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:

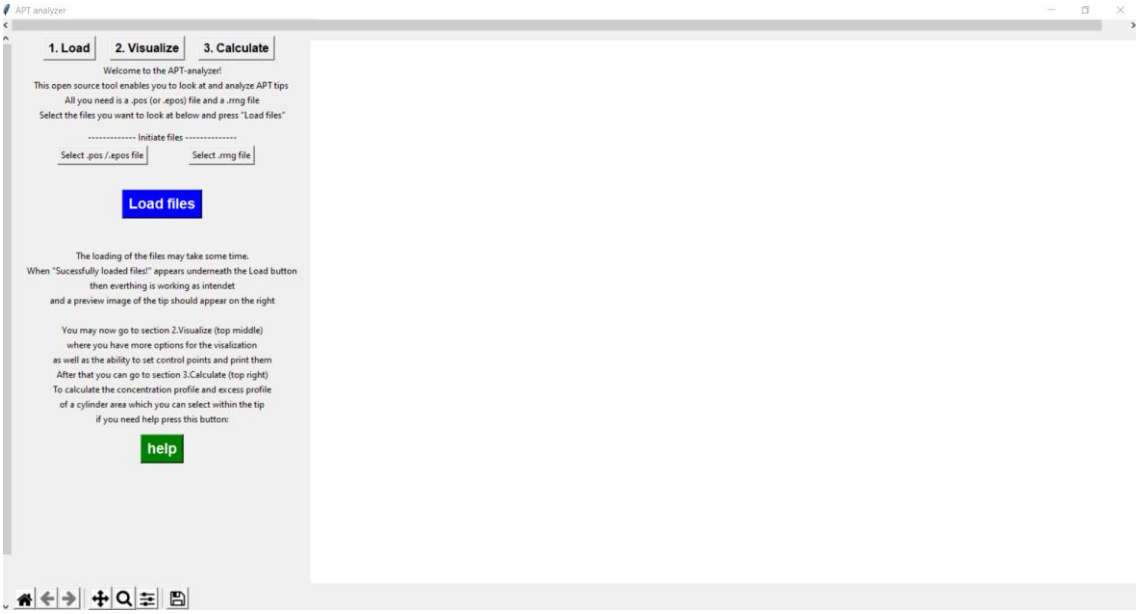


Fig.1 How the GUI should look like after starting the APT-anylzer

As can be seen in the upper left side, the Gui contains 3 pages:

1. Load
2. Visualize
3. Calculate

The APT-analyzer starts of in page 1. Load in which the input files are selected and loaded in. In order to visualize a APT tip using the APT-analyzer, two files are necessary:

- .pos file (instead of a .pos file also a .epos file 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 and a label saying "pos file selected" /"rrng file selected" can be seen underneath the search button, the blue button **Load files** may be pressed.

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:

