HyperSpy: open-source multidimensional analysis software for electron microscopy

Håkon Wiik Ånes[1,*], P. Crout[2], N. Cautaerts[3], K.E. MacArthur[4], E. Prestat[5], J. Hjelen[1], A.T.J. van Helvoort[6] and K. Marthinsen[1]

[1]NTNU, Dept. of Materials Science and Engineering, Trondheim, Norway
[2]Uni. of Cambridge, Dept. of Materials Science and Metallurgy, Cambridge, UK
[3]Flemish Institute for Technological Research, Boeretang, Belgium
[4]Oxford Instruments Nanoanalysis, High Wycombe, UK
[5]Culham Centre for Fusion Energy, Abingdon, UK
[6]NTNU, Dept. of Physics, Trondheim, Norway
*email: hakon.w.anes@ntnu.no

EMAS 2023 - 17th European Workshop on Modern Developments and Applications in Microbeam Analysis

NTNU

Logo by Stefano Mazzucco based on figure by Wikipedia user Goffrie

FAIR MAS

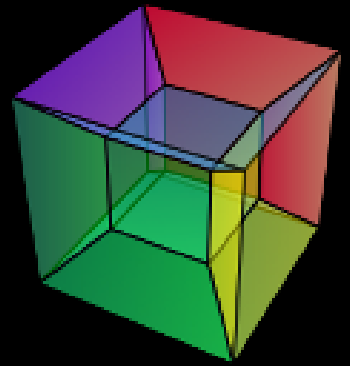
… assess the state-of-the-art and
reliability of microbeam analysis techniques

FAIR guiding principles
Findable
Accessible
Interoperable
Reproducible

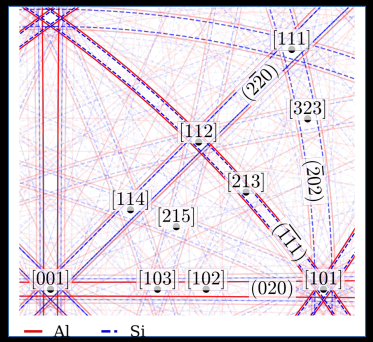
Data

Algorithms
Tools
Workflows

1



2



Why open-source? Why HyperSpy?

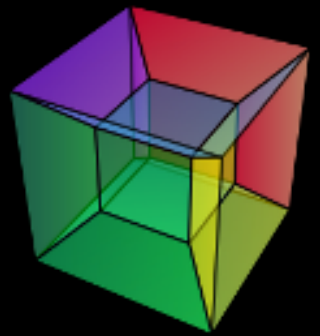
Collect data → Write new code to analyse data → Analyse data → Publish result in journal

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



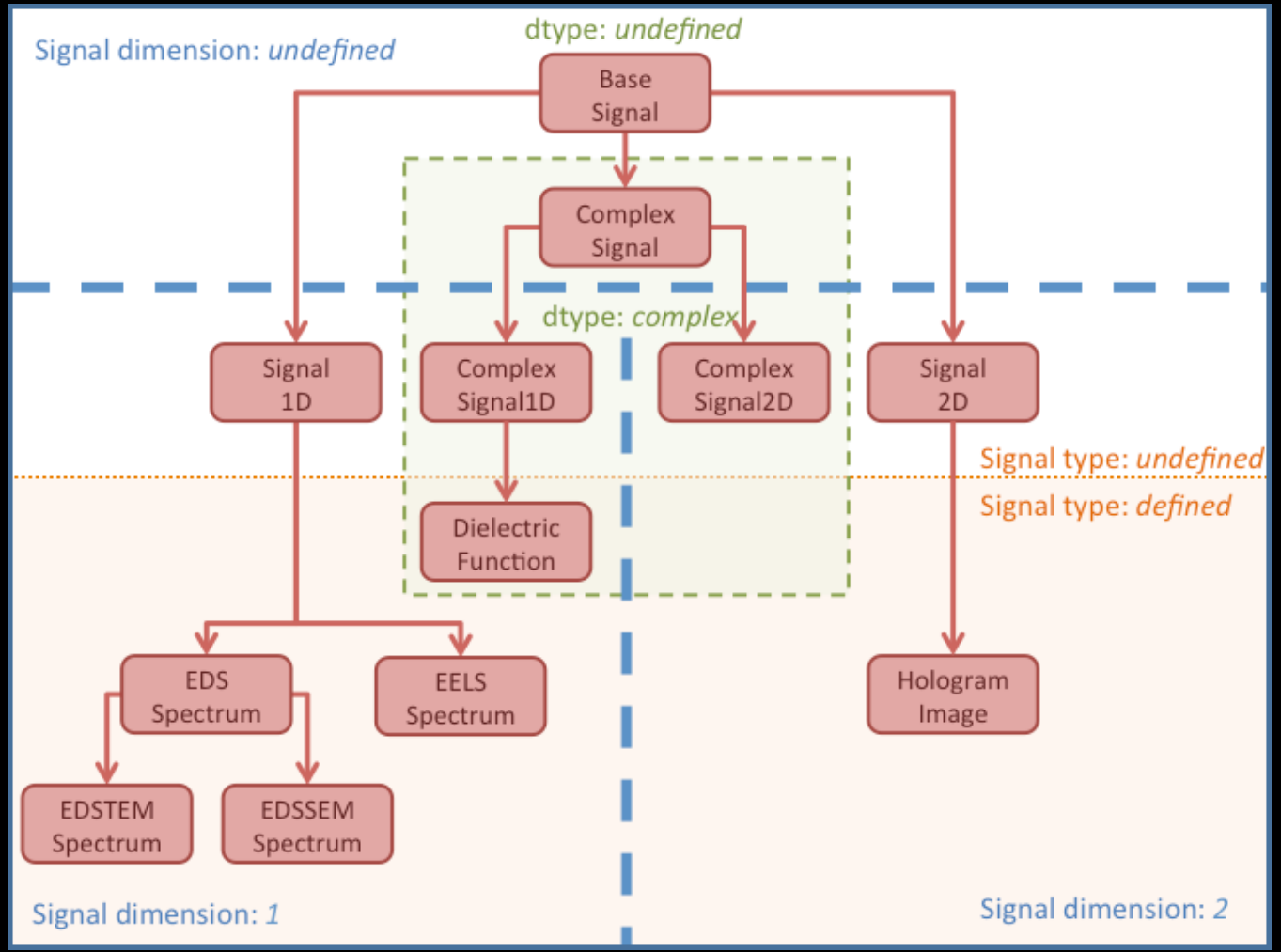
"I hope no-one else thought of this before I did...."

