Indices (excel file)
        - Growth Rate Function APAP (excel file)
        - Document (pdf file)
    - KAP Folder
        - Miller Indices (excel file)
        - Growth Rate Function KAP (excel file)
        - Document (pdf file)
- Miller Indices Template
- Growth Rate Function Template

MATLAB Compiler Runtime (MCR) version 7.16 is a prerequisite for this application. A copy of MCR is available on http://web.ics.purdue.edu/~singh2/MCRInstaller.exe

#### 2.1.1 Installing MCR

Please refer to the Read Me notepad file to know more about installation procedure.

### 2.2 Starting the Application

Once you have MCR version 7.16 installed or if you have it installed already, run the MorphologyDomain.exe file. It is a standalone application and you do not need MATLAB to run it. You can execute it directly by double clicking or through command prompt.

You may also try MATLAB command window to run this application. Select the path for MorphologyDomain directory and type "!MorphologyDomain" (without quotes) on the command window. This will open the graphical user interface (GUI) of MorphologyDomain.

# 3.0 Creating Database

## 3.0 CREATING DATABASE

*Creating database for Miller Indices and Growth Rate Function*

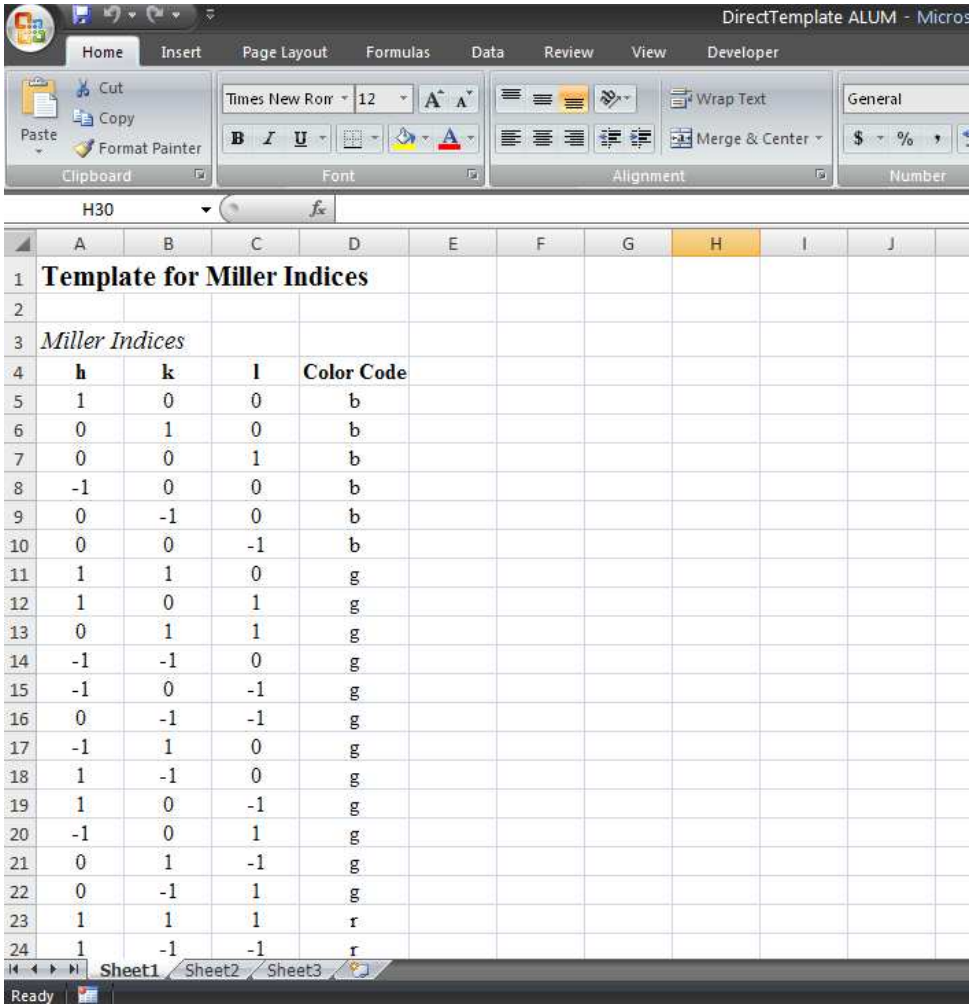
### 3.1 Miller Indices Database

Before getting the desired output, you need to create input data in the right format. The format of the input for Miller indices and color code of the F-face is given in the excel template which you will find in MorphologyDomain folder. Once you open the template excel file, you will be able to see the format in which the input needs to be given. You can create your own database anywhere on your computer and can give any name to the excel file. But make sure that your input data is always on SHEET 1 of the excel file. Once you have made your own template in the format given, type in the Miller indices such that Miller indices of one family of faces are consecutive. Make sure that every family of faces has ONE single color code which you will type in next to the Miller indices of every face. Different families can have different color codes depending on what you want. The allowable color codes are the following:

| Colour Code | Colour |
|---|---|
| y | Yellow |
| m | Magenta |
| c | Cyan |
| r | Red |
| g | Green |
| b | Blue |
| w | White |
| k | Black |

Once you have created the complete dataset for one crystal, save the excel file with any name you want.

On the next page you will see a screenshot of the excel file. The data shown there is that of Alum crystal.



| | A | B | C | D |
|---|---|---|---|---|
| 1 | **Template for Miller Indices** | | | |
| 2 | | | | |
| 3 | *Miller Indices* | | | |
| 4 | **h** | **k** | **l** | **Color Code** |
| 5 | 1 | 0 | 0 | b |
| 6 | 0 | 1 | 0 | b |
| 7 | 0 | 0 | 1 | b |
| 8 | -1 | 0 | 0 | b |
| 9 | 0 | -1 | 0 | b |
| 10 | 0 | 0 | -1 | b |
| 11 | 1 | 1 | 0 | g |
| 12 | 1 | 0 | 1 | g |
| 13 | 0 | 1 | 1 | g |
| 14 | -1 | -1 | 0 | g |
| 15 | -1 | 0 | -1 | g |
| 16 | 0 | -1 | -1 | g |
| 17 | -1 | 1 | 0 | g |
| 18 | 1 | -1 | 0 | g |
| 19 | 1 | 0 | -1 | g |
| 20 | -1 | 0 | 1 | g |
| 21 | 0 | 1 | -1 | g |
| 22 | 0 | -1 | 1 | g |
| 23 | 1 | 1 | 1 | r |
| 24 | 1 | -1 | -1 | r |

**Figure1:** Excel sheet of Miller indices of F-faces with their representative color code.

### 3.2 Growth Rate Function Database

Once you are done with creating database for the Miller indices, you can create face-specific growth rate function for "Accessible Region Analysis". You will find a sample template in the main folder. Follow the template pattern. The cell B3 takes input of % supersaturation from the MorphologyDomain. The cell C3 converts B3 to the necessary form for the growth rate functions. The cells B6, B7, … are the face-specific growth rates that are functions of C3. Starting from A6, all the cells in A will have the family color codes and the cell just next to it will be a function of C3. Remember that this should be SHEET 1 of your excel file. You can name the excel file anything and save it anywhere on your computer.

On the next page you will see a screenshot of the excel file. The data shown here is that of Alum crystal.

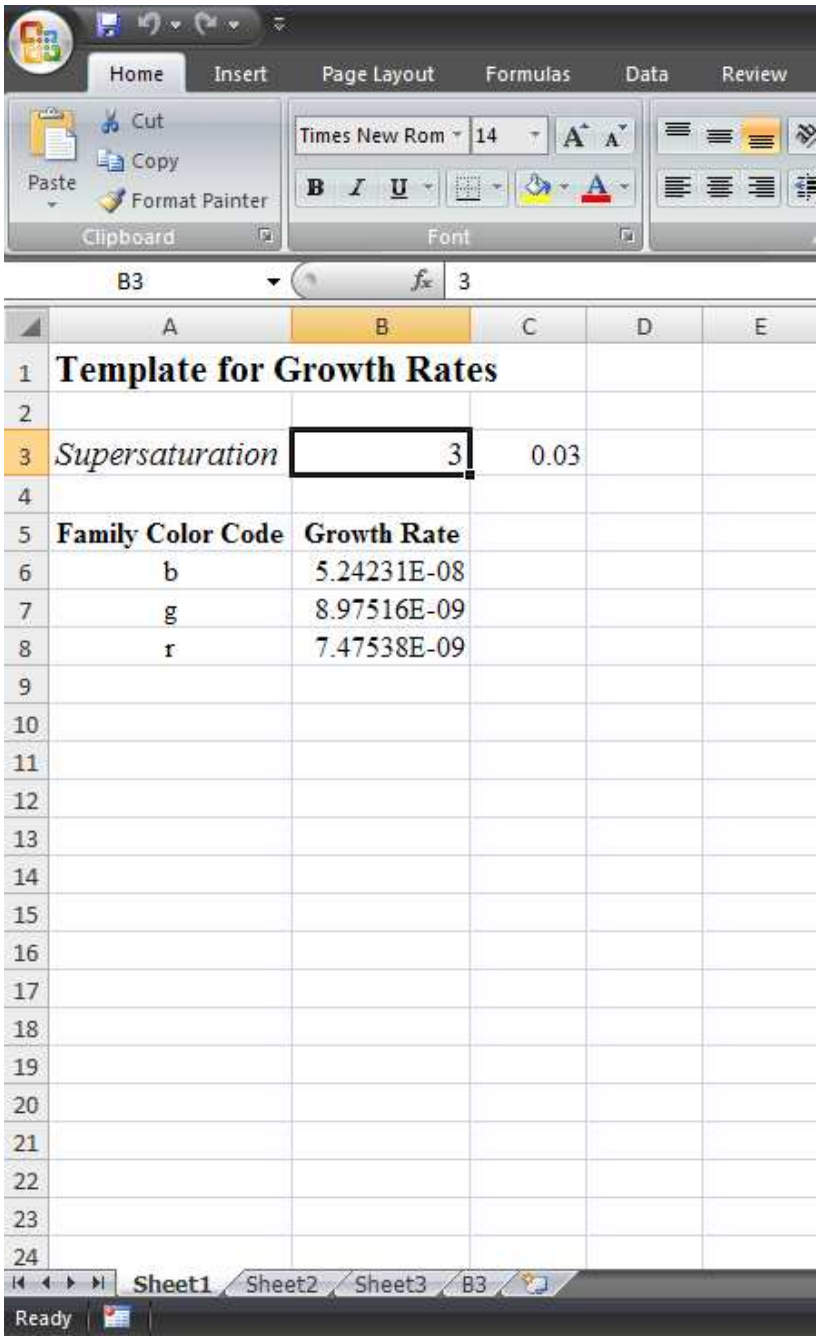



**Figure 2:** Growth Rate Functions of Alum crystal

# 4.0 Using the Application

## 4.0 USING THE APPLICATION

Please read the following step-wise instructions on using MorphologyDomain application. Alternatively, you can also see the video tutorial in the main folder.

