

HyperSpy: open-source multidimensional analysis software for electron microscopy

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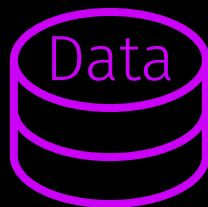




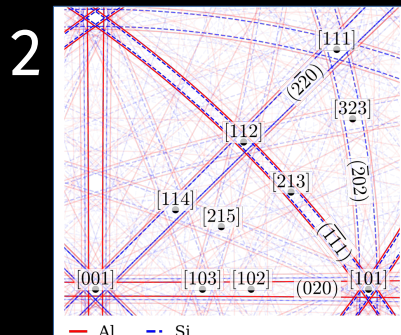
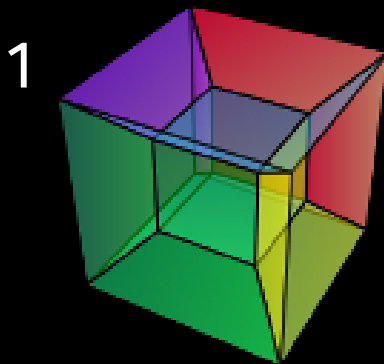
... assess the state-of-the-art and reliability of microbeam analysis techniques

FAIR guiding principles

- Findable
- Accessible
- Interoperable
- Reproducible



Algorithms
Tools
Workflows



Why open-source? Why HyperSpy?



Why open-source? Why HyperSpy?

Collect data

Write new
code to
analyse data

Analyse
data

Publish
result in
journal



Community driven

Source code,
issues, discussions

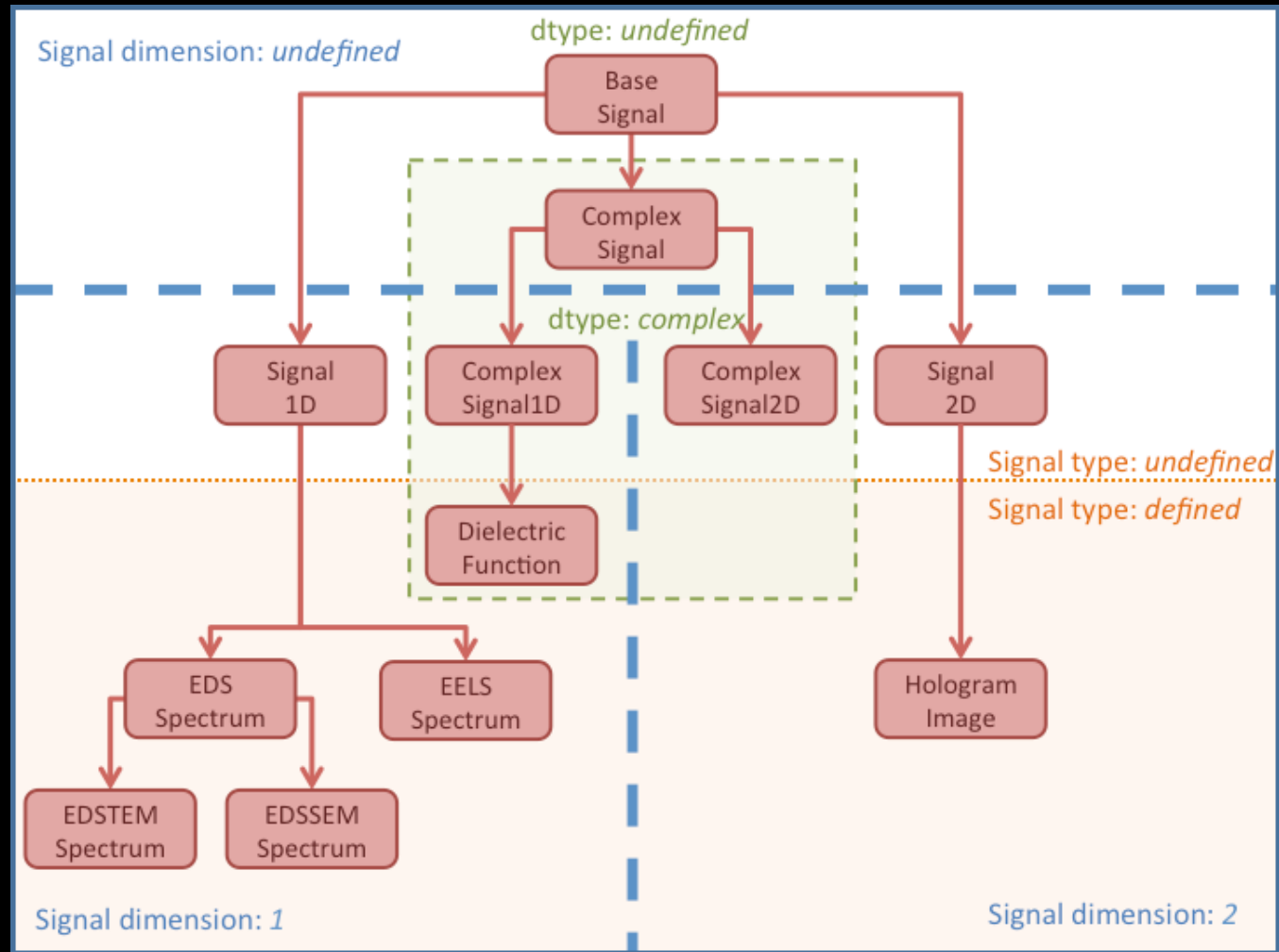


*"I hope no-one else thought
of this before I did..."*

*"I'm glad someone coded this already,
now I don't have to!"*

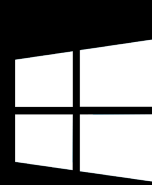
Format	Read	Write	lazy
Gatan's dm3	Yes	No	Yes
Gatan's dm4	Yes	No	Yes
FEI's emi and ser	Yes	No	Yes
hspy	Yes	Yes	Yes
zspy	Yes	Yes	Yes
Image: e.g. jpg, png, tif, ...	Yes	Yes	Yes
TIFF	Yes	Yes	Yes
MRC	Yes	No	Yes
MRCZ	Yes	Yes	Yes
EMSA/MSA	Yes	Yes	No
NetCDF	Yes	No	No
Ripple	Yes	Yes	Yes
SEMPER unf	Yes	Yes	Yes
Blockfile	Yes	Yes	Yes
DENSsolutions' Impulse log	Yes	No	No
DENSsolutions' Digiheater log	Yes	No	No
Bruker's bcf	Yes	No	Yes
Bruker's spx	Yes	No	No
EMD (NCEM)	Yes	Yes	Yes
EMD (Velox)	Yes	No	Yes
Protochips log	Yes	No	No
EDAX spc and spd	Yes	No	Yes
h5USID h5	Yes	Yes	Yes
Phenom elid	Yes	No	No
DigitalSurf's sur and pro	Yes	No	No
Nexus nxs	Yes	Yes	Yes
EMPAD xml	Yes	No	Yes
JEOL asw, map, img, pts, eds	Yes	No	No
TVIPS .tvips	Yes	Yes	Yes

Analyse your own data



How do I get it?