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

Supported file formats

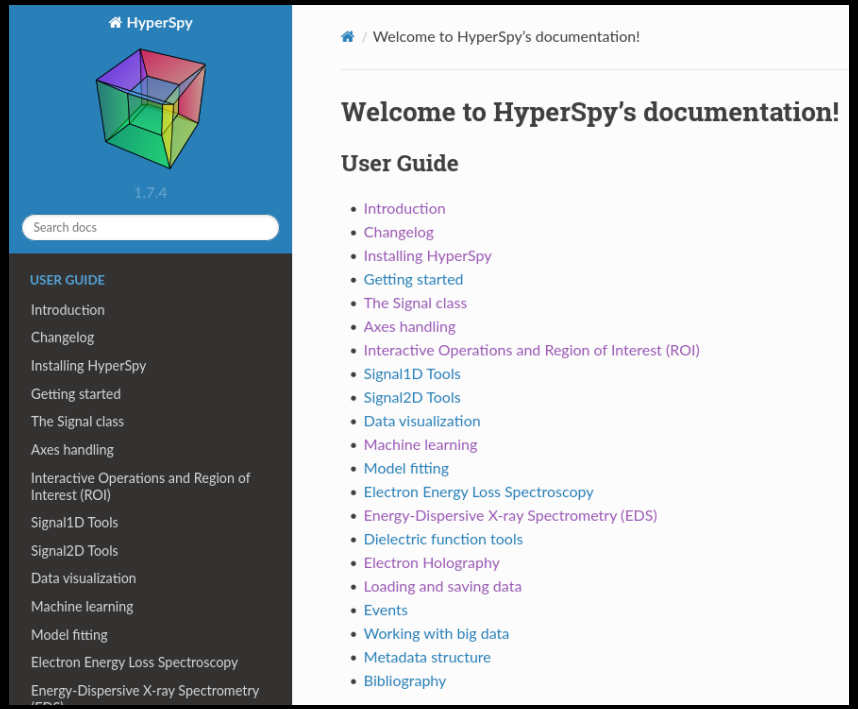
Format	Read	Write	lazy
Gatan's dm3	Yes	No	Yes
Gatan's dm4	Yes	No	Yes
FEI's emi and ser	Yes	No	Yes
hspy	Yes	Yes	Yes
zspy	Yes	Yes	Yes
Image: e.g. jpg, png, tif, ...	Yes	Yes	Yes
TIFF	Yes	Yes	Yes
MRC	Yes	No	Yes
MRCZ	Yes	Yes	Yes
EMSA/MSA	Yes	Yes	No
NetCDF	Yes	No	No
Ripple	Yes	Yes	Yes
SEMPER unf	Yes	Yes	Yes
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



```
> pip install hyperspy
```

HyperSpy Bundle (installation wizard)

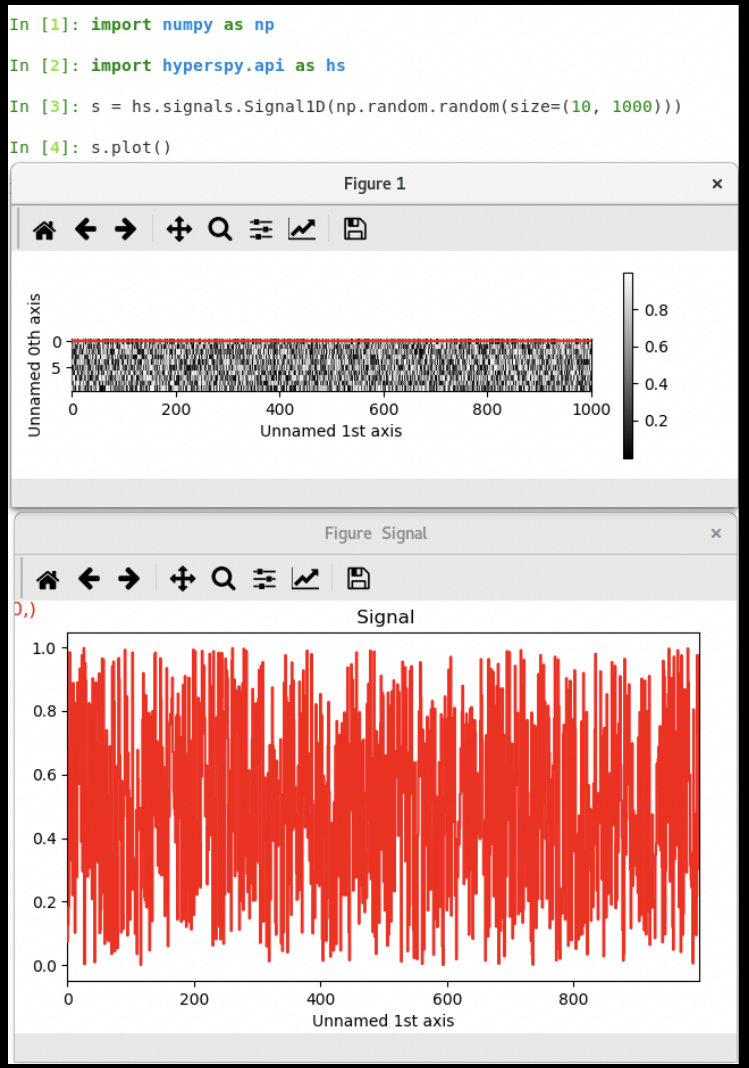
Anaconda Navigator (GUI)

How do I use it?

→ hyperspy.org

```
> ipython
```

In your terminal



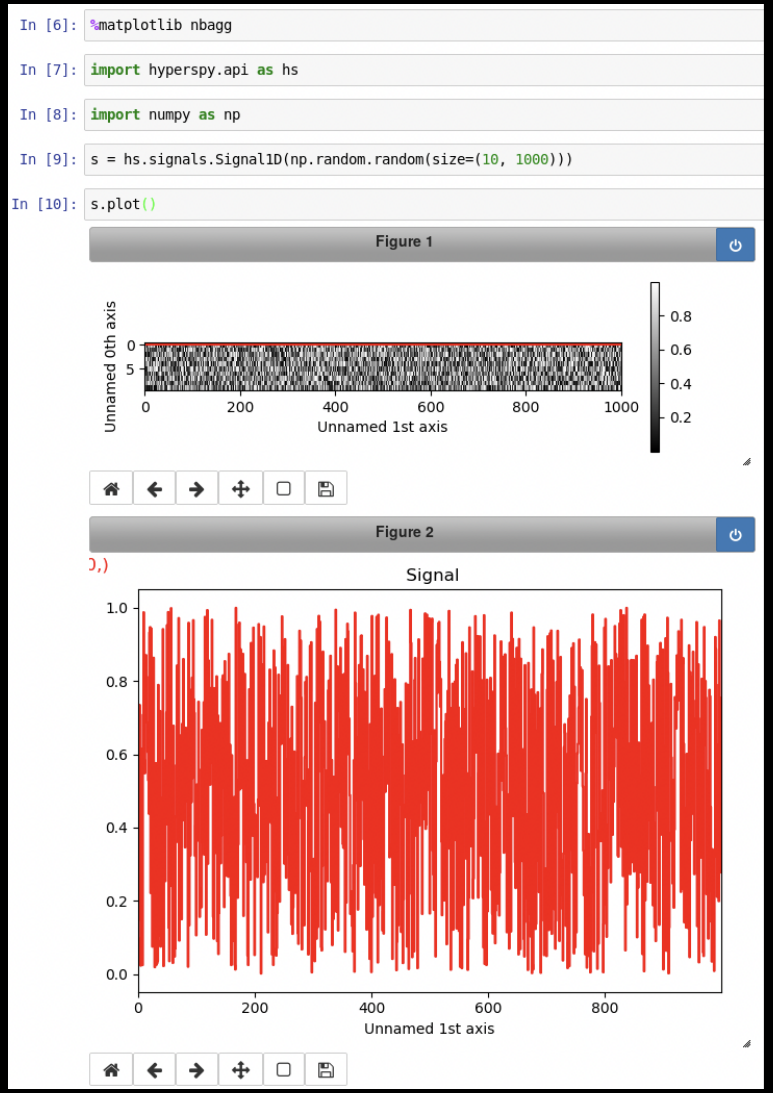
How do I use it?

