An Introduction to HyperSpy:

The multi-dimensional data analysis toolbox

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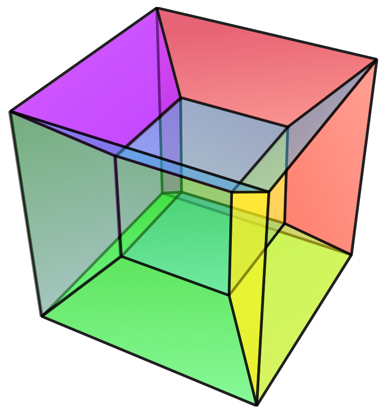
April 5, 2018



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A quick note first:

This isn't your parents' Powerpoint...

...because everything is interactive!

In [3]:

```
import datetime
import time
datestring = datetime.datetime.now().strftime('%B %d, %Y')
for c in 'Today is {}!'.format(datestring):
    print(c, end='')
    time.sleep(.1)
```

```
Today is April 05, 2018!
```

Made possible with:

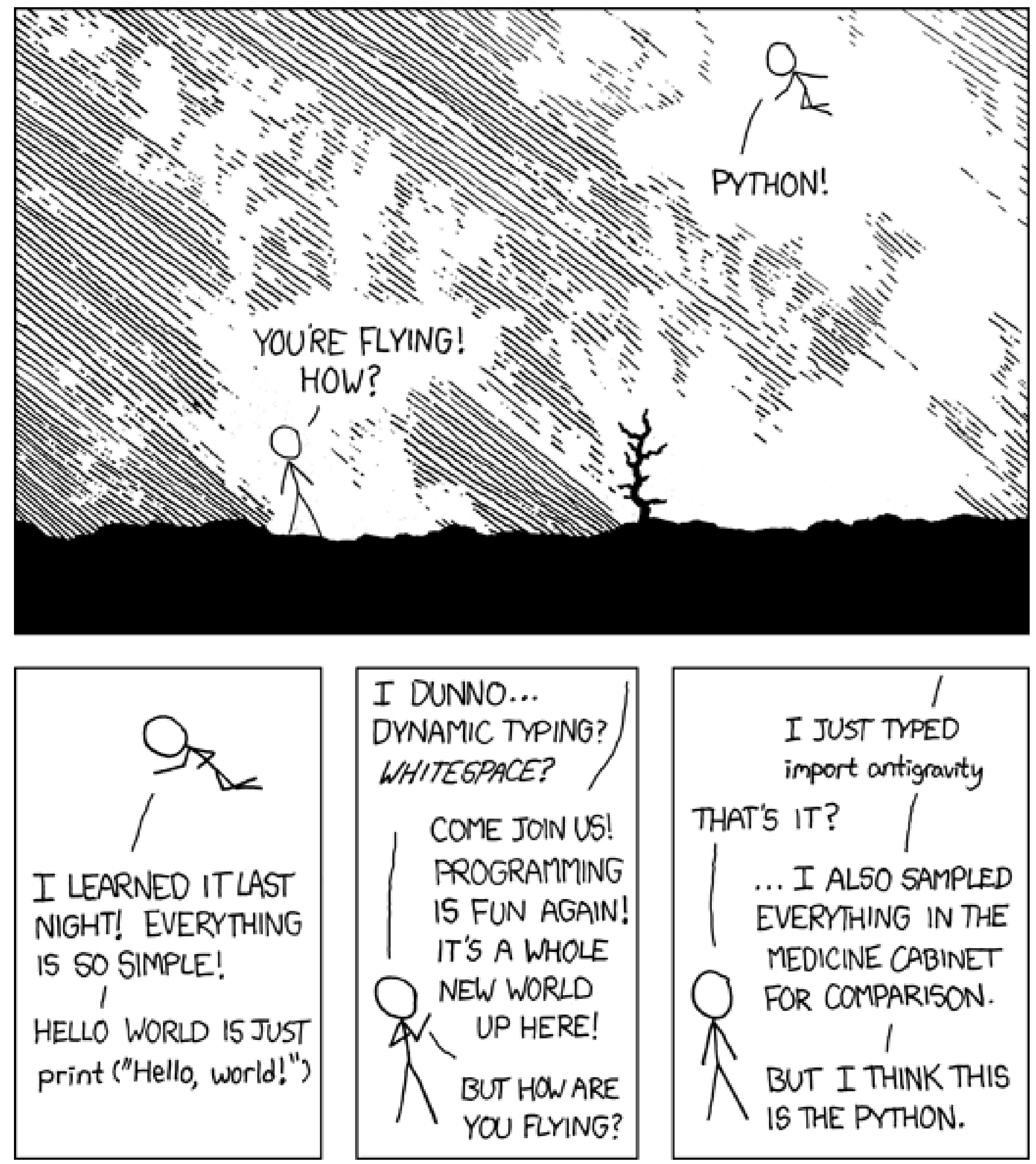
- Jupyter notebook — https://jupyter.org/
- RISE (Reveal.js IPython/Jupyter Slideshow Extension) — https://github.com/damianavila/RISE

Introduction

What is HyperSpy?

- Open-source Python library for interactive data analysis of multi-dimensional datasets
- Makes it easy to operate on multi-dimensional arrays as you would a single spectrum (or image)
- Easy access to cutting-edge signal processing tools
- Modular structure makes it easy to add custom features

Why python™?



Courtesy of XKCD: https://xkcd.com/353/

Why python™?