→ hyperspy.org



HyperSpy

1.7.4

Search docs

USER GUIDE

- Introduction
- Changelog
- Installing HyperSpy
- Getting started
- The Signal class
- Axes handling
- Interactive Operations and Region of Interest (ROI)
- Signal1D Tools
- Signal2D Tools
- Data visualization
- Machine learning
- Model fitting
- Electron Energy Loss Spectroscopy
- Energy-Dispersive X-ray Spectrometry (EDS)

Welcome to HyperSpy's documentation!

User Guide

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- Dielectric function tools
- Electron Holography
- Loading and saving data
- Events
- Working with big data
- Metadata structure
- Bibliography

```
> pip install hyperspy
```

HyperSpy Bundle (installation wizard) 

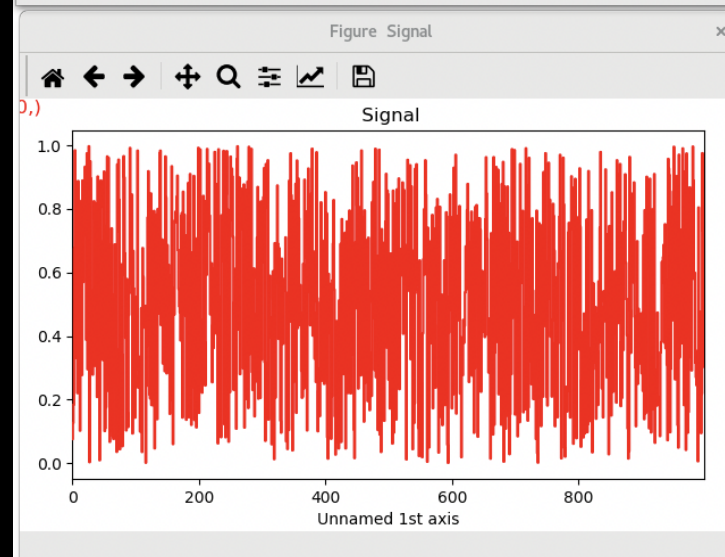
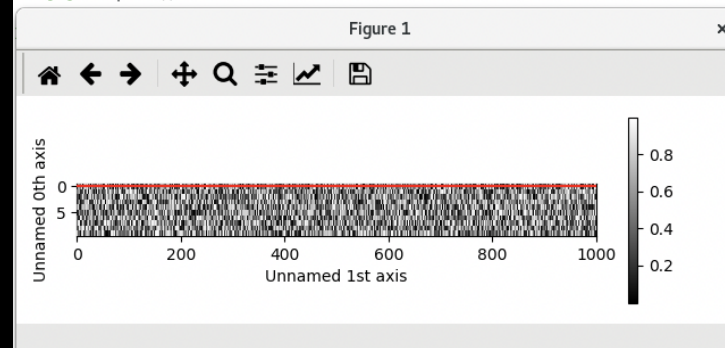
Anaconda Navigator (GUI) 

How do I use it?

→ hyperspy.org

> ipython

```
In [1]: import numpy as np
In [2]: import hyperspy.api as hs
In [3]: s = hs.signals.Signal1D(np.random.random(size=(10, 1000)))
In [4]: s.plot()
```



In your terminal

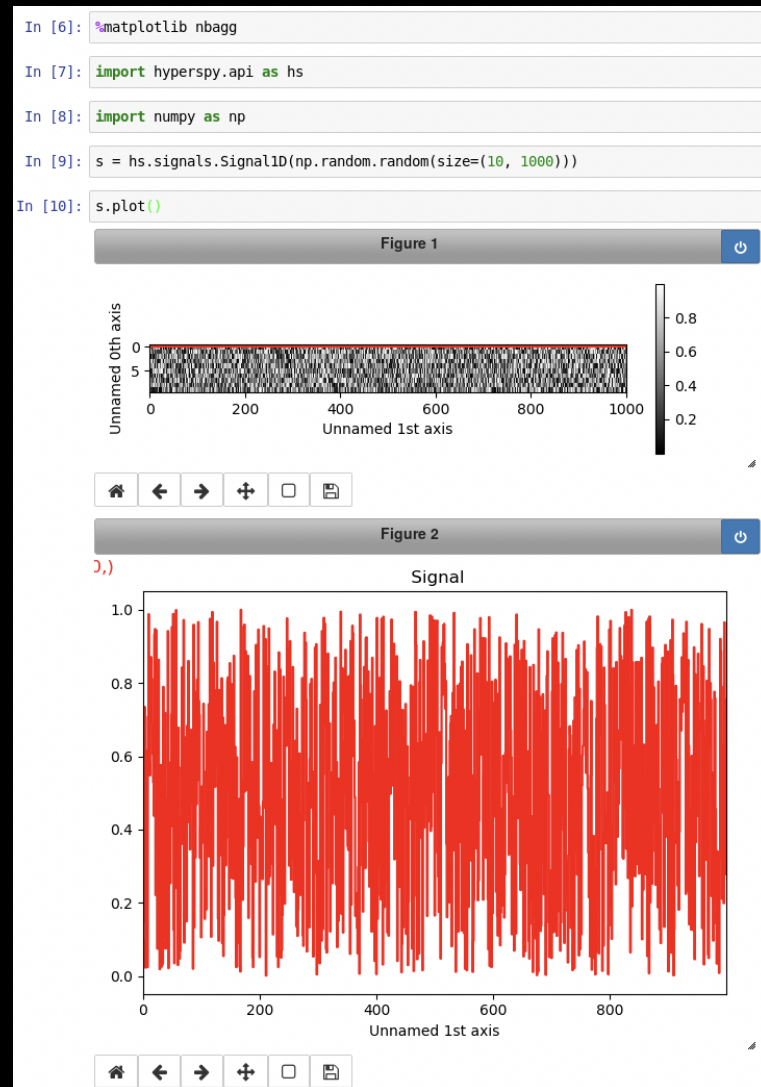
How do I use it?

