tutorial

April 6, 2023

[27]:

```
import sys
sys.path.append('./test')
import pylab as pl
import numpy as np
import xarray as xr
from rhkpy import rhkpy
```

1 Loading dI/dV map

[28]:

```
filename_map = './test/dI-dV_ABC_Graphite-Sample5_9K_2021_08_24_11_54_33_632.
  ↪sm4'
specmap = rhkpy.stmdata(filename_map)
```

There are two xarray Datasets in the file: `image` and `spectra`. One can access these using the dot . notation

[9]:

```
specmap.image
```

[9]:

```
<xarray.Dataset>
Dimensions:     (x: 512, y: 512, scandir: 2)
Coordinates:
  * x           (x) float64 -563.6 -563.4 -563.2 -563.0 … -464.2 -464.0 -463.8
  * y           (y) float64 -828.9 -828.7 -828.5 -828.3 … -729.5 -729.3 -729.1
  * scandir     (scandir) <U8 'forward' 'backward'
Data variables:
    topography  (x, y, scandir) float64 0.2228 0.5587 0.3199 … 1.126 1.268
    current     (x, y, scandir) float64 105.2 95.93 108.6 … 99.23 92.91 96.35
    lia         (x, y, scandir) float64 -0.05732 -0.1006 … -0.09234 -0.1453
Attributes:
    filename:          ./test/dI-dV_ABC_Graphite-Sample5_9K_2021_08_24_11_54_…
    xoffset:           -563.5723326555265
    yoffset:           -828.9023483917802
    xoffset_units:     nm
    yoffset_units:     nm
    bias:              0.5
    bias units:        V
    setpoint:          100.0000013351432
    setpoint units:    pA
    measurement date:  08/23/21
    measurement time:  19:46:50
```

Both the `spectra` and `image` have attributes, which can be accessed like so:

```
[39]: specmap.image.attrs
```

```
[39]: {'filename': './test/dI-dV_ABC_Graphite-Sample5_9K_2021_08_24_11_54_33_632.sm4',
       'xoffset': -563.5723326555265,
       'yoffset': -828.9023483917802,
       'xoffset_units': 'nm',
       'yoffset_units': 'nm',
       'bias': 0.5,
       'bias units': 'V',
       'setpoint': 100.0000013351432,
       'setpoint units': 'pA',
       'measurement date': '08/23/21',
       'measurement time': '19:46:50'}
```

`image` has data variables: ‘topography’, ‘current’ and ‘lia’. It has coordinates: ‘x’, ‘y’, ‘scandir’

Plotting the topography data, we select the `forward` scan direction. This can be done using the `isel` function

```
[40]: fwscan = specmap.image.isel(scandir=0)
```

Now we can see that the coordinate `scandir` is gone, leaving only `x` and `y`

```
[41]: fwscan
```

```
[41]: <xarray.Dataset>
      Dimensions:      (x: 512, y: 512)
      Coordinates:
        * x            (x) float64 -563.6 -563.4 -563.2 -563.0 … -464.2 -464.0 -463.8
        * y            (y) float64 -828.9 -828.7 -828.5 -828.3 … -729.5 -729.3 -729.1
          scandir      <U8 'forward'
      Data variables:
          topography   (x, y) float64 0.2228 0.3199 0.4098 0.348 … 1.181 1.199 1.126
          current      (x, y) float64 105.2 108.6 94.26 95.62 … 106.6 98.58 92.91
          lia          (x, y) float64 -0.05732 -0.09757 0.2002 … 0.01556 -0.09234
      Attributes:
          filename:          ./test/dI-dV_ABC_Graphite-Sample5_9K_2021_08_24_11_54_…
          xoffset:           -563.5723326555265
          yoffset:           -828.9023483917802
          xoffset_units:     nm
          yoffset_units:     nm
          bias:              0.5
          bias units:        V
```

```
    setpoint:           100.0000013351432
    setpoint units:     pA
    measurement date:   08/23/21
    measurement time:   19:46:50
```

Selecting the 'topography' DataArray from the set. This has coordinates 'x' and 'y' and values as a numpy array, which can be accessed by `fwscan['topography'].data`