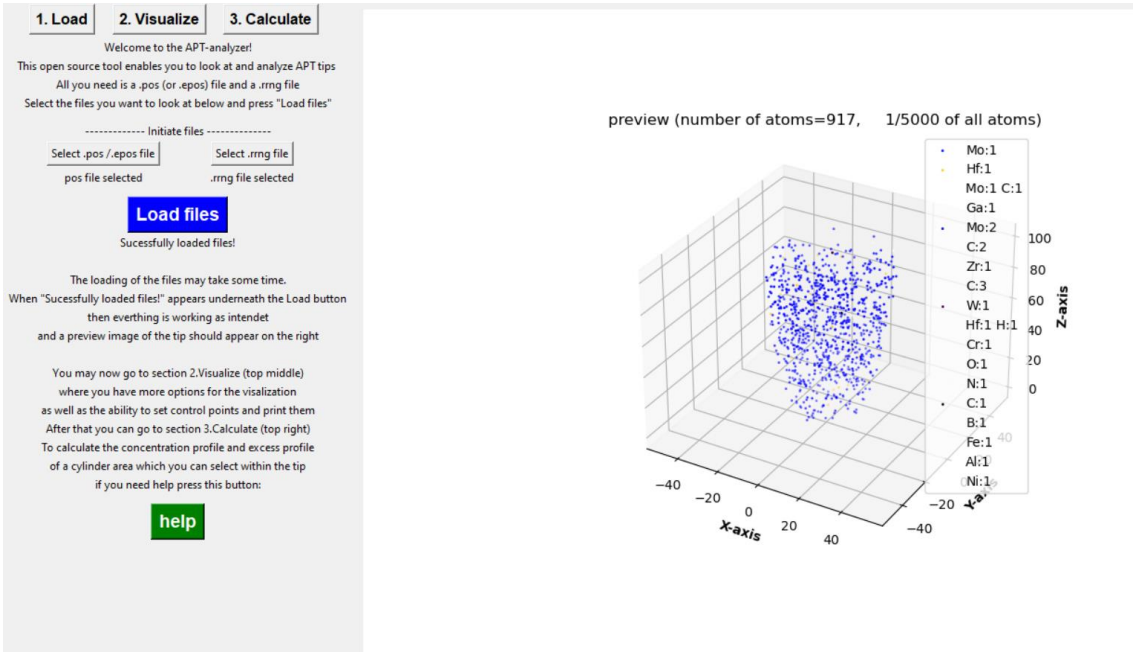


Fig. 2 After successfully loading in a tip.

If the loading of the files did not work as intendent, 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 in the middle, you will open the visualization page. How this page should look like including a short description of each feature can be seen below:

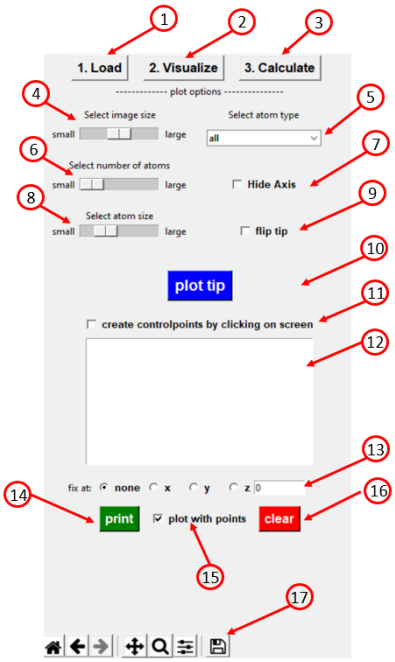


Fig 3 The features of page 2. Visualize

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. Plot the tip
11. Checkbox for creating control points
12. Textbox in which the control points are saved, you can also write in their to your liking, but be careful of the format
13. Fix one direction in space at set location (this will also create a plane in the fixed direction and rotate the plot accordingly)
14. Print the Textbox into a .txt file
15. Checkbox for plotting the tip with/without control points
16. Clear the entire content of the textbox
17. Toolbar to save the plot

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 without changing any setting the window may appear in the following settings:

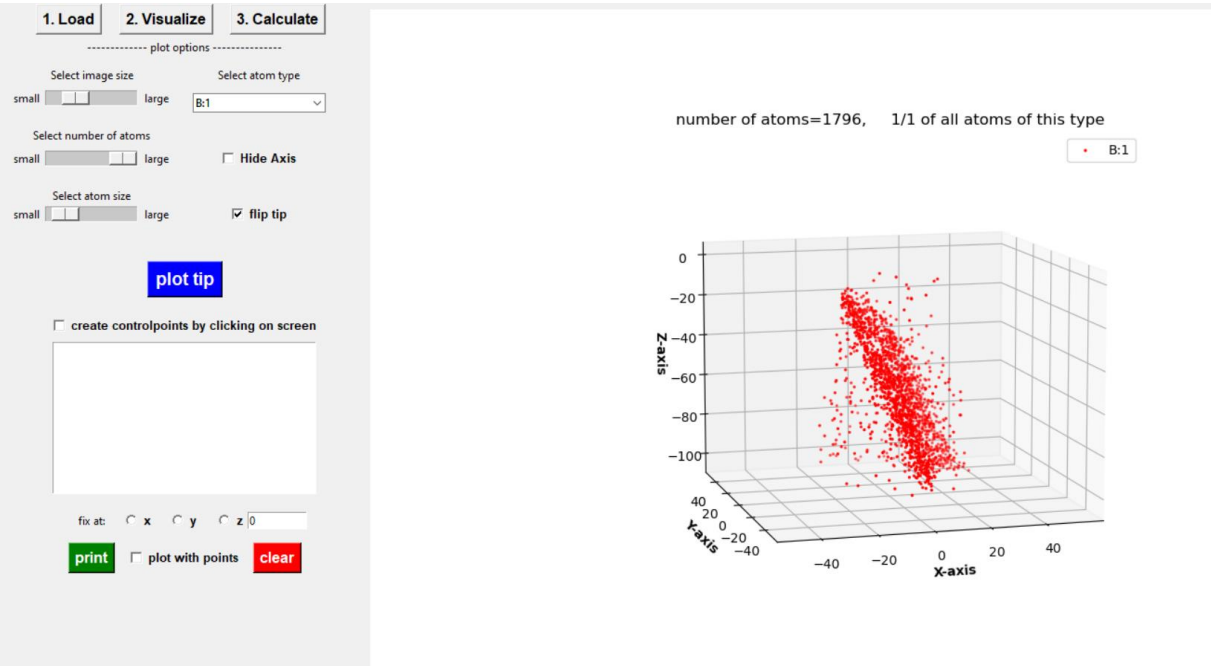


Fig 4 An example for an adjusted plot

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 your 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 may 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 click on screen" checkbox and afterwards press **plot tip**. If you don't plot the tip again it won't be updated. Now each time you press the screen the x,y and z coordinates of your mouse are put into the textbox and a black cross should appear on the screen where you pressed the mouse button. This should look as follows:

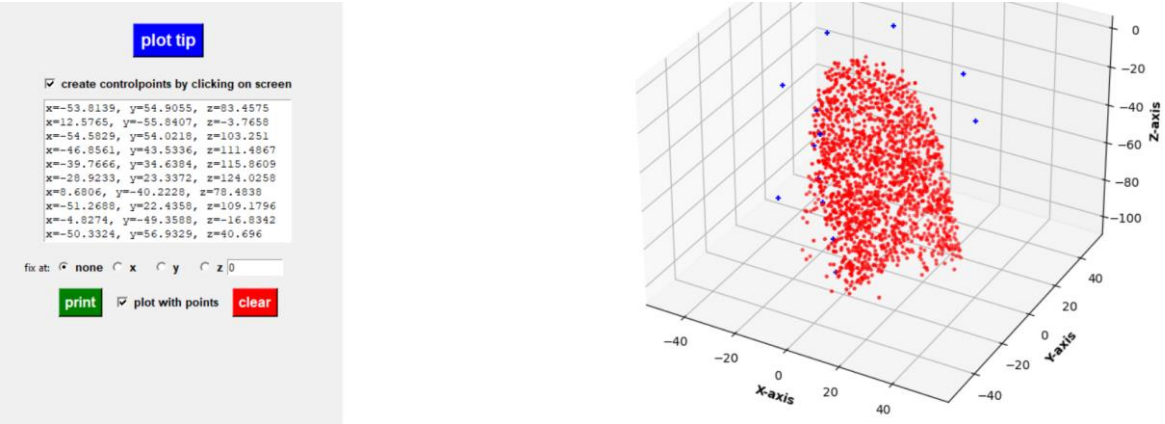


Fig. 5 selecting control points without fixing a direction.

The problem with selecting points in 3d, while looking at it from a 2d plane is that there are infinitely many points the program can choose from along the direction looking at the plane. In order to make it possible to accurately select points you need to fix one coordinate by the **fix at:** function below. By selecting either x,y or z and setting the fixed value, a plane along this direction is created and the 3d plot is rotated to look directly on it. Now if you create control points you can adjust the other two directions with your mouse while the fixed value stays the same. Be careful not to rotate the plot however otherwise the point selection may be not as accurate anymore. You can then decide if you want to show the plot with or without the control points below.

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. However, you need to be careful of using 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 .txt file you may press the button **print**.

