Curve fitting in HyperSpy:

Applications to EELS data analysis

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Create some test data

- 50x50 array of Gaussians with randomly varying A, mu, and sigma

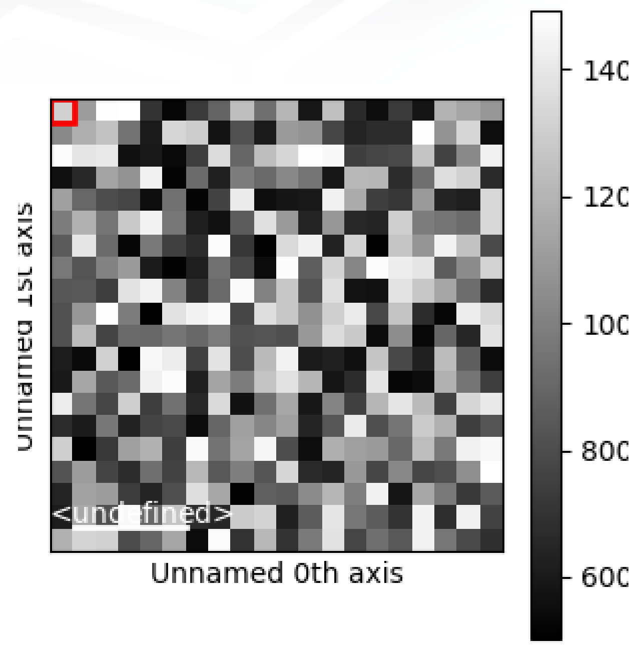
In [2]:

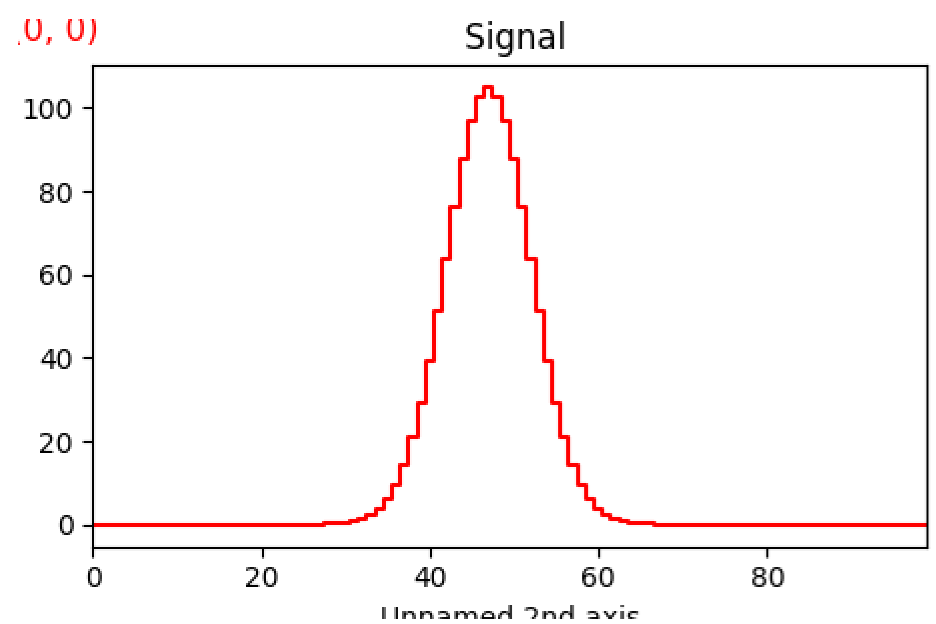
```
amps = hs.signals.Signal2D(np.random.randint(500,1500,size=[20,20]))
centers = hs.signals.Signal2D(np.random.randint(45,55,size=[20,20]))
sigmas = hs.signals.Signal2D(np.random.randint(5,10,size=[20,20]))

xaxis = np.tile(np.arange(0,100),20**2)
xaxis = xaxis.reshape([20,20,100])
xaxis = np.rollaxis(xaxis,2)
curves = amps.data/np.sqrt(2*np.pi*sigmas.data**2)*np.exp(-(xaxis-centers.data)**2/(2*sigmas.data**2))
curves = np.rollaxis(curves,0,3)
gaussians = hs.signals.Signal1D(curves)

gaussians
```

