Welcome to 2019 M&M Short Course X-15

Data Analysis in Materials Science with

HyperSpy
multi-dimensional data analysis

Presented by (a selection of) the HyperSpy developers:

- Duncan Johnstone
- Katherine MacArthur
- Magnus Nord
- Eric Prestat
- Joshua Taillon

Session 5:
An Introduction to Machine Learning in Electron Microscopy

Electron Microscopy in the age of "Big Data"

Josh Taillon

August 4, 2019

1:15 - 1:30 PM

NIST Disclaimer

Certain commercial equipment, instruments, materials, vendors, and software are identified in this talk for example purposes and to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

What types of machine learning are we talking about?

- For the most part, ***unsupervised*** learning:
  - *i.e.* no training or validation of models
  - Goal is to find previously unknown patterns in data set without pre-existing label
  - Many algorithms for this are built-in with HyperSpy

- Distinct from supervised learning, reinforcement learning, or deep learning
  - Not covered here — not included in HyperSpy directly
  - Using `scikit-learn`, TensorFlow, pyTorch, etc.

What can unsupervised learning do for you?

- The primary use for unsupervised learning is in *signal separation*
    - Sometimes called *hyperspectral unmixing* as well

- Ideally, we can automatically determine what signals are present in the data, and where they are located
    - This is the basis of most vendors' *phase mapping* offerings

- Can also be used for *dimensionality reduction* and denoising:
    - Picking out only the "interesting" features and discarding the rest of the noise

What techniques is this used on?

- Most typically in the EM fields, signal separation is performed on raster-based ***hyperspectral mapping*** methods:
  - STEM-EELS and STEM-EDS
  - SEM-EDS
  - (μ-)XRF mapping
  - FTIR mapping
  - Cathodoluminescence mapping

- Otherwise, these techniques can be used on any type of data:
  - Images, time series, etc.

What *is* hyperspectral unmixing?

- Start with some hyperspectral data:

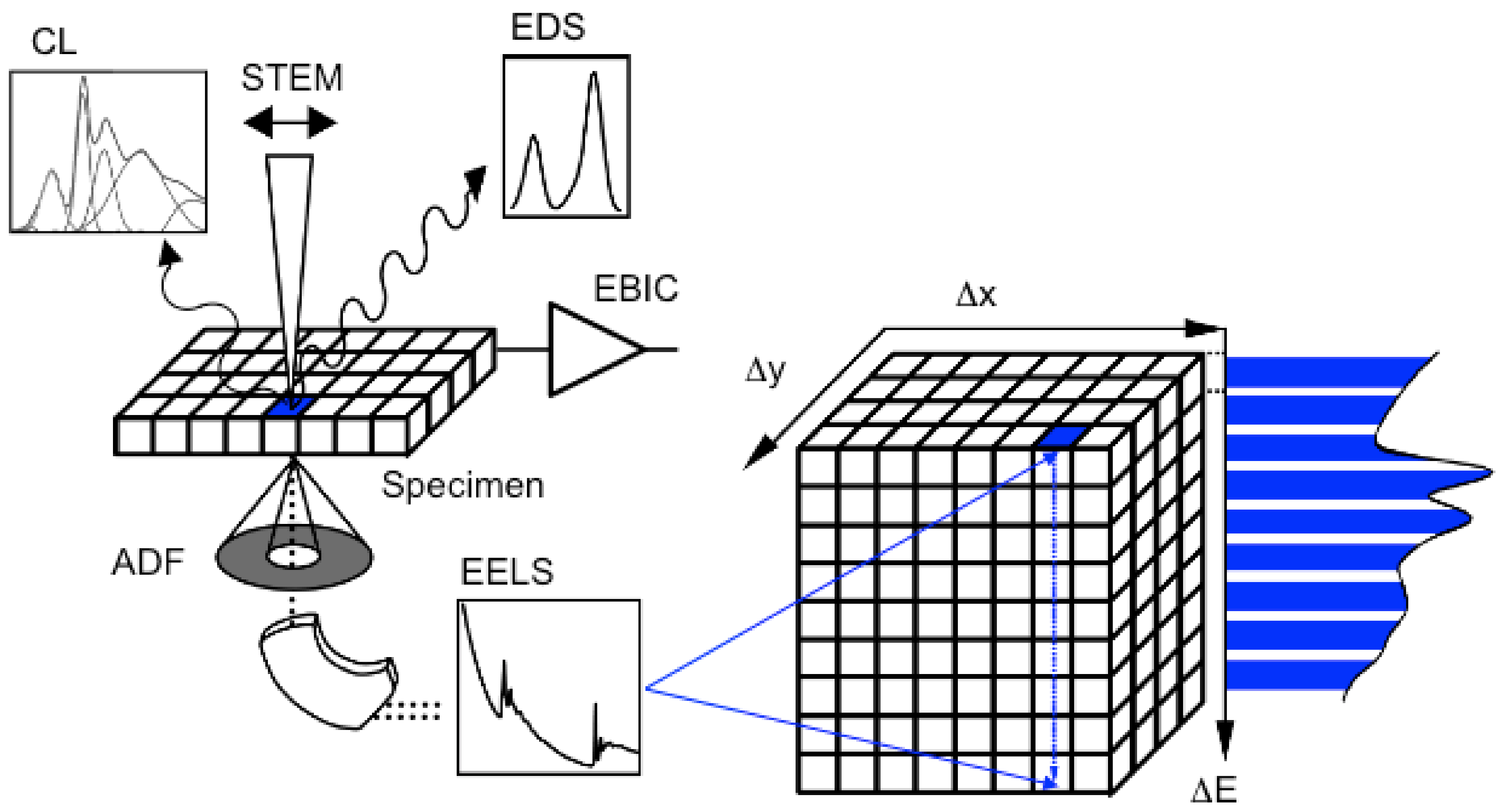
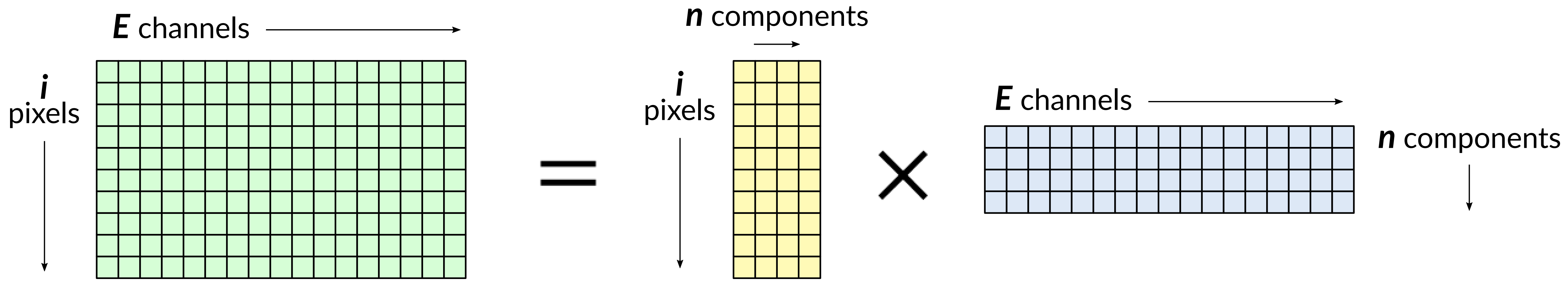


Image courtesy of Gatan, Inc.

What *is* hyperspectral unmixing?