[18]:
```
fwscan['topography']
```

[18]:
```
<xarray.DataArray 'topography' (x: 512, y: 512)>
array([[ 0.22277586,  0.31985992,  0.40975636, …,  0.1738827 ,
         0.25653668,  0.21637588],
       [ 0.42118773,  0.49016015,  0.49237385, …,  0.55386099,
         0.4927506 ,  0.47112197],
       [ 0.66517782,  0.67569847,  0.68743548, …,  0.68594219,
         0.71097722,  0.65945614],
       …,
       [-0.04212871, -0.02539763,  0.02653675, …,  1.07600668,
         1.05096369,  1.07442425],
       [-0.1272415 , -0.10926353, -0.07156714, …,  1.10464527,
         1.05920205,  1.02997055],
       [ 0.05461745,  0.07771955,  0.08524178, …,  1.18111791,
         1.19945448,  1.12606963]])
Coordinates:
  * x        (x) float64 -563.6 -563.4 -563.2 -563.0 … -464.2 -464.0 -463.8
  * y        (y) float64 -828.9 -828.7 -828.5 -828.3 … -729.5 -729.3 -729.1
    scandir  <U8 'forward'
Attributes:
    units:       nm
    long units:  nanometer
```

[43]:
```
fwscan['topography'].data
```

[43]:
```
array([[ 0.22277586,  0.31985992,  0.40975636, …,  0.1738827 ,
         0.25653668,  0.21637588],
       [ 0.42118773,  0.49016015,  0.49237385, …,  0.55386099,
         0.4927506 ,  0.47112197],
       [ 0.66517782,  0.67569847,  0.68743548, …,  0.68594219,
         0.71097722,  0.65945614],
       …,
       [-0.04212871, -0.02539763,  0.02653675, …,  1.07600668,
         1.05096369,  1.07442425],
       [-0.1272415 , -0.10926353, -0.07156714, …,  1.10464527,
         1.05920205,  1.02997055],
       [ 0.05461745,  0.07771955,  0.08524178, …,  1.18111791,
         1.19945448,  1.12606963]])
```

The coordinates in the Dataset are accessed by `.coords`, for example in the 'x' direction:

`fwscan.coords['x']`. The values can be directly acessed as: `fwscan.coords['x'].data`

```
[46]: fwscan.coords['x']
```

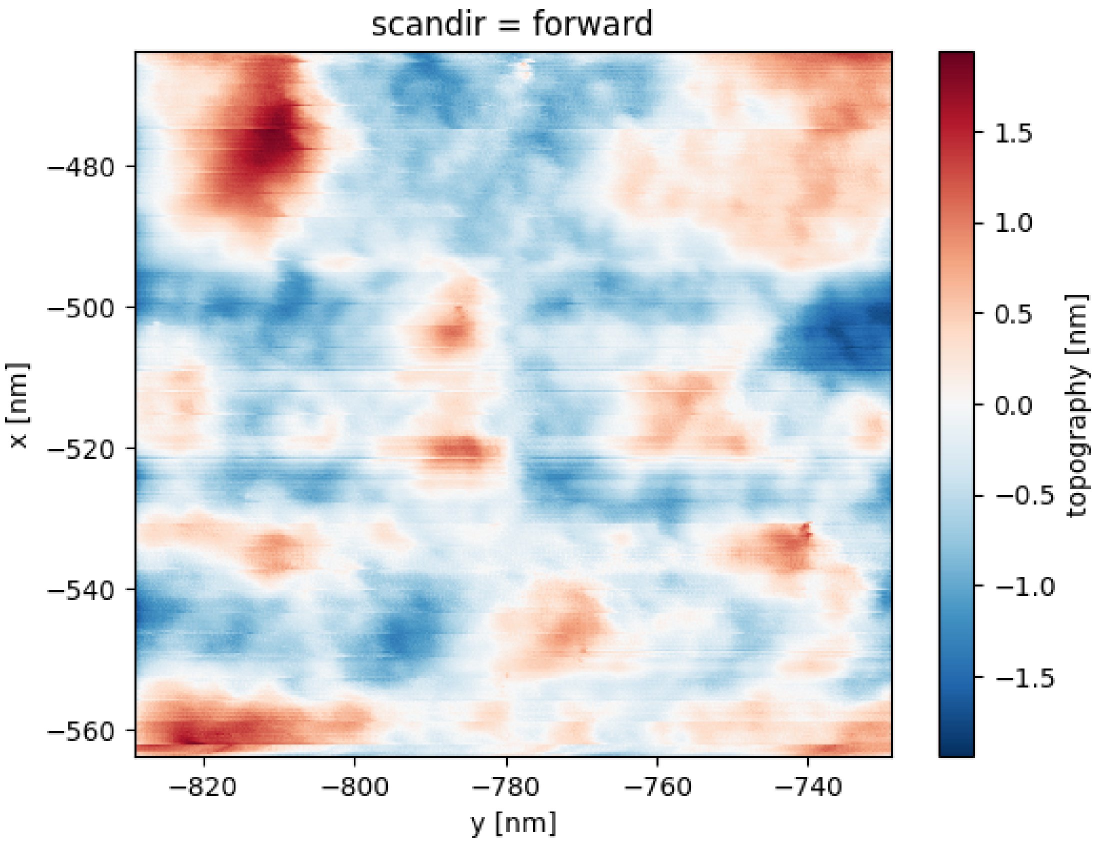
```
[46]: <xarray.DataArray 'x' (x: 512)>
      array([-563.572333, -563.37702 , -563.181708, …, -464.158269, -463.962956,
             -463.767644])
      Coordinates:
        * x        (x) float64 -563.6 -563.4 -563.2 -563.0 … -464.2 -464.0 -463.8
          scandir  <U8 'forward'
      Attributes:
          units:       nm
          long units:  nanometer
```