→ hyperspy.org

```
> jupyter-lab
```

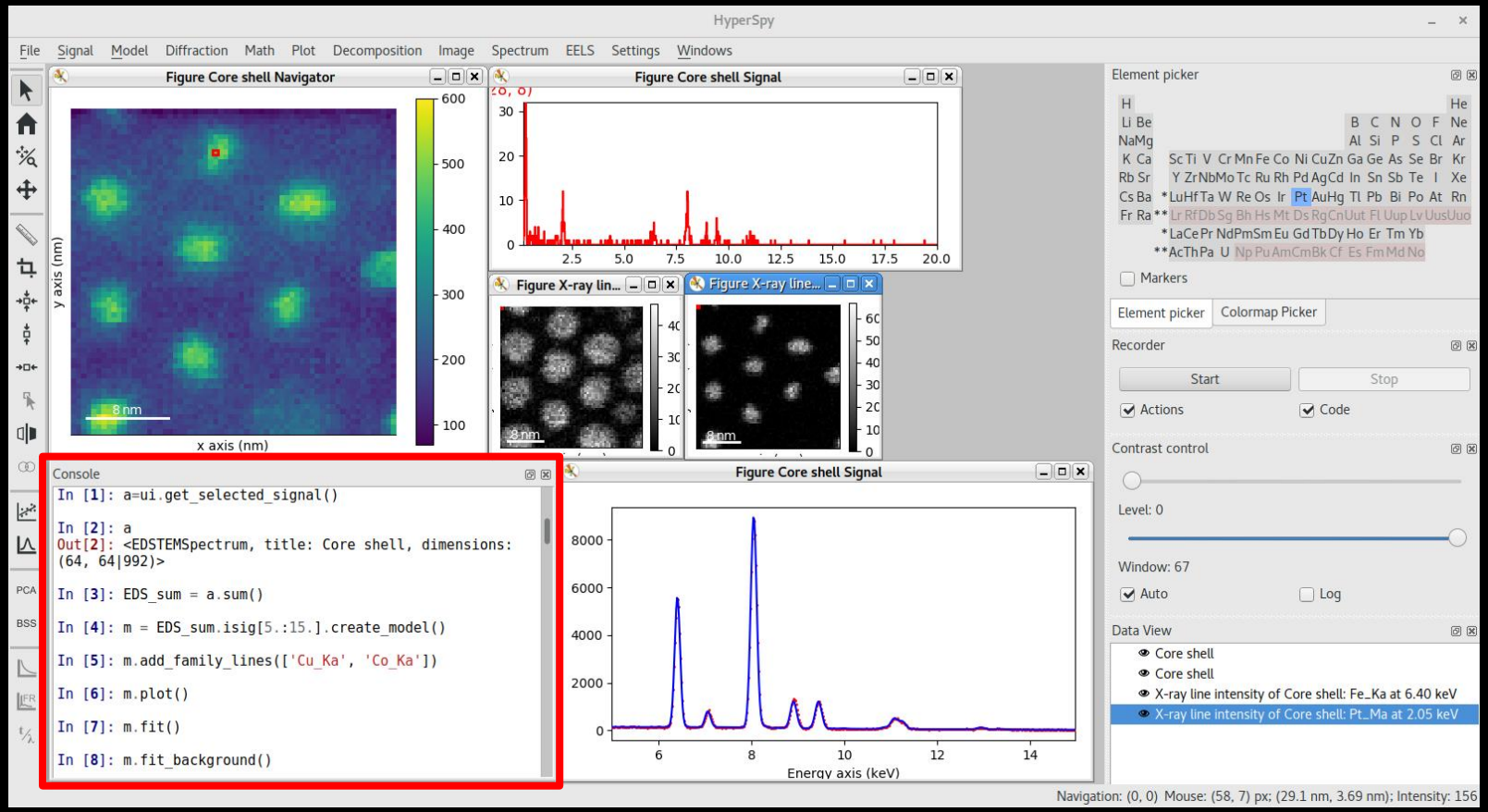
```
> jupyter-notebook
```

In your browser



How do I use it?

