The APTyzer Tutorial Version 1.2

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The APTyzer is a python based tool for visualizing and analyzing Atom-Probe-Tomography (APT) data, with a focus on calculating concentration and excess profiles of elements. It uses the .pos and .rrng file formats to load in APT data. It is also compatible with the Nexus file format, NXapm.

The APT specimen used in this tutorial were created by [1].

Contents

1 Getting started / Loading files

First, run the APTyzer code with jupyter notebook. If successful, the GUI should look like, as in fig. 1. If the appearing GUI has a different format one possibility how to solve this issue is to restart the kernel of jupyter notebook.

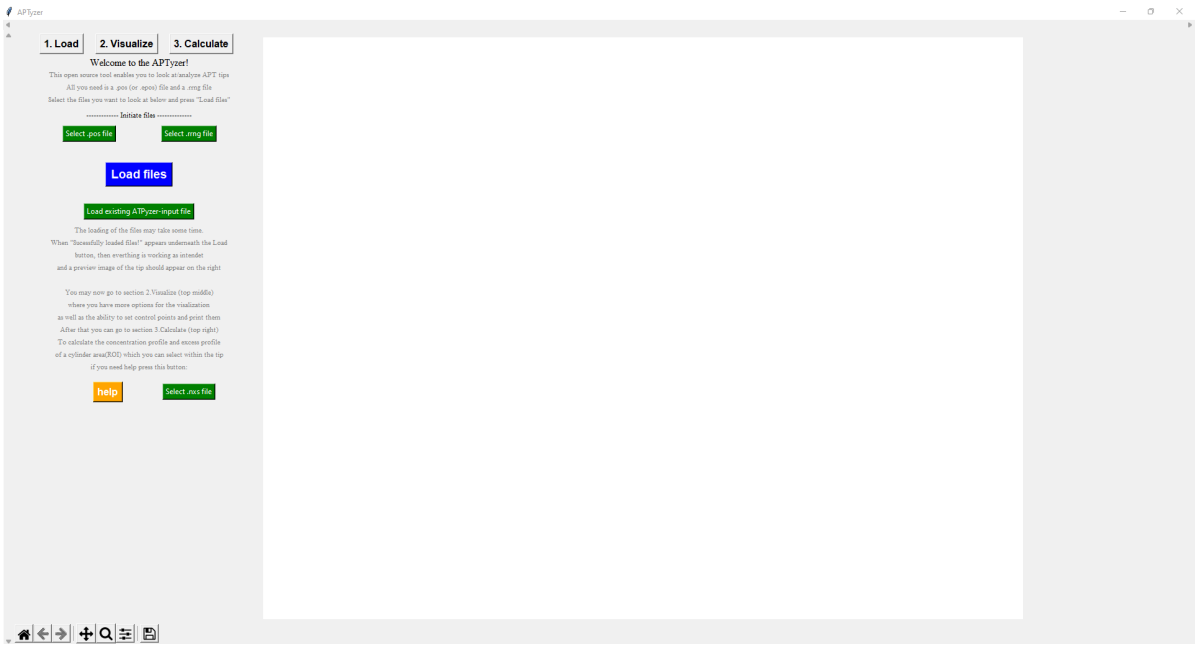


Figure 1: How the GUI should look like after starting the APT-analyzer.

As can be seen in the upper left side, the GUI contains 3 buttons representing 3 pages:

1. Load
2. Visualize
3. Calculate

The APT-analyzer starts on page ”1. Load” in which the input files are selected and loaded in. In order to visualize an APT specimen using the APT-analyzer, two files are necessary:

- .pos file (also .epos files can be used)
- .rrng file

So the first step is to load in a .pos/.epos file and a .rrng file from your directory. (Note that the APTyzer will only recognize the file as such if .pos/.epos or .rrng is written in them, also .POS/.EPOS and .RRNG are valid, everything else will result in the program not recognizing the file).After you successfully selected the files a label saying ”pos file selected” / ”rrng file selected” can be seen underneath the search buttons.

Alternatively a NXapm file in the format .nxs can also be loaded by using the button **Select .nxs file**. Now you may press the button **Load files**. It may take a while to load in the files and calculate the tip. If everything worked as it should, the message ”successfully loaded tip” will appear underneath the load button and a preview image of the tip will appear on the right side, including a description what kind of atoms and how many atoms are inside the specimen.

This may look as follows:

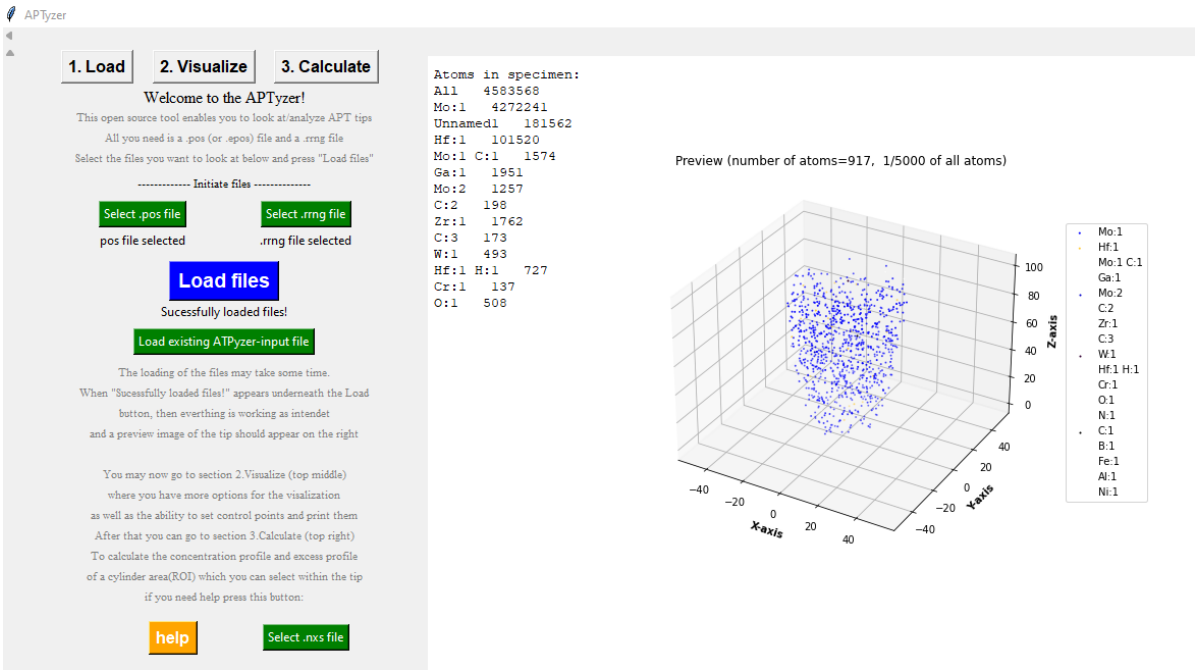


Figure 2: GUI after successfully loading in a tip.

If loading the files did not work as intended, the problem may be with the format of the files. In the case all atoms loaded in appear all white and have no label attached, the format of the rrng file might be in a format not recognized by the APT-analyzer. The rrng format loaded into the APT-analyzer has to be as in the following example file:

```
[Ions]
Number=2
Ion1=Mo
Ion2=Hf
[Ranges]
Number=3
Range1=30.5820 30.8770 Vol:0.01558 Mo:1 Color:0000FF
Range2=45.8259 46.2670 Vol:0.01558 Mo:1 Color:0000FF
Range3=59.5660 59.7500 Vol:0.02232 Hf:1 Color:FFCC33
```

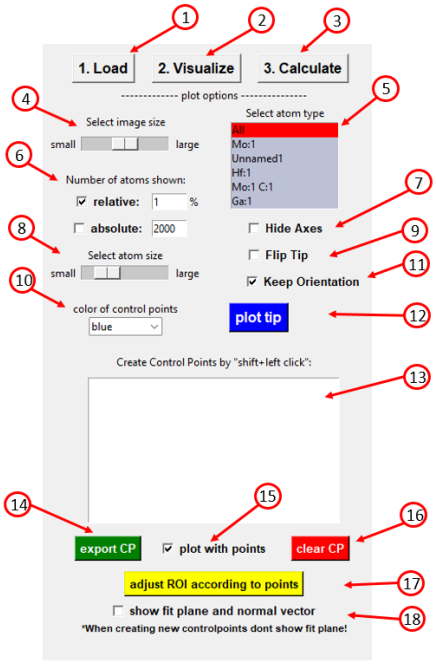
Below the button for loading your files is a short explanation how to proceed as well as the **help** button. If you press this button, it will open the Github page for the APT-analyzer where you can ask questions, point out bugs or suggest features. Please always include the version of the APTyzer you are using.

By clicking the button **Load existing APTyzer-input file** you can also load an input file, which was saved by a previous APTyzer session. This include all settings for the Region of interest (ROI), all control points (CPs) and all fit points. This files format is .txt and is written out in a specific way using the APTyzer. If the file is changed it may not be able to read it in again.

2 Visualize

2.1 Adjust plot

If you press the button labelled ”2.Visualize” at the top, you will open the visualization page. How this page should look like including a short description of each feature can be seen below:



1. Change to page 1. Load
2. Change to page 2.Visualize
3. Change to page 3. Calculate
4. Adjust the size of the figure
5. Select the atom types you want to show
6. Select the number of atoms
7. Checkbox for hiding the axes
8. Adjust the size of the atoms points
9. Turn the whole tip upside down
10. Selection box for choosing the colors of the control points
11. Checkbox to keeping the orientation of specimen when plotting
12. Plot the tip
13. Textbox in which the control points are saved, you can also write your own control points in there, but be careful of the format
14. Export the content of the textbox to hdf5
15. Checkbox to make controlpoints visible/invisible in the plot
16. Clear the entire content of the textbox
17. Button for adjusting the ROI used for concentration/excess calculation according to the control points
18. Checkbox for showing the fit plane of the control points in addition to the normal vector to the fit plane

Figure 3: The features of page 2. Visualize

If you want to plot the tip now you may press the blue button **plot tip** .

Important to note is that whenever you **change something** in the settings the plot button needs to be **pressed again** in order to update.

When you press it after having changed some of the settings, the window may appear as follows:

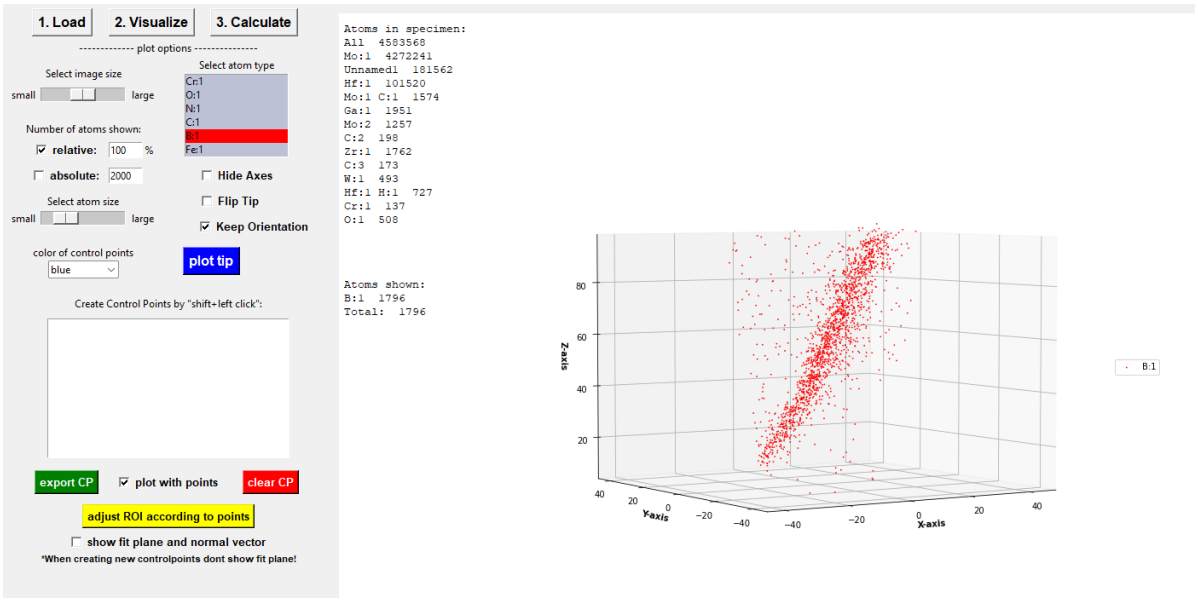


Figure 4: An example for an adjusted plot

Inside the 3d plot you can **adjust the angle** from which you are looking at the object and you can **zoom in**, depending on your mouse button configurations. The default setting in Windows 10 is that by holding the left mouse button you can rotate the 3d plot and look at it from different angles and by holding the right mouse button and moving your mouse up and down you can zoom in and out of the image.

As can be seen in fig. 4 it is possible to select and display single atom types. In the listbox (Fig.3 Nr.5) multiple atom types can be selected to be shown.

! It is important to note that the listbox and all the other boxes are **scrollable**!

If no atom type is selected "All" will automatically be selected and all atom types will be shown. At the left side of the plot the number of atoms plotted is visible as well as the amount compared to the total number of atoms in the .pos file. The number of atoms can be selected under "Number of atoms shown:", which can be either set in relative terms, in which a % amount of atoms from the total amount can be selected. When selecting absolute terms, a set amount of atoms can be shown. This is then applied on each atom type, so for example, if you select 2000, then up to 2000 atoms of each atom type will be depicted (if there are less than 2000 atoms in the specimen then the total amount of atoms will be depicted). Since the number of atoms shown is calcualted by rounding, depending on how many atoms are in the specimen of the selected type, not the exactly selected amount may be depicted. **You need to be careful not to display too many atoms at once**, because it may cause long loading times. The best way would be to set the "Number of atoms shown" rather low at the start (maybe 0.1 % or less

depending on how many atoms are in your specimen) gradually increase the number of atoms that are loaded in the plot. By continuously pressing plot tip the plot can be updated with the new settings.

2.2 Creating Control points (CPs)

The APTzer also lets you mark points of interest (control points). Creating CPs can also be used to locate the orientation of a grain boundary, which will be explained later on.

If you want to create CPs you simply click on the plot while holding the ”shift” key. This will select the coordinates of the nearest atom to your mouse curser and save them inside the control point text box. It is also marked in the plot by a ”+” which is in the color selected in the selection box labelled ”color of control points”.

! It has to be noted however that if your plot becomes out of focus, by either selecting a specific element in the listbox or by writing inside your text box, you need to press **plot tip** again before selecting control points. This will put the plot back into focus and selecting control points will be possible again. Also if you show the plane which is fitted by your CPs, the creation of the control points is deactivated and you have to deselect ”show fit plane and normal vector”, underneath the adjust button to be able to create CP again. Generally if the creating of the CP doesnt work, first thing to try it pressing **plot tip** again!

This should look as follows:

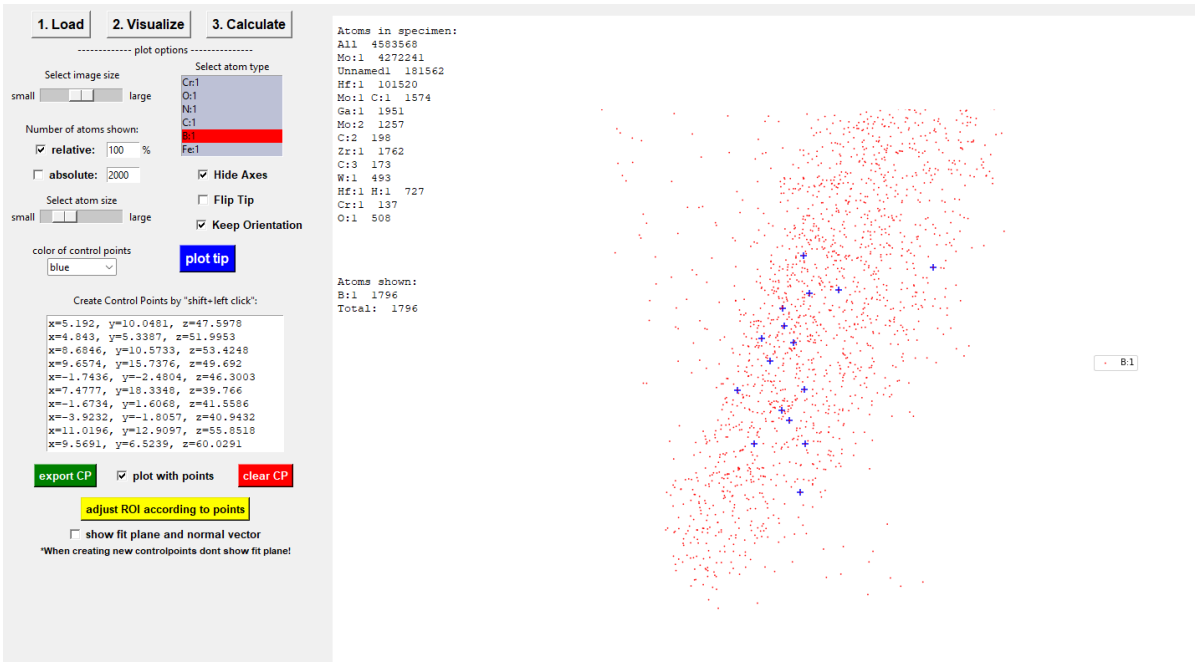


Figure 5: Selecting control points along the grain boundary of an APT tip.

It is important to note that the **textbox** can be customized to **your liking**. You can **delete** and **add** points also by just **using** the text box. You can even create new control points which are not already points of the APT specimen, by simply writing the x,y and z coordinates you want and seeing where the new point is plotted.
However, you need to be careful and only use the exact same format as shown in fig. 5 otherwise the APT-analyser may have problems reading in the points. You can also quickly clear all control points by pressing **clear CP** . If you want to print your control points into a .hdf5 file you may press the button **export CP** . This will automatically create a hdf5 file with the name "controlpoints.h5" in the same folder you selected the .pos file.