Plotting the ‘topography’ DataArray. When plotting the ‘topography’ the data has been plane and line fitted.

The coordinates `x` and `y` are in the absolute tip positions

```
[16]: fwscan['topography'].plot()
```

```
[16]: <matplotlib.collections.QuadMesh at 0x22cdf402c20>
```



Let's see the spectra Dataset

```
[29]: specmap.spectra
```

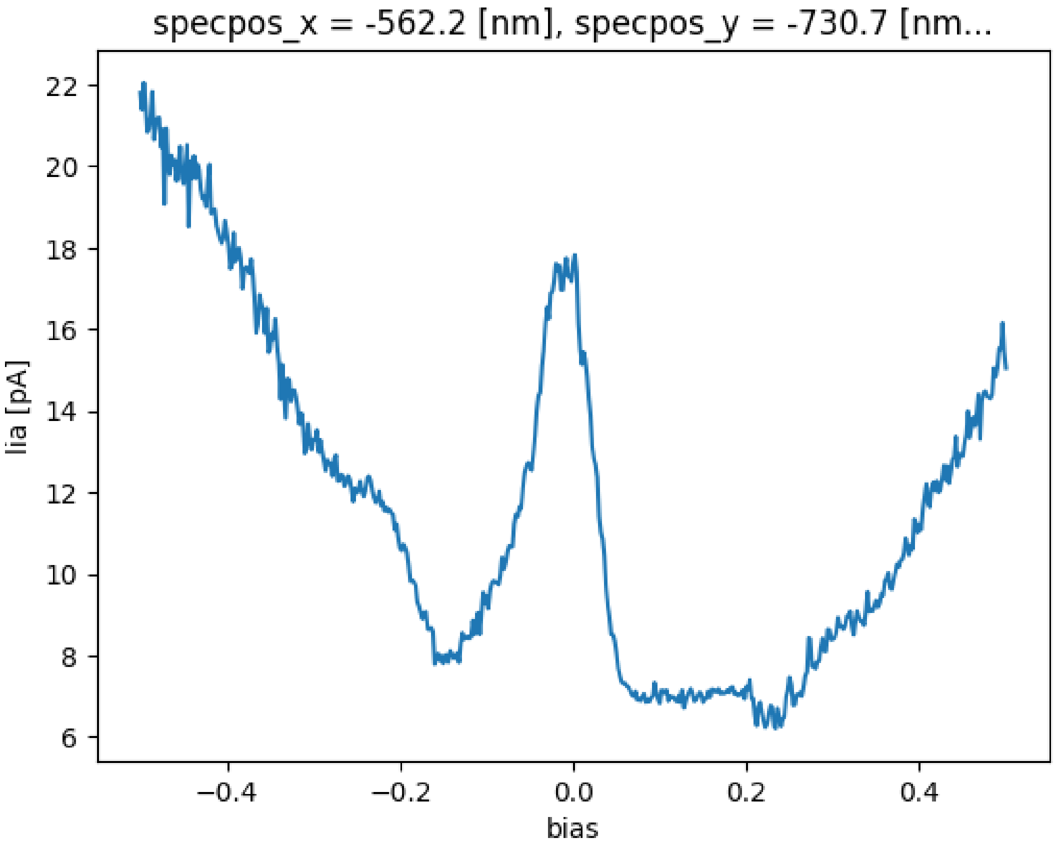
```
[29]: <xarray.Dataset>
      Dimensions:      (bias: 501, specpos_x: 32, specpos_y: 32, repetitions: 1,
                        biasscandir: 2)
      Coordinates:
        * bias         (bias) float64 0.5 0.498 0.496 0.494 … -0.496 -0.498 -0.5
        * specpos_x    (specpos_x) float64 -465.3 -468.5 -471.6 … -559.1 -562.2
        * specpos_y    (specpos_y) float64 -730.7 -733.8 -736.9 … -824.4 -827.5
        * repetitions  (repetitions) int32 0
        * biasscandir  (biasscandir) <U5 'left' 'right'
      Data variables:
          lia          (bias, specpos_x, specpos_y, repetitions, biasscandir) float64
      …
          current      (bias, specpos_x, specpos_y, repetitions, biasscandir) float64
      …
          x            (specpos_x, specpos_y) float64 -465.3 -468.5 … -559.1 -562.2
          y            (specpos_x, specpos_y) float64 -730.7 -730.7 … -827.5 -827.5
      Attributes:
          filename:          ./test/dI-dV_ABC_Graphite-Sample5_9K_2021_08_24_11_54_…
          bias:              0.5
          bias units:        V
          setpoint:          100.0000013351432
          setpoint units:    pA
          measurement date:  08/23/21
          measurement time:  19:50:01
```