From your desktop

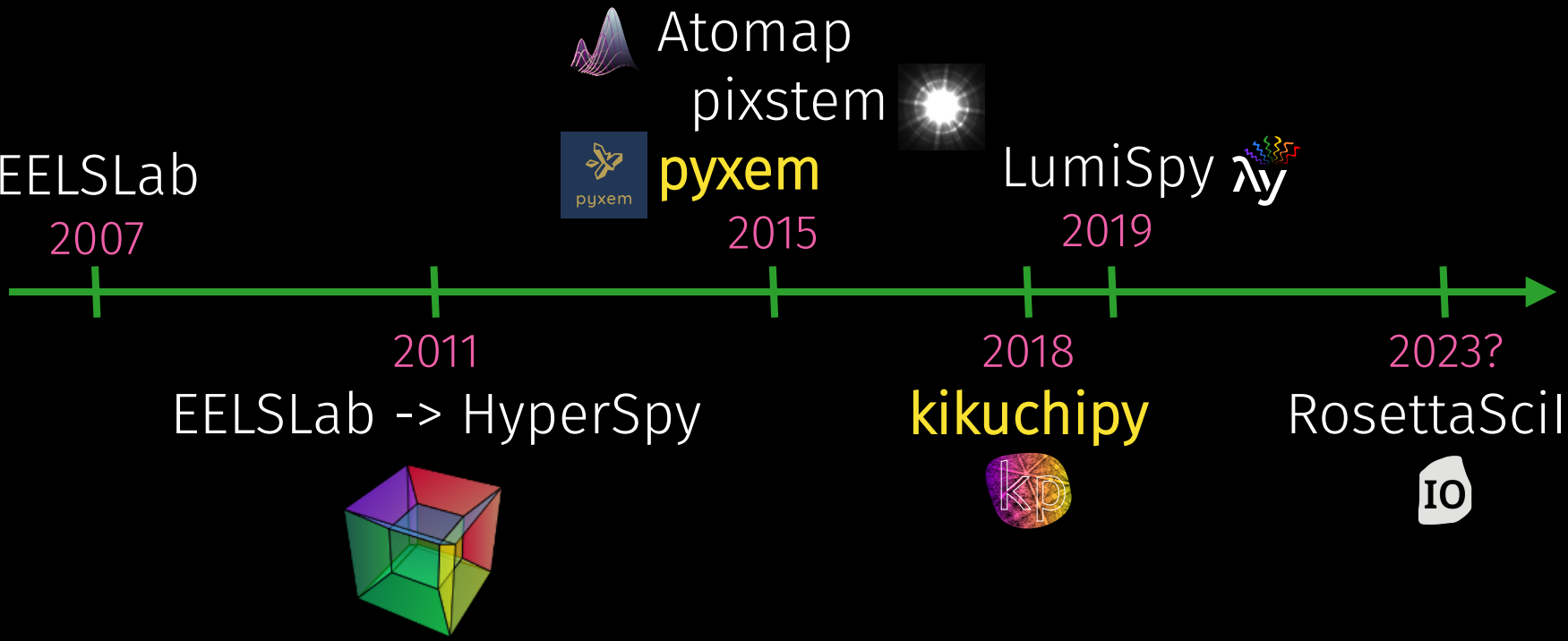


Visualisation
Maths
'Slicing'
Generic fitting

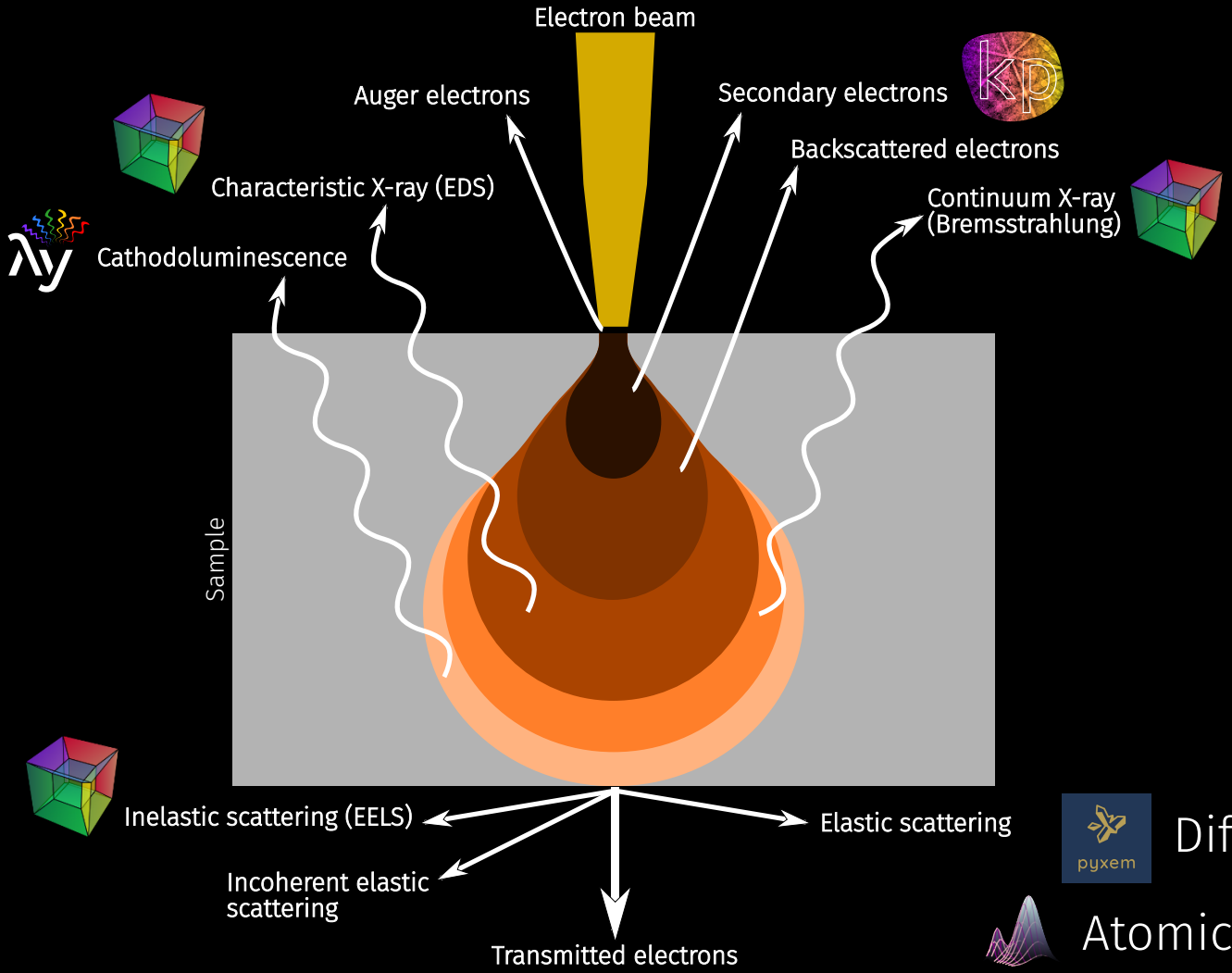
Mapping ops.
Metadata
ML
Big data

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

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



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



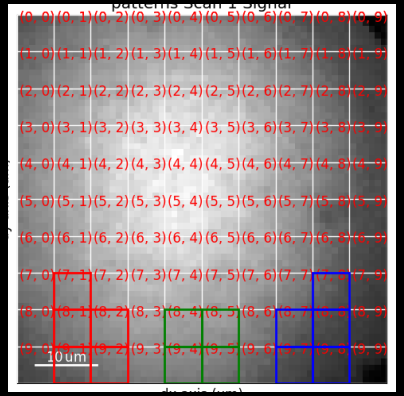
pyxem

Diffraction

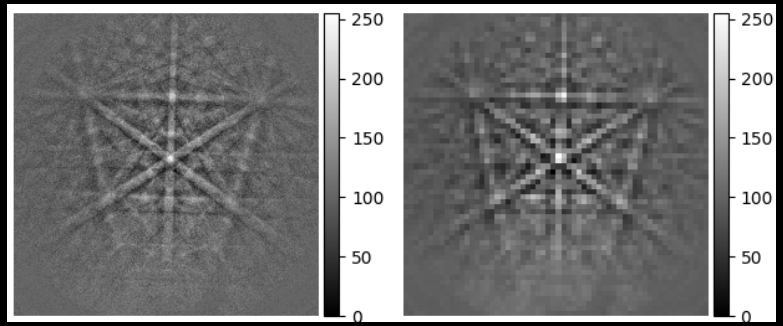
Atomic resolution images

kikuchipy: diffraction in SEM

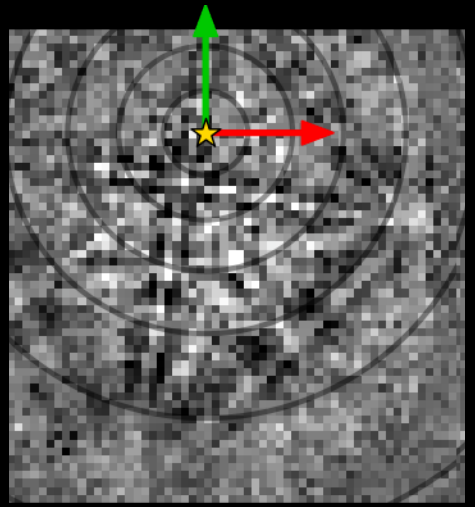
Virtual imaging



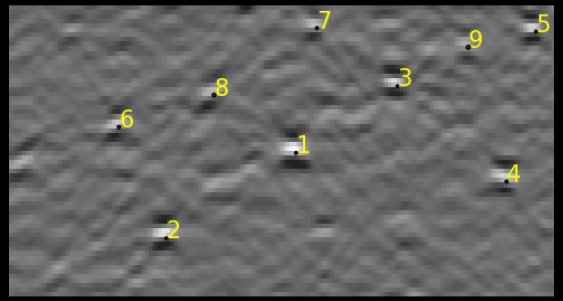
Pattern processing



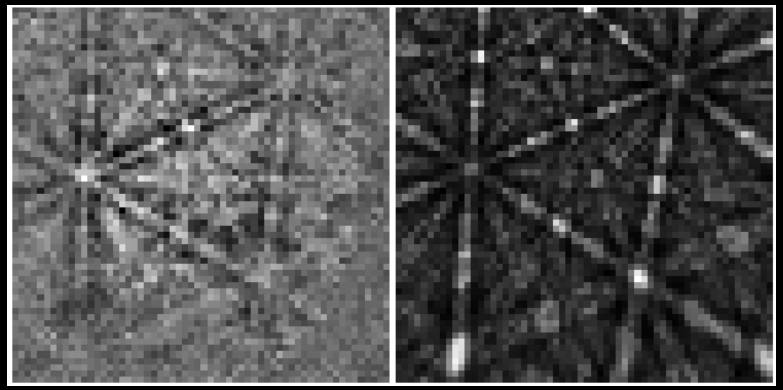
Calibration



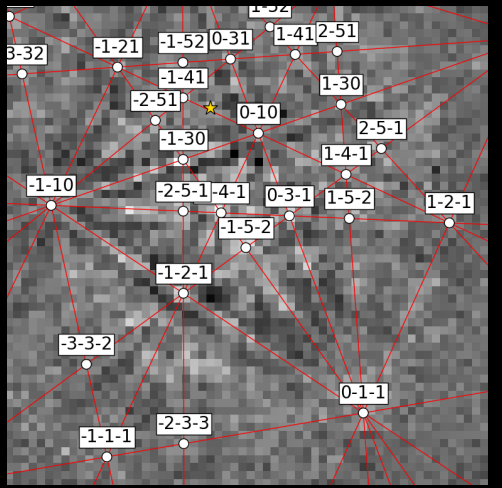
Hough indexing



Pattern matching



Geo./kin. simulations

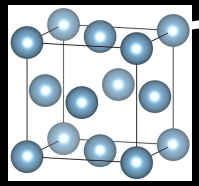


Differentiate between two similar cubic crystals

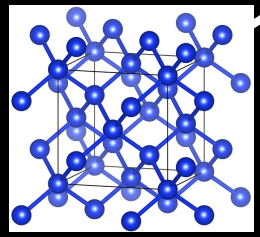
	Structure	Atomic positions	*a* [Å]	Space group
Al	FCC	4a	4.05	Fm-3m (225)
Si	Diamond	8a	5.43	Fd-3m (227)