Out[2]:

```
<Signal1D, title: , dimensions: (20, 20|100)>
```

```
In [3]: gaussians.plot()
```





Create a model

In [4]:
```
gaussians_model = gaussians.create_model()
gaussians_model.components
```

Out[4]:
```
   # |       Attribute Name |       Component Name |       Component Type
---- | -------------------- | -------------------- | --------------------
```

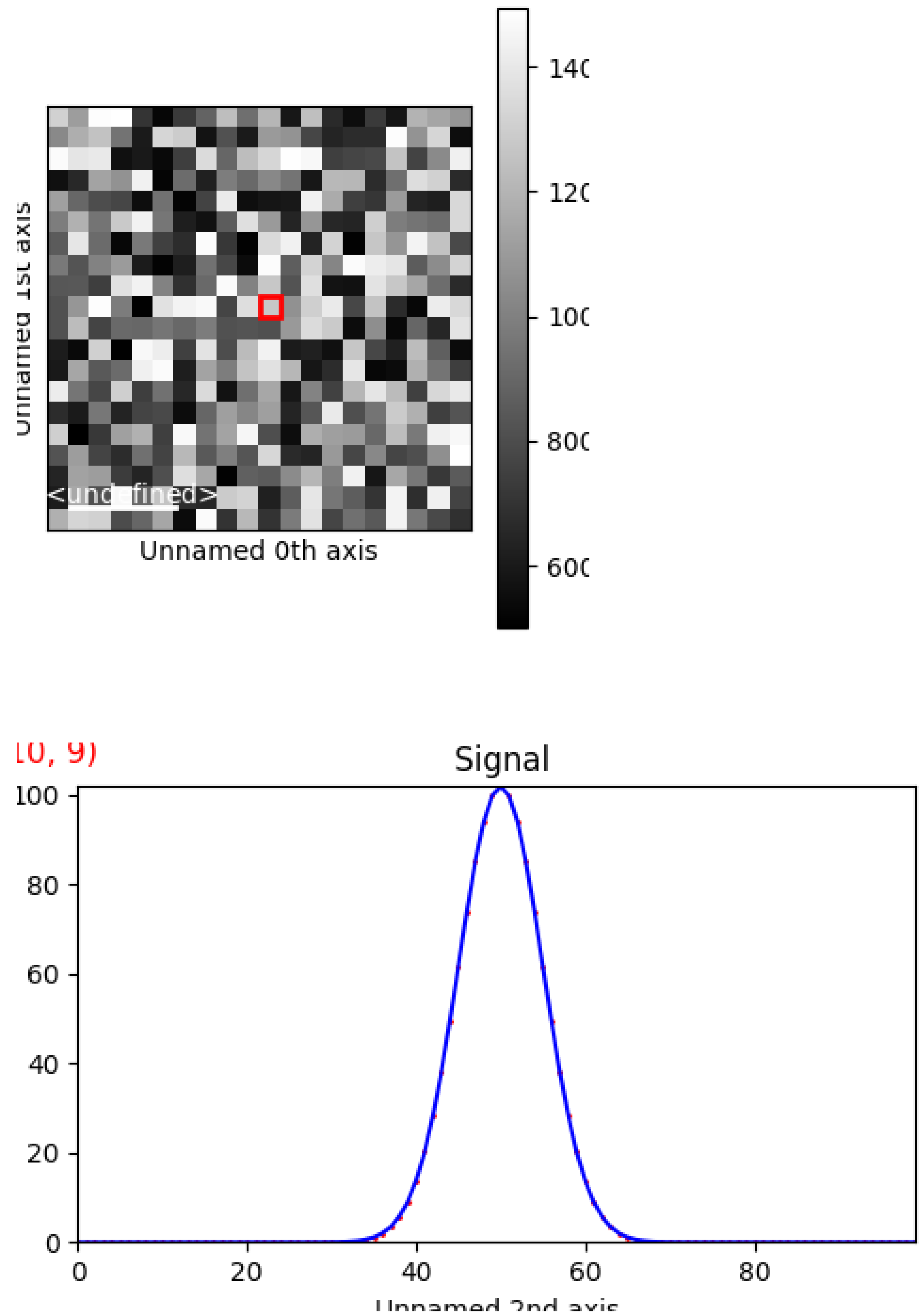
Add single Gaussian component:

In [5]:
```
gaussians_model.append(hs.model.components1D.Gaussian())
gaussians_model[0].estimate_parameters(gaussians,10,90,False)
gaussians_model.components
```

Out[5]:
```
   # |       Attribute Name |       Component Name |       Component Type
---- | -------------------- | -------------------- | --------------------
   0 |             Gaussian |             Gaussian |             Gaussian
```

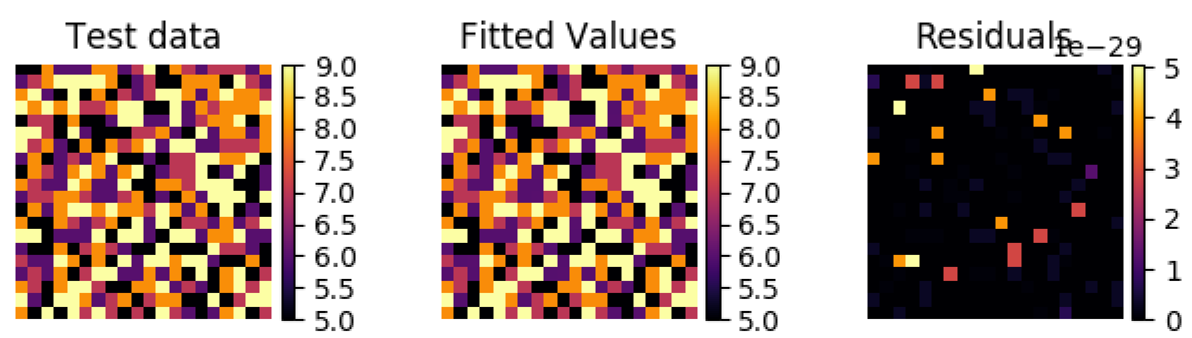
Perform fit at all pixel locations:

In [6]:
```
gaussians_model.multifit()
gaussians_model.plot()
```



Compare fitted values to test data

In [7]:
```
sig_results = gaussians_model.components.Gaussian.parameters[1].as_signal()
residuals = (sig_results-sigmas)**2

hs.plot.plot_images([sigmas, sig_results, residuals], cmap='inferno',
                    axes_decor='off', tight_layout=True,
                    label=['Test data', 'Fitted Values', 'Residuals'])
plt.tight_layout()
```



Add some noise to the test data

In [8]:

```
noisy = gaussians.deepcopy()
noisy.unfold()

for i in range(0,20**2):
    noisy.data[i,:] =noisy.data[i,:] + np.random.poisson(np.sqrt(noisy.data[i,:].max()),100)
noisy.fold()
```

Modeling the noisy data

Create model and add a single Gaussian component:

In [9]:
```
noisy_model = noisy.create_model()
noisy_model.append(hs.model.components1D.Gaussian())
```

Add a linear offset to account for 'background' from adding noise:

In [10]:
```
noisy_model.append(hs.model.components1D.Offset())
```

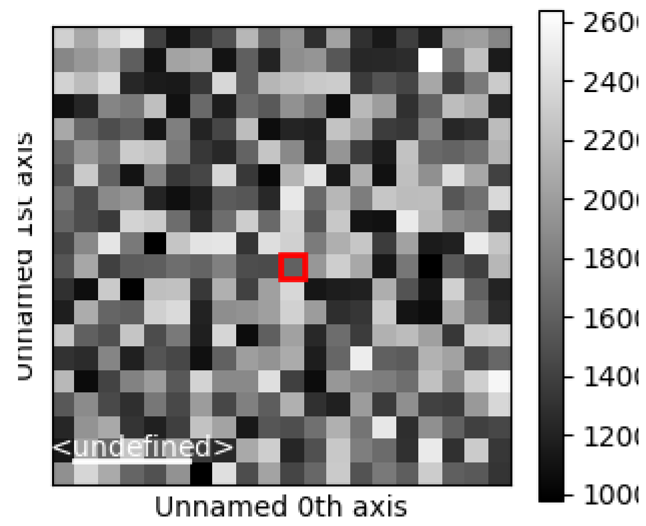
Estimate model parameters using a quick arithmetic estimation:

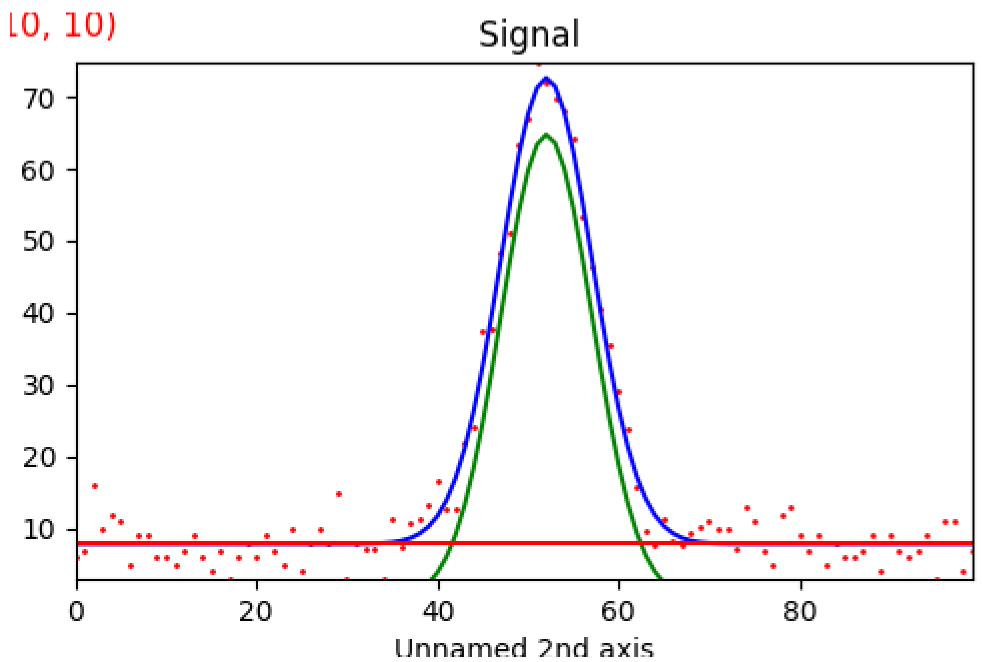
In [11]:
```
noisy_model['Gaussian'].estimate_parameters(signal=noisy, x1=10, x2=90, only_current=False)
noisy_model['Offset'].estimate_parameters(signal=noisy, x1=10, x2=90, only_current=False);
```

Perform fit at all image pixels:

In [12]:
```
noisy_model.multifit(show_progressbar=True)
noisy_model.plot(plot_components=True)
```

100% 400/400 [00:03<00:00, 124.82it/s]





More Realistic Application:

Fitting EELS Fine Structure

Useful aside: The EELS Database

EELS Data Base
Inner & Outer Shell Excitation Spectrum Repository

- https://eelsdb.eu/
  - Largest open-access repository of EELS and X-ray absorption spectra
  - Nearly 300 spectra covering 43 elements and growing
- Database can be directly queried by:
  - `title` — "Hexagonal Boron Nitride"
  - `formula` — "BN"
  - `element` — "B,N"
  - `edge` — "K" or "L1"
  - Etc., many other options

Spectra can be pulled directly from database into HyperSpy (requires internet connection):