- Quickly becoming the *de facto* standard of scientific computing

- Free (as in speech and as in beer)
  - No pesky licenses to checkout

- Vast array of scientific libraries available:
  - `pip install antigravity`

- Thanks to `numpy` and other libraries, similar (or often better) performance than MATLAB

History of HyperSpy

- Developed by [Francisco de la Peña] in 2007 — 2012 as part of Ph.D. Thesis
- Originally called EELSLab:

Talk EELSLab: a Python toolbox for (hyper)spectroscopy data analysis

Presented by Francisco de la Peña in Poster and Demo Session 2011

Abstract

EELS*Lab*: a Python toolbox for (hyper)spectroscopy data analysis

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Modern scientific instruments from several disciplines now yield multidimensional spectroscopic data. As an example, a modern transmission electron microscope (TEM) can acquire spectral data from sub-atomic volumes that ultimately could reveal the position and nature of each atom of a material [1]. However, such datasets are usually quite large and difficult to work with.

EELS*Lab* [2] has been developed as a tool to facilitate hyperspectral data analysis. Originally it was intended for TEM data analysis, but it has been successfully used in other domains. Specifically, it provides easy access to multidimensional curve fitting, peak analysis and machine learning algorithms, as well as a viewing framework for navigating data and reading and writing capabilities for several popular hyperspectral formats.

This talk will discuss how Python has been used to implement these features, with demonstrations of applications to both spatially-resolved spectroscopic data (so-called spectrum images) [3] and to structural analysis of atomic resolution image stacks [4]. The blend of intuitiveness, power, and availability of high-quality scientific libraries that Python offers has allowed the creation of a simple, natural tool that scientists from many disciplines can both use and easily extend into new scientific domains.

References

[1] Sandra Van Aert et al., « Three-dimensional atomic imaging of crystalline nanoparticles », *Nature* 470, n°. 7334 (17th of February, 2011): 374-377.

[2] http://www.eelslab.org

[3] R. Arenal et al., « Extending the analysis of EELS spectrum-imaging data, from elemental to bond mapping in complex nanostructures », *Ultramicroscopy* 109, n°. 1 (December 2008): 32-38.

[4] Michael C. Sarahan et al., « Point defect characterization in HAADF-STEM images using multivariate statistical analysis », *Ultramicroscopy* 111, n°. 3 (February 2011): 251-257.

- Open-sourced (on Github) in 2010
- Renamed to HyperSpy in 2011
- Now... over 100 citations, and rapidly growing!

Design philosophy of HyperSpy

- HyperSpy is a Python library, rather than standalone program
    - Part of the greater scientific Python ecosystem
- Data storage is in an open hierarchical format (HDF5)
- Analysis done via reproducible notebooks
- Feature development is completely open-source

How we came to love HyperSpy

Josh:

- Became interested in multivariate statistical analysis of EELS spectrum images
- No easy way to do that in commercial software
- The entire scientific Python ecosystem is available from HyperSpy — machine learning, clustering, signal separation, etc.
- Came for the data analysis, stayed because of the community

Andy:

- Needed a way to efficiently and objectively process chemical tomography data based on hyperspectral images
- No available commercial options except brute force
- Quickly realized that HyperSpy was ideally set up to enable reproducible and well documented data analysis
    - You know, science!

Getting Started

Installation

- Easiest method on Windows — HyperSpy bundle
  - http://hyperspy.org/download.html#windows-bundle-installers
  - Installs a Python distribution with HyperSpy included
  - Best method if you have no prior Python experience

- For more control (on Windows, Mac, and Linux) — Anaconda Python
  - https://www.anaconda.com/download/
  - After installing Anaconda, simply run `conda install hyperspy`
  - This method is preferred by the developers

How to use HyperSpy?

- Console/Command line
- Integrated development environment (IDE)
- **Jupyter Notebook** (and JupyterLab)
- HyperSpyUI

Important note:

Because HyperSpy is a library, all of these are just generic ways to access Python, and not specific to HyperSpy!
(except the last one)

Console/Command line

The simplest way to run is with a pre-written script directly from the command line:

```
$ python analysis_script.py
```

There are also "advanced Python interpreters", such as Jupyter QTConsole, `bpython`, `ipython`, etc.

Integrated Development Environments

- Spyder (live example)
- PyCharm
- NetBeans

Jupyter Notebook

The Jupyter project (https://jupyter.org) exists to:

"...develop open-source software, open-standards, and services for interactive computing across dozens of programming languages."

The "Notebook" is a human-readable format for storing both the inputs and outputs of code (see https://en.wikipedia.org/wiki/Notebook_interface)...

Inspired by Mathematica and Maple; has been adopted in many languages

Features of the notebook:

- Separation of the kernel (for calculation) and the front-end (for display)
- Runs completely in the web-browser (no special software needed)
- Kernel can be run on a central server — users connect with a web browser
- `.ipynb` files are JSON format and can be versioned
- Language-agnostic (can be used with Python, R, Java, Julia, etc.)

Jupyter Lab

- An exciting new project that is more fully-featured and will eventually replace the Notebook interface
- Aims to be an IDE like Spyder or RStudio, but running within the browser
- Incorporates notebooks, the terminal, text editor, file browser, rich outputs, etc. into one interface

HyperSpyUI (https://github.com/hyperspy/hyperspyui)

- Developed in parallel to HyperSpy as a more "user-friendly" experience
- Many commonly used features from HyperSpy are available
- Deviation for a short view of HyperSpyUI (loading EELS signal, view metadata, signal separation, macro recorder)
- Most use Jupyter notebooks, but the UI is useful for quick investigations, or for those without programming experience

How to get help?

