

APT- analyzer Tutorial

The APT-analyzer 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.

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1. Getting started / Loading files

Run the APT-analyzer code with jupyter note. If successful following window should appear:

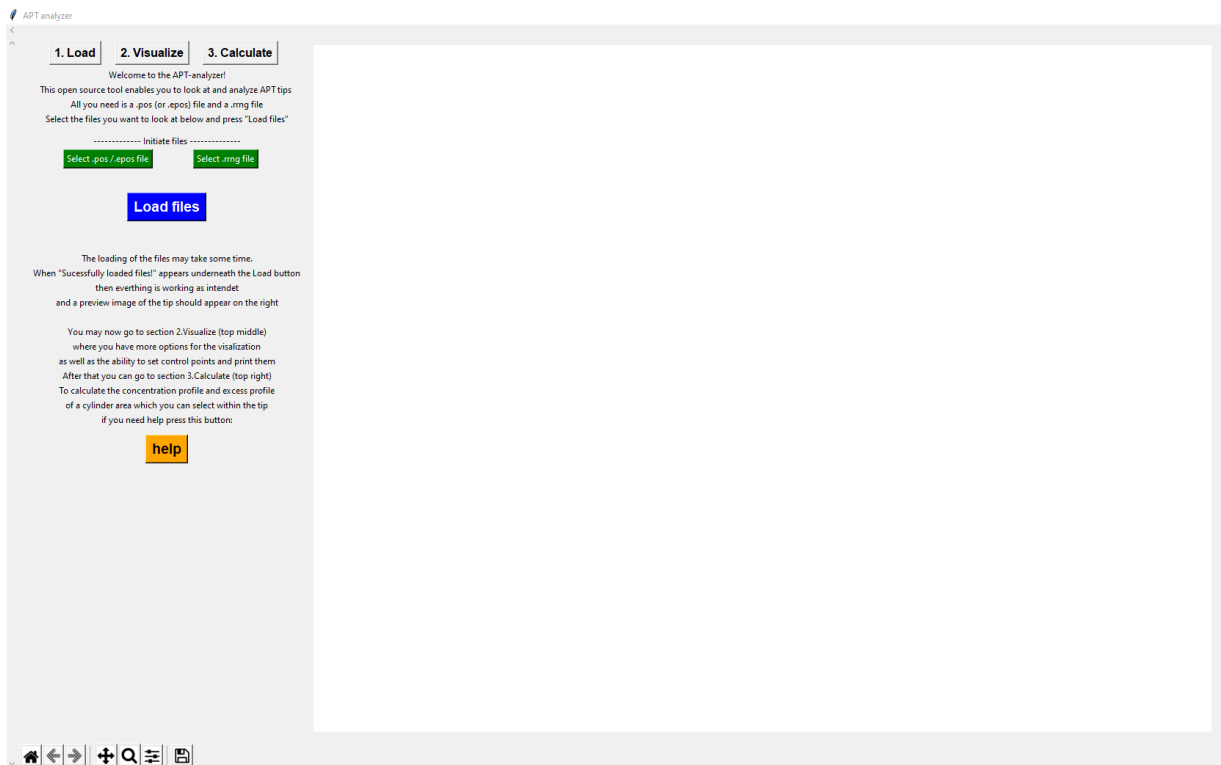


Fig.1 How the GUI should look like after starting the APT-analyzer

If the GUI does not look as in Fig.1, but has a different format with overlapping icons, one possibility how to solve this issue is to restart the kernel of jupyter note.

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

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 tip 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 APT-analyzer 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. 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.

This may look as follows:

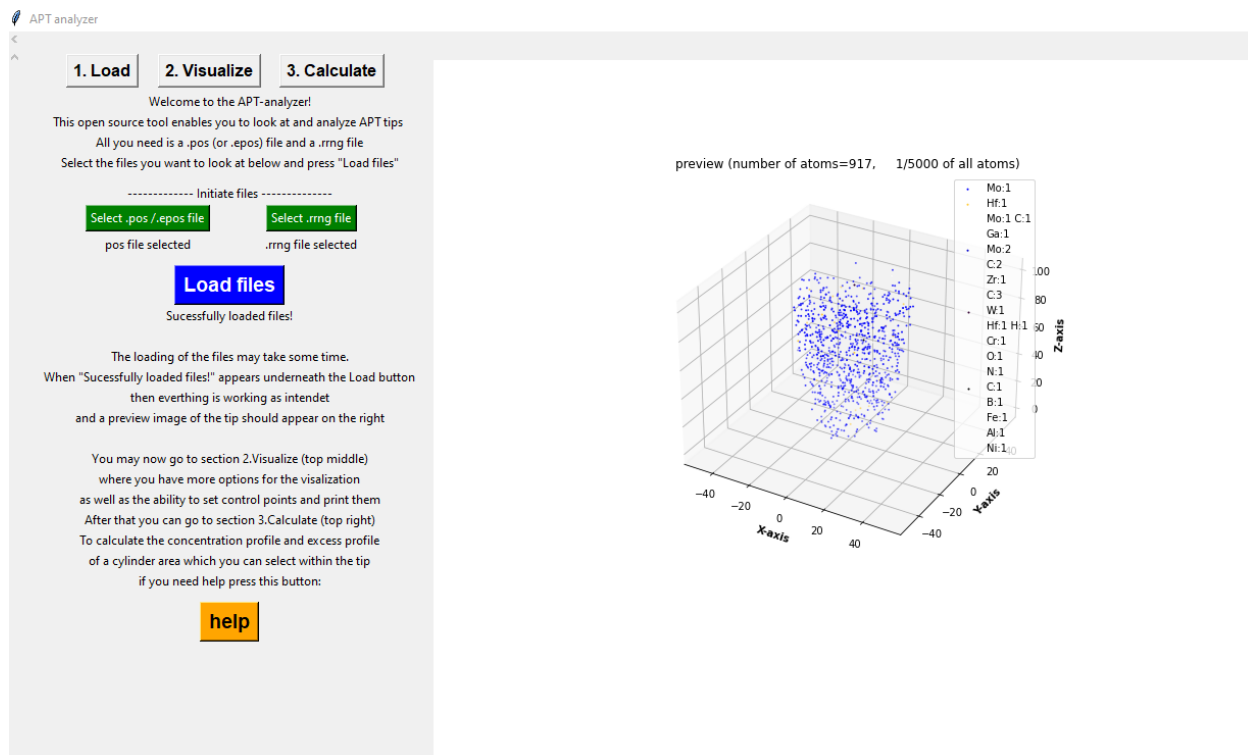


Fig. 2 GUI after successfully loading in a tip.

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:

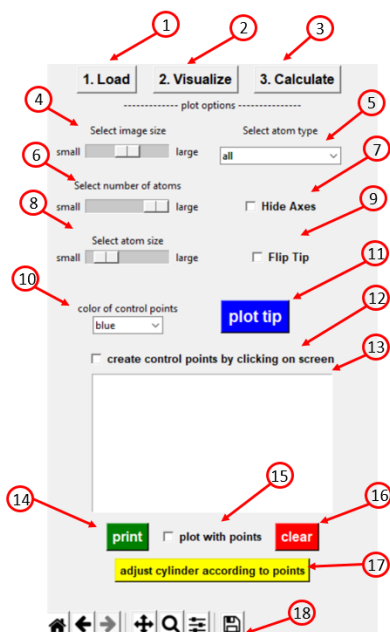
```
[Ions]
Number=2
Ion1=Mo
Ion2=Hf
[Ranges]
Number=3
Range1=30.5820 30.8770 Vol:0.01558 Mo:1 Color:0000FF
Range2=45.8259 46.2670 Vol:0.01558 Mo:1 Color:0000FF
Range3=59.5660 59.7500 Vol:0.02232 Hf:1 Color:FFCC33
```

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.

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 type
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. Plot the tip
12. Checkbox for making it possible to create control points
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. Print the content of the Textbox
15. Checkbox to make controlpoints visible/invisible in the plot
16. Clear the entire content of the textbox
17. Button for adjusting the cylinder used for concentration/excess Calculation according to the control points
18. Toolbar to save the plot

Fig.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 changing some of the settings, the window may appear as follows:

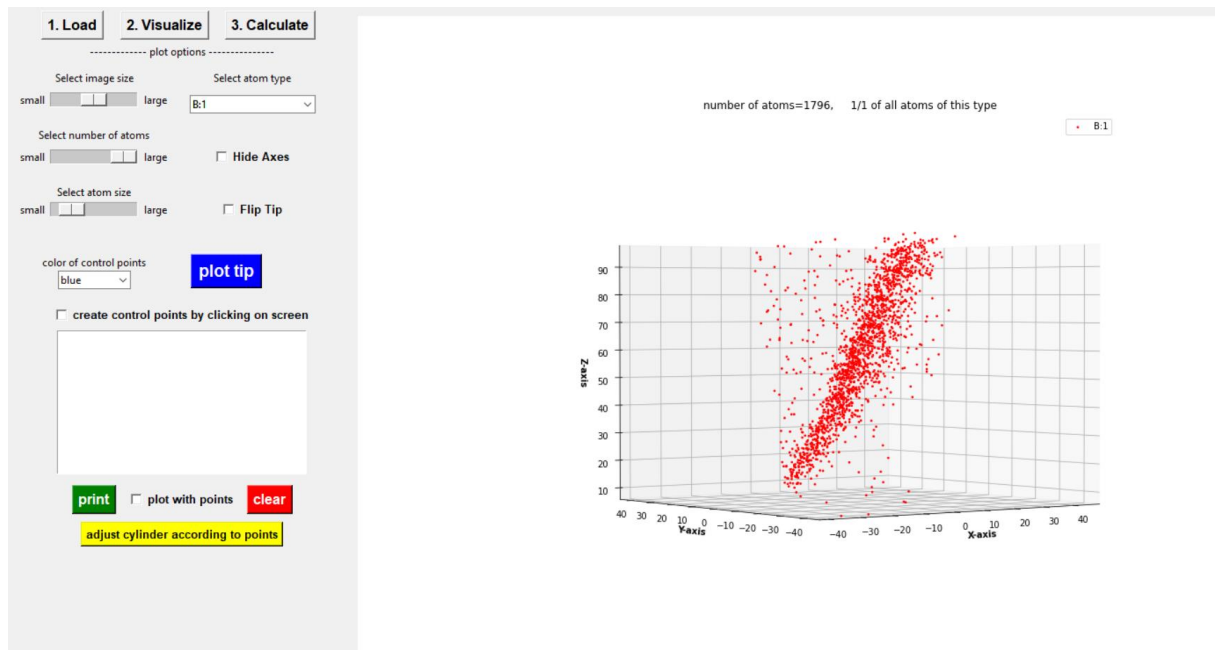


Fig.4 An example for an adjusted plot

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 should be 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 you saw in Fig. 4 you can select single atom types. At the top 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. In the example of Fig. 4, 1796 atoms of B are displayed which is all the B atoms in the .pos files. **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 “Select number of atoms” slider to small at first and gradually make it larger when you see that not enough atoms are loaded in the plot. By continuously pressing **plot tip** the plot can be updated with the new settings.

2.2 Creating Control points

If you want to create control points, you need to check the “create control points by clicking on screen” checkbox and afterwards press **plot tip**. If you don’t plot the tip again it won’t be updated with the ability to make control points. Now each time you press the screen the atom which is closest to your mouse cursor is selected as a control point and saved 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”. This should look as follows:

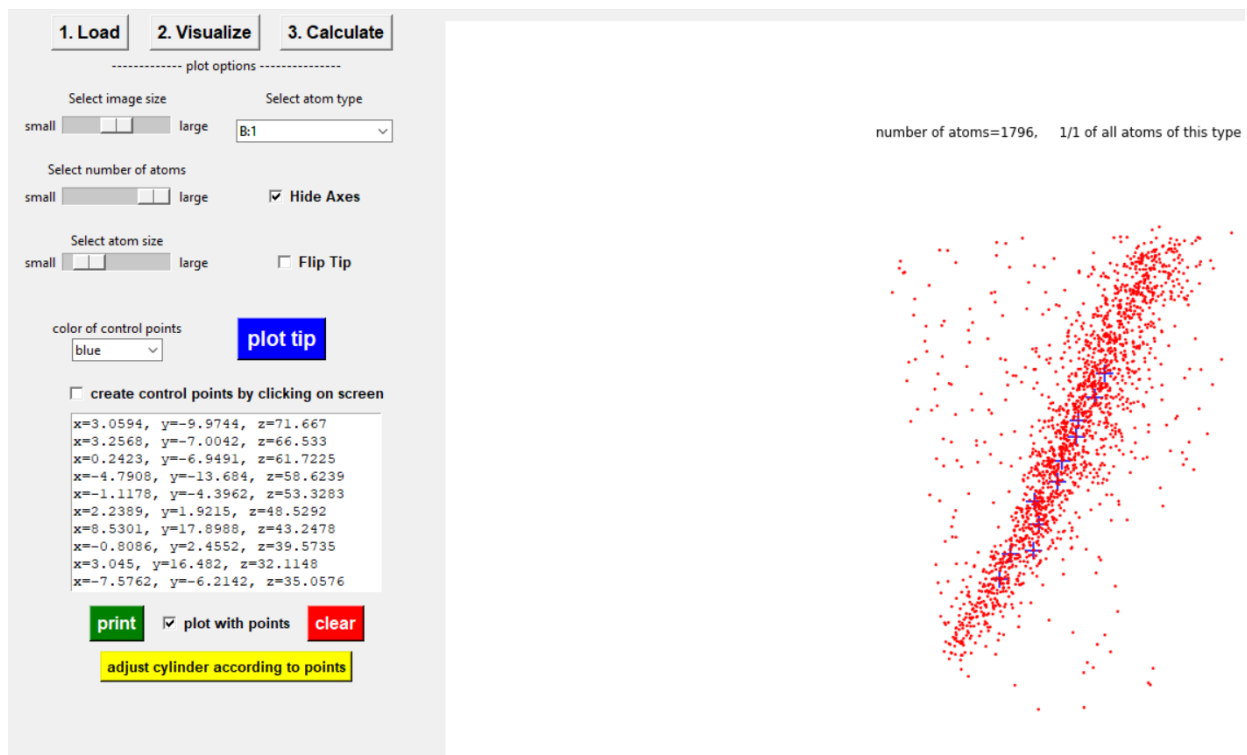


Fig. 5 Selecting control points along the grain boundary of an APT tip.

If you adjust the screen while the “create controlpoints” checkbox is checked, each time you press the screen a control point will be created, so it is better to **adjust the screen before** you want to create control points. **Note** that each time you **check/uncheck** the “create control points” checkbox, **you need to press **plot tip**** again in order to **update** the screen with/without the mechanic.

If you want to change the angle or zoom in to better locate the control point you want to select, uncheck the “create controlpoints” , press the plot button and adjust your screen, then check the “create controlpoints” checkbox and press the plot button again. This will keep the plot in the adjustment selected before.

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 tip, 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**. If you want to print your control points into a .hdf5 file you may press the button **print**. This will automatically create a hdf5 file in the folder of the APT_analyzer named “controlpoints.h5”

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 cylinder 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 be automatically be checked and you just need to plot the tip again to show the aligned cylinder. An example on how this would look like can be seen in Fig. 6.

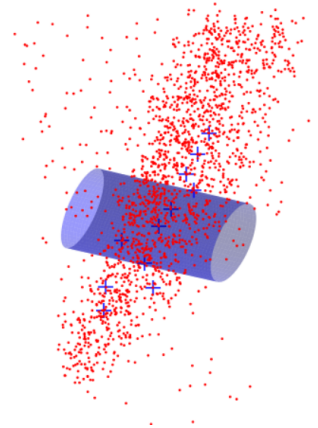
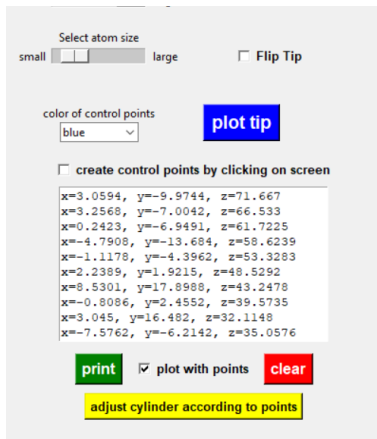


Fig. 6 Adjusting the cylinder along the control points

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 Fig7. This image is just for illustrative purposes and does not show a feature of the APT-analyzer, so you won't be able to replicate it with the default version of the APT-analyzer. If you want me to include the option to show the fit plane and its normal vector, please write me and I can include it in future updates.