How this could look like can be seen below:

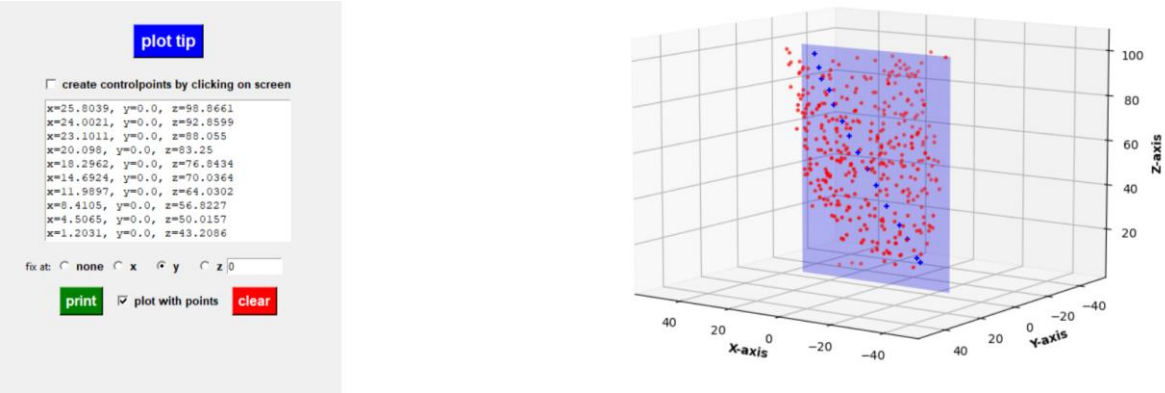


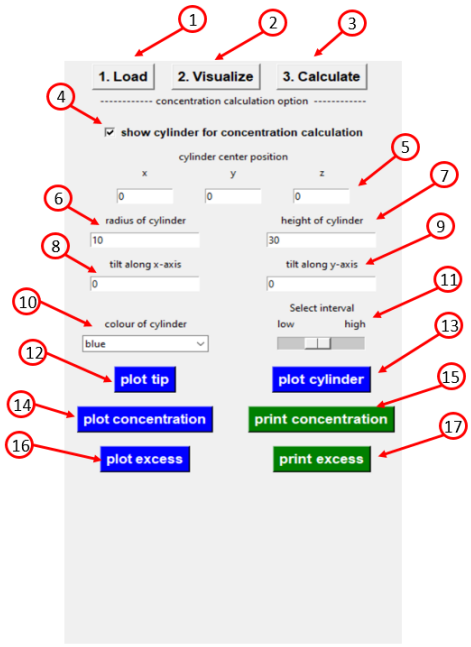
Fig 6. Selecting control points by fixing one direction in space.

It should also be noted that the **color** of both the plane and the points can be changed by going to page "3. Calculation" and selecting the preferred colour in the "color of cylinder" selection box.

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. Calculation which can be found on the top left corner of the GUI. How page 3.Calculation should look like and the description of each button can be seen below:



1. Change to page 1. Load
2. Change to page 2.Visualize
3. Change to page 3. Calculate
4. Checkbox to select if 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 the tip as before, all adjustments on page 2 will also appear
13. Plot a close up of the atoms inside the cylinder
14. Plot the concentration profile along the cylinder with set interval
15. Print out the plotted concentration profile in a .txt file
16. Plot the excess profile along the cylinder with set interval
17. Print out the excess profile in a .txt file

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.