### 4.1 Choosing File

Once you have opened the application, the first thing you need to do is choose an excel file as an input with Miller indices and color codes. For that, click on “File” button. Then choose the excel file which you want as the input. Then, click on “Open”. Then, wait for sometime till the application reads the excel file. As soon as the excel file is read, you will be able to see the excel file path on the edit box beside the “File” button. After this, you can proceed further.

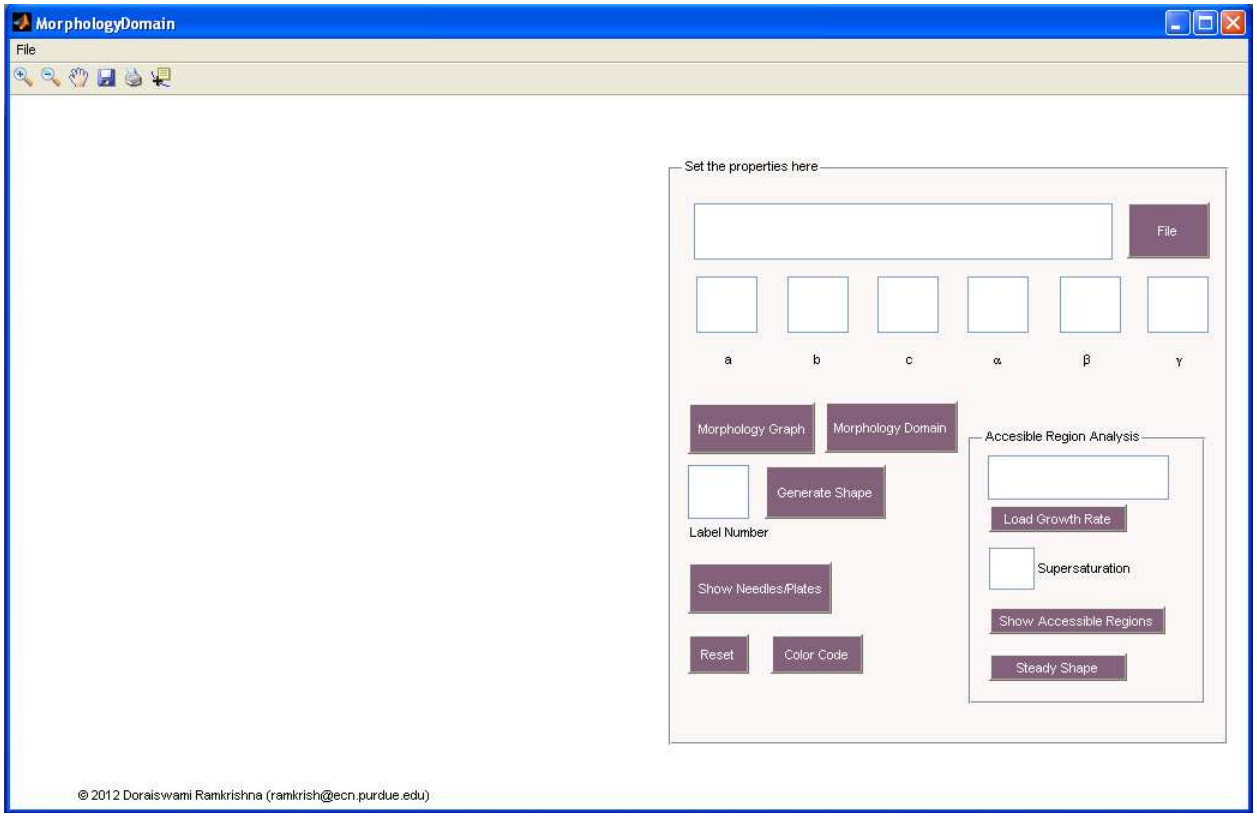



**Figure 3:** Main window of MorphologyDomain application

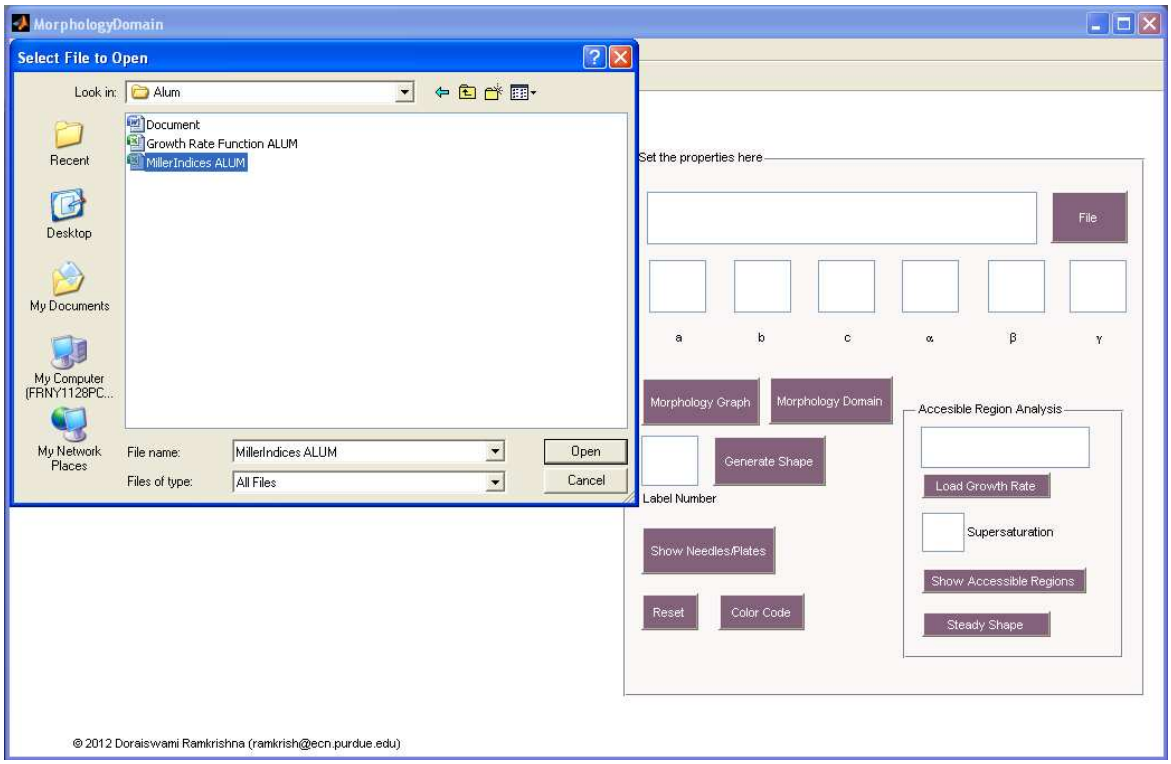



**Figure 4:** Choosing Miller indices excel file

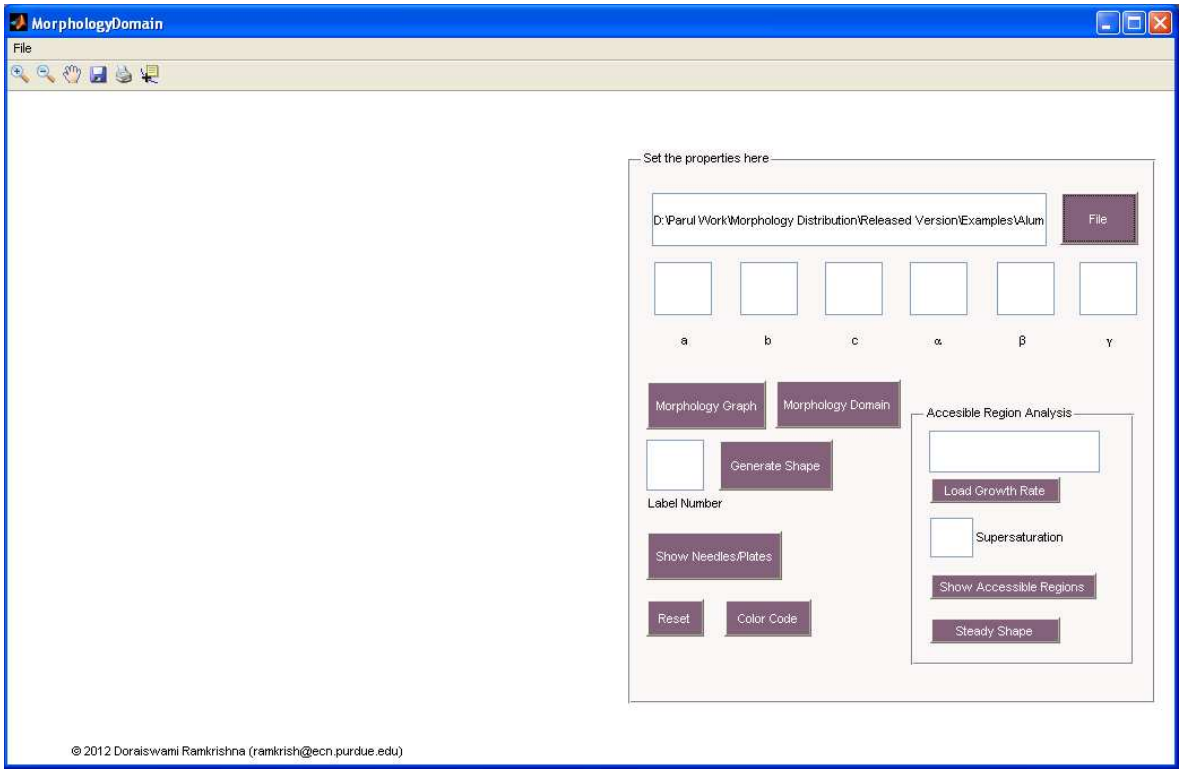



**Figure 5:** The path name will be displayed after the excel file has been read

### 4.2 Lattice parameter input

After file selection, you need to give lattice parameter input. In the 6 edit boxes below the push button “File”, type a, b, c, alpha, beta, and gamma in the order given.

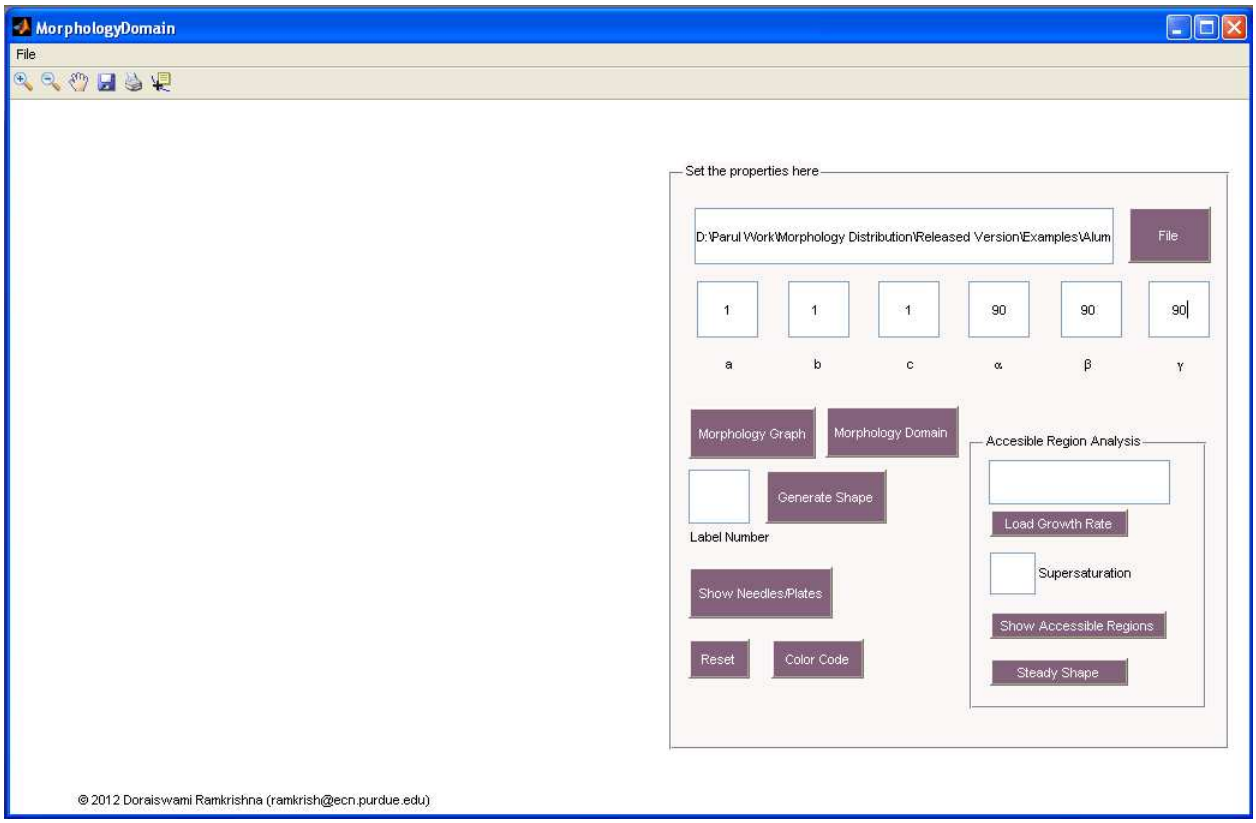



**Figure 6:** Typing Lattice parameters

### 4.3 Viewing the Morphology Graph

After you are done with all the inputs, click on “Morphology Graph” button. A bidirected graph of Morphology Set is produced with first order transitions. Each node of the graph is associated with a label number and the corresponding element of Morphology set. The edges of the Morphology Graph represent the conditions for morphology transformations. The different kinds of face transitions can be identified from the edges of the Morphology Graph. Each edge connects a set with its subset and the difference in the cardinality of the connected sets determines the order of transition. The higher order transitions involve different kinds of faces disappearing or appearing simultaneously, which can also be explained by the linear combinations of first order transitions. To see the relation among the families for every possible domain, click on “Morphology Domain” button. On clicking, a table will pop up. It will be a matrix with dimension ‘number of edges of the graph’ x ‘number of families + 3’. The third last column shows the edge number for every relation in the plot. The last two columns will show the label numbers of the two nodes forming that edge.

Every possible domain on the plot has a label number associated with it which is written to the left side of the point. Now, if you want to see the crystal shape for a possible morphology, type its label number in the label number edit box and then click on “Generate Shape”. Upon clicking, a waitbar and a figure will pop up. Wait till the waitbar closes (Or you can click on cancel to close it if you don’t want to see the shape). Once the waitbar closes automatically, you will be able to see a representative crystal morphology corresponding to the Morphology domain on the new figure window.

To check potential needles/plates, click on “Show Needles/Plates” button. Upon clicking, all potential needles/plates morphologies will be circled red. If no morphology is a potential needle/plate, nothing will be circled.

To check which geometric family corresponds to which color, click on “Color Code” button.