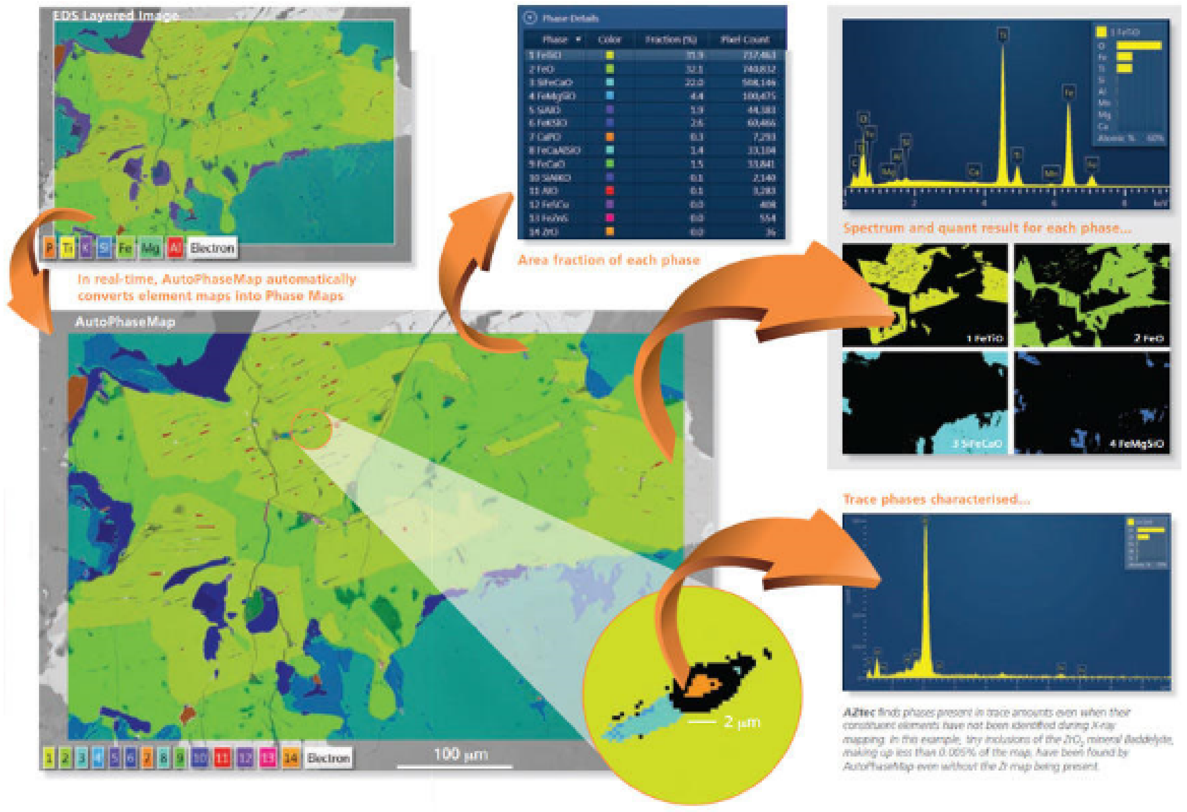


$$(i \times E) = (i \times n) \quad (n \times E)$$

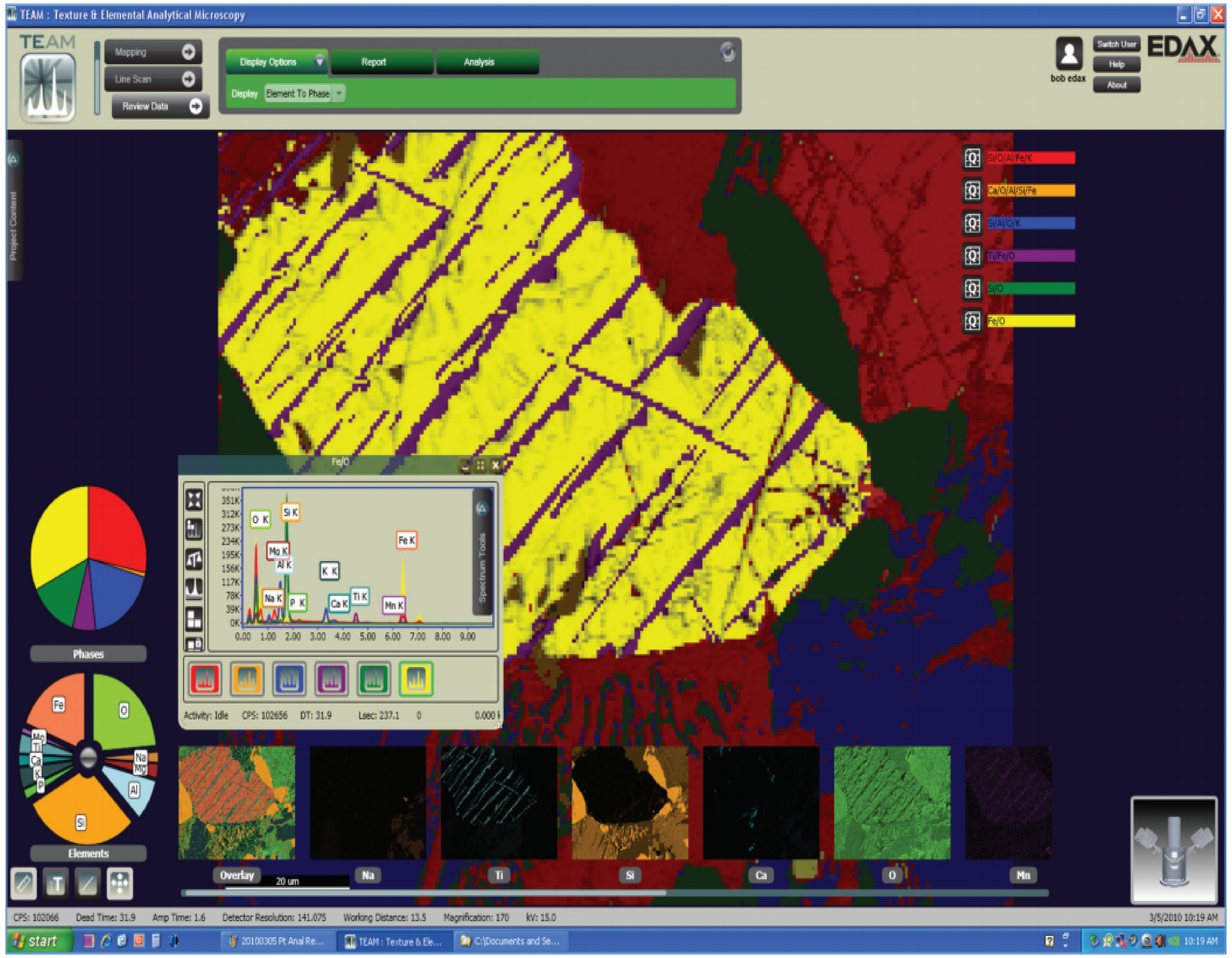
A linear algebra problem!

What do the vendors offer?

- If you've used a modern EDS software package, you probably have done hyperspectral unmixing (they usually call it *phase mapping*)...



Oxford — *AutoPhaseMap*



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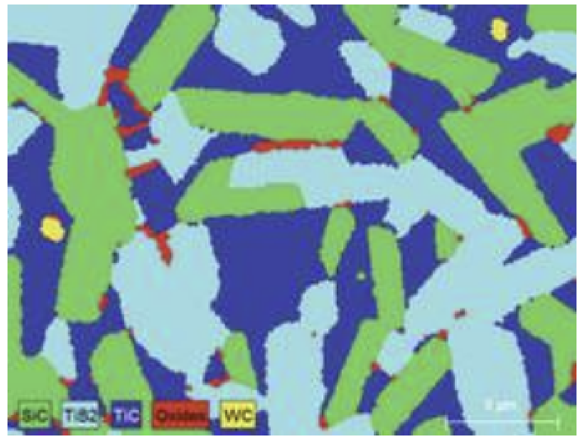
ESPRIT AutoPhase