In [13]:
```python
# Search by formula:
hs.datasets.eelsdb(formula='BN')
```

Out[13]:
```
[<EELSSpectrum, title: Boron nitride, dimensions: (|1002)>,
 <EELSSpectrum, title: boron nitride, dimensions: (|837)>,
 <EELSSpectrum, title: Boron Nitride single wall nanotube, dimensions: (|1256)>,
 <EELSSpectrum, title: Boron Nitride multiwall nanotube, dimensions: (|786)>,
 <EELSSpectrum, title: Boron Nitride multiwall nanotube, dimensions: (|792)>,
 <EELSSpectrum, title: Boron Nitride single wall nanotube, dimensions: (|561)>,
 <EELSSpectrum, title: Boron Nitride triple wall nanotube, dimensions: (|546)>,
 <EELSSpectrum, title: Hexagonal Boron Nitride, dimensions: (|1024)>,
 <EELSSpectrum, title: Hexagonal Boron Nitride, dimensions: (|1024)>,
 <EELSSpectrum, title: Cubic boron nitride, dimensions: (|946)>,
 <EELSSpectrum, title: Cubic boron nitride, dimensions: (|812)>]
```

In [14]:
```
# Search my element and spectrum type:
hs.datasets.eelsdb(element=('Fe','O'), spectrum_type='coreloss')
```

Out[14]:
```
[<EELSSpectrum, title: Iron (III) oxide, hematite, dimensions: (|1024)>,
 <EELSSpectrum, title: Iron Oxide, dimensions: (|1024)>,
 <EELSSpectrum, title: Hematite, dimensions: (|1024)>,
 <EELSSpectrum, title: Iron Oxide Hematite, dimensions: (|926)>,
 <EELSSpectrum, title: Iron Oxide Hematite, dimensions: (|620)>,
 <EELSSpectrum, title: Ti-ferrite (spinel), dimensions: (|780)>,
 <EELSSpectrum, title: Ti-ferrite (spinel), dimensions: (|780)>,
 <EELSSpectrum, title: Iron Oxide Magnetite, dimensions: (|911)>,
 <EELSSpectrum, title: Iron Oxide Magnetite, dimensions: (|629)>,
 <EELSSpectrum, title: Iron Oxide Siderite, dimensions: (|826)>,
 <EELSSpectrum, title: Iron Oxide Siderite, dimensions: (|605)>,
 <EELSSpectrum, title: Iron Oxide 2-lines ferrihydrite, dimensions: (|671)>,
 <EELSSpectrum, title: Iron Oxide 2-lines ferrihydrite, dimensions: (|660)>,
 <EELSSpectrum, title: Iron Oxide Goethite, dimensions: (|1024)>,
 <EELSSpectrum, title: Iron Oxide Goethite, dimensions: (|704)>,
 <EELSSpectrum, title: Iron Oxide Cl-containing akaganeite, dimensions: (|427)>,
 <EELSSpectrum, title: Iron Oxide Cl-containing akaganeite, dimensions: (|552)>,
 <EELSSpectrum, title: ferrous Titanate, dimensions: (|1024)>,
 <EELSSpectrum, title: Iron titanium oxide, dimensions: (|1024)>,
 <EELSSpectrum, title: LaFeO3 thin film, dimensions: (|209)>,
 <EELSSpectrum, title: LaFeO3 thin film, dimensions: (|209)>,
 <EELSSpectrum, title: Strontium ferrite, dimensions: (|1024)>]
```

Back to the demo...

Load data downloaded from EELS Database

Core-loss and low-loss boron nitride spectra:

In [15]:
```
s = hs.datasets.eelsdb(title="Hexagonal Boron Nitride", spectrum_type="coreloss")[0]
ll = hs.datasets.eelsdb(title="Hexagonal Boron Nitride", spectrum_type="lowloss")[0]

### If no internet:
#s = hs.load("examples/BN_(hex)_B_K_Giovanni_Bertoni_100.msa")
#ll = hs.load("examples/BN_(hex)_LowLoss_Giovanni_Bertoni_96.msa")
```

Set microscope parameters:

In [16]:
```
s.set_microscope_parameters(beam_energy=100, convergence_angle=0.2, collection_angle=2.55)
```

Add Boron and Nitrogen to model:

In [17]:
```
s.add_elements(('B', 'N'))
```

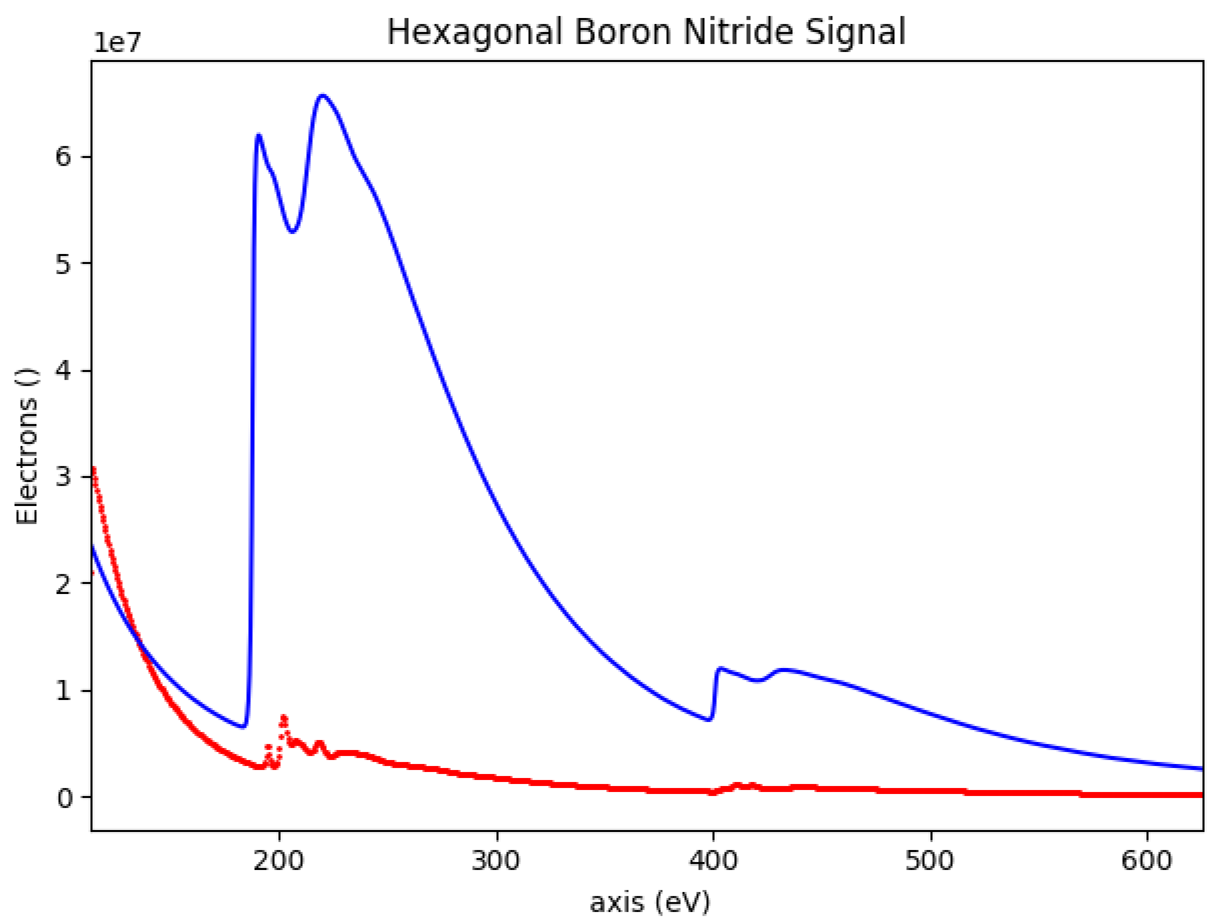
Create model:

- Automatically adds PowerLaw component to fit background
- Automatically adds relevant edges in the energy range of the spectrum

In [18]:
```
m = s.create_model(ll=ll)
m.components
```

Out[18]:
```
   # |       Attribute Name |       Component Name |       Component Type
---- | -------------------- | -------------------- | --------------------
   0 |             PowerLaw |             PowerLaw |             PowerLaw
   1 |                  N_K |                  N_K |           EELSCLEdge
   2 |                  B_K |                  B_K |           EELSCLEdge
```