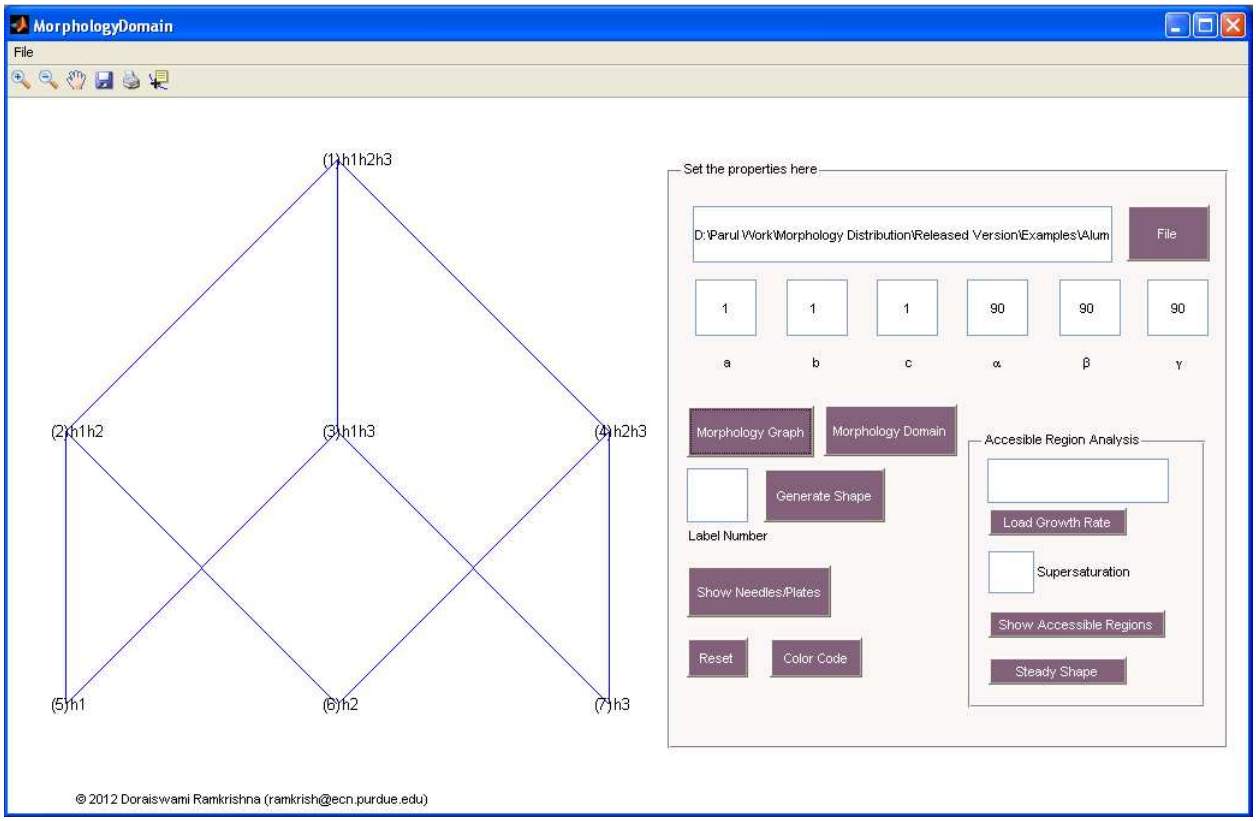



**Figure 7:** A bidirected graph generated after clicking on “Morphology Graph”

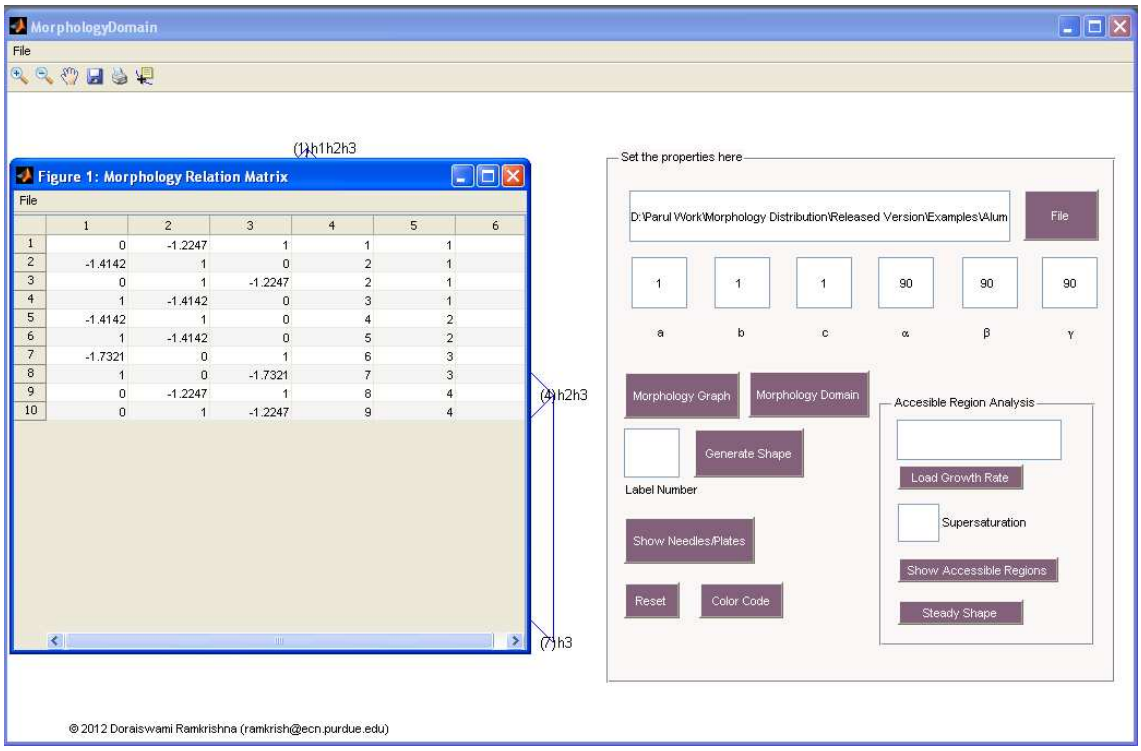



**Figure 8:** First three elements of a row vectors are the components of Normal vectors of Morphology Domain and the last three elements are the indices of edge and the connected nodes.