- Well-documented user guide and documentation: http://hyperspy.org/hyperspy-doc/current/user_guide/index.html
- Tutorials and demos: https://github.com/hyperspy/hyperspy-demos
- User group list: hyperspy-users@googlegroups.com
- Gitter chat: https://gitter.im/hyperspy/hyperspy
- If all else fails, Andy and Josh

HyperSpy's `Signal` Class

- The "heart" of HyperSpy's data structure
- Every dataset stored within HyperSpy is a sub-class of `Signal`

Structure of a `Signal`

- `Signal` is a wrapper around the raw data
- Data is stored in a `numpy` array
- Calibration information is stored in two types of `Axes` objects:
  - Navigation and Signal dimensions

In [4]:
```
hs.signals.Signal1D(np.random.random((10, 20, 30))).axes_manager
```

Out[4]:

< Axes manager, axes: (20, 10|30) >

Navigation axis name	size	index	offset	scale	units
	20	0	0.0	1.0	
	10	0	0.0	1.0	

Signal axis name	size	offset	scale	units
	30	0.0	1.0	

Structure of a `Signal`

Examples of signal dimensionality:

	Navigation	Signal
Single spectrum	0	1
Line scan spectrum image	1	1
Areal spectrum image	2	1
Single image	0	2
Time series image stack	1	2
4D STEM diffraction image	2	2

Structure of a `Signal`

- `Signal`s can be sliced by index, or by axis units, on either type of axis

- Signal axis slicing:

In [5]:
```
s = hs.datasets.example_signals.EDS_SEM_Spectrum()
print(s)

# Slice by axis units with floats:
print(s.isig[1.0:5.0])

# Slice by index with integers:
print(s.isig[20:100])
```

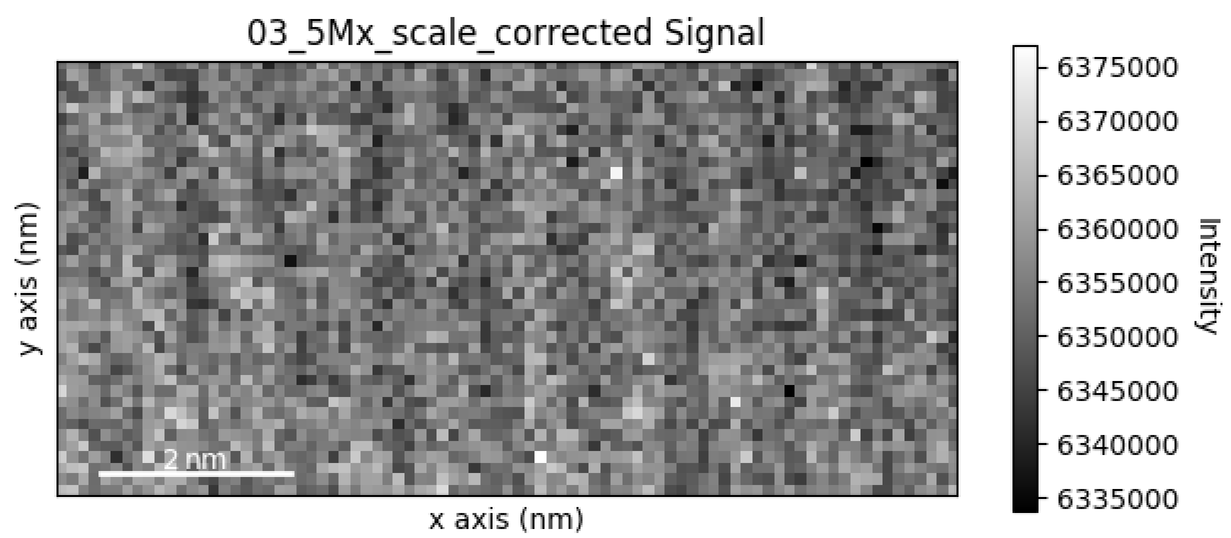
```
<EDSSEMSpectrum, title: EDS SEM Spectrum, dimensions: (|1024)>
<EDSSEMSpectrum, title: EDS SEM Spectrum, dimensions: (|400)>
<EDSSEMSpectrum, title: EDS SEM Spectrum, dimensions: (|80)>
```

- Navigation axis slicing:

```
In [6]: im = hs.load('examples/HRSTEM.dm3')
        print(im)

        # Slice by axis units and index:
        im_crop = im.isig[1.0:10.5, 20:60]
        print(im_crop)
        im_crop.plot()
```

```
<Signal2D, title: 03_5Mx_scale_corrected, dimensions: (|512, 512)>
<Signal2D, title: 03_5Mx_scale_corrected, dimensions: (|83, 40)>
```



Getting your data in (and out) of HyperSpy

Many data readers have been written for experimental tools:

Format	Read	Write	lazy	Format	Read	Write	lazy
Gatan's dm3/dm4	Yes	No	Yes	**SEMPER unf**	Yes	Yes	Yes
FEI's emi and ser	Yes	No	Yes	**Blockfile**	Yes	Yes	Yes
HDF5	Yes	Yes	Yes	**DENS heater log**	Yes	No	No
Image: jpg, TIFF, etc.	Yes	Yes	Yes	**Bruker's bcf**	Yes	No	Yes
MRC	Yes	No	Yes	**EMD (Berkley Labs)**	Yes	Yes	Yes
EMSA/MSA	Yes	Yes	No	**Protochips log**	Yes	No	No
NetCDF	Yes	No	No	**EDAX .spc and .spd**	Yes	No	Yes
Ripple	Yes	Yes	Yes				

Loading data is simple!

Example of Gatan's `dm3` format:

```
In [7]: im = hs.load('examples/HRSTEM.dm3')
```

```
In [8]: im
```

```
Out[8]: <Signal2D, title: 03_5Mx_scale_corrected, dimensions: (|512, 512)>
```

```
In [9]: im.metadata
```

```
Out[9]: ├── Acquisition_instrument
        │   └── TEM
        │       ├── acquisition_mode = STEM
        │       ├── beam_current = 0.0
        │       ├── beam_energy = 200.0
        │       ├── camera_length = 20.0
        │       ├── dwell_time = 0.00012989999389648437
        │       ├── magnification = 5000000.0
        │       └── microscope = JEOL COM
        ├── General
        │   ├── date = 2016-05-07
        │   ├── original_filename = HRSTEM.dm3
        │   ├── time = 12:58:18
        │   └── title = 03_5Mx_scale_corrected
        └── Signal
            ├── Noise_properties
            │   └── Variance_linear_model
            │       ├── gain_factor = 1.0
            │       └── gain_offset = 0.0
            ├── binned = False
            ├── quantity = Intensity
            └── signal_type =
```