If you have created **more than 3 control points** and you want to align the area (cylinder shape) in which the excess and concentration calculation is performed according to the control points you may press the button, **adjust ROI according to points** . This will fit a plane through all your selected control points inside the text box and calculate the normal vector of this plane, which will be used to set the cylinders angles. It also calculates the centre of all selected points in x,y and z and sets this centre as the centre of the cylinder. After you press the yellow adjust button, the checkbox to show the cylinder on page " 3.Calculate " will automatically be checked and you just need to plot the tip again to show the aligned cylinder. An example on how this should look like can be seen in fig. 6.

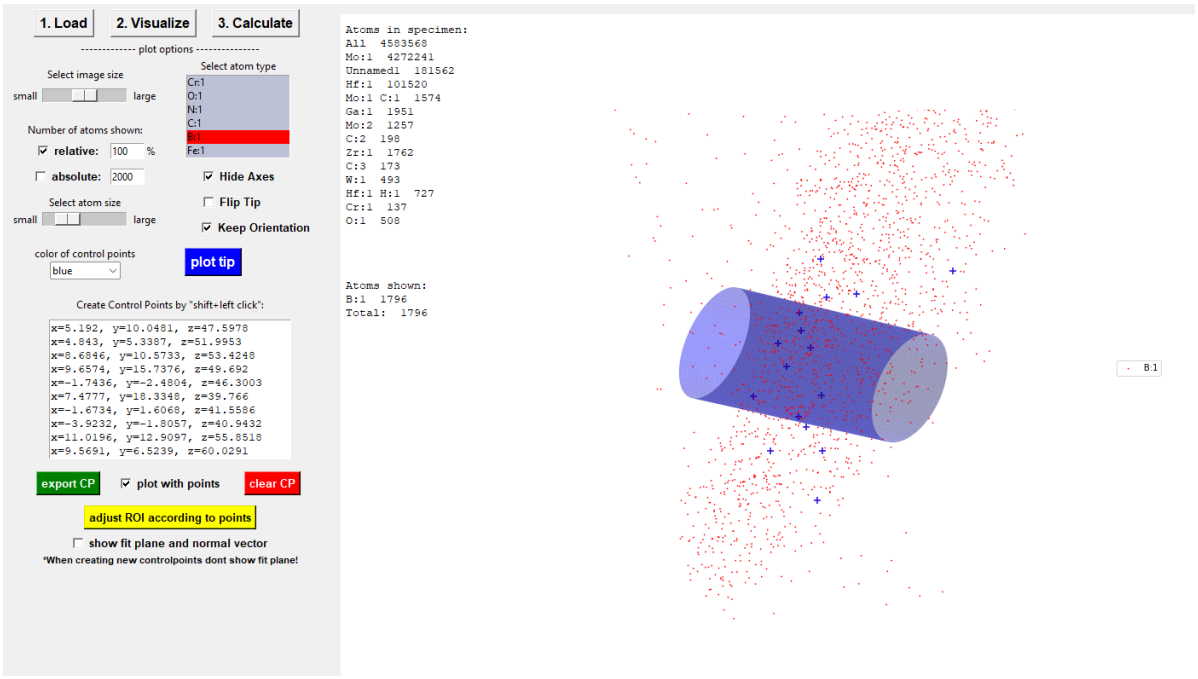


Figure 6: Adjusting the cylinder along the control points

An illustration how the fit plane looks like as well as its normal vector in the centre of the fitted control points (in red) can be seen in fig. 7 . The plane fitting all control points can be made visible by checking the checkbox **"show fit plane and normal vector"**. It has to be noted that the checkbox **"plot with points"** has to be checked, so the control points also have to be shown in order for the fit plane to appear.

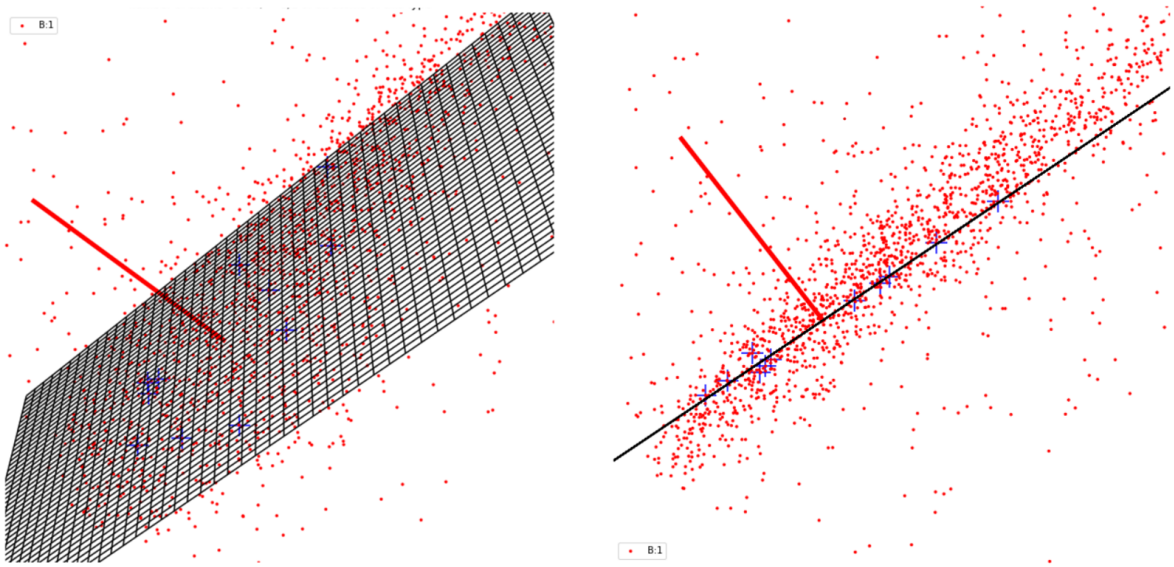


Figure 7: An illustration of the fit plane through all control points including the normal vector of the plane.