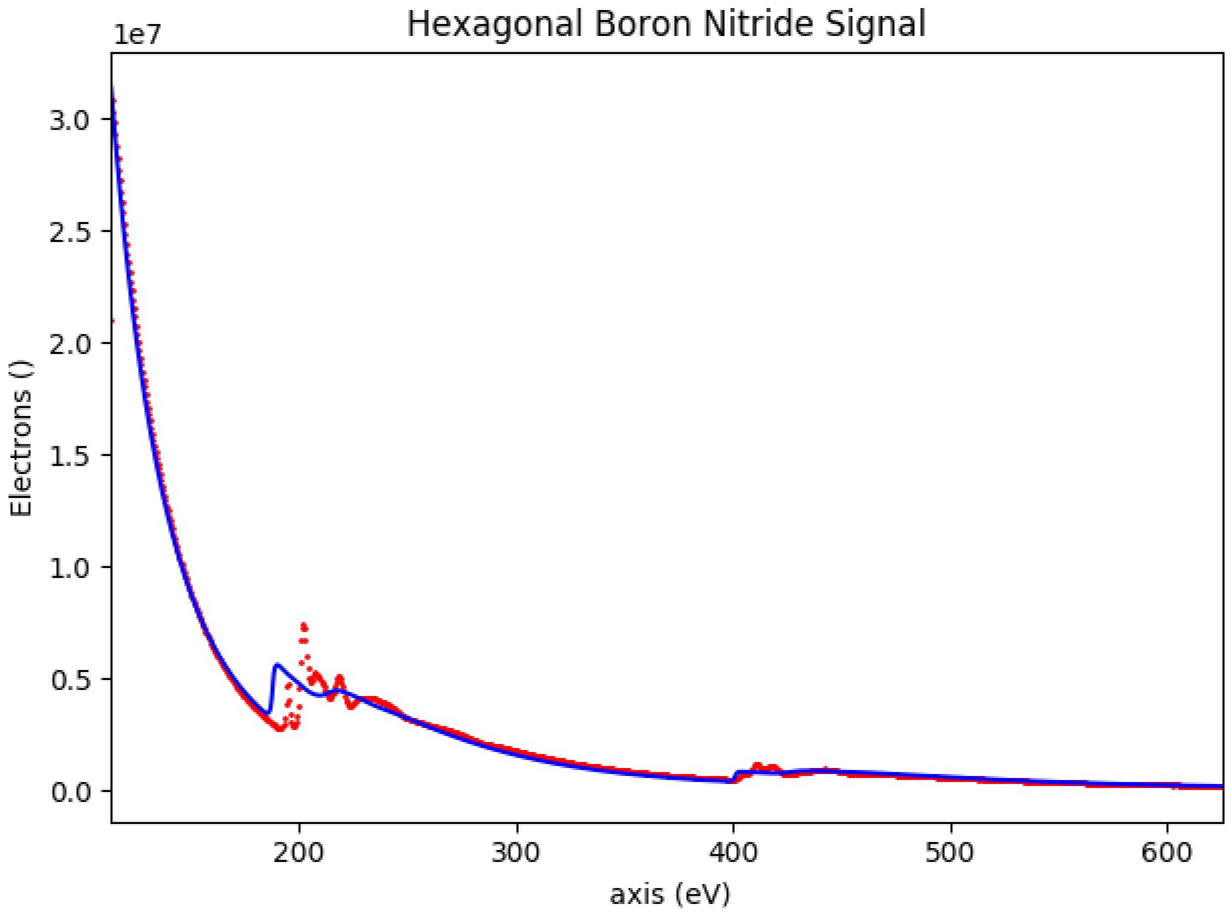
In [19]:
```
m.plot()
```



Hexagonal Boron Nitride Signal
1e7
6
5
4
3
2
1
0
Electrons ()
200
300
400
500
600
axis (eV)