Δa = 25%

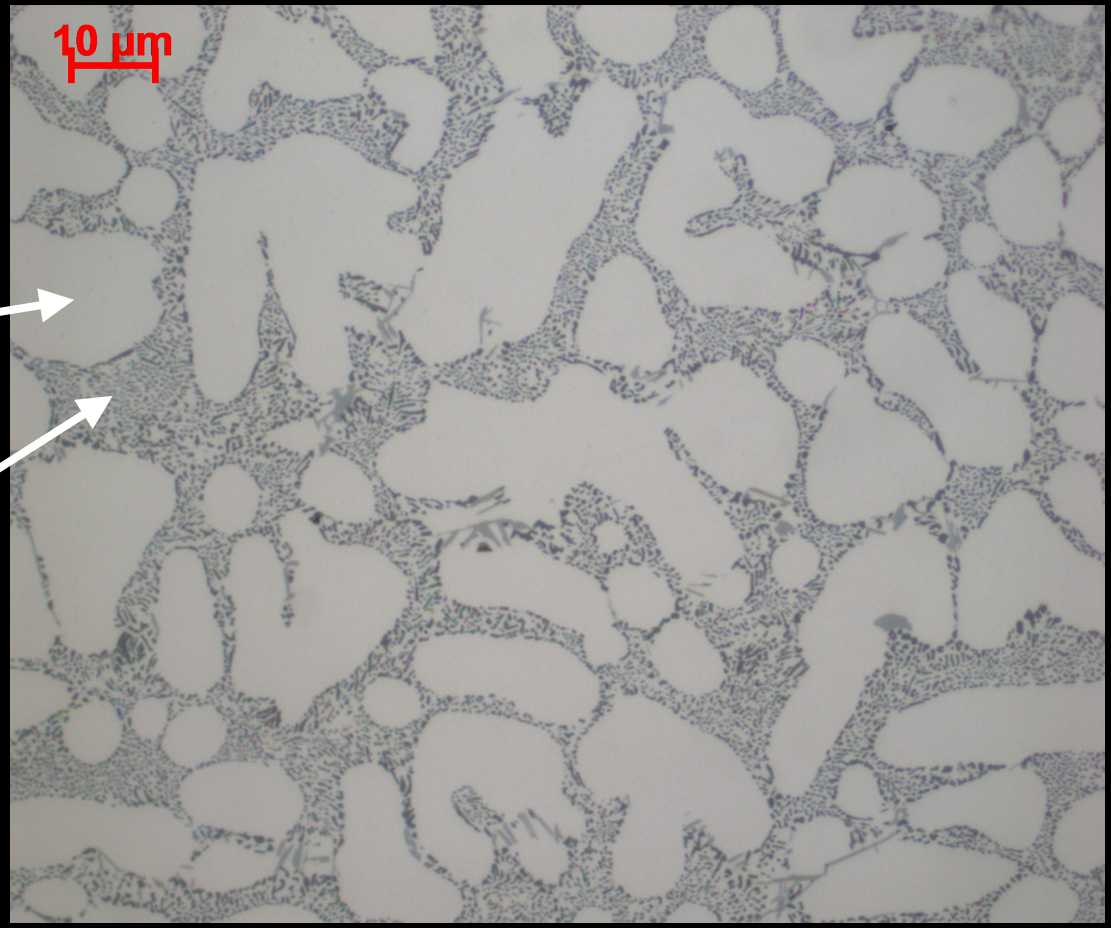
Al



Si



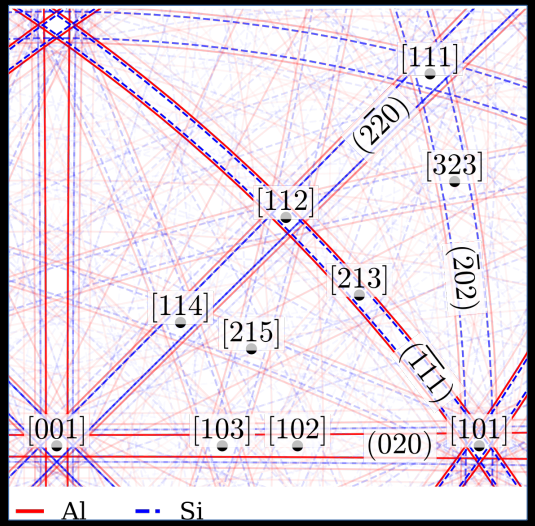
Al-10wt.%Si

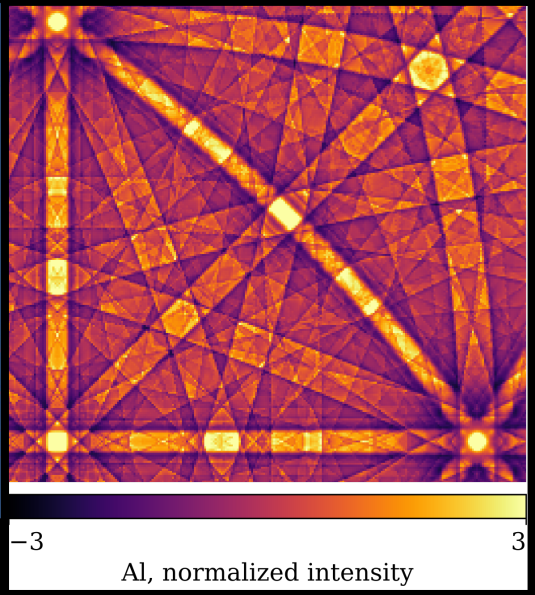


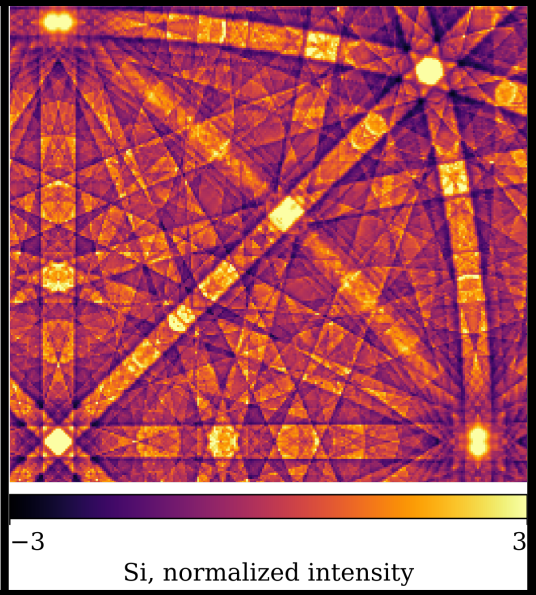
Ånes *et al.* (2023) In preparation

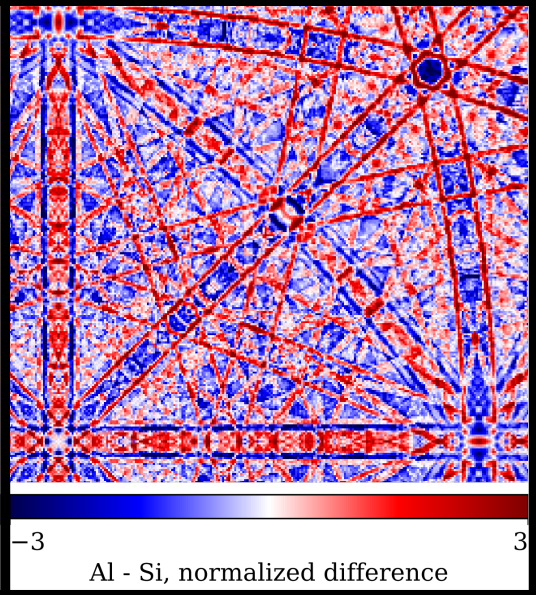
How similar is Al and Si?

r = 0.3256





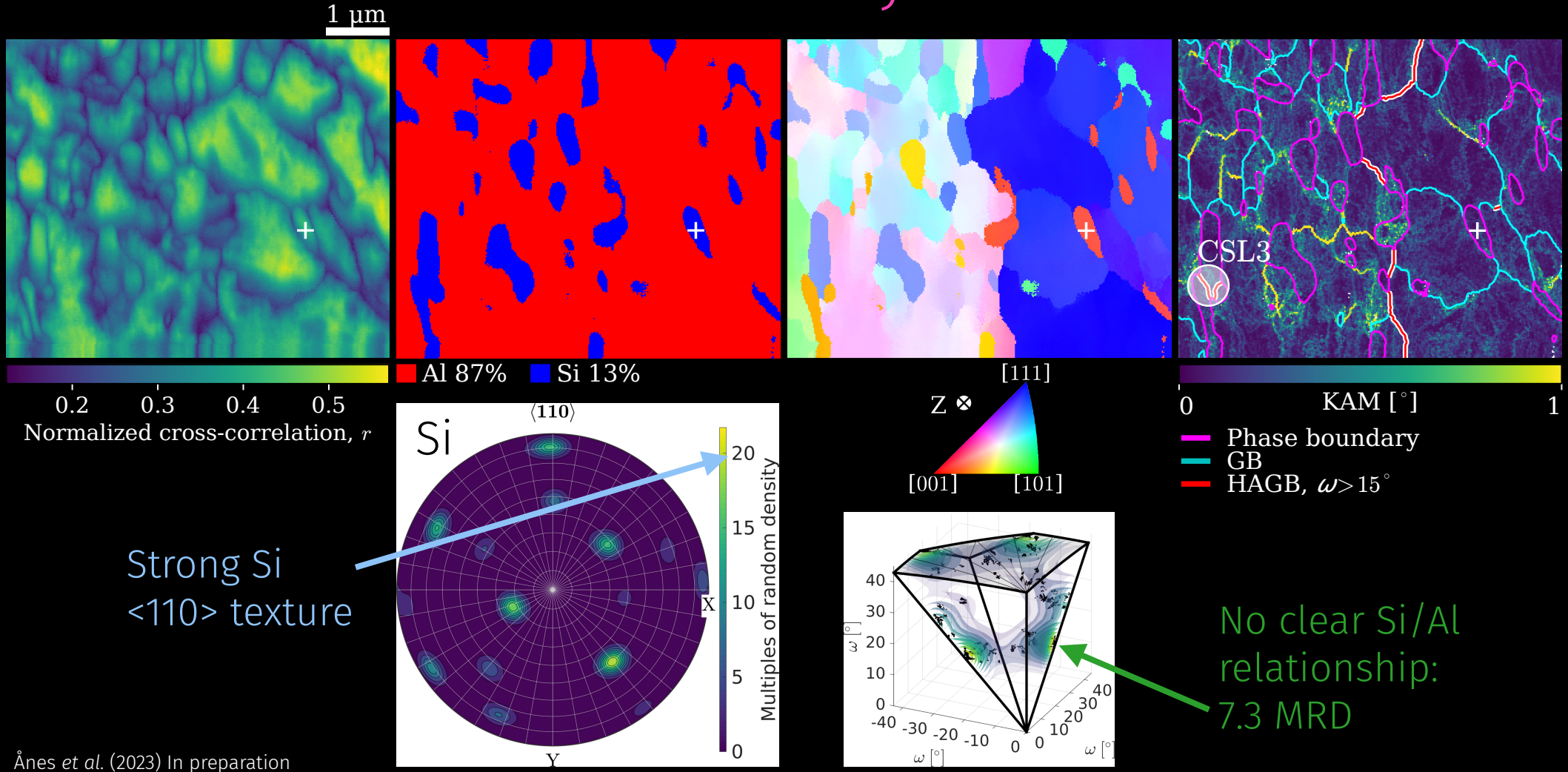