Now in order to actually perform the excess and concentration calculations you may go to the page ”3.Calculate”.

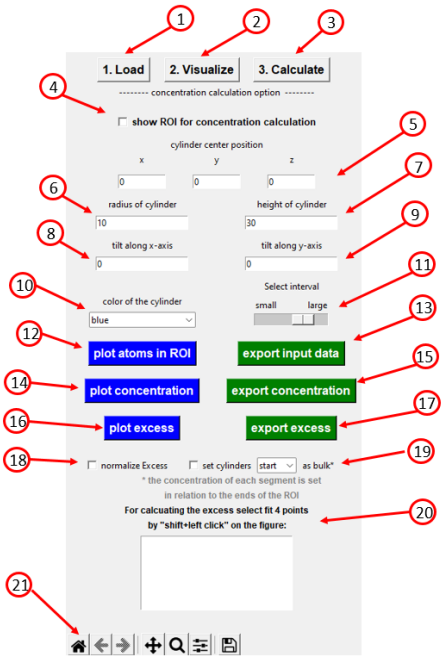
3 Calculate

3.1 Choose cylinder for calculation

In order to calculate, plot and print the concentration data of all or single atom types, you need to go to page ”3.Calculate” which can be found on the top left corner of the GUI. How page ”3.Calculate” should look like and the description of each button can be seen in fig. 8 .

When you check the checkbox **”show cylinder for concentration calculation”**, and press the **plot tip** button, a cylinder will appear in the 3d plot of the tip. This cylinder indicates the area in which the concentration and excess calculation will take place. You can change the position of the cylinders centre by changing the x,y and z values. Also the radius and the height of the cylinder can be adjusted, as well as the cylinder’s tilt along the x and y-axis. Lastly the colour in which the cylinder appears and the length of the interval of the concentration / excess calculation can be adjusted.

All the adjustments you did on page ”3.Calculate” regarding the position, size and orientation of your ROI are visible when you press **plot tip** on page ”2.Visualize”.



1. Change to page 1. Load
2. Change to page 2. Visualize
3. Change to page 3. Calculate
4. Checkbox to select if ROI (cylinder) should be shown in plot
5. Adjust the x,y and z coordinates of the cylinders center
6. Adjust the cylinders radius
7. Adjust the cylinders height
8. Adjust the cylinders tilt along the x-axis
9. Adjust the cylinders tilt along the y-axis
10. Adjust the color of the cylinder
11. Select the size of the interval in which the concentration and excess will be calculated and plotted
12. Plot a close up of the atoms inside the cylinder
11. Export all input data to .txt file, including all adjustments to the ROI, all control points and all fit points
14. Plot the concentration profile along the cylinder with set interval
15. Export the plotted concentration profile in a .csv file
16. Plot the excess profile along the cylinder with set interval
17. Export the plotted excess profile in a .csv file
18. Checkbox for normalizing the excess calculations (going from 0 to 1)
19. Checkbox for setting a bulk value either at the start of the cylinder or at the end. This is to set a reference concentration in the concentration profile
20. Text box for selecting fit points for excess calculations
21. Toolbar to save the plot

Figure 8: General description of features on page 3.Calculate.

An example of a tip with a cylinder can be seen in fig. 9.

If you want to see a close up of the cylinder, as seen in fig. 10, you may press **plot atoms in ROI**. This will show you exactly how the atoms inside the selected ROI (cylinder) are arranged and may be useful when the ROI is tilted. It has to be noted that currently the feature of selecting CPs is only implemented when plotting the whole tip not when plotting the close up of the atoms inside the ROI.

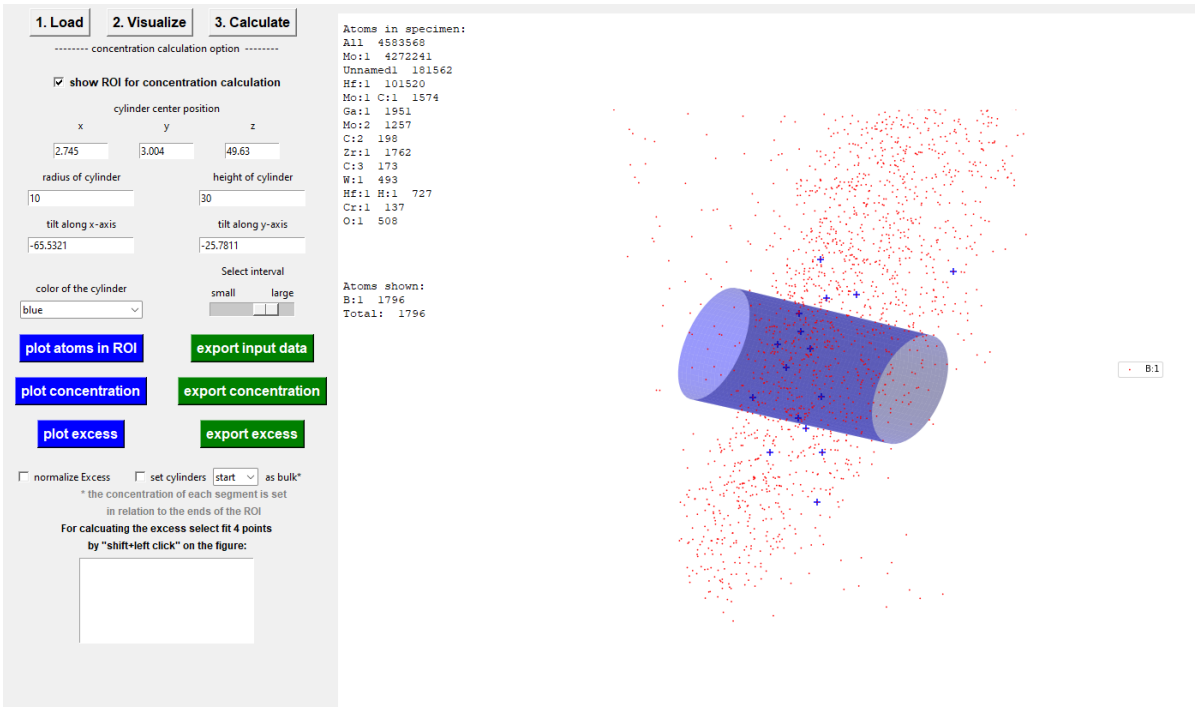


Figure 9: Example plot a tip with a cylinder area for concentration calculation.