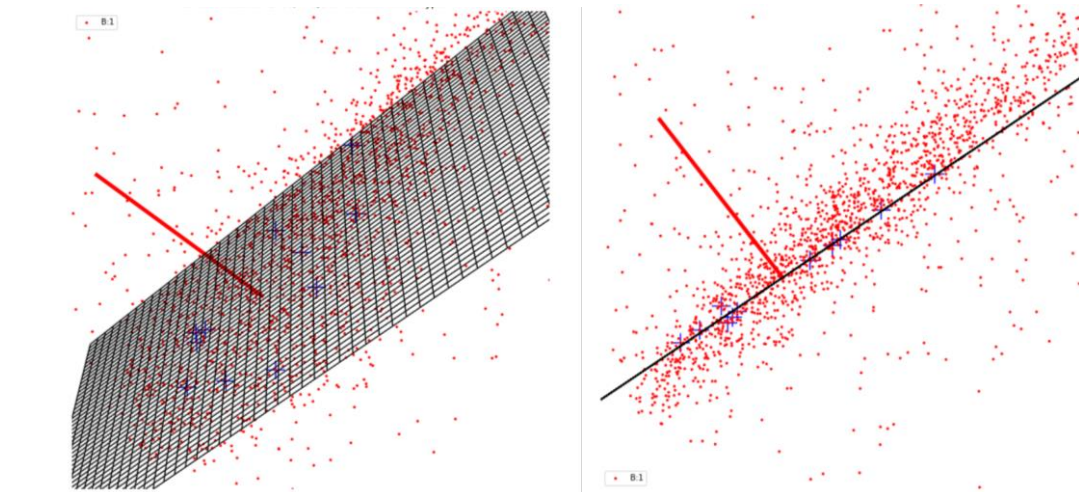


Fig.7 An illustration of the fit plane through all control points including the normal vector of the plane. Take note that the visualization of the plane is not a feature of the APT-analyzer.

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 below:

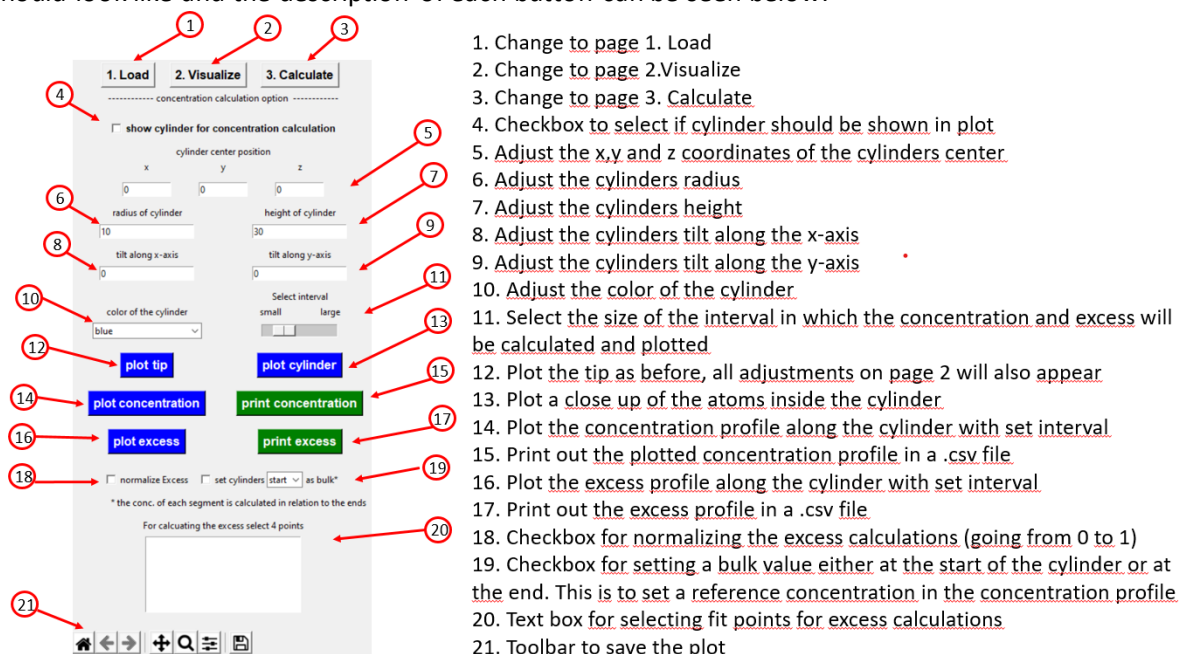


Fig. 7 General description of features on page 3.Calculate.

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 2. Visualize should be also visible here when you press **plot tip** and likewise if you set something on page 3 you can also see it when you press **plot tip** on page 2.

An example of a tip with a cylinder can be seen in Fig. 8.