→ hyperspy.org

> `jupyter-lab`

> `jupyter-notebook`

In your browser



How do I use it?

From your desktop

The screenshot displays the HyperSpy software interface with several windows open:

- Figure Core shell Navigator:** A heatmap showing spatial distribution of signals across a grid.
- Figure Core shell Signal:** A plot of signal intensity versus energy (keV), showing peaks at approximately 6.4 and 8.0 keV.
- Figure X-ray line...:** Two smaller plots showing X-ray line intensity for different elements.
- Console:** A terminal window with a red border containing the following Python code:

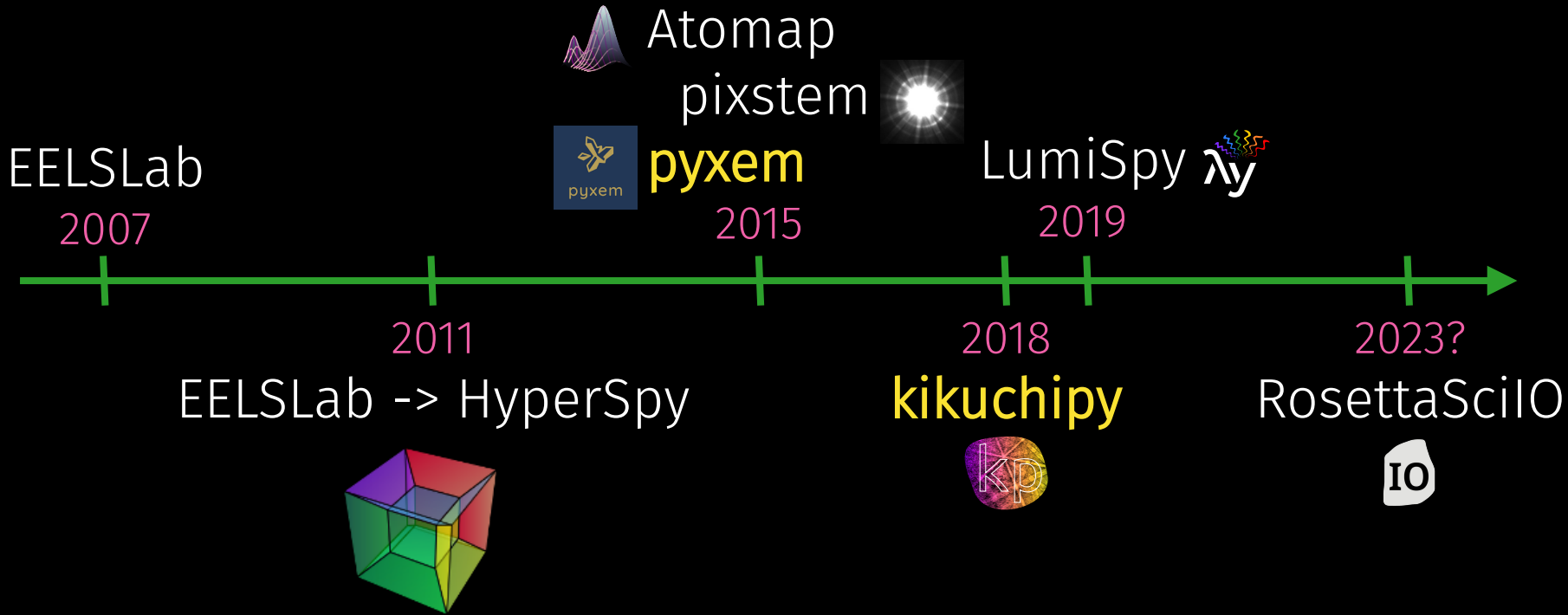
```
In [1]: a=ui.get_selected_signal()
In [2]: a
Out[2]: <EDSTEMSpectrum, title: Core shell, dimensions:
(64, 64|992)>
In [3]: EDS_sum = a.sum()
In [4]: m = EDS_sum.isig[5.:15.].create_model()
In [5]: m.add_family_lines(['Cu_Ka', 'Co_Ka'])
In [6]: m.plot()
In [7]: m.fit()
In [8]: m.fit_background()
```
- Figure Core shell Signal (bottom):** A plot of signal intensity versus energy (keV) with a fitted curve, showing peaks at approximately 6.4 and 8.0 keV.
- Element picker:** A window showing a periodic table with elements highlighted in blue.
- Recorder:** A window with 'Start' and 'Stop' buttons and checkboxes for 'Actions' and 'Code'.
- Contrast control:** A window with a slider and 'Level: 0'.
- Data View:** A window showing a list of data series, including 'Core shell', 'Core shell', 'X-ray line intensity of Core shell: Fe_Ka at 6.40 keV', and 'X-ray line intensity of Core shell: Pt_Ma at 2.05 keV'.

Visualisation
Maths
'Slicing'
Generic fitting

Mapping ops.
Metadata
ML
Big data

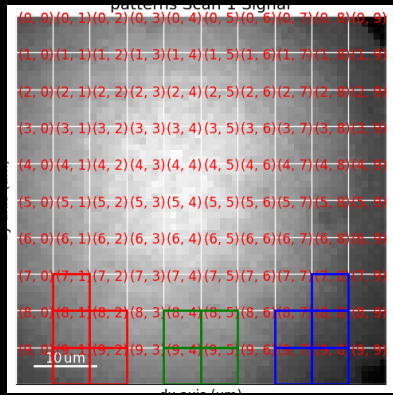
Limited functionality.. unless you use the built-in console!