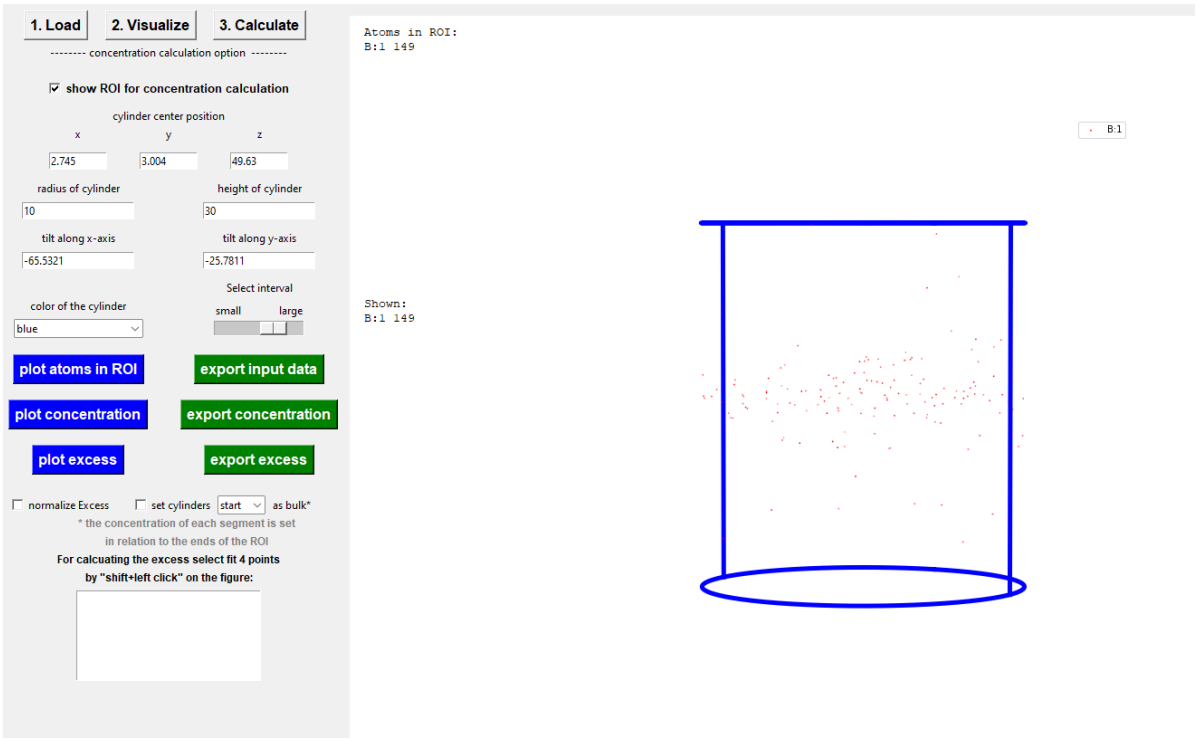


Figure 10: Close up plot of the atoms inside the cylinder area

3.2 Concentration and Excess calculation

When you want to see the concentration profile along your cylinder you may press the button **plot concentration** . This creates a 2d plot which should look similar to fig. 11.

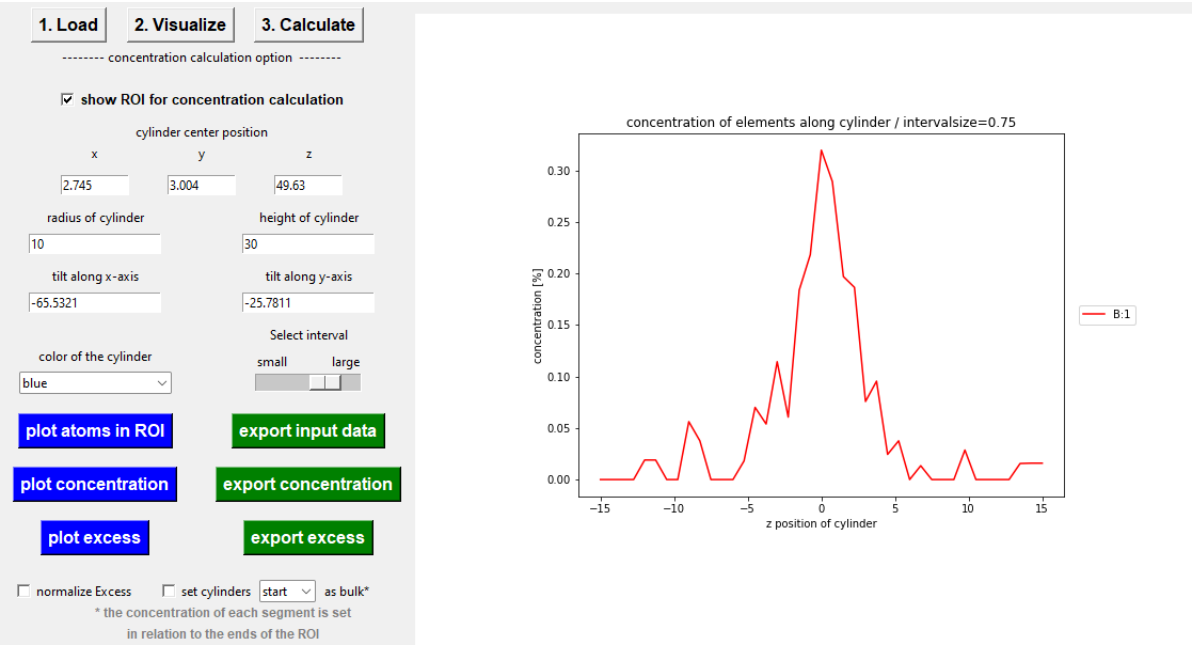


Figure 11: Example of a Concentration profile plot. In this case the boron accumulation in the Grain boundary can be seen.