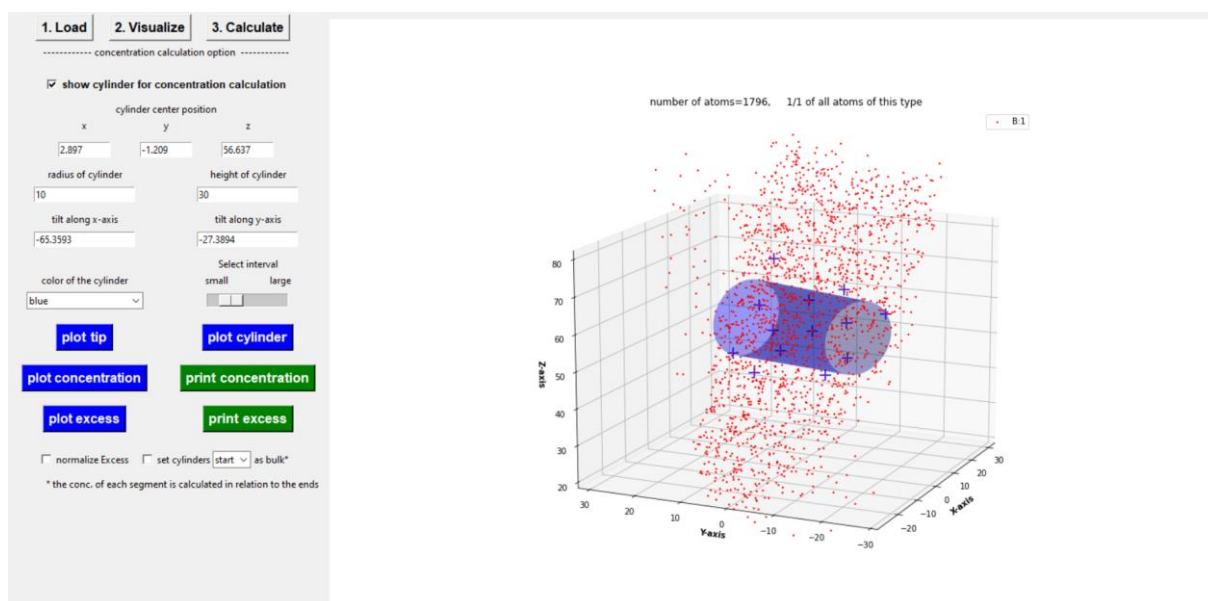


Fig. 8 Example plot a tip with a cylinder area for concentration calculation.

If you want to see a close up of the cylinder you may press **plot cylinder**. This will show you exactly how the atoms inside the selected cylinder are arranged and may be useful when the cylinder is tilted. It has to be noted that currently the feature of selecting control points is only implemented when plotting the whole tip not when plotting the close up of the atoms inside the cylinder.

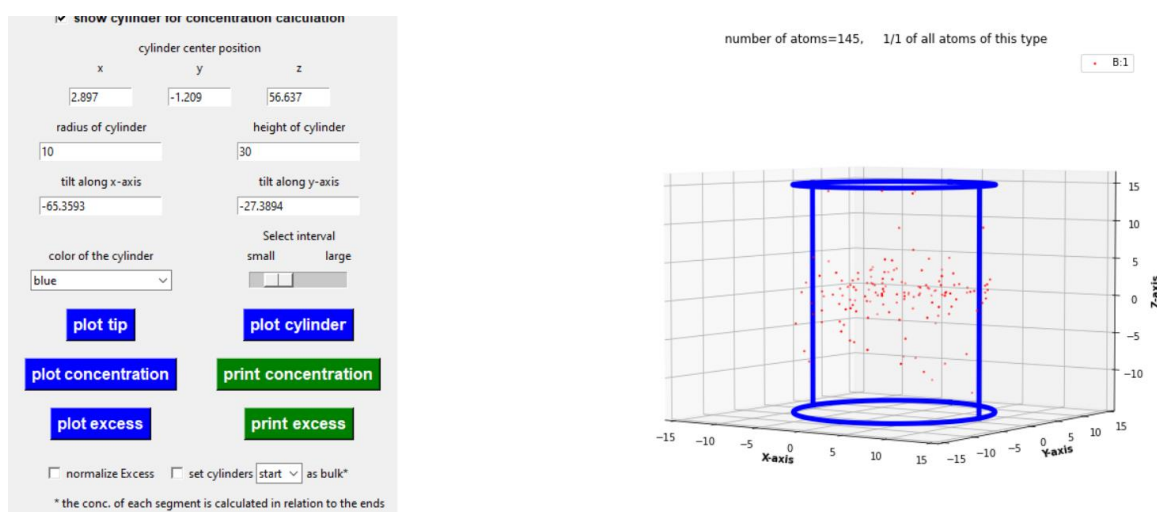


Fig. 9 Close up plot of the atoms inside the cylinder area

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.10.