A brief history of HyperSpy and (some) of its extensions

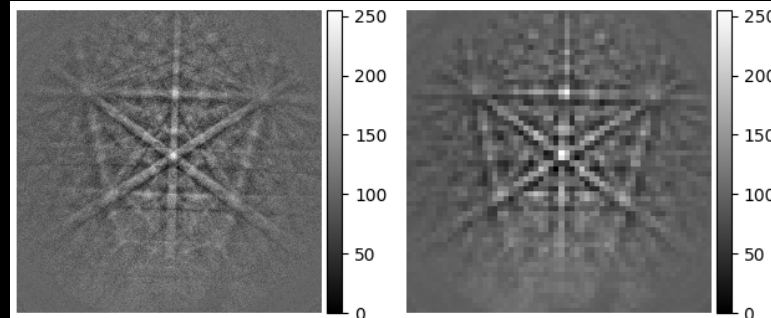


kikuchipy: diffraction in SEM

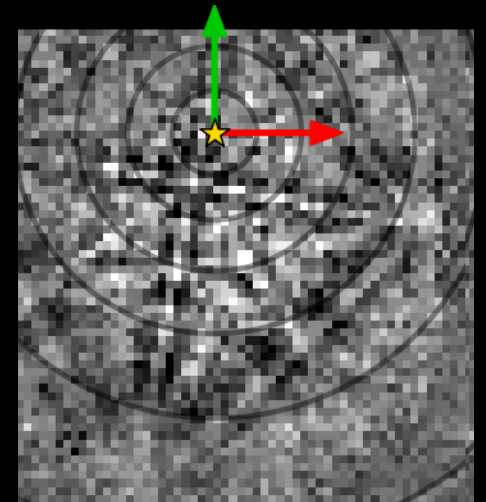
Virtual imaging



Pattern processing

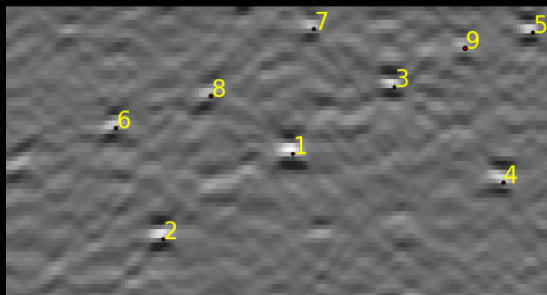


Calibration

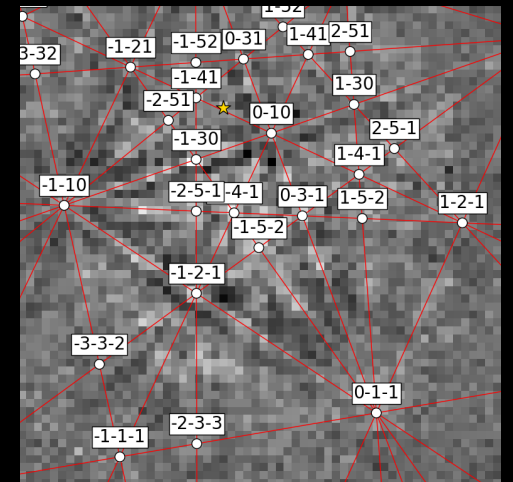
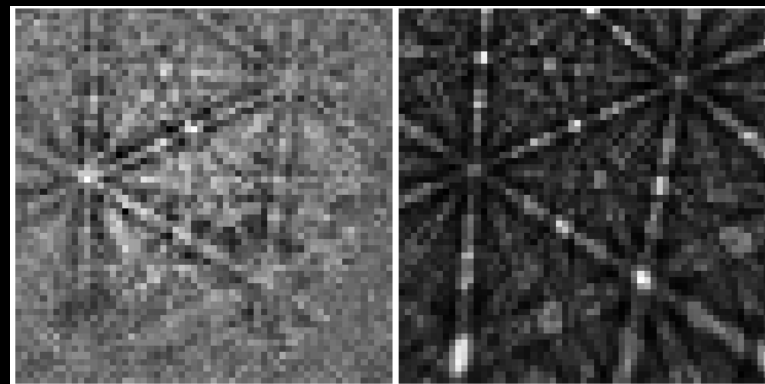


Geo./kin. simulations

Hough indexing



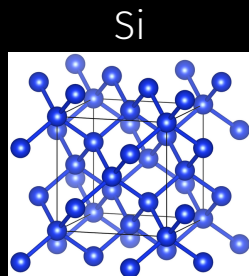
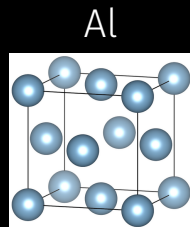
Pattern matching



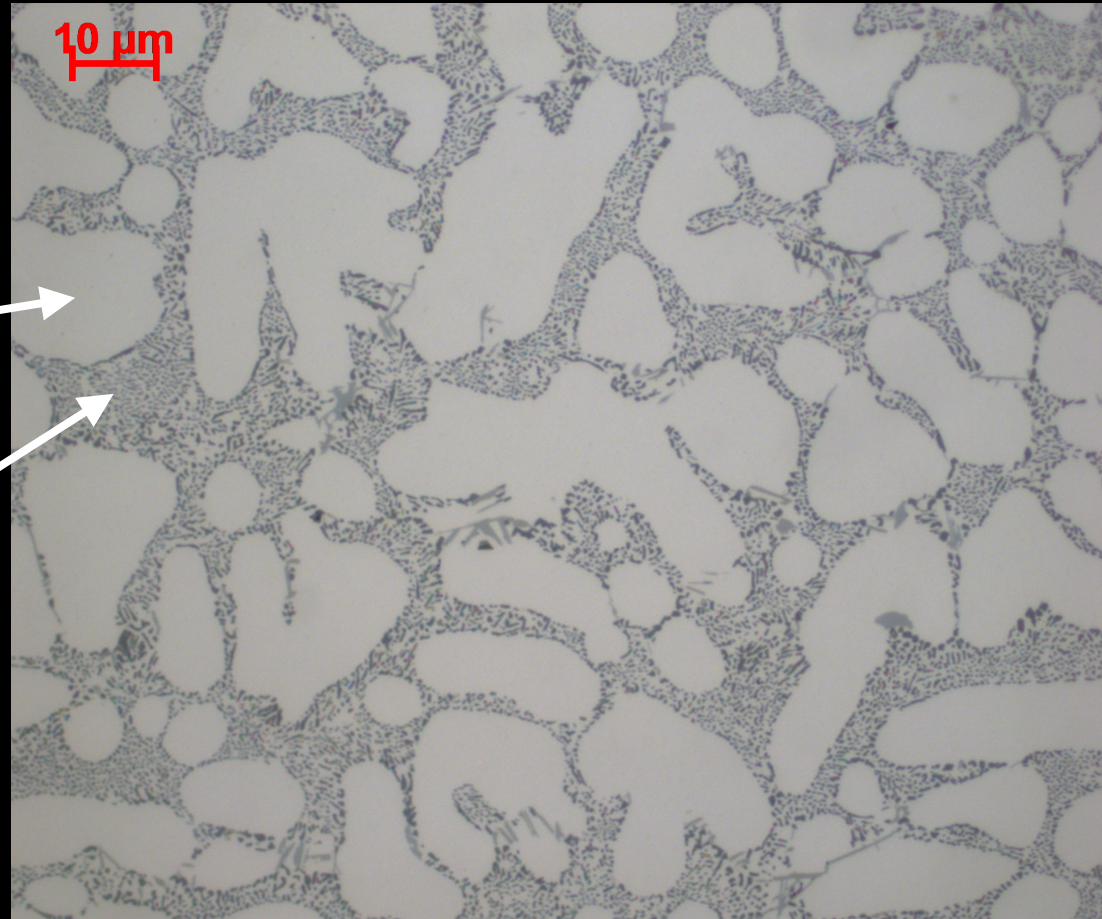
Differentiate between two similar cubic crystals