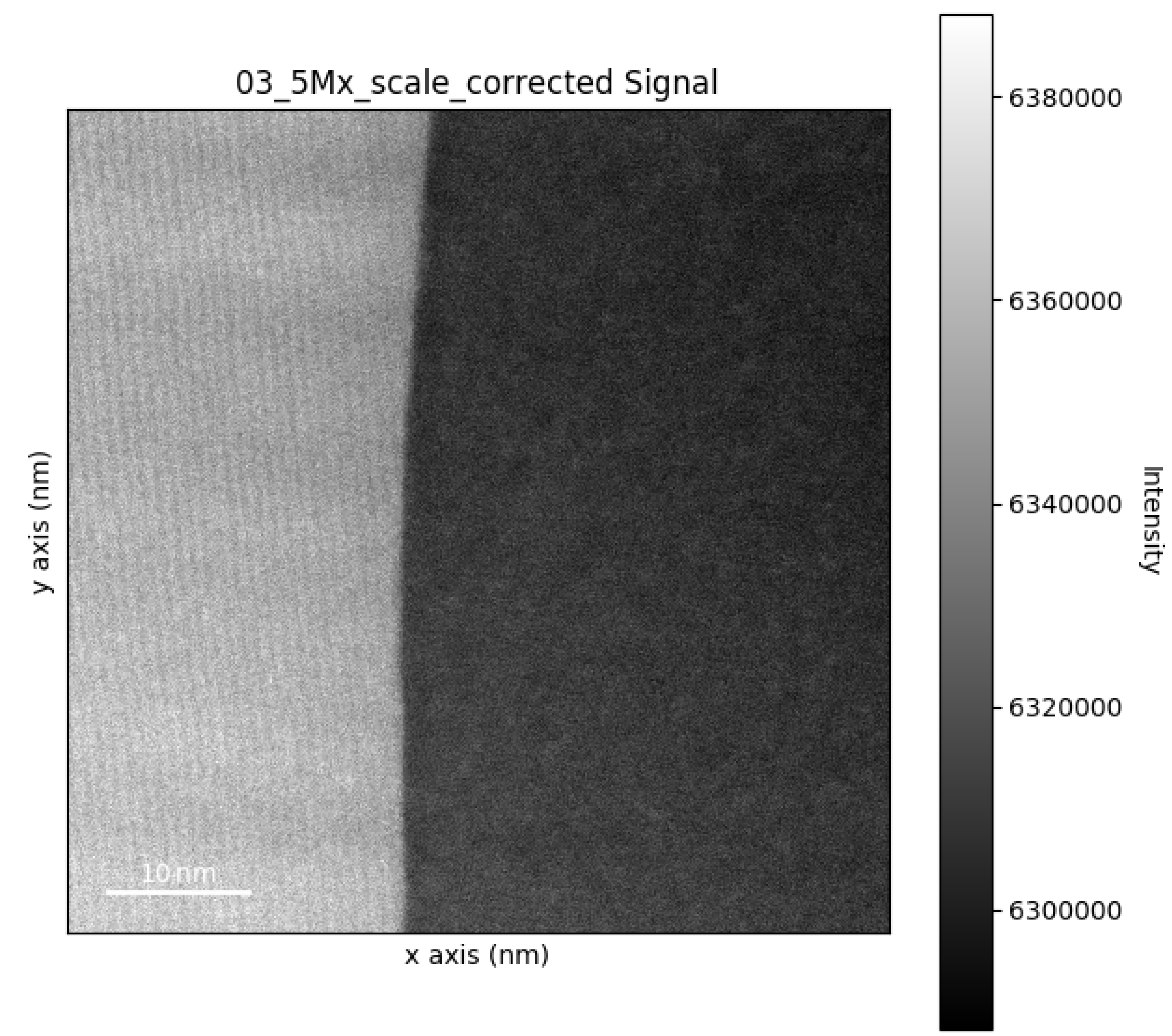
Original metadata is maintained:

In [10]:
```
im.original_metadata
```

Out[10]:
```
├── ApplicationBounds = (0, 0, 984, 1920)
├── DocumentObjectList
│   └── TagGroup0
│       ├── AnnotationGroupList
│       │   └── TagGroup0
│       │       ├── AnnotationType = 31
│       │       ├── BackgroundColor = (0, 0, 0)
│       │       ├── BackgroundMode = 2
│       │       ├── FillMode = 2
│       │       ├── Font
│       │       │   ├── Attributes = 0
│       │       │   ├── FamilyName = Microsoft Sans Serif
│       │       │   └── Size = 7
│       │       ├── ForegroundColor = (-1, -1, -1)
│       │       ├── HasBackground = 0
│       │       ├── IsMoveable = 1
│       │       ├── IsResizable = 1
│       │       ├── IsSelectable = 1
│       │       ├── IsTranslatable = 1
│       │       ├── IsVisible = 1
│       │       ├── ObjectTags
│       │       ├── Rectangle = (482.0, 16.0, 496.0, 142.0)
```

Plotting is also simple within the notebook:

In [11]:
```
im.plot()
```



EDAX EDS mapping data

In [12]:
```
s = hs.load('examples/SEM_EDS_map.spd')
```

In [13]:
```
s
```

Out[13]: <EDSSEMSpectrum, title: EDS Spectrum Image, dimensions: (256, 231|2000)>