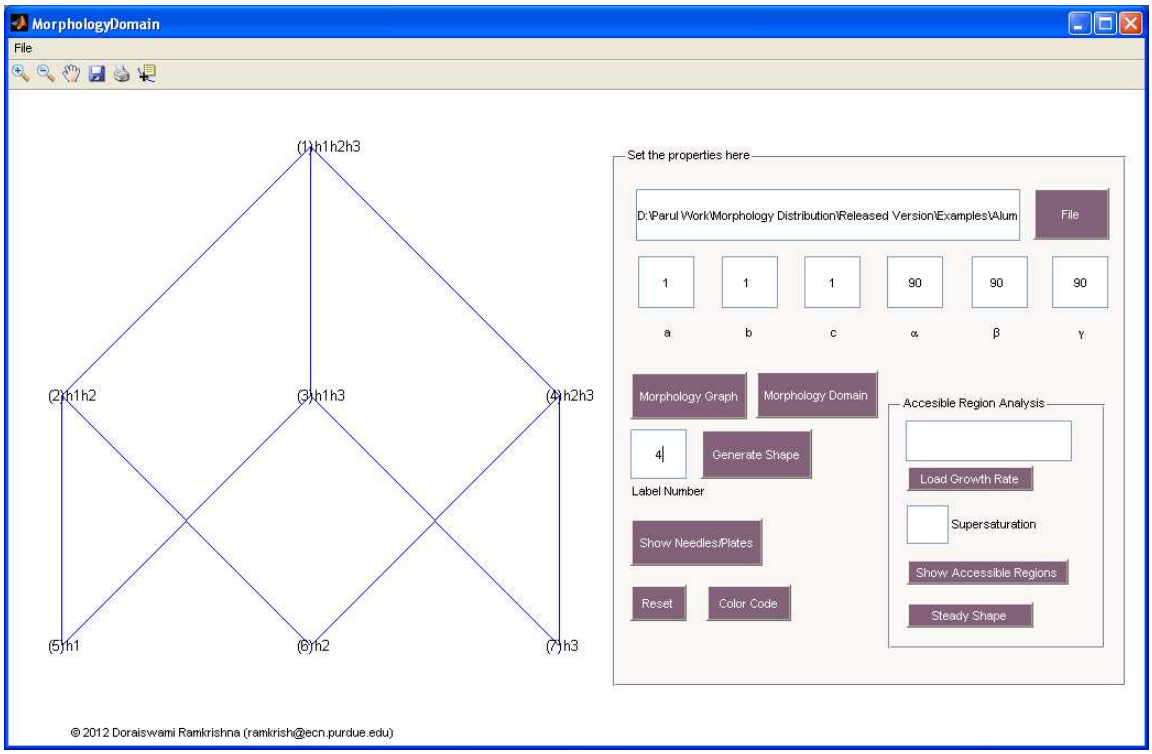



**Figure 9:** Typing a label number to see the corresponding shape

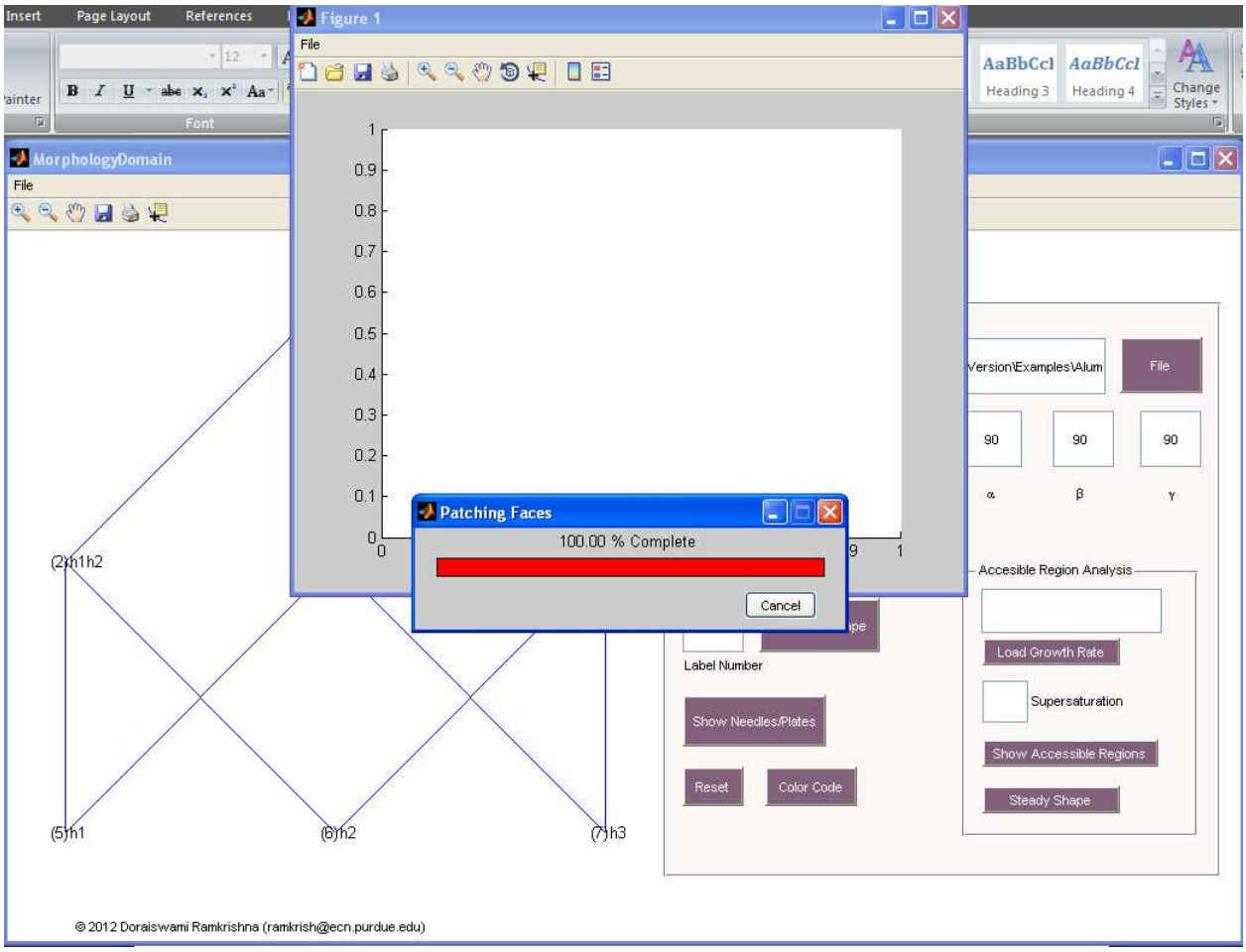



**Figure 10:** Waitbar for generating shape corresponding to the label number

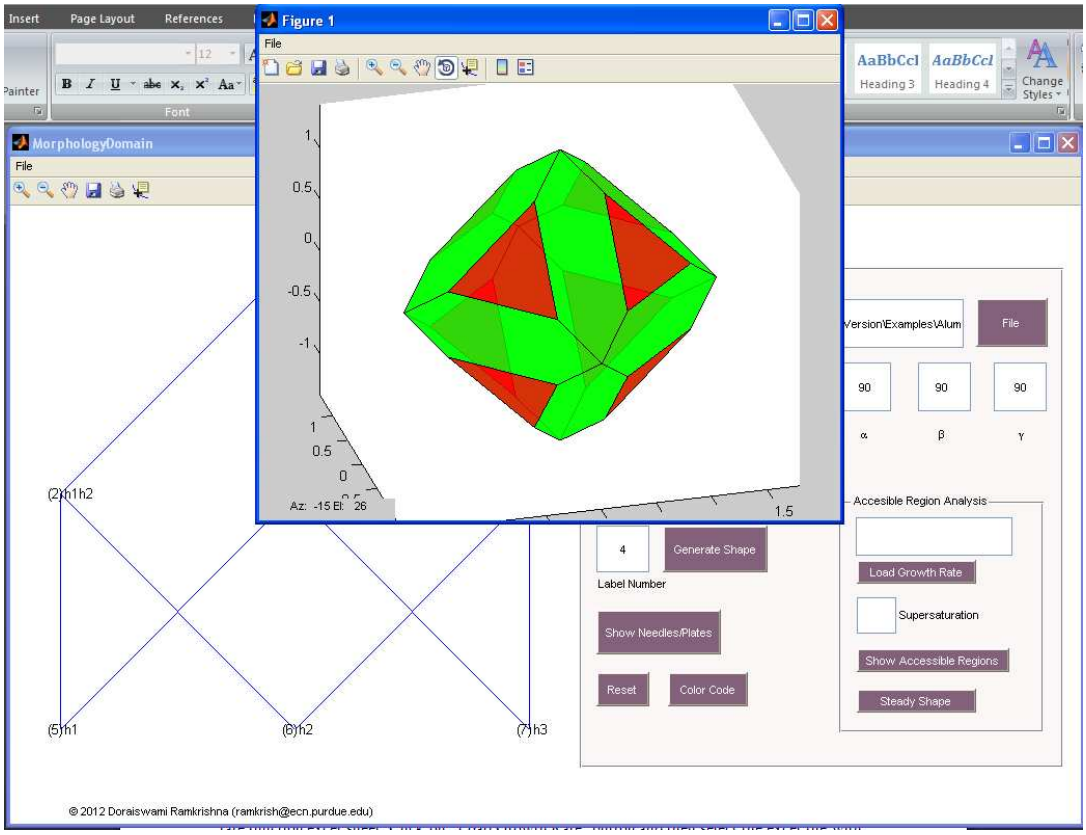



**Figure 11:** Shape generated corresponding to the label number

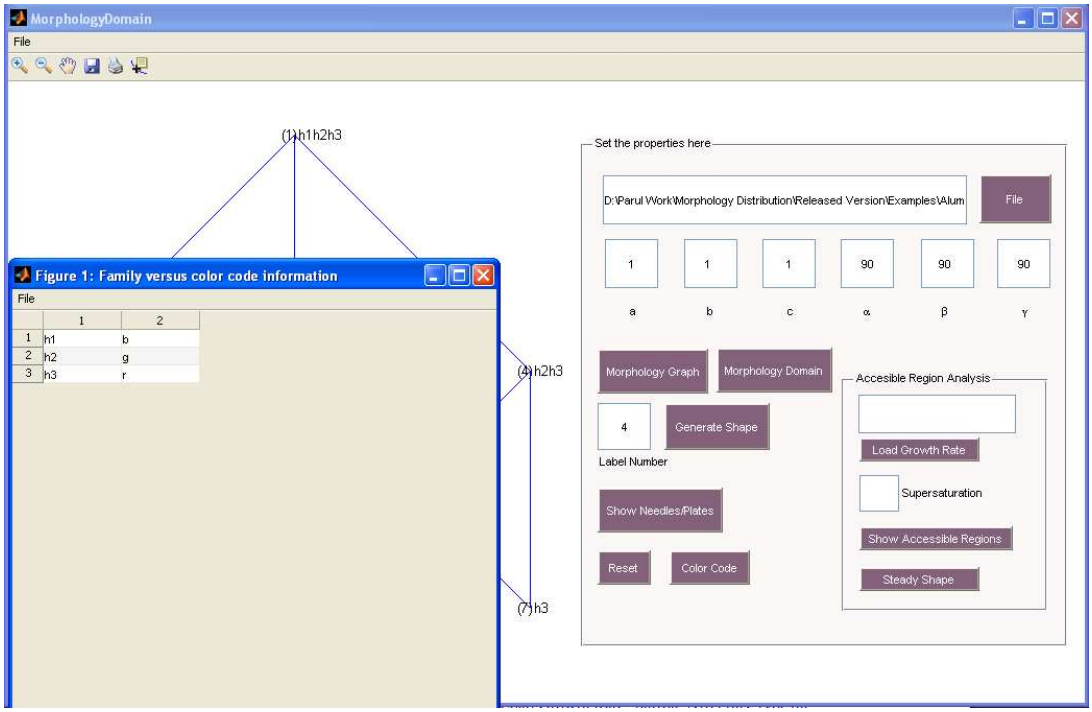



**Figure 12:** Family versus color code information for Alum crystal

### 4.4 Accessible Region Analysis

If you want to find out what all morphologies are accessible for a particular supersaturation, you need to do the accessible region analysis. The Accessible Region of steady-state morphologies in the Morphology Domain can be determined from the growth rate functions alone. For this, you firstly need to give an input of the growth rate function excel sheet. Click on "Load Growth Rate" button and then select the excel file with the growth rate function. Click on "Open" button. Once the excel file has been read, the file path will be shown on the edit box just above "Load Growth Rate" button. After this, type a valid supersaturation value on the edit box "supersaturation". After typing, click on "Show Accessible Regions" button. Wait for sometime till a new Morphology Graph is plotted with green lines joining the nodes which are the accessible morphology domains for that supersaturation value. If no green lines appear then the accessible domain is the Morphology Domain corresponding to label 1.

You can see the steady shape (shape attained after steady state is reached for that supersaturation) by clicking on "Steady Shape" button. A new figure will pop up after a waitbar. Wait till the waitbar closes after which the shape will be generated on the figure.