Plotting the dI/dV spectra.

We can use the `sel` function for this, by specifying the coordinates in nm. Finally selecting the 'lia' data variable to plot as a function of the `bias` coordinate. To do this we first select the one value in repetitions coordinate, because there are only two spectra (left and right bias scan) at each tip position. We also can use the `isel` and `sel` functions together.

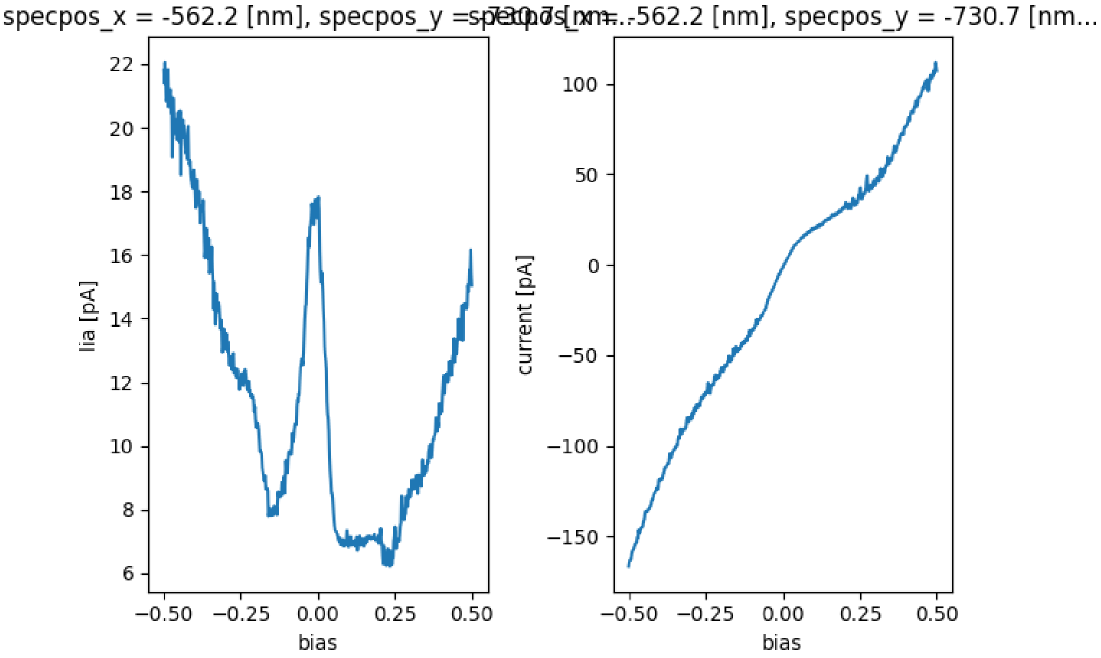
```
[36]: specmap2 = specmap.spectra.isel(repetitions=0)
      specmap2.isel(biasscandir=0).sel(specpos_x=-782, specpos_y=-521,␣
       ↪method='nearest')['lia'].plot()
```

```
[36]: [<matplotlib.lines.Line2D at 0x22ce4e5f7c0>]
```