Perform least squares fitting to data

In [20]:
```
m.smart_fit()
m.plot()
```



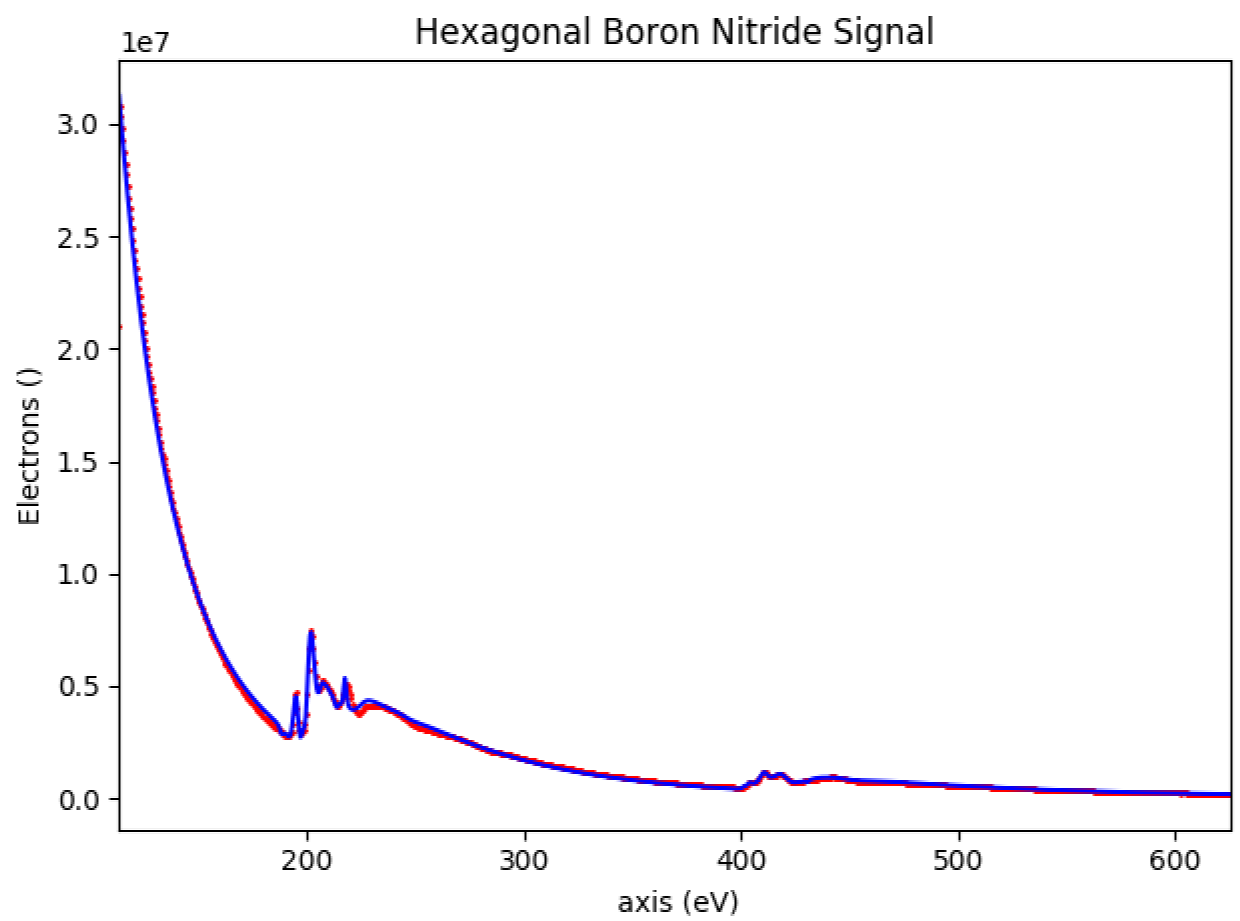
Perform least-squares fitting with fine structure

- Requires local database of ionization cross-sections
- HyperSpy uses values calculated using Egerton's `sigmak3` and `sigmal3` routines
- Better ones come with DigitalMicrograph, and HyperSpy can use those files:
  - Not open-source, so cannot be distributed

In [ ]:
```
# To change to Gatan's GOS files:
### hs.preferences.EELS.eels_gos_files_path = <path to GOS tables>
```

In [21]:
```
m.enable_fine_structure()
m.smart_fit()
```

```
In [22]: m.plot()
```



Hexagonal Boron Nitride Signal
1e7
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Electrons ()
200
300
400
500
600
axis (eV)

Questions?

Next demo: Processing TEM EDS data