Al-10wt.%Si

	Structure	Atomic positions	a [Å]	Space group
Al	FCC	4a	4.05	Fm-3m (225)
Si	Diamond	8a	5.43	Fd-3m (227)

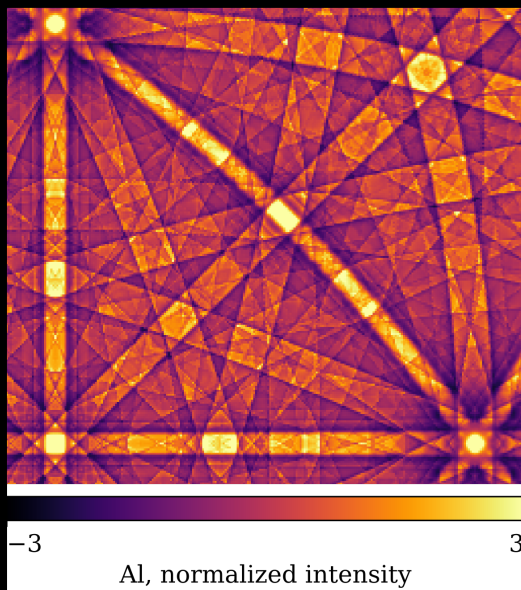
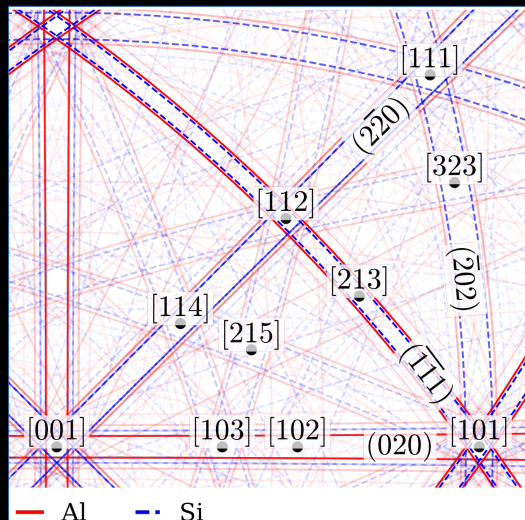
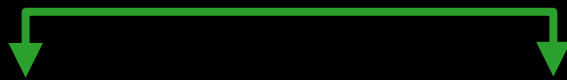


$$\Delta a = 25\%$$

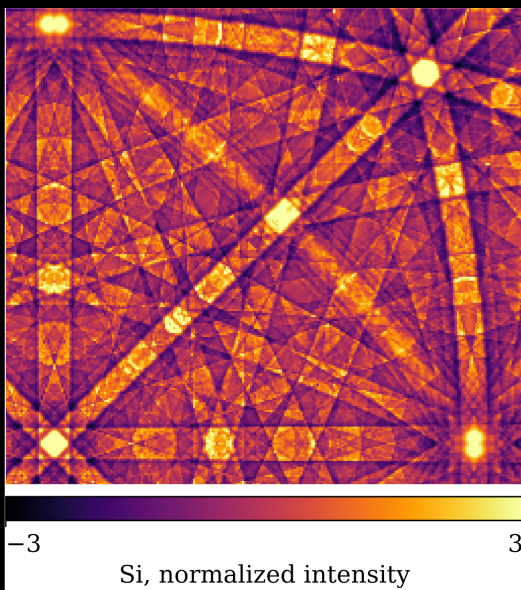


How similar is Al and Si?

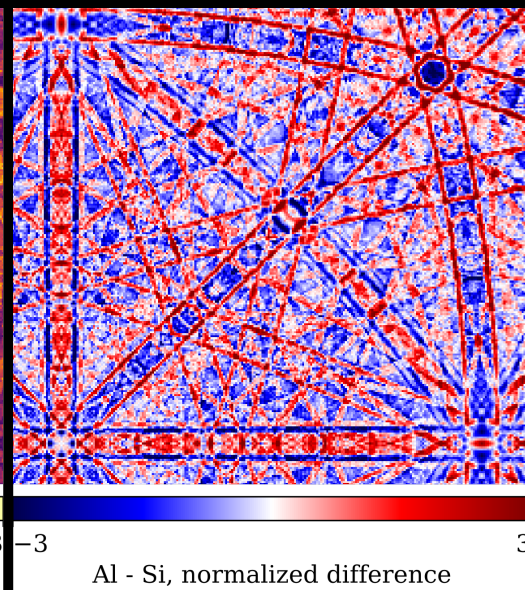
$$r = 0.3256$$



Al, normalized intensity



Si, normalized intensity

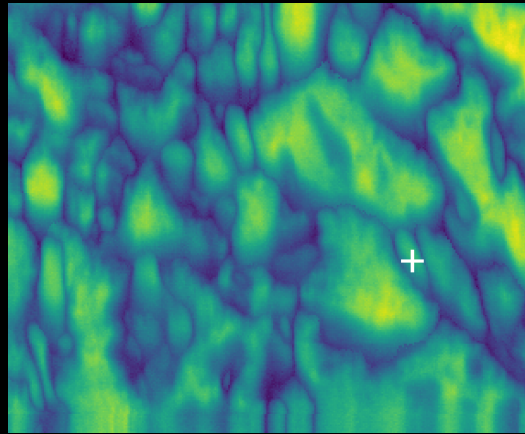


Al - Si, normalized difference

Use *relative intensities*

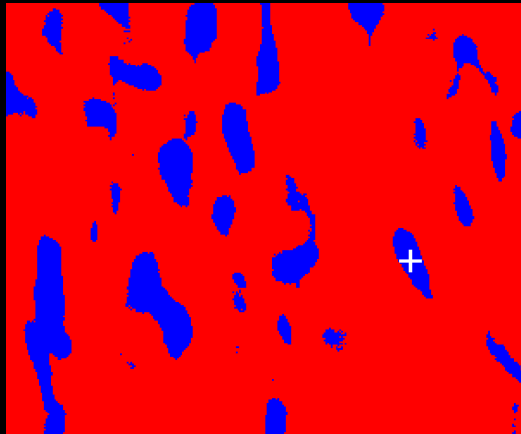
Microstructure of one Si colony in Sr-modified Al-10Si