Plot both the current and Lock-In

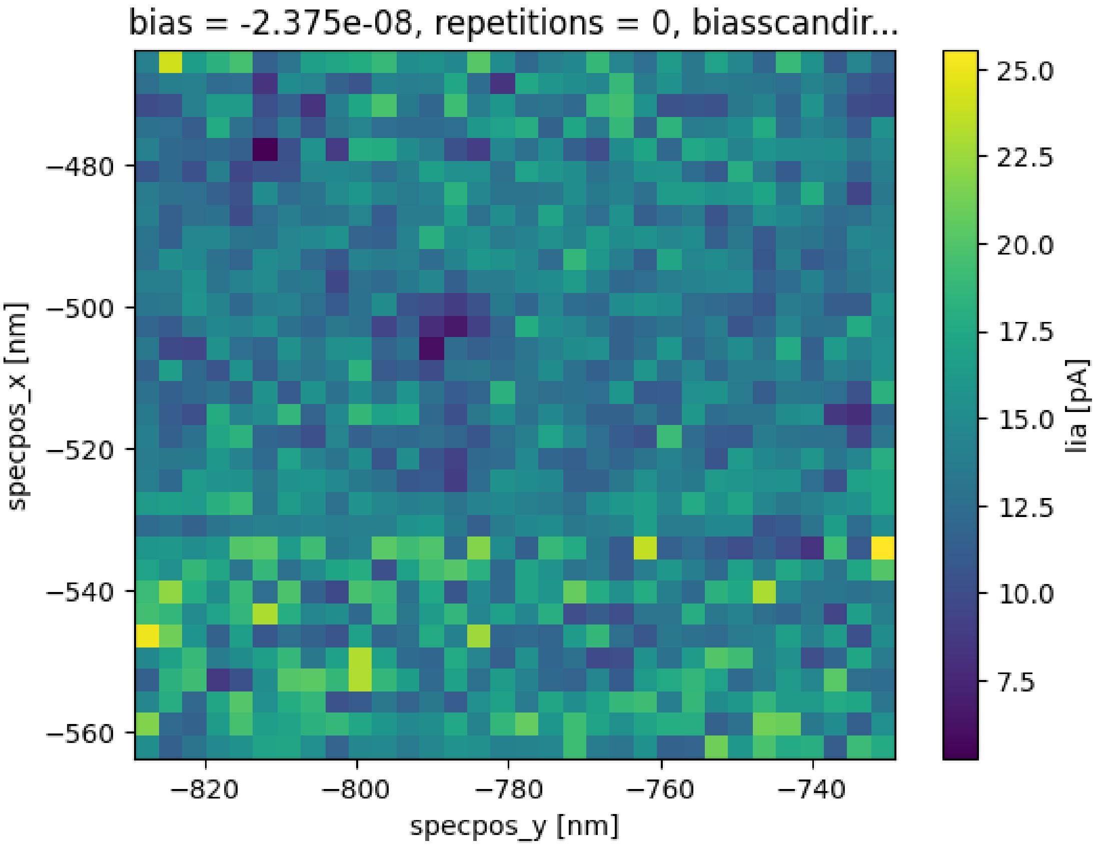
[38]:
```
fig, (ax1, ax2) = pl.subplots(1, 2)
specmap2.isel(biasscandir=0).sel(specpos_x=-782, specpos_y=-521,␣
 ↪method='nearest')['lia'].plot(ax=ax1)
specmap2.isel(biasscandir=0).sel(specpos_x=-782, specpos_y=-521,␣
 ↪method='nearest')['current'].plot(ax=ax2)
pl.tight_layout()
```



Plot the dI/dV value at zero bias.