Use *relative intensities*

Ånes *et al.* (2023) In preparation

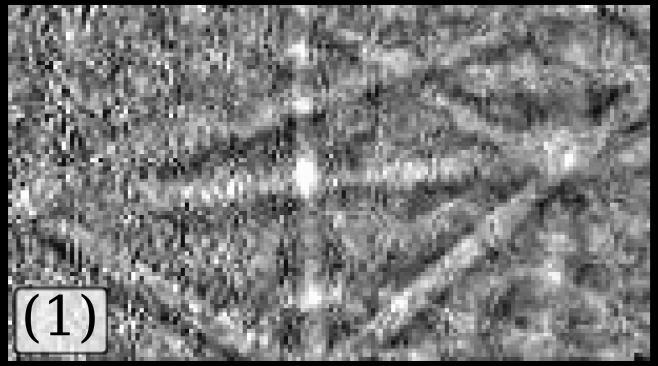
Microstructure of one Si colony in Sr-modified Al-10Si

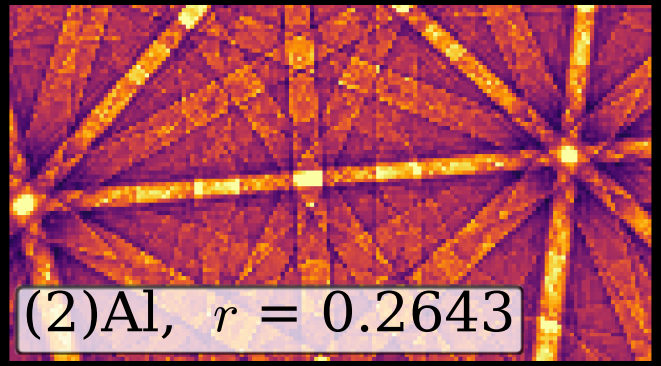


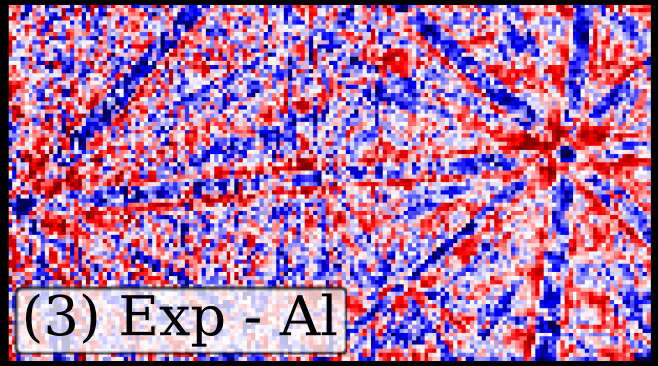
Ånes *et al.* (2023) In preparation

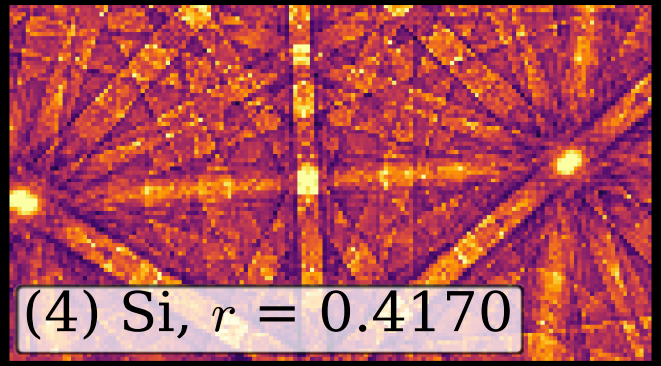
Reliable results? Evaluate patterns!