1 μm

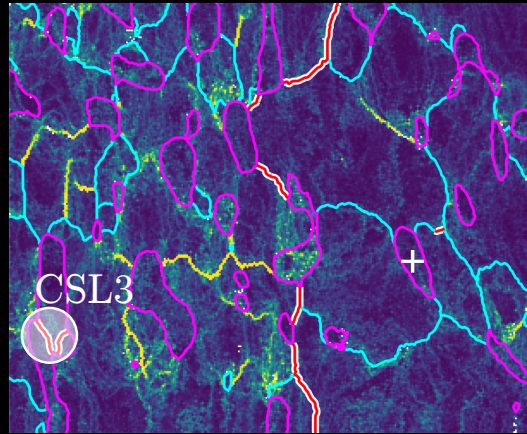
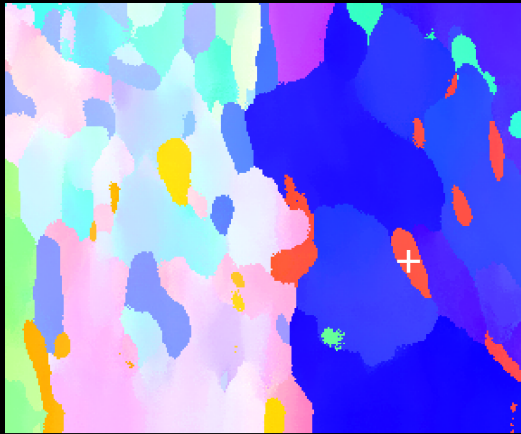


Normalized cross-correlation, r

0.2 0.3 0.4 0.5



Al 87% Si 13%

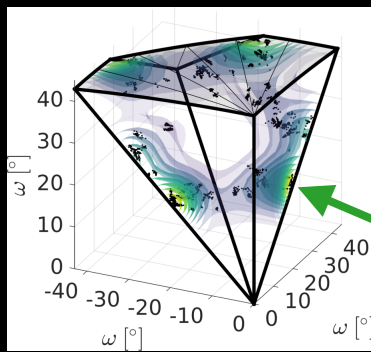
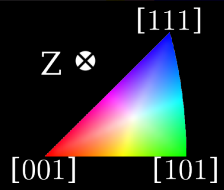
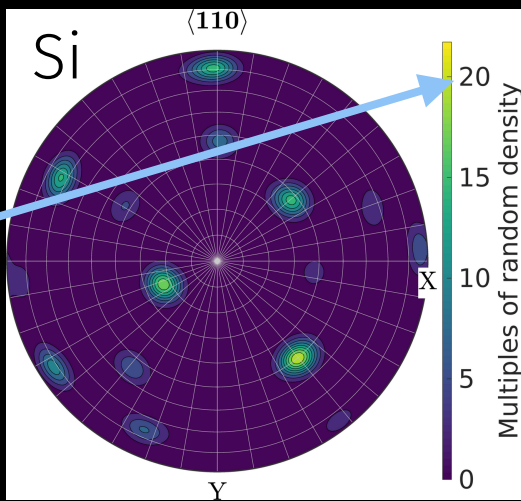


KAM [$^{\circ}$]

0 1

- Phase boundary
- GB
- HAGB, $\omega > 15^{\circ}$

Strong Si
<110> texture



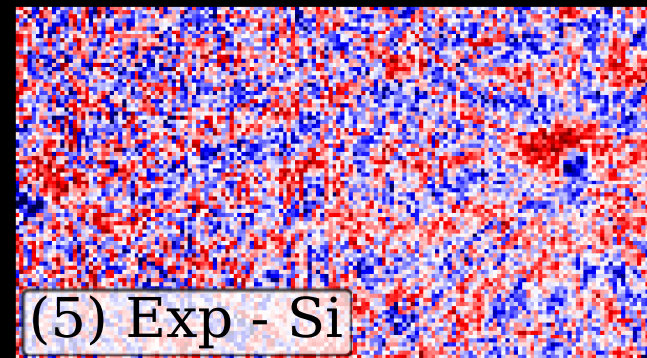
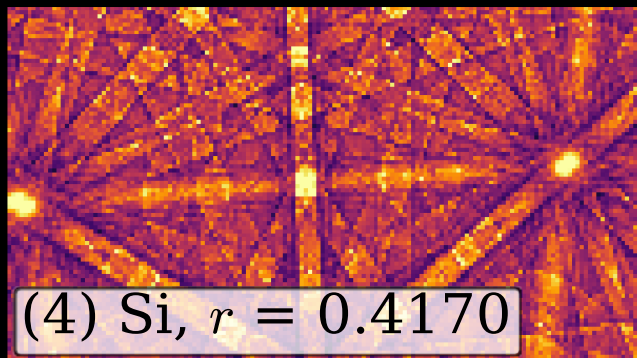
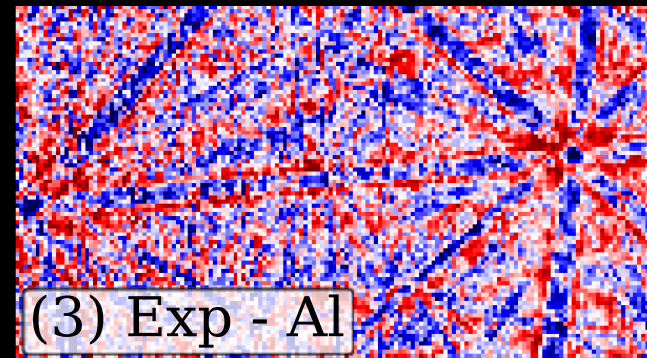
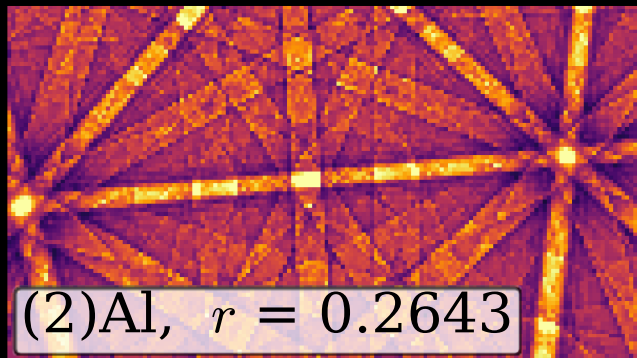
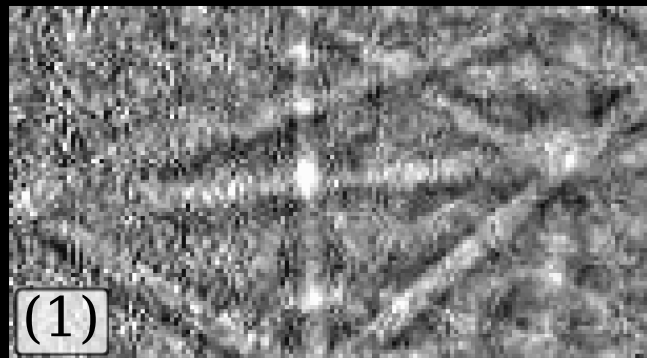
No clear Si/Al
relationship:
7.3 MRD

Reliable results? Evaluate patterns!