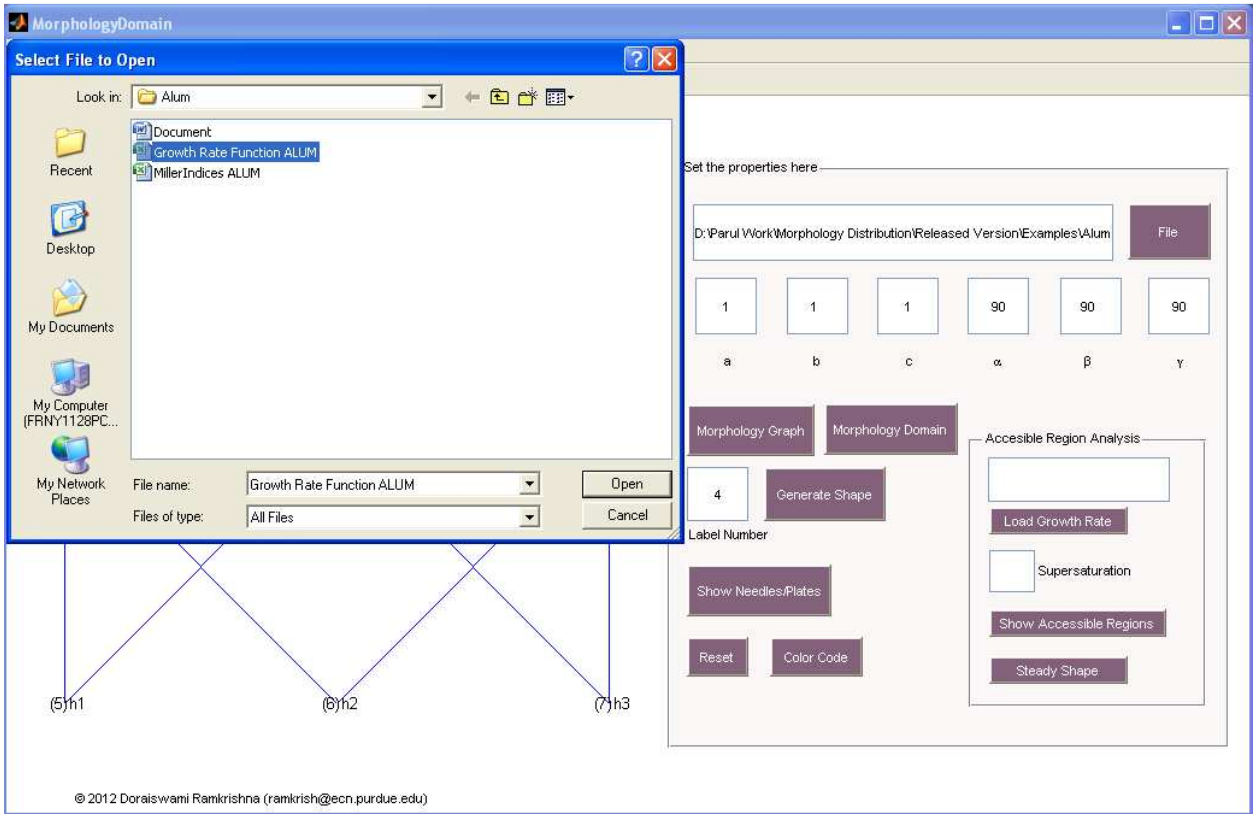



**Figure 13:** Choosing the Growth Rate Function excel file

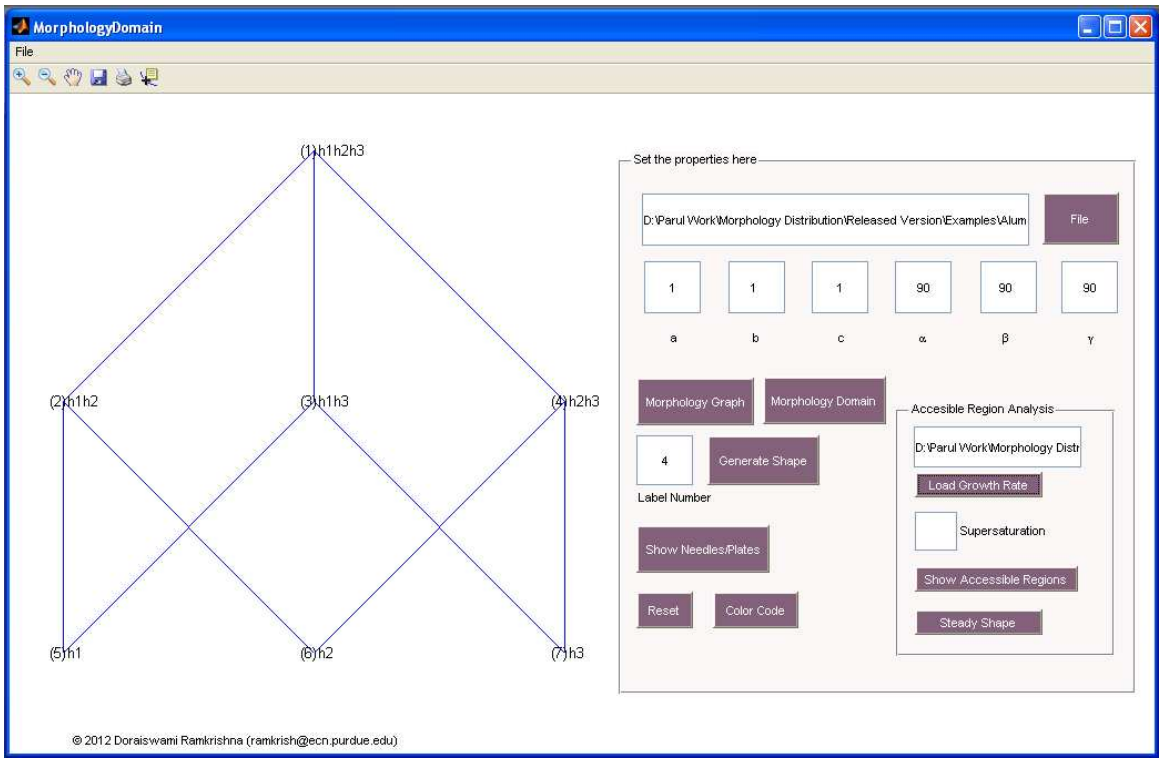



**Figure 14:** A path name will be displayed after the excel file has been read

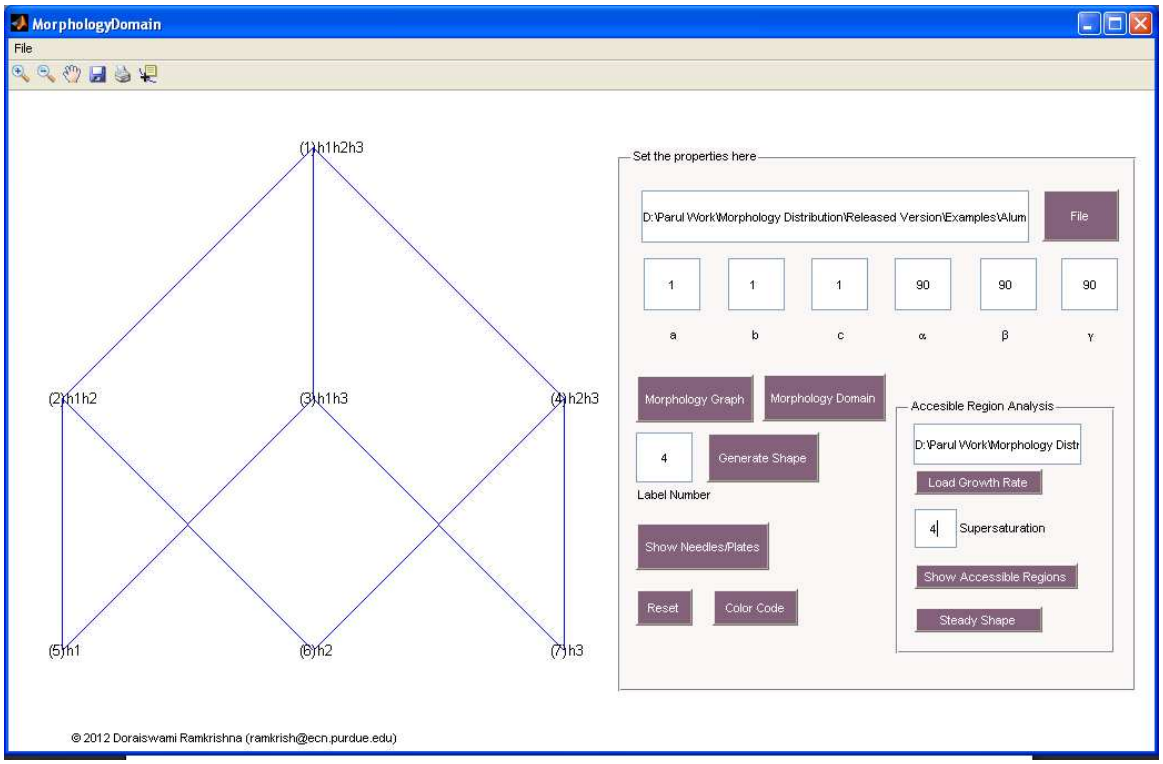



**Figure 15:** Typing a value of Supersaturation

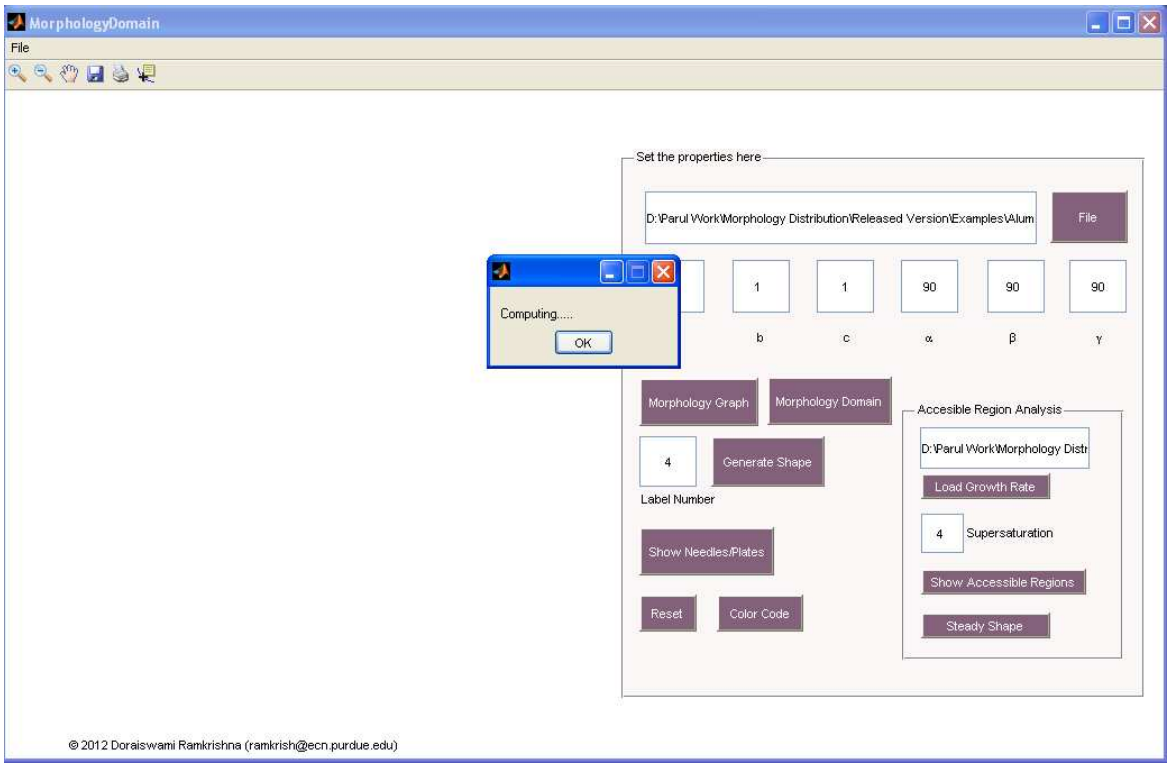



**Figure 16:** Waitbar for computing a new Morphology Graph

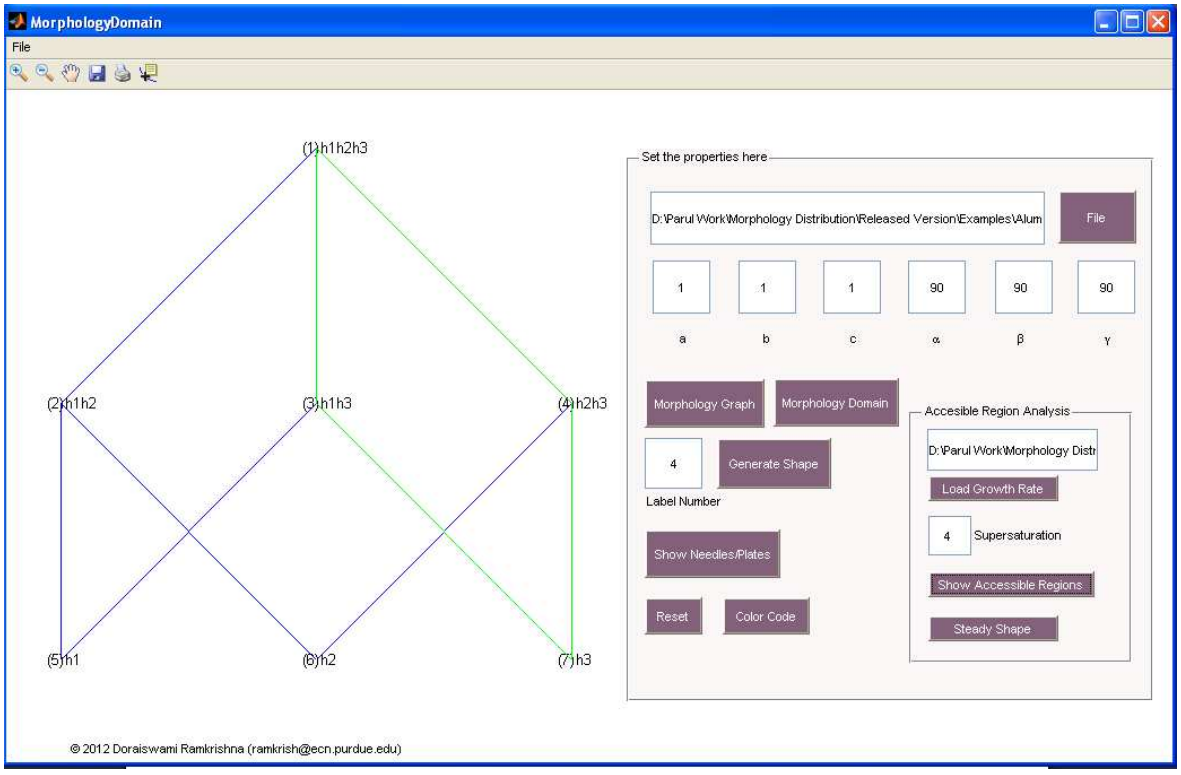



**Figure 17:** Morphology Graph with accessible domains connected with green edges

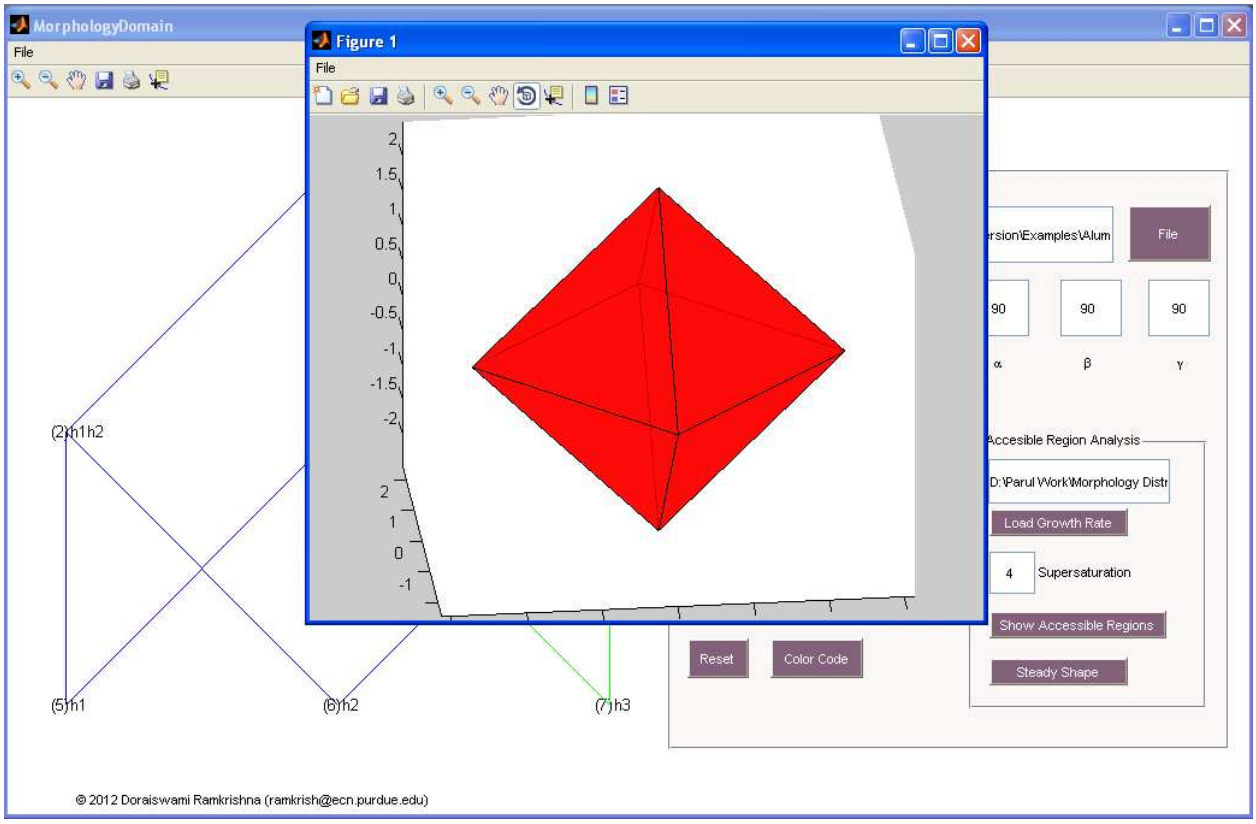



**Figure 18:** Steady state shape at the given supersaturation value

### 4.5 Using toolbar options

You can zoom in, zoom out and pan the plot image using the toolbar options.

You can also save the graph as an image in the format you want. Note that if you save, the whole window image will be saved along with the plot. To save, go to “file” in the menu bar and then click on “Save as”.

To resume back to the original setup of the image, double click on the graph image with any of the toolbar options. This means that select any of the tool bar options, and then double click on the plot image. Then, the plot image will go back to its original size and placing.