In [14]:
```
s.axes_manager
```

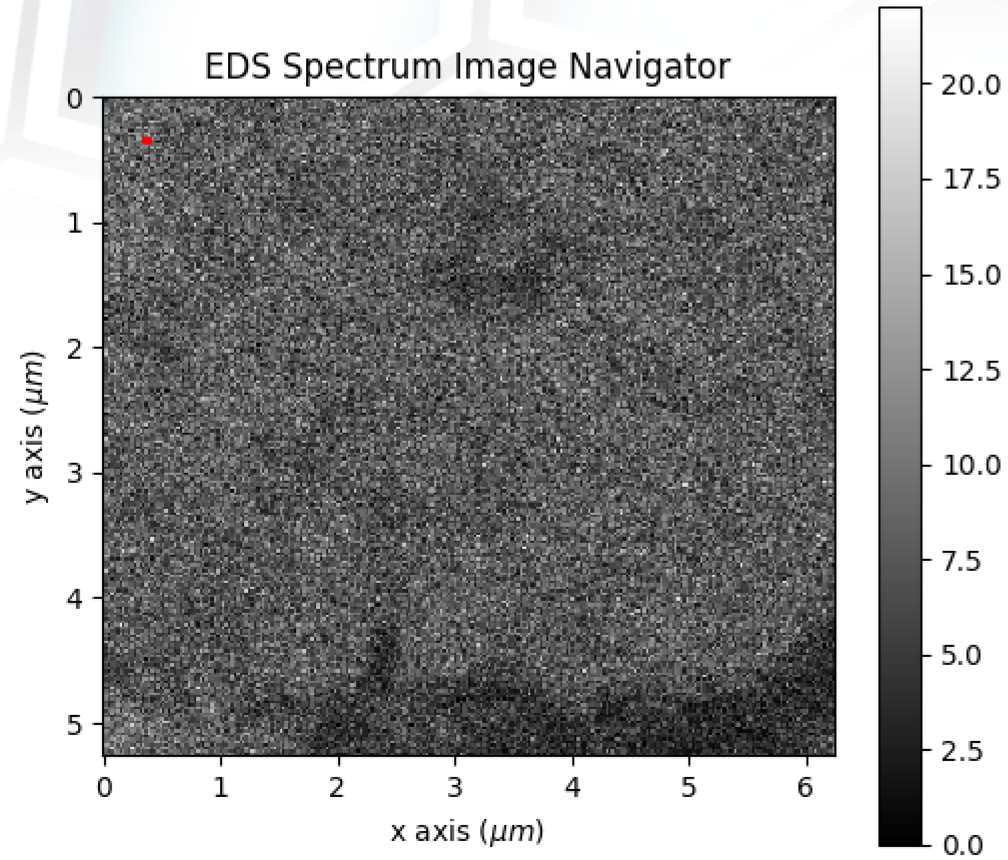
Out[14]:

< Axes manager, axes: (256, 231|2000) >

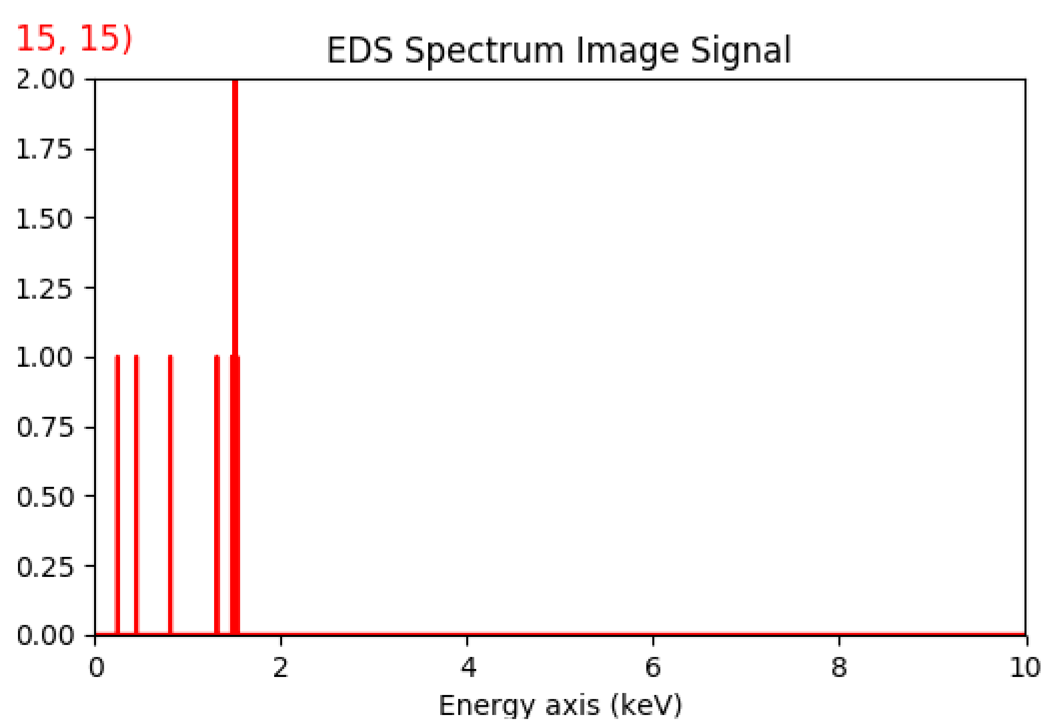
Navigation axis name	size	index	offset	scale	units
x	256	0	0.0	0.02440594509243965	μm
y	231	0	0.0	0.022832725197076797	μm