The concentration profile is usually calculated by splitting the cylinder into many segments and then calculate the concentration of each element of each individual segment separately. Another option would be to set one end of the cylinder as the bulk and calculate the concentration compared to the bulk concentration. This can be done by checking the ”set cylinder as bulk” checkbox and selecting either the ”start” or the ”end” as your comparison point. Then the concentration profile will be calculated depending on the concentration of one of the cylinders ends. In the case that the cylinder goes outside the APT specimen then you would see the concentration going down, while in the normal case the concentration generally stays constant until no more points are inside a segment of the cylinder, at which point the concentration will drop to zero.

After you plotted the concentration you can export the concentration in a .csv file by pressing the **export concentration** button. The csv. File will automatically be generated with the name ”APTyzer-concentration.csv” into the folder, where you have chosen the .pos file . In it the concentration data of each selected atom type will be written as well as the length scale of the cylinder. Similar to the concentration, also the excess can be exported by using the **export excess** button. This may look similar as in fig. 12.

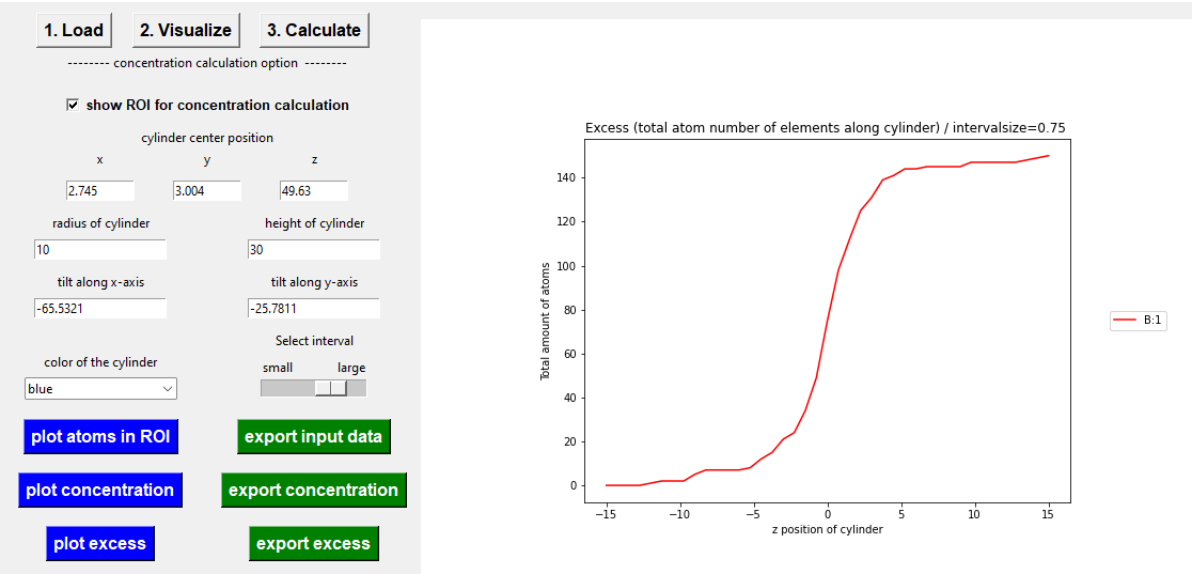


Figure 12: An example of an excess plot. This shows the excess referring to the same boron grain boundary accumulation.

!It has to be noted that you first need to plot the excess before you can export it, otherwise you will export the excess from your previous settings. Same is true for the concentration plot/print. Also important to note is that the calculated excess and concentration always relate to all the atoms of the selected type, no matter how many are depicted on screen by the plot, the concentration/excess calculation always considers all of them!

The excess can also be normalized (going from 0 to 1) instead of displaying the total amount of atoms. This is done by checking the normalize checkbox. This may help seeing grain boundary accumulation while looking at multiple elements with different amounts of total elements.

To actually calculate the interfacial excess, you need to select 4 points on the excess plot in order to fit two lines. The first two points you place will fit the first line while the third and fourth point you place will fit the second line. To select points you have to press the left mouse button on the screen while holding the ”shift” button. This should look as in fig. 13.

!When you want to calculated the interfacial excess only show one atom type, otherwise the center of the GB will not be correctly selected!