Exp.

Sim.

Exp. - Sim.



HyperSpy: open-source multidimensional analysis software for electron microscopy

Support and use open-source software

Contributes to assessing the reliability of microbeam analysis techniques

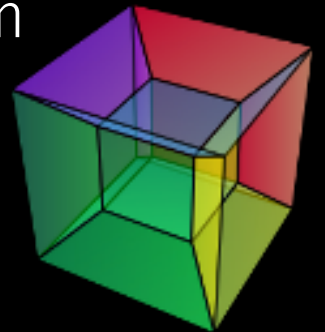
Thanks to contributors of HyperSpy's ecosystem

Special thanks to originators:

Francisco de la Peña (HyperSpy)

Duncan Johnstone (pyxem)

Thank you!



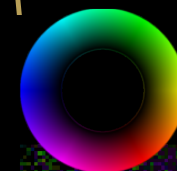
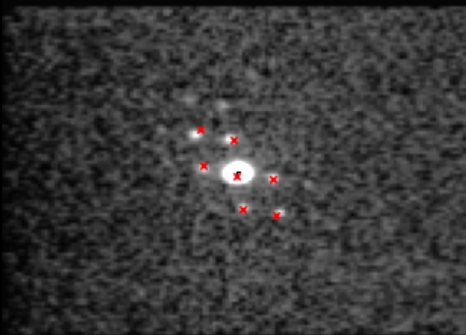
Virtual imaging



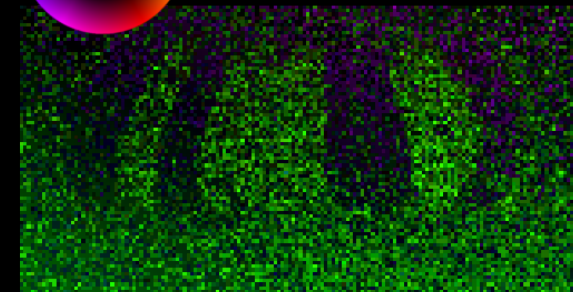
60 <undefined>

pyxem: diffraction in TEM

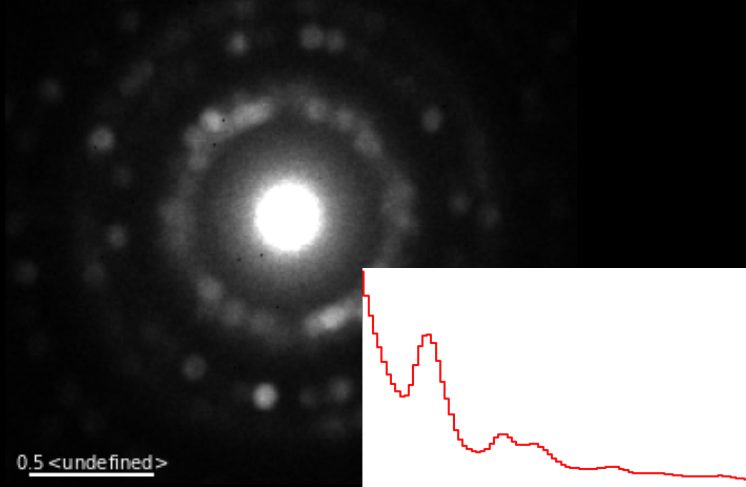
Peak finding



Differential phase contrast



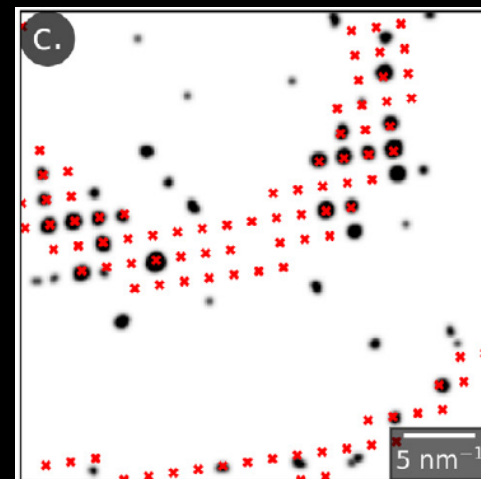
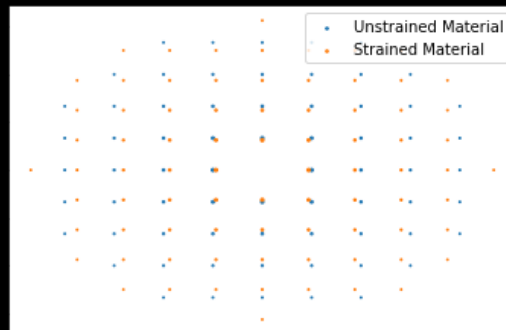
Radial integration