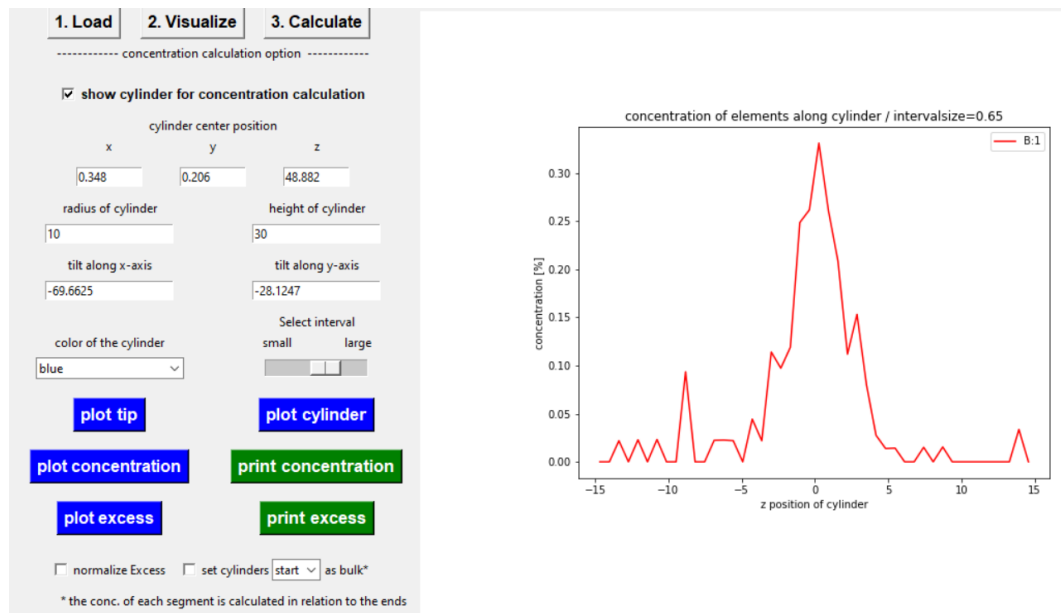


Fig. 10 Example of a Concentration profile plot. In this case the boron accumulation in the Grain boundary can be seen.

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 tip 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 print the concentration in a .csv file by pressing the **print concentration** button. The csv. File will automatically be generated into the folder, where you have the APT-analyzer with the name “APT_analyzer_concentration.csv”. 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 plotted by using the **plot excess** button. This may look similar to this:

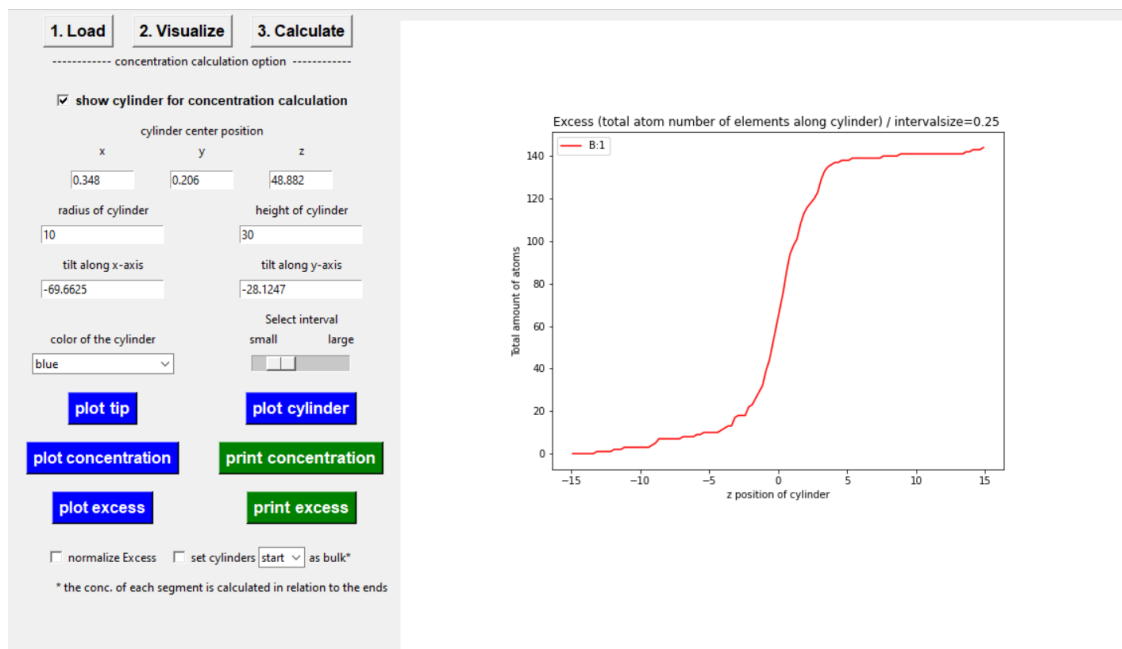


Fig. 11 An example of an excess plot. This shows the excess referring to the same boron grain boundary accumulation.

By pressing the **print excess** button the excess can then be printed into a .txt file.

It has to be noted that you first need to plot the excess before you can print it, otherwise you will print 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. This should look as follows:

☒ show cylinder for concentration calculation

cylinder center position

x	y	z
3.885	-5.662	62.512

radius of cylinder: 10 height of cylinder: 30

tilt along x-axis: -62.7992 tilt along y-axis: -26.7613

color of the cylinder: blue

Select interval: small large

plot tip **plot cylinder**

plot concentration **print concentration**

plot excess **print excess**

☐ normalize Excess ☐ set cylinders start as bulk*

* the conc. of each segment is calculated in relation to the ends

For calculating the excess select 4 points

```

x=-14.11, y=1.44
x=-3.53, y=9.79
x=6.33, y=134.07
x=14.66, y=141.95
  
```

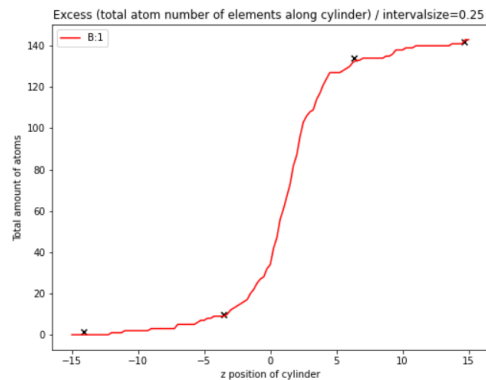


Fig. 12 Selecting points on the excess plot in order to fit the interfacial excess value

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.13.

cylinder center position

x	y	z
3.885	-5.662	62.512

radius of cylinder: 10 height of cylinder: 30

tilt along x-axis: -62.7992 tilt along y-axis: -26.7613

color of the cylinder: blue

Select interval: small large

plot tip **plot cylinder**

plot concentration **print concentration**

plot excess **print excess**

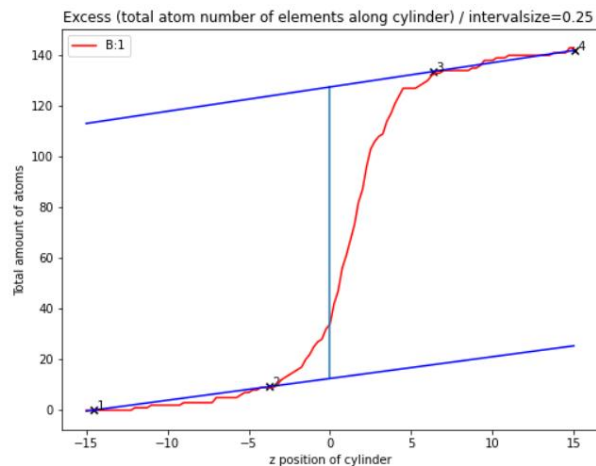
☐ normalize Excess ☐ set cylinders start as bulk*

* the conc. of each segment is calculated in relation to the ends

For calculating the excess select 4 points

```

x=-14.54, y=0.05
x=-3.74, y=9.32
x=6.33, y=133.6
x=15.03, y=141.95
  
```



Calculated with the following 4 points:

point 1: x = -14.54 y = 0.05

point 2: x = -3.74 y = 9.32

point 3: x = 6.33 y = 133.6

point 4: x = 15.03 y = 141.95

the interfacial excess atoms = 114.994 atoms

the interfacial excess = 0.366 atoms/nm²

Fig. 13 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!**