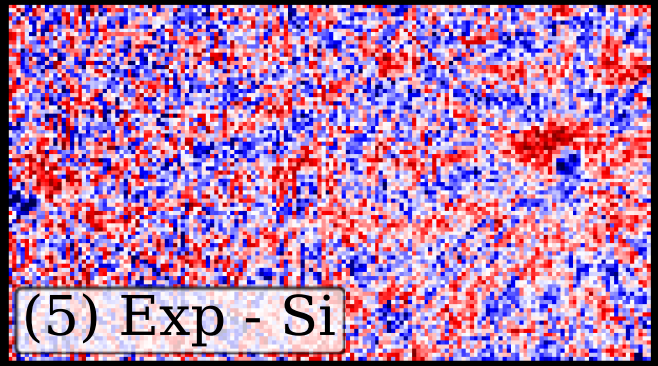
Exp. | Sim. | Exp. - Sim.











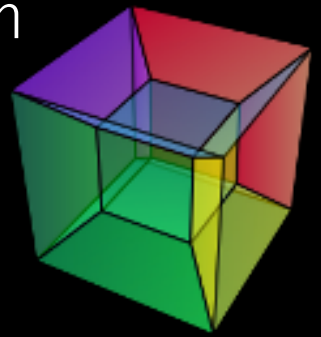
Ånes *et al.* (2023) In preparation

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)

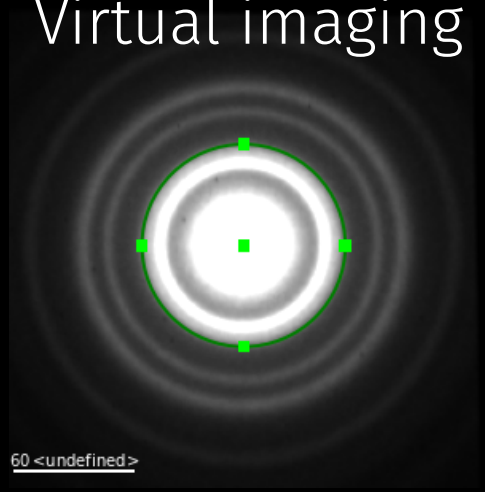


NTNU

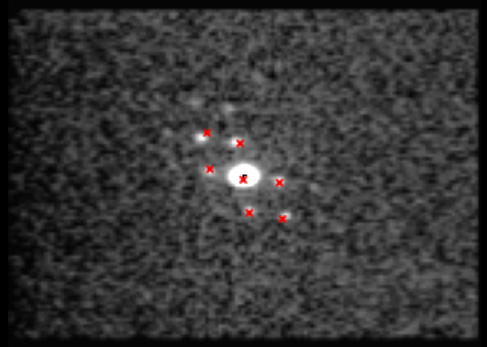
Thank you!