[33]:
```
specmap.spectra.isel(repetitions=0, biasscandir=0).sel(bias=0,␣
  ↪method='nearest')['lia'].plot()
```

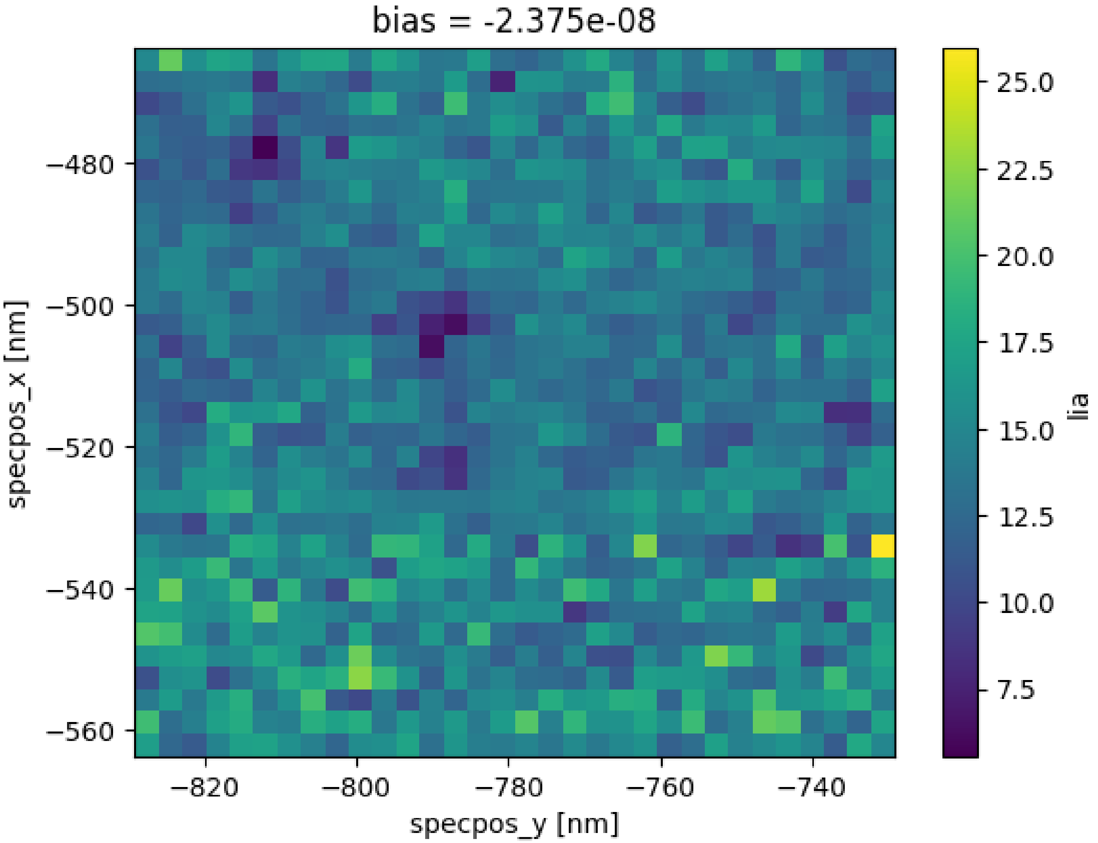
[33]:
```
<matplotlib.collections.QuadMesh at 0x22cdf2046d0>
```



Average over the forward and backward directions of the bias sweep

```
[35]: specmap.spectra.mean(dim=['repetitions', 'biasscandir']).sel(bias=0,␣
      ↪method='nearest')['lia'].plot()
```

```
[35]: <matplotlib.collections.QuadMesh at 0x22ce6b5bcd0>
```



Let’s do something more fancy, like plotting spectra across a line, parallel to the ‘y’ axis at ‘x’=-542 nm

```
[48]: specmap_avg = specmap.spectra.mean(dim=['repetitions', 'biasscandir'])
```

```
[50]: spec_along_line = specmap_avg.sel(specpos_x=-542, method='nearest')
```