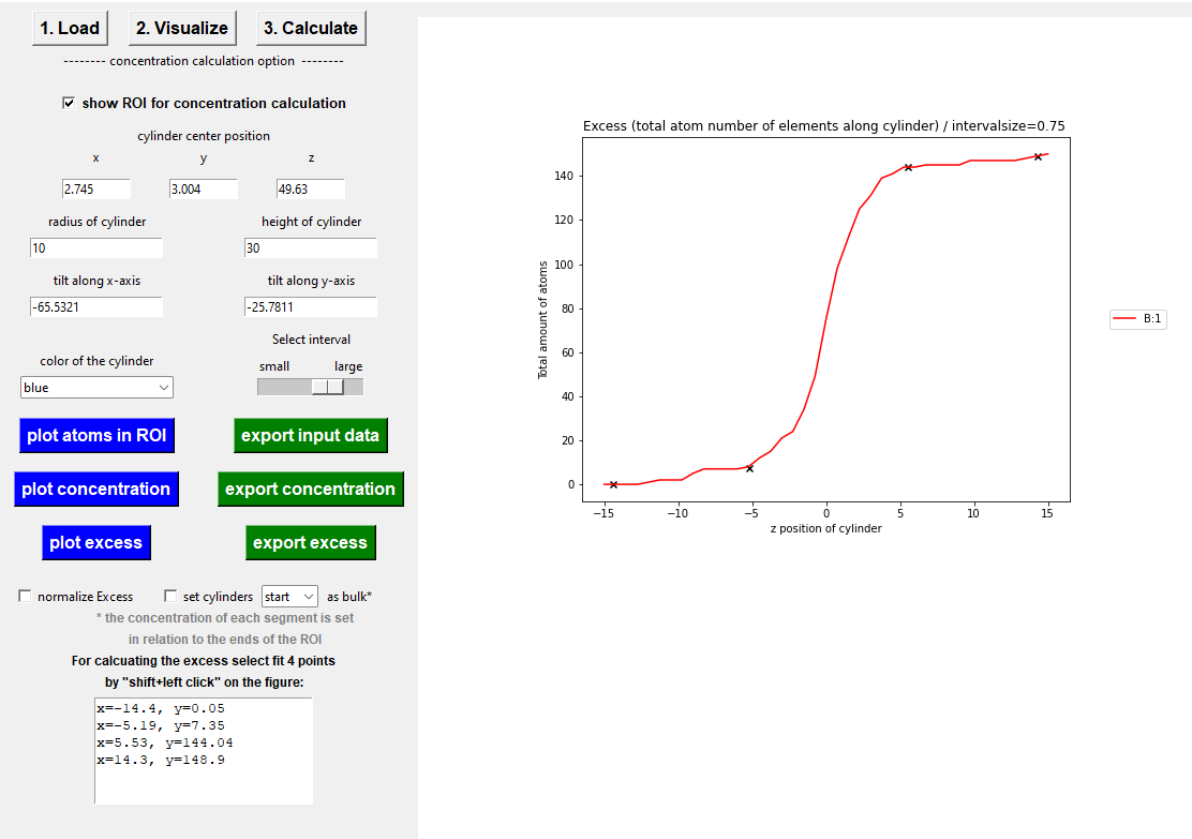


Figure 13: Selecting points on the excess plot in order to fit the interfacial excess value

After you selected exactly 4 points (it will not work if you select more or less than 4 points), press plot excess again in order to perform the calculation. Then the two lines and the interfacial excess will be plotted. An example of this can be seen in fig. 14.

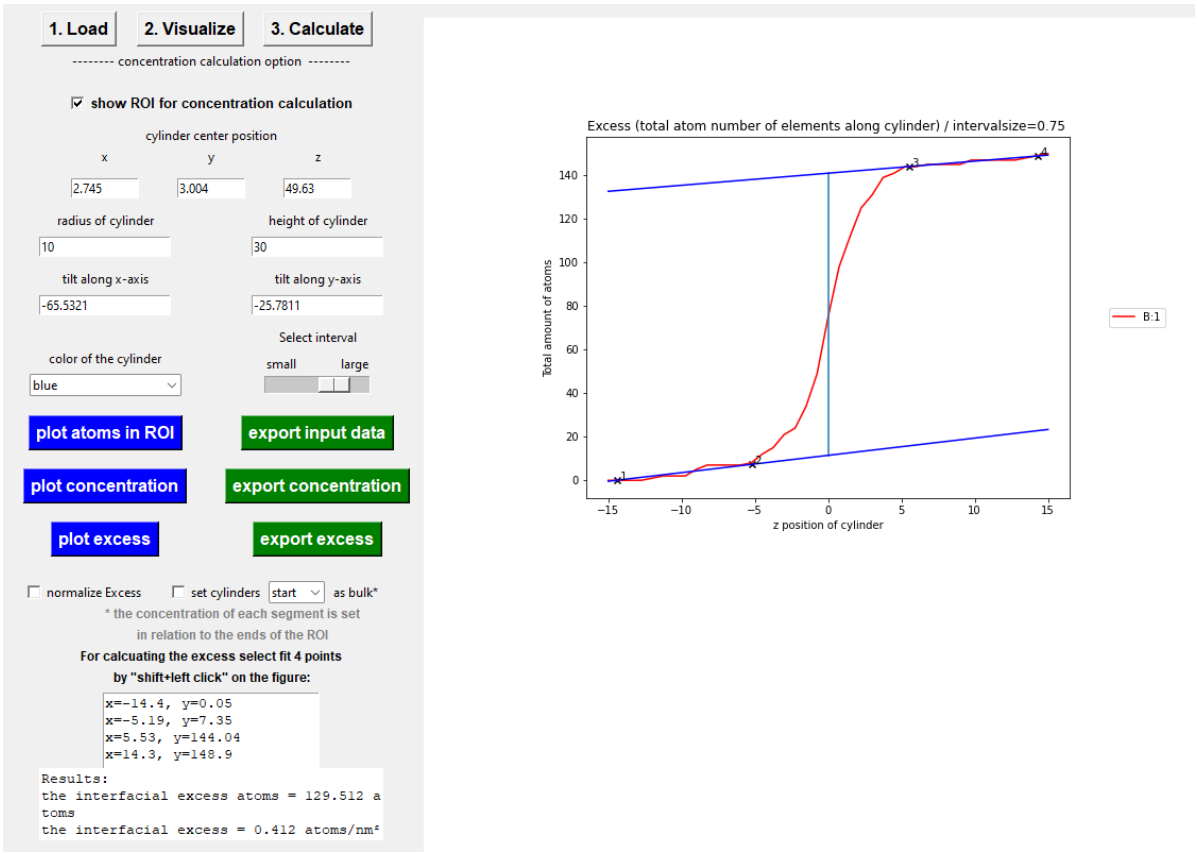


Figure 14: Calculation of interfacial excess

Be adjusting the cylinder along control points, it should be guaranteed that the excess is around the 0 value, so if the slopes of the two lines are different it can still be fitted using this method. That's it for the tutorial. If you have any questions, feel free to contact me. **Enjoy using the APT-analyzer!**

4 List of Versions

The APT-analyzer was written using Python 3.8.8 using following package versions:

- numpy 1.20.1
- tkinter 8.6 TkVersion
- matplotlib 3.3.4
- pandas 1.3.4

References

[1] K. Leitner et al. “How grain boundary chemistry controls the fracture mode of molybdenum”. In: *Materials & Design* 142 (Mar. 2018), pp. 36–43. DOI: 10.1016/j.matdes.2018.01.012.