0.5 <undefined>

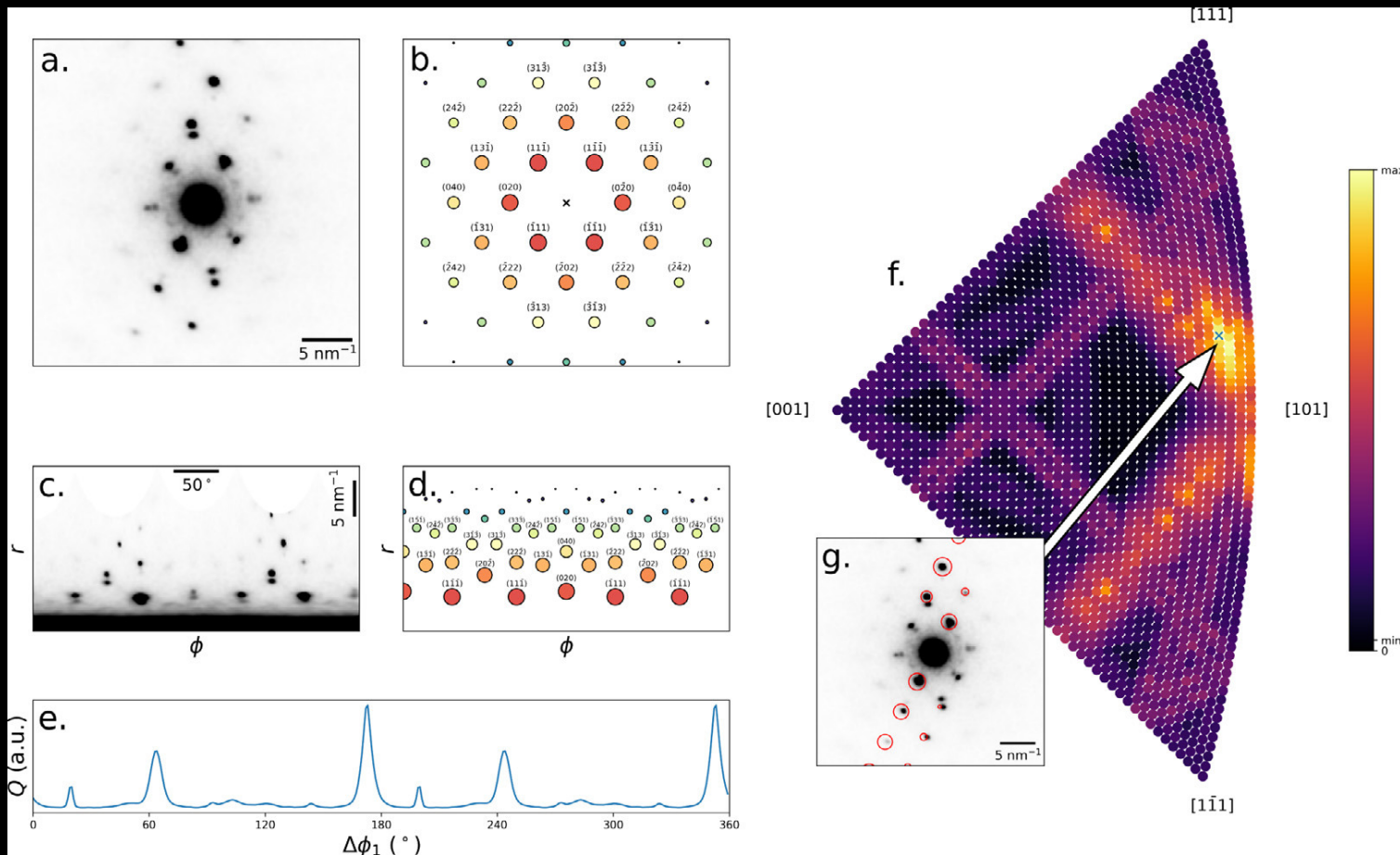
Phase/orientation mapping

Lattice strain mapping



Template matching with pyxem

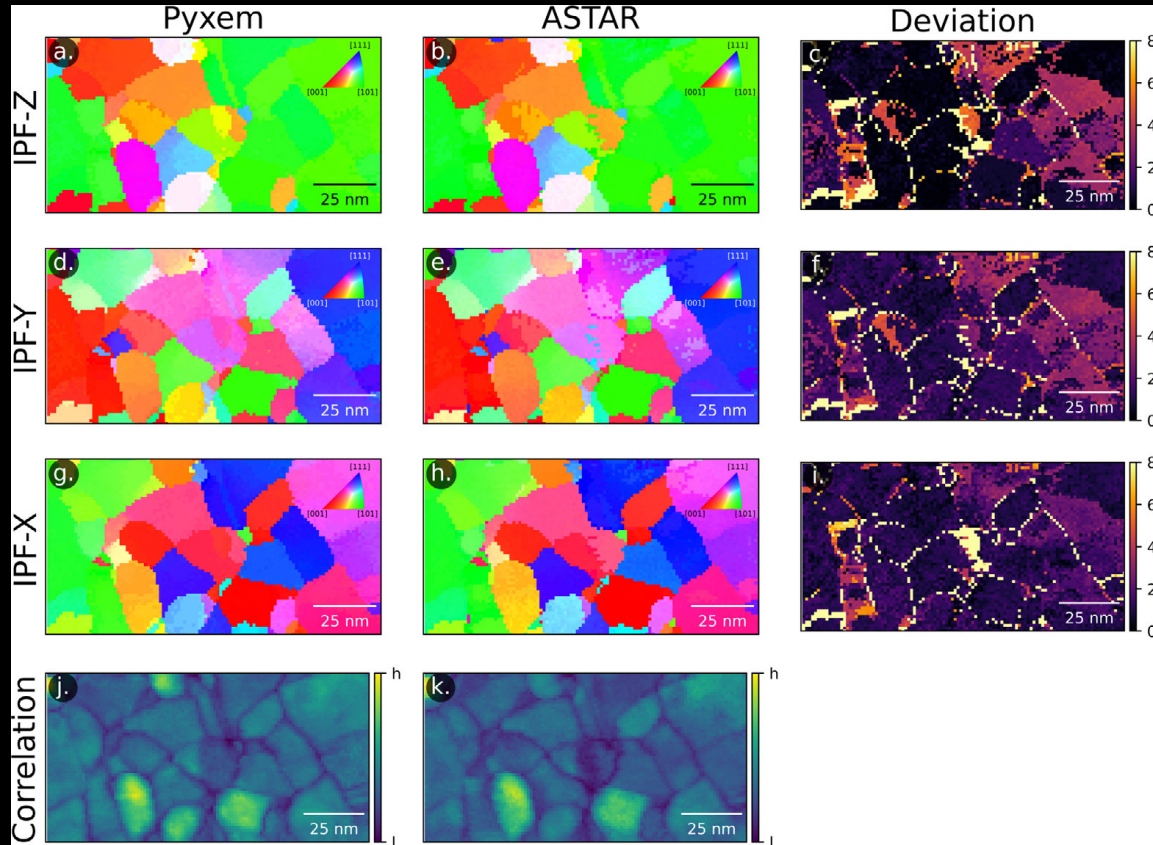
γ -Fe



Based on work by E. Rauch and co-workers

Template matching with pyxem... reliable results?

Cu-Ag



GPU -> Fast



Modular -> Flexible

Benefit of open-source

Pros:

- Good analysis methods are not lost
- Anyone can evaluate the code
- Bugs can be fixed quickly
- Works on any OS

Cons:

- Developed part time in between other work
- Documentation/manual might be lacking