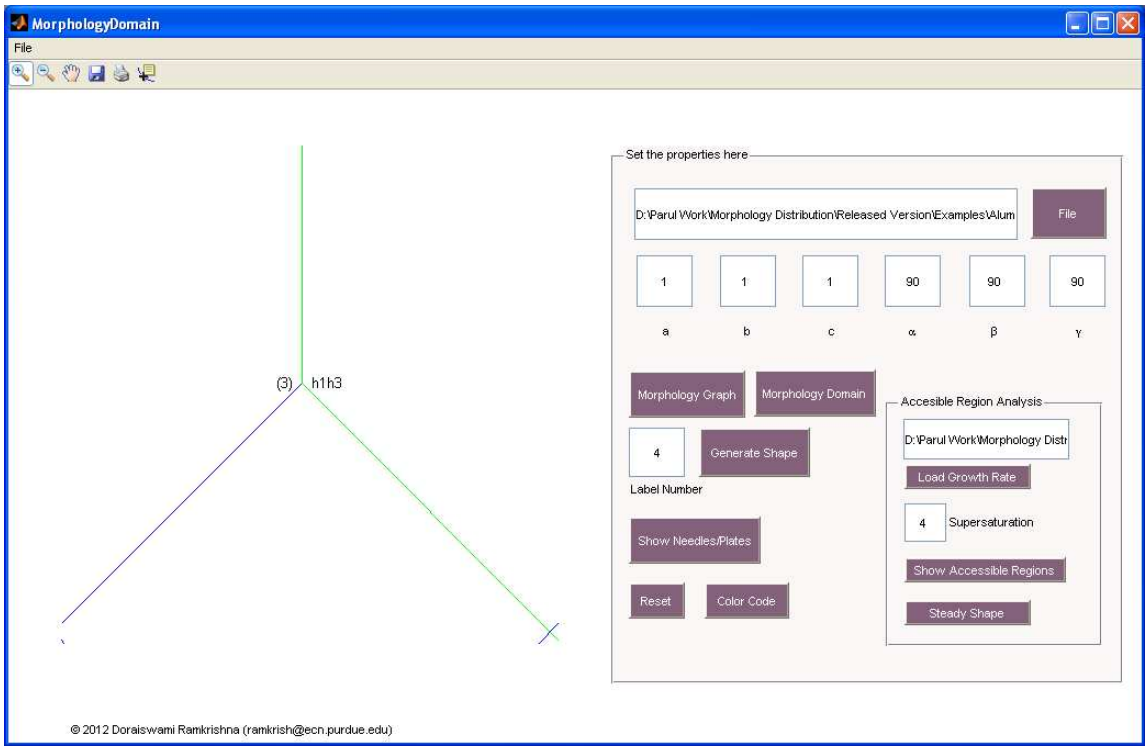



**Figure 19:** Zoomed-in plot image

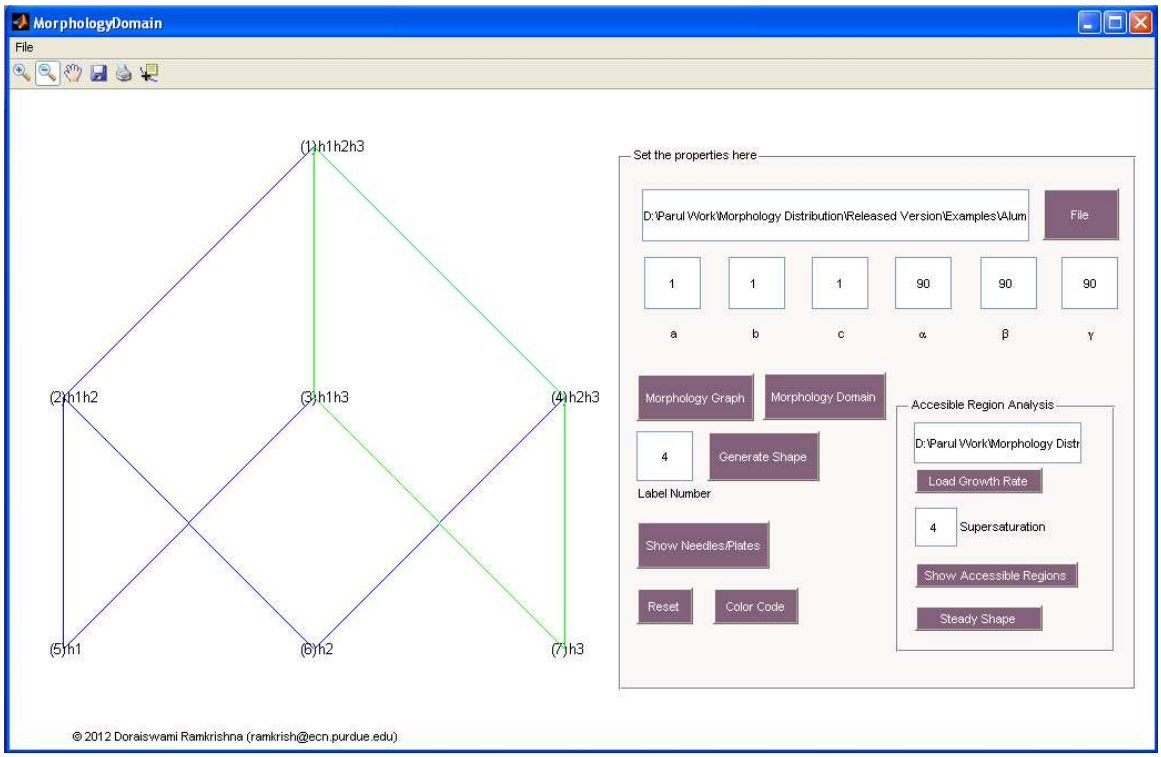



**Figure 20:** Zoomed-out plot image

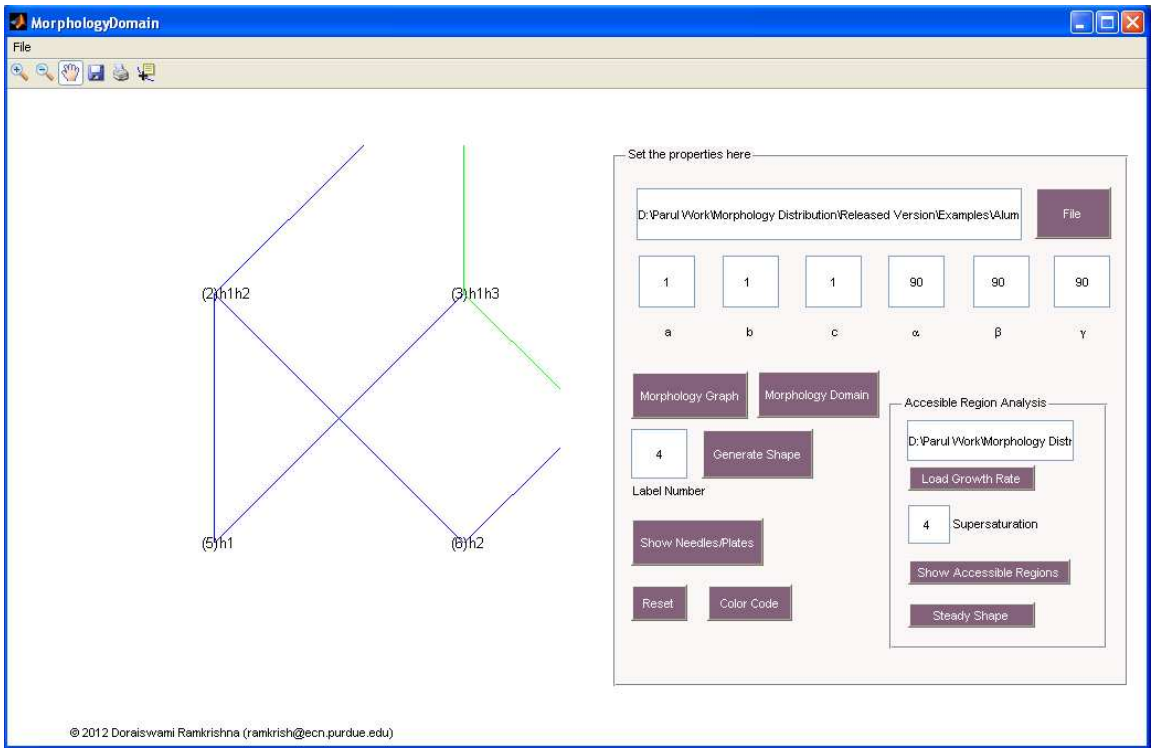



**Figure 21:** Panning plot image to the right

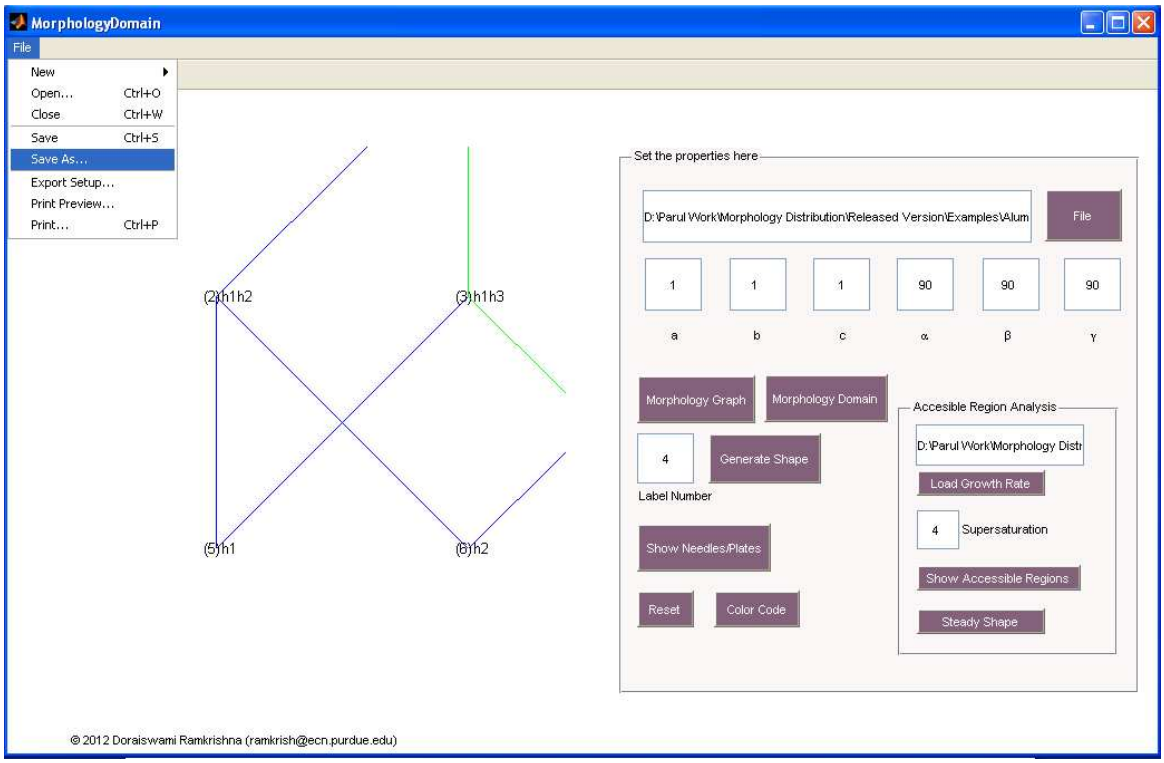



**Figure 22:** Saving the figure

# 5.0 Glossary

**5.0 GLOSSARY**

| Word | Meaning |
|---|---|
| Morphology | Shape or Habit of a crystal |
| Miller Indices | Miller indices are a notation system in crystallography for planes and directions in crystal (Bravais) lattices. |
| Lattice Parameters | Parameters defining the unit cell of a crystal lattice, that is, the length of one of the edges of the unit cell or an angle between edges. |
| Supersaturation | The term supersaturation refers to a solution that contains more of the dissolved material than could be dissolved by the solvent under the solubility amount. |
| Steady State | A state or condition of a system or process (as one of the energy states of an atom ) that does not change in time |

## **Reference**:

1. Meenesh R. Singh, Parul Verma, Hsien-Hsin Tung, Shailendra Bordawekar and Doraiswami Ramkrishna, “A Novel Method for Crystal Morphology Screening,” *submitted*.