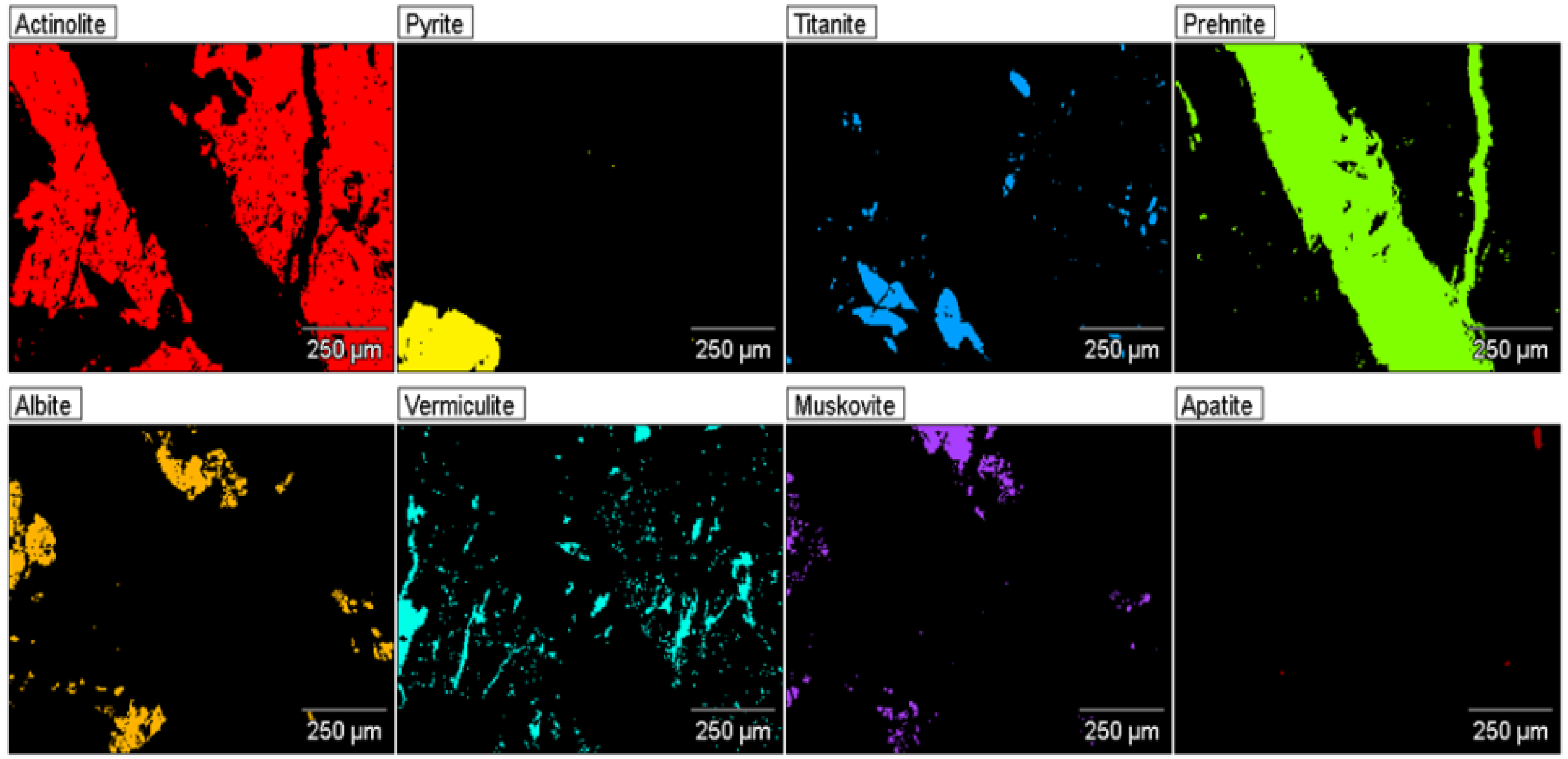
The Automatic Phase Analysis Tool



- Fully automatic search for phases in maps
- Works with all types of ESPRIT maps
- Adjustable sensitivity and adjustable minimal phase area

Chemical phase map of a hard ceramic material

Bruker — *AutoPhase*



COMPASS

ThermoFisher SCIENTIFIC

Thermo Fisher — *COMPASS*

Strengths/challengs with *vendor* options?

The Good

- **Simple point-and-click operation**
- **Tight integration**
    - Collection, visualization, reporting, etc.
- **Usually runs in real-time**
- **Integration with other data sources (*e.g.* EBSD)**
- **Generally "just works"**

The Not So Good

- **Extremely "black box"**
- **Reproducibility (!)**
    - Configurable options with little understanding of why
- **What are the uncertainties?**
- **Tied to software ($)**
- **Choice of vendor should not change the scientific result**

Strengths/challengs with *open-source* options?

The Not So Good

- Usually not point-and-click
- (Can be) difficult to access raw data from the vendor software
- Generally only post-processing
- Learning curve can be substantial
- Can take a lot more fiddling

The Good

- You know what's happening
- Reproducibility (!)
    - Anyone can recreate your analysis (including you!)
- Uncertainty can be understood
- Usually free
- Results do not depend on vendor

Open-source "phase mapping"

- Many algorithms exist to solve: $\mathbf{D}_{(x,y),E} = \mathbf{W}_{(x,y)} \times \mathbf{S}_E$
  - Assumptions implicit in each affect their suitability for EDS, EELS, etc.
- Primary methods (built into HyperSpy):
  - Principal component analysis (PCA) — finds non-physical spectra that describe the most variance in the datacube
  - Independent component analysis (ICA) — maximizes independence between spectral results
  - Non-negative matrix factorization (NMF) — enforces positivity in spectral components and weights

A simple example:

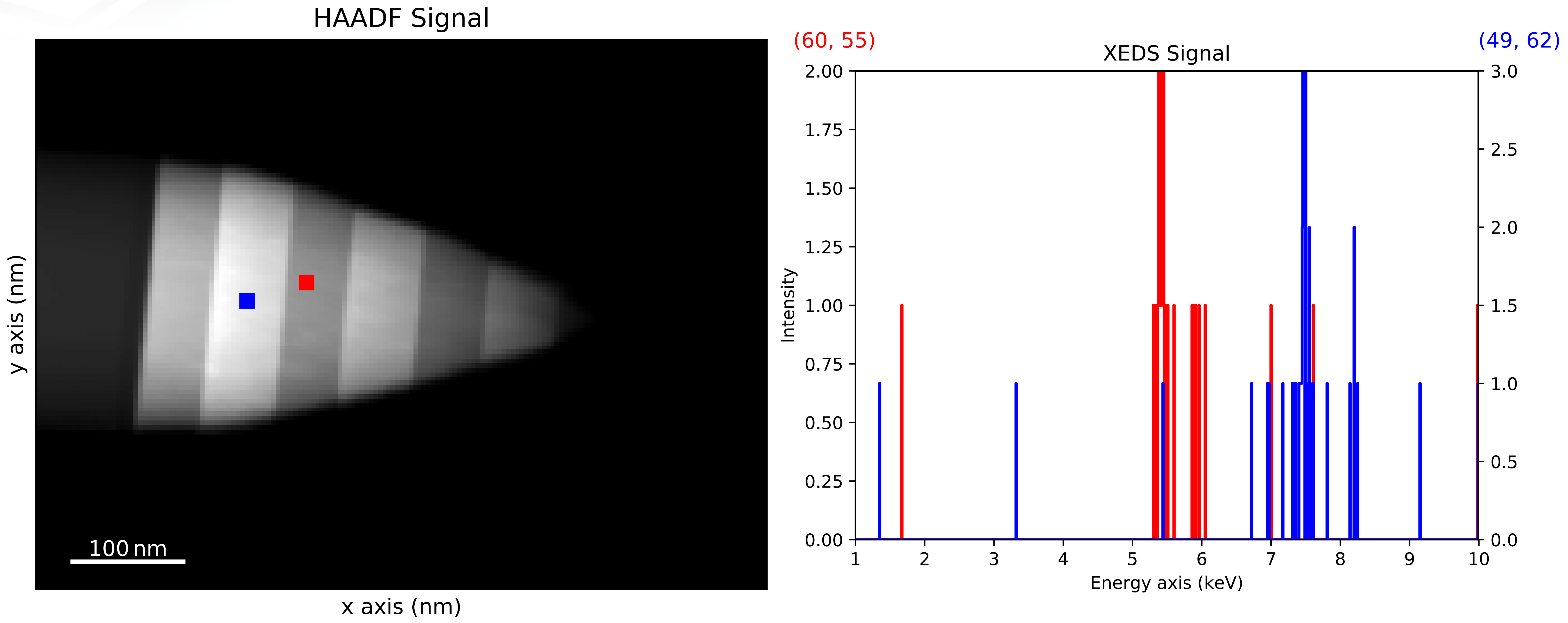
- Signal separation enabling EDS tomography

- Atom probe specimen fabricated from NIST SRM 2135c
  - Ni/Cr thin film depth profile standard (on Si substrate)
  - Layer thicknesses are approximately 56 nm
  - Data collected by Andrew Herzing (NIST)

- Data collected from 0 to 360 degrees tilt in increments of 5 degrees
  - Dataset is 165 x 124 x 73 x 900

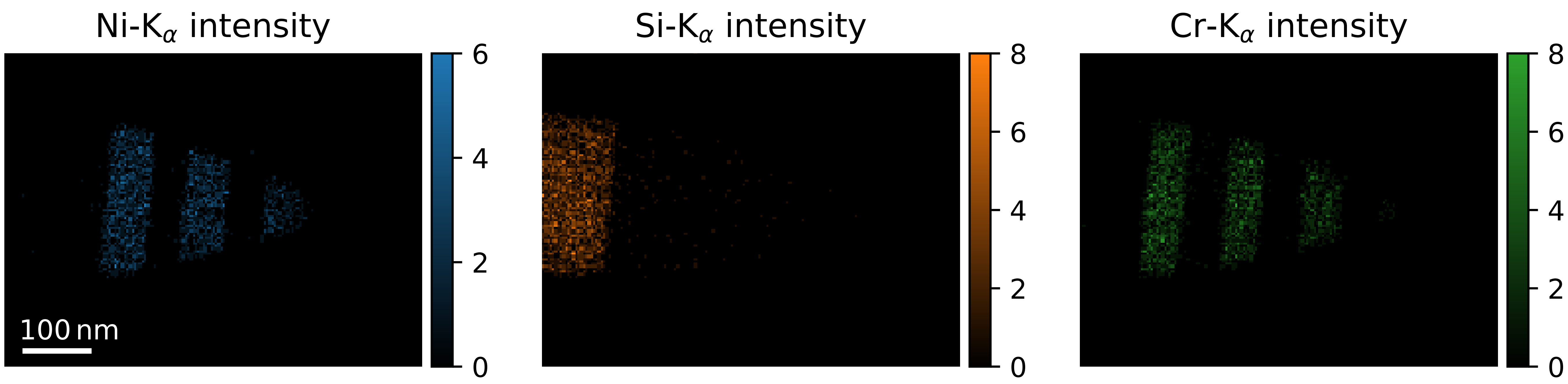
- HAADF and XEDS SI data collected simultaneously

A simple example:



Single pixel counts in the single digits
Cr and Ni visible, but noisy