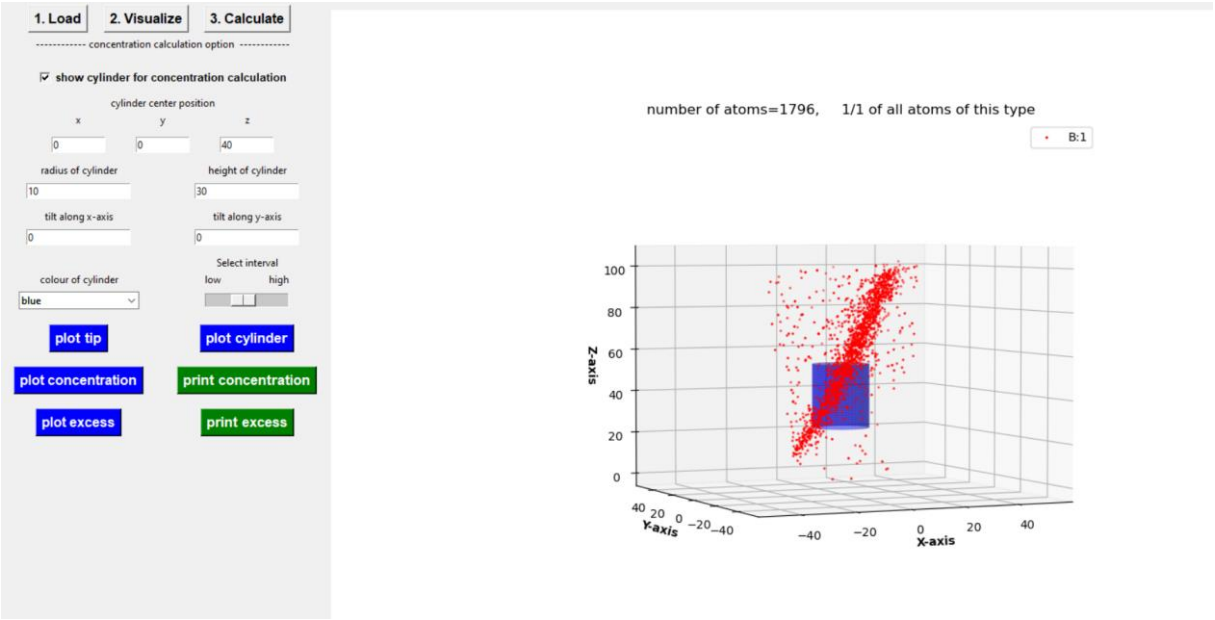


Fig. 8 Example plot a tip with a cylinder area for concentration calculation.

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.

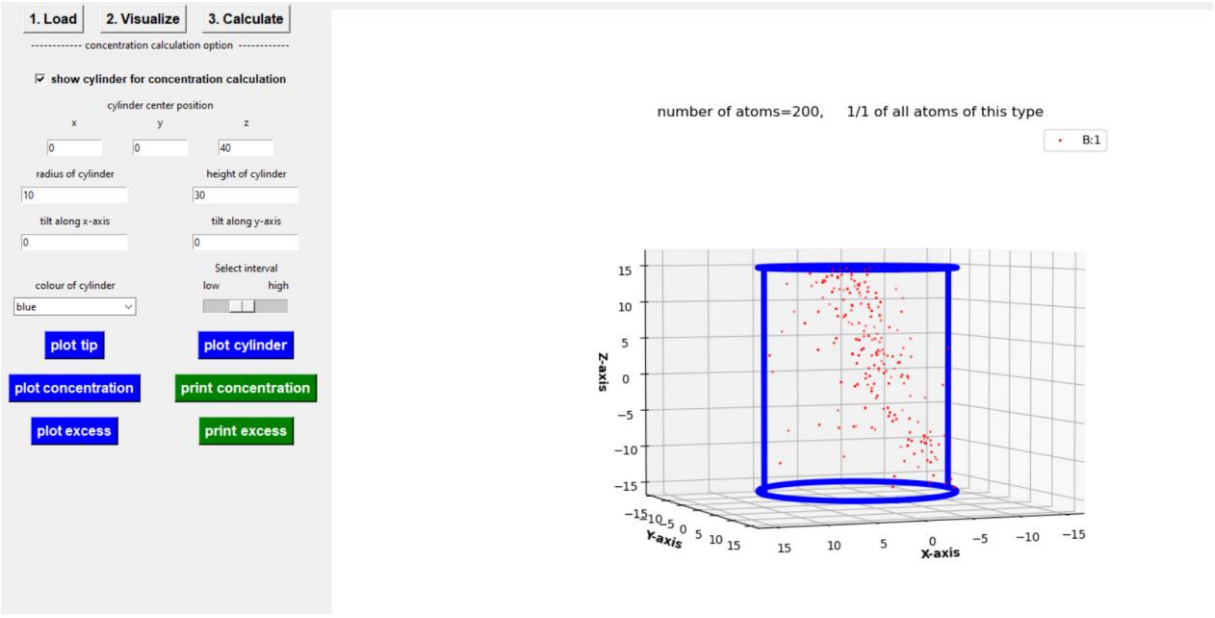


Fig. 9 Close up plot of the atoms inside the cylinder area

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 this:

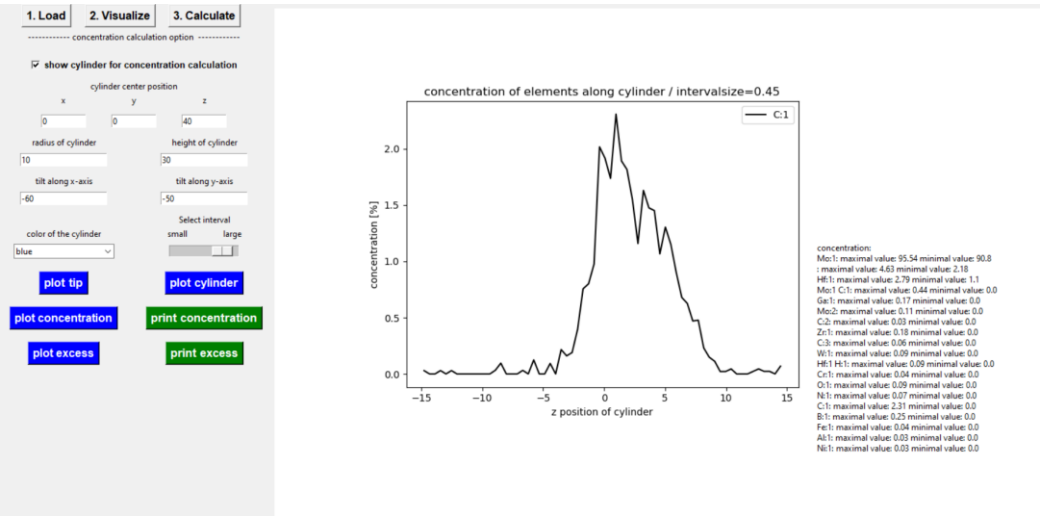


Fig. 10 Example of a Concentration profile plot. In this case the Carbon accumulation in the Grain boundary can be seen.

After you plotted the concentration you can print the concentration in a .txt file by pressing the **print concentration** button. Similar to the concentration, also the excess can be plotted by using the **plot excess** button. This may look similar to this:

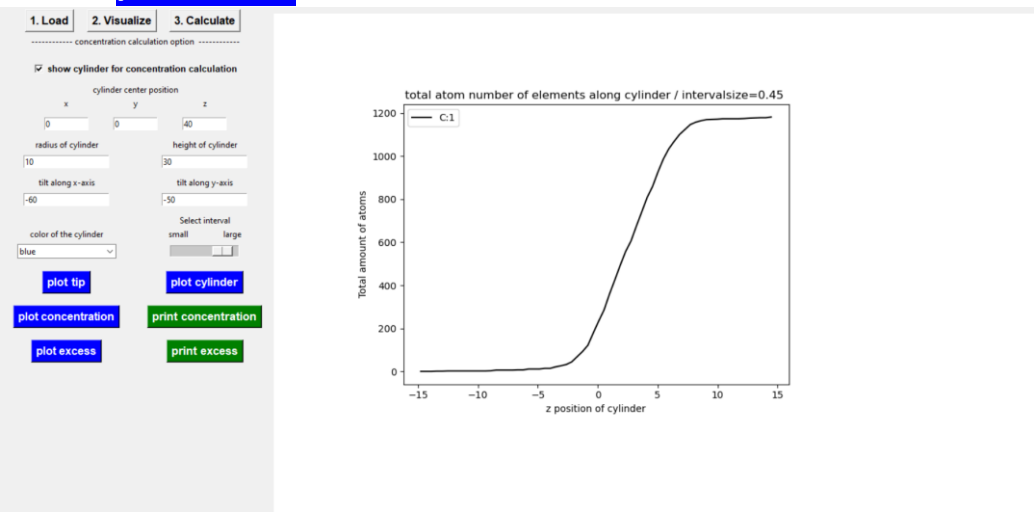


Fig. 11 An example of an excess plot. This shows the excess referring to the same carbon grain boundary accumulation.

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.

That's it for the tutorial. If you have any questions, feel free to contact me. **Enjoy using the APT-analyzer!**