The selected data now has coordinates of `bias` and `specpos_y`.

```
[51]: spec_along_line
```

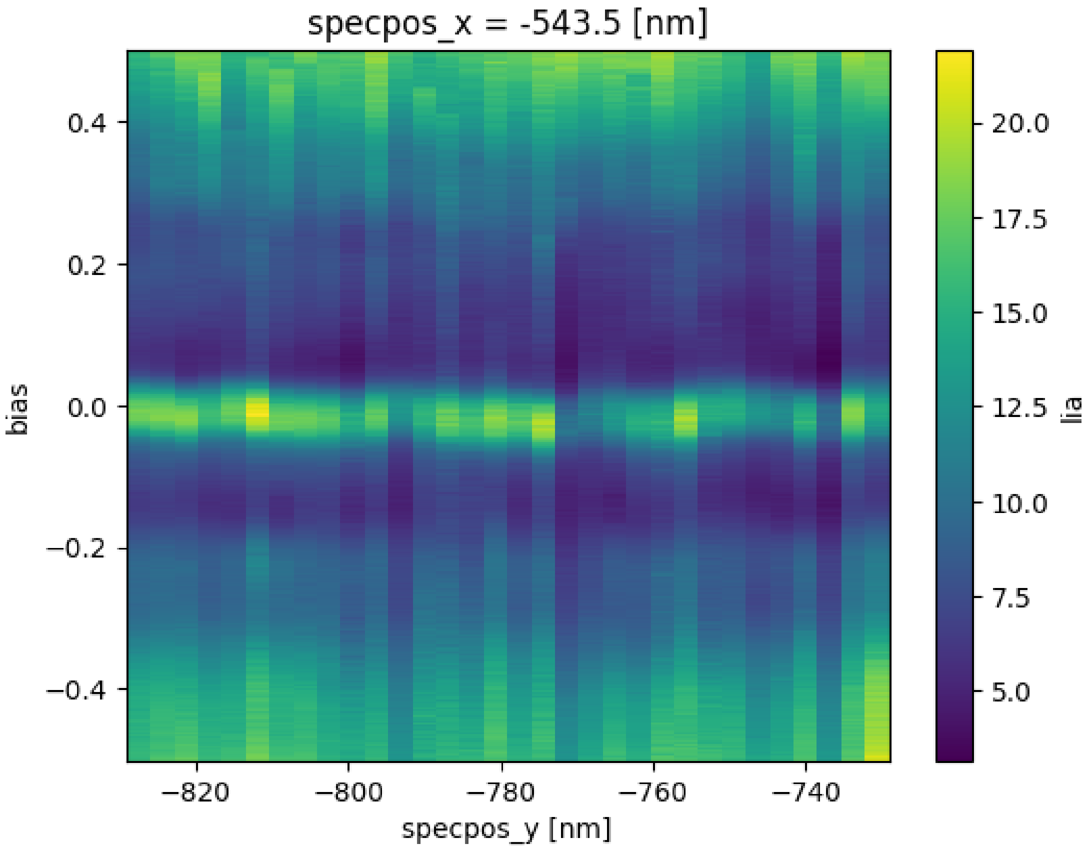
```
[51]: <xarray.Dataset>
      Dimensions:    (bias: 501, specpos_y: 32)
      Coordinates:
        * bias       (bias) float64 0.5 0.498 0.496 0.494 … -0.496 -0.498 -0.5
          specpos_x  float64 -543.5
        * specpos_y  (specpos_y) float64 -730.7 -733.8 -736.9 … -821.3 -824.4 -827.5
      Data variables:
          lia        (bias, specpos_y) float64 18.12 19.5 15.82 … 17.33 16.82 15.61
          current    (bias, specpos_y) float64 122.6 130.2 95.7 … -136.6 -129.6
          x          (specpos_y) float64 -465.3 -468.5 -471.6 … -556.0 -559.1 -562.2
```

```
    y            (specpos_y) float64 -808.8 -808.8 -808.8 … -808.8 -808.8 -808.8
```

We can plot this on a density plot.

```
[53]: spec_along_line['lia'].plot()
```

```
[53]: <matplotlib.collections.QuadMesh at 0x22ce7177c70>
```



```
[ ]:
```