pyxem: diffraction in TEM

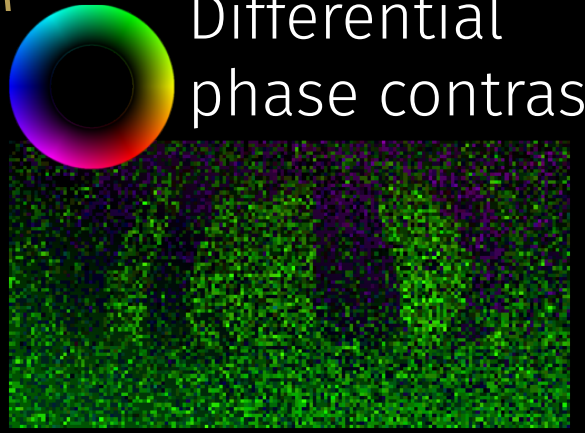
Virtual imaging



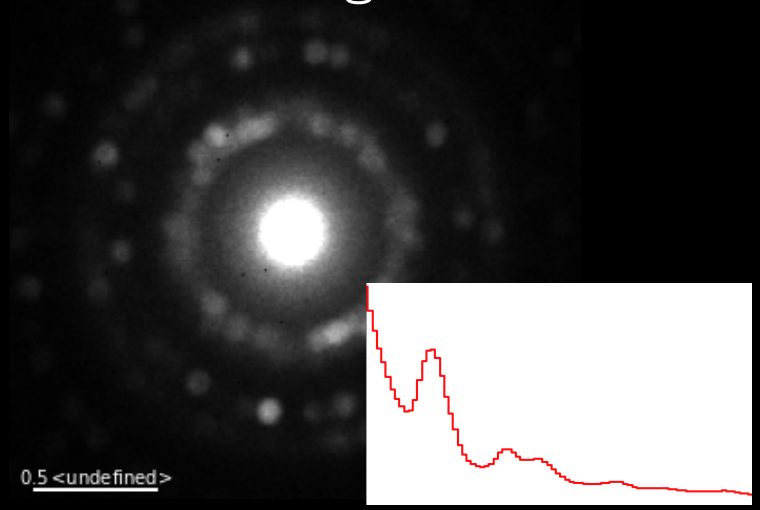
Peak finding



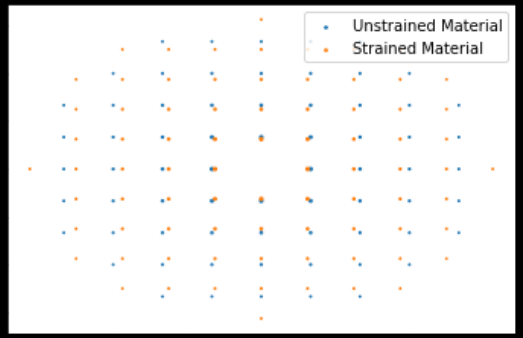
Differential phase contrast



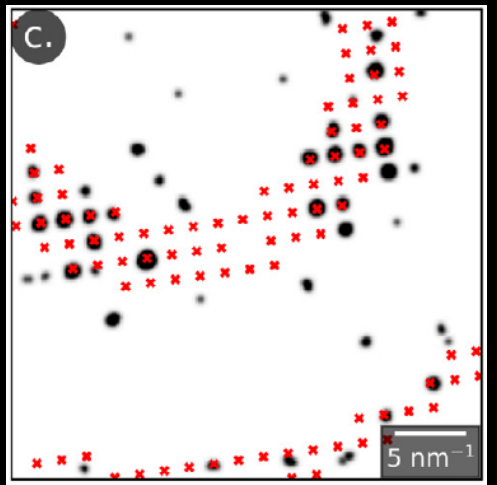
Radial integration



Lattice strain mapping

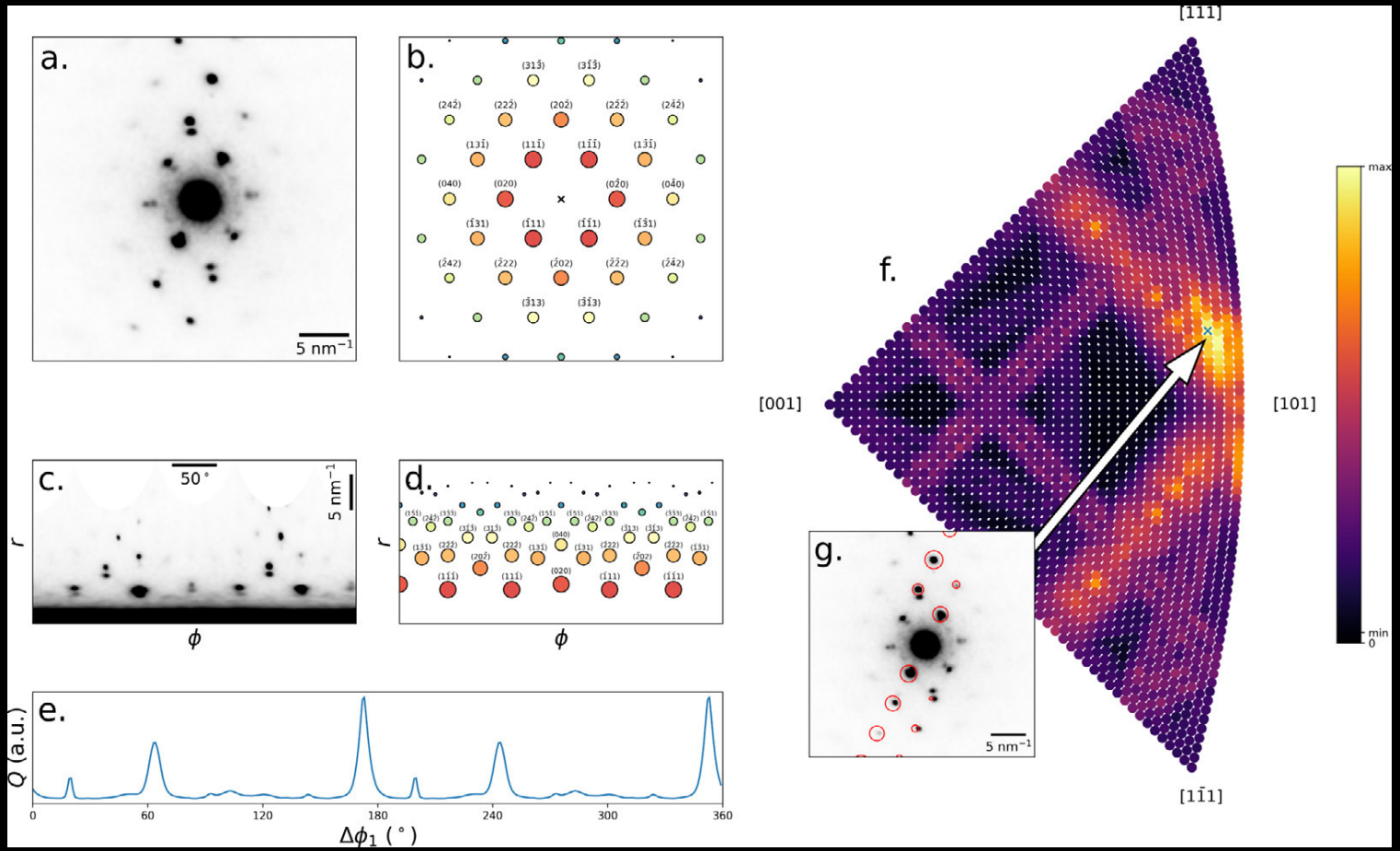


Phase/orientation mapping



Template matching with pyxem

γ-Fe

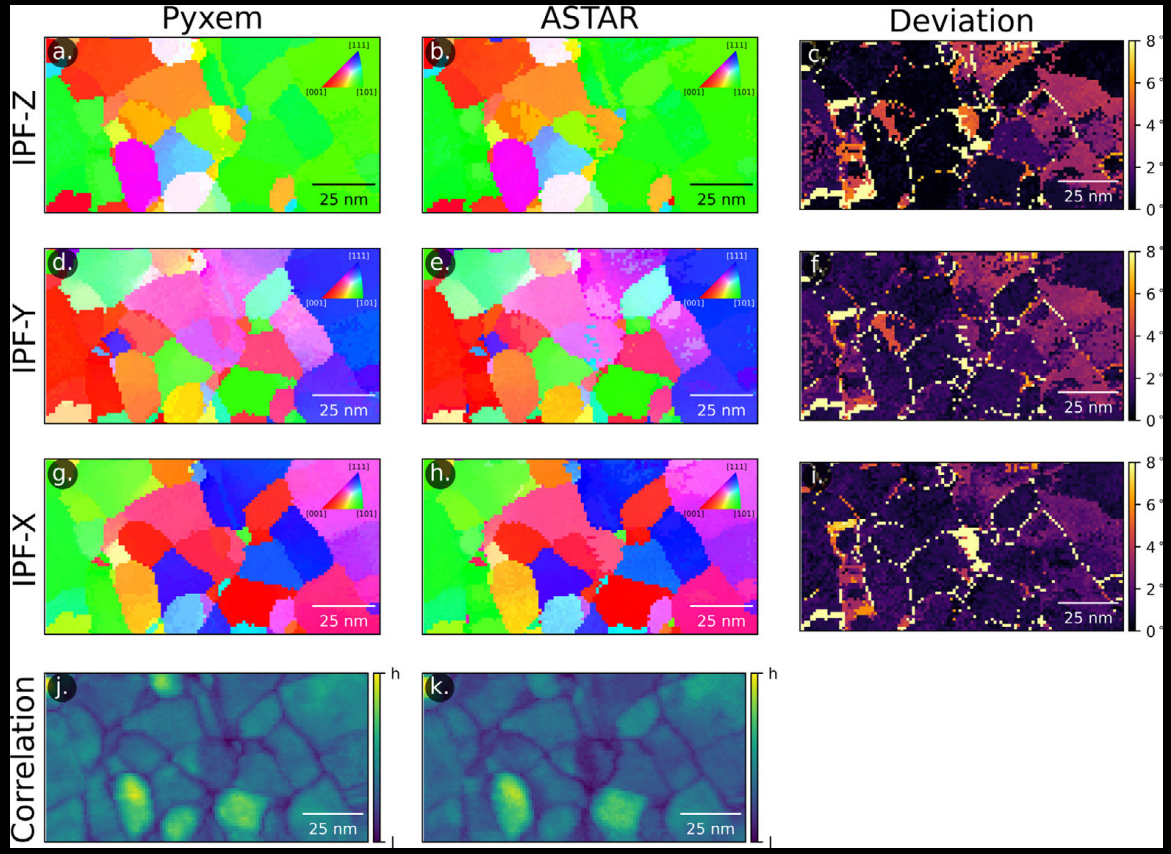


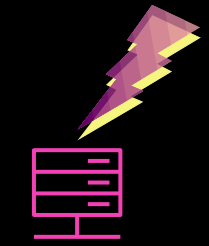
Based on work by E. Rauch and co-workers

Cautaerts *et al.* (2022) *Ultramicroscopy* **237**

Template matching with pyxem... reliable results?

Cu-Ag





GPU -> Fast

Modular -> Flexible

Cautaerts *et al.* (2022) *Ultramicroscopy* **237**

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