Signal axis name	size	offset	scale	units
Energy	2000	0.0	0.005	keV

In [15]:
```
s.plot()
```

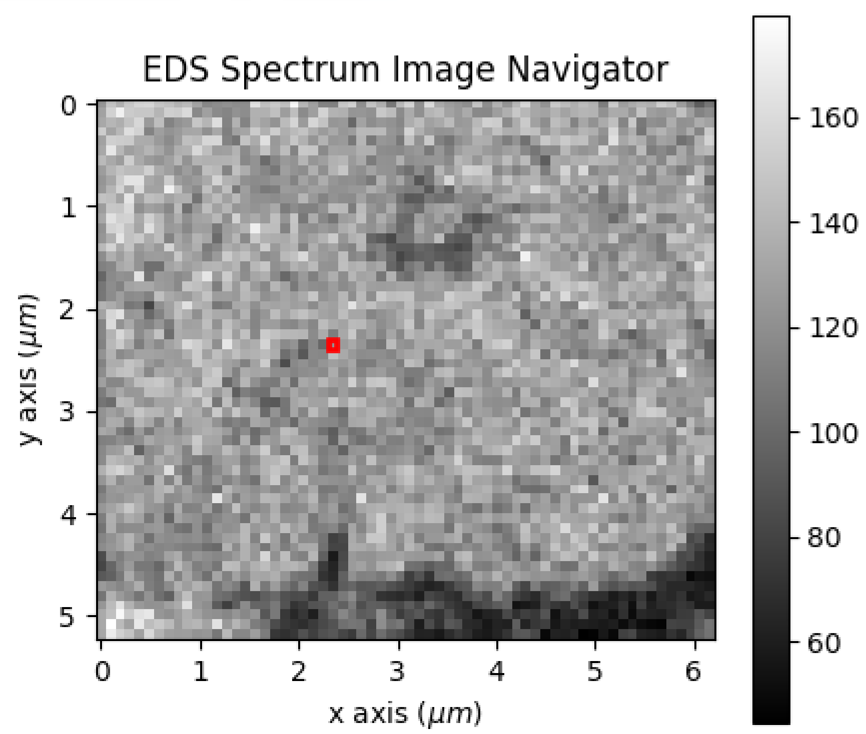


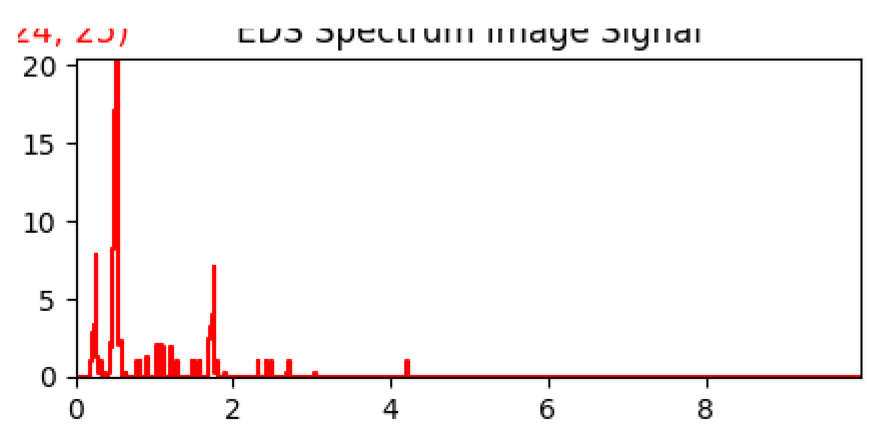
EDS Spectrum Image Navigator
y axis (μm)
x axis (μm)
0
1
2
3
4
5
6
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0



15, 15)
EDS Spectrum Image Signal
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
2
4
6
8
10
Energy axis (keV)

```
In [16]: sbin = s.rebin(new_shape=[64, 56, 500])
         sbin.plot()
```





Generic data access

- A `Signal` can be created from any data that can be expressed as a `numpy` array
- If your tool can output raw data, it can be loaded into HyperSpy with little fuss
- Using general Python features, data from other sources can be loaded easily as well

Loading a `.csv` spectrum file

In [17]:

```
# Print the first few lines of the .csv file for inspection:
with open('examples/spectrum.csv', 'r') as f:
    for i in range(10):
        print(f.readline(), end='')
```

```
# Energy (eV), Counts
9.000000134110450745e+01,1.090600000000000000e+04
9.020000134408473969e+01,1.090400000000000000e+04
9.040000134706497192e+01,1.069800000000000000e+04
9.060000135004520416e+01,1.044400000000000000e+04
9.080000135302543640e+01,1.038000000000000000e+04
9.100000135600566864e+01,1.030400000000000000e+04
9.120000135898590088e+01,1.019400000000000000e+04
9.140000136196613312e+01,1.022700000000000000e+04
9.160000136494636536e+01,1.006700000000000000e+04
```

In [18]:
```
# Load the data into a numpy array from the .csv file:
d = np.loadtxt("examples/spectrum.csv", delimiter=',')

# Create a signal from the second column of data (the spectral counts)
s = hs.signals.Signal1D(d[:,1])
s
```

Out[18]:
```
<Signal1D, title: , dimensions: (|2041)>
```

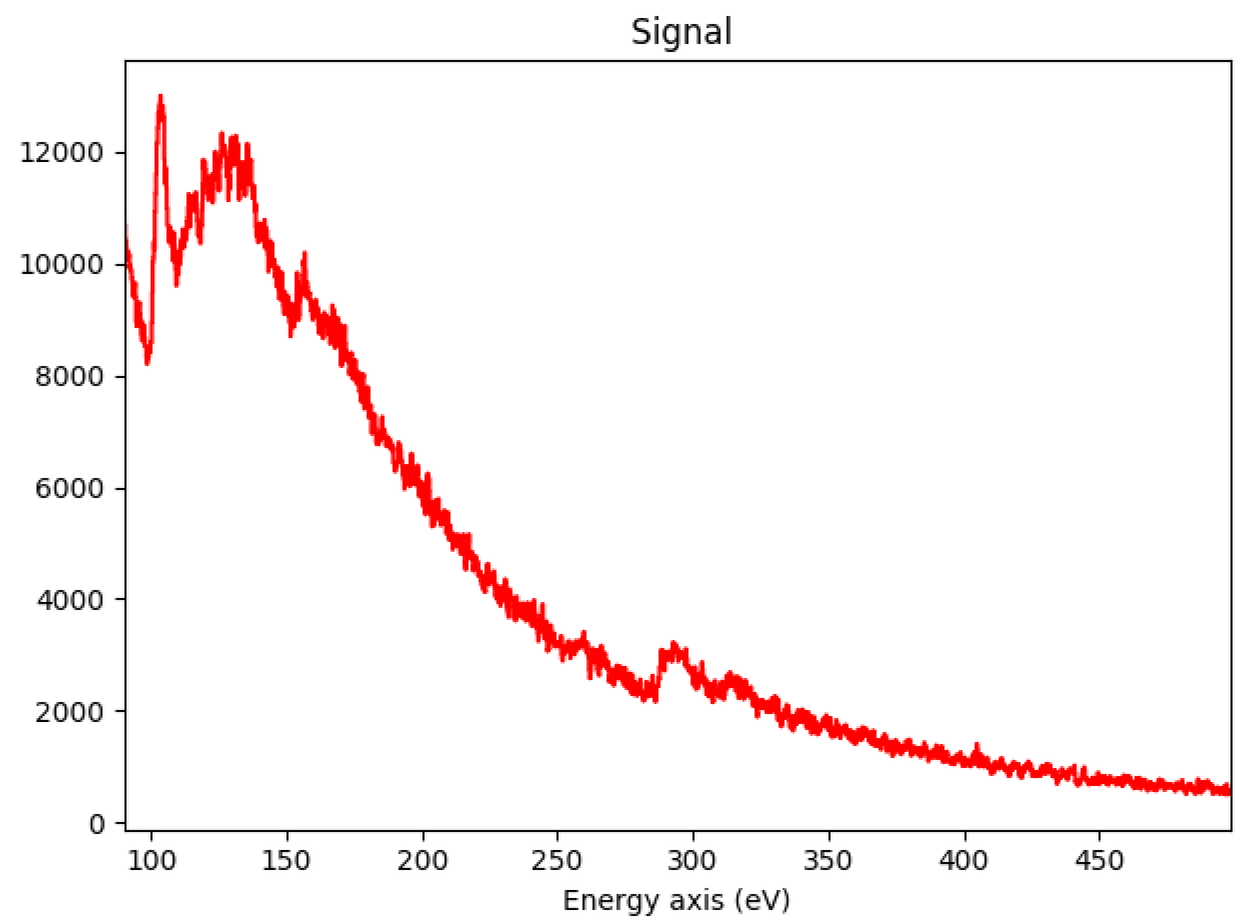
In [19]:
```
# Take the first column of values and set the energy axis accordingly:
energy_data = d[:,0]
s.axes_manager[0].scale = np.diff(energy_data).mean()
s.axes_manager[0].units = 'eV'
s.axes_manager[0].offset = energy_data[0]
s.axes_manager[0].name = 'Energy'
s.axes_manager
```

Out[19]:

< Axes manager, axes: (|2041) >

Signal axis name	size	offset	scale	units
Energy	2041	90.00000134110451	0.20000000298023224	eV

In [21]:
```
s.plot()
```


Signal
12000
10000
8000
6000
4000
2000
0
100
150
200
250
300
350
400
450
Energy axis (eV)

Loading and saving MATLAB files

The SciPy project provides a Matlab reader and saver that makes this easy:

In [22]:
```
from scipy.io import loadmat, savemat
house = loadmat('examples/house_image.mat')
print(house['__header__'])
```

```
b'MATLAB 5.0 MAT-file, Platform: PCWIN64, Created on: Mon Sep 11 14:27:46 2017'
```

In [23]:
```
s = hs.signals.Signal2D(house['IMin0'])
print(s.metadata)
s.axes_manager
```

```
├── General
│   └── title =
└── Signal
    ├── binned = False
    └── signal_type =
```

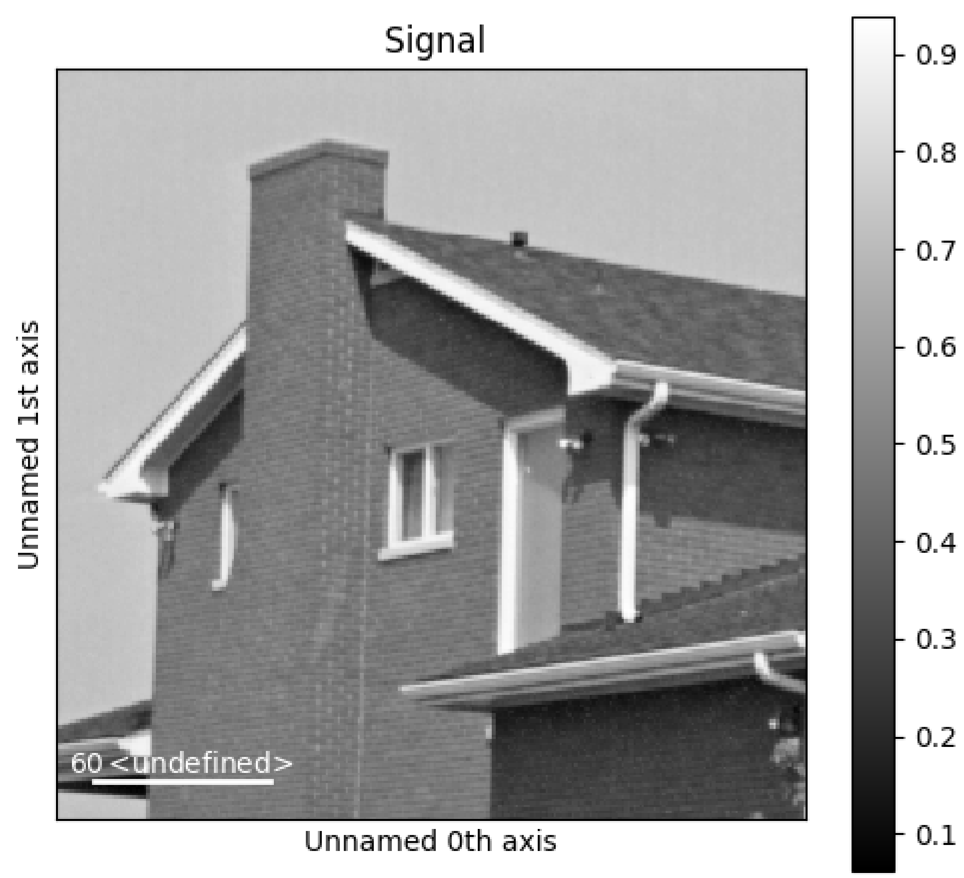
Out[23]:

< Axes manager, axes: (|256, 256) >

Signal axis name	size	offset	scale	units
	256	0.0	1.0	
	256	0.0	1.0	

In [24]:

```
s.plot()
```



Signal
Unnamed 1st axis
Unnamed 0th axis
60 <undefined>
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

"Lazy" signal access

- HyperSpy makes it easy to work with big data (bigger than your system's memory)
- Uses the excellent `dask` library for chunking operations
- Almost all the regular features of HyperSpy can operate on "lazy" signals (see User Guide)

Comparison with normal loading:

In [25]:
```
# Load the EDS map lazily:
s = hs.load('examples/SEM_EDS_map.spd', lazy=True)
print(type(s.data))
```

```
<class 'dask.array.core.Array'>
```

In [26]:
```
# Print some statistics about memory usage
print("Full dataset should consume:", s.data.nbytes / 1e6, 'MB')
print("Chunk sizes are:", s.data.chunks)
one_chunk = s.data[:s.data.chunks[0][0], :s.data.chunks[1][0],:s.data.chunks[2][0]]
print("Memory use from one chunk: ", one_chunk.nbytes / 1e6, "MB")
```

```
Full dataset should consume: 236.544 MB
Chunk sizes are: ((77, 77, 77), (128, 128), (2000,))
Memory use from one chunk:  39.424 MB
```

Saving data from HyperSpy — HDF5

- The default format for HyperSpy data is an `.hspy` file in HDF5 format
- Open, hierarchical data format supporting compression and full read/write capability
- All HyperSpy signals can be saved as `.hspy` files
- Saves full metadata about signal, including critical processing parameters
  - Modeling, signal separation, elemental information

Saving data from HyperSpy — data interchange

- Other formats can be easily written:
    - Single spectra — `.msa` format
    - Images — TIFF, JPG, etc.
    - Spectrum images — Lispix-style `.rpl`/`.raw` pairs

Electron microscopy-specific tools

- HyperSpy is incredibly flexible, but was developed from a microscopy perspective
- Has in-depth features related to image, EDS, and EELS processing
  - Many of the tools are applicable to multiple modalities
- Some other EM tools available:
  - Dielectric function analysis (for plasmon EELS)
  - Electron holography
  - "Extension" projects that build upon HyperSpy (like Andy's `tomotools`)
- Provides a robust framework on which to develop new processing pipelines

EDS Processing

- EDS support is implemented as `EDSSpectrum`, a subclass of `Signal` for EDS-specific features

- Open metadata structure holds relevant info about instrument and detectors:

In [27]:
```
s = hs.datasets.example_signals.EDS_TEM_Spectrum()
s.metadata.Acquisition_instrument.TEM.Detector
```

Out[27]:
```
└── EDS
    ├── azimuth_angle = 0.0
    ├── detector = Super-X 4 detectors Brucker
    ├── elevation_angle = 22.0
    └── energy_resolution_MnKa = 133.312296
```

- Also holds all the compositional information:

In [28]:
```
print(s.metadata.Sample.elements)

# Elements can be added easily:
s.add_elements(['Cu'])
print(s.metadata.Sample.elements)
```

```
['Fe' 'Pt']
['Cu', 'Fe', 'Pt']
```

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Processing tools

- All the "basic" EDS processing tools are included:
  - Background removal
  - Net intensity line map extraction
  - Quantification using Cliff-Lorimer (k-factors), ζ-factors, and ionization cross sections

- Can also use the general HyperSpy tools for more advanced analysis:
  - Curve fitting
  - Machine learning
    - Factor reduction
    - Signal separation ("phase mapping")

- Look to the extensive documentation in the User Guide and Tutorials for help

EELS Processing

- EELS is a "first-class citizen" — software was originally called "EELSLab"
- EELS support is implemented as `EELSSpectrum`, a subclass of `Signal` for EELS-specific features
- Like EDS, open metadata structure holds relevant info about instrument and detectors:

In [29]:
```
s = hs.load('examples/signal_separation_EELS_SI.hdf5')
s.metadata.Acquisition_instrument
```

Out[29]:
```
└── TEM
    ├── Detector
    │   └── EELS
    │       └── collection_angle = 20.829999923706055
    ├── beam_energy = 200.0
    ├── convergence_angle = 12.0
    └── dwell_time = 0.20000000000000001
```

Processing tools

- Almost all of Egerton's EELS methods are built in:
    - Core-loss background subtraction
    - Estimating thickness
    - Low-loss deconvolution
    - Estimating elastic scattering threshold
    - Kramers-Kronig analysis

- Can also use the general HyperSpy tools for more advanced analysis:
    - Curve fitting
    - Machine learning
        - Factor reduction
        - Signal separation ("phase mapping")

- Look to the extensive documentation in the User Guide and Tutorials for help

Extensibility of HyperSpy

- For most, HyperSpy already does everything a microscopist might need
- Open framework means if it doesn't, you can make it so!
- Some examples:
  - Andy's `tomotools`
  - pyXem — Pythonic Crystallographic Electron Microscopy
  - Atomap — Quantifying atomic columns in ADF STEM images
  - fpd_data_processing — Fast Pixelated Detector processing

Interactive demos

- Curve fitting (and it's application to EELS spectrum images)
- Processing TEM EDS data (including source separation)
- Extensibility (Andy's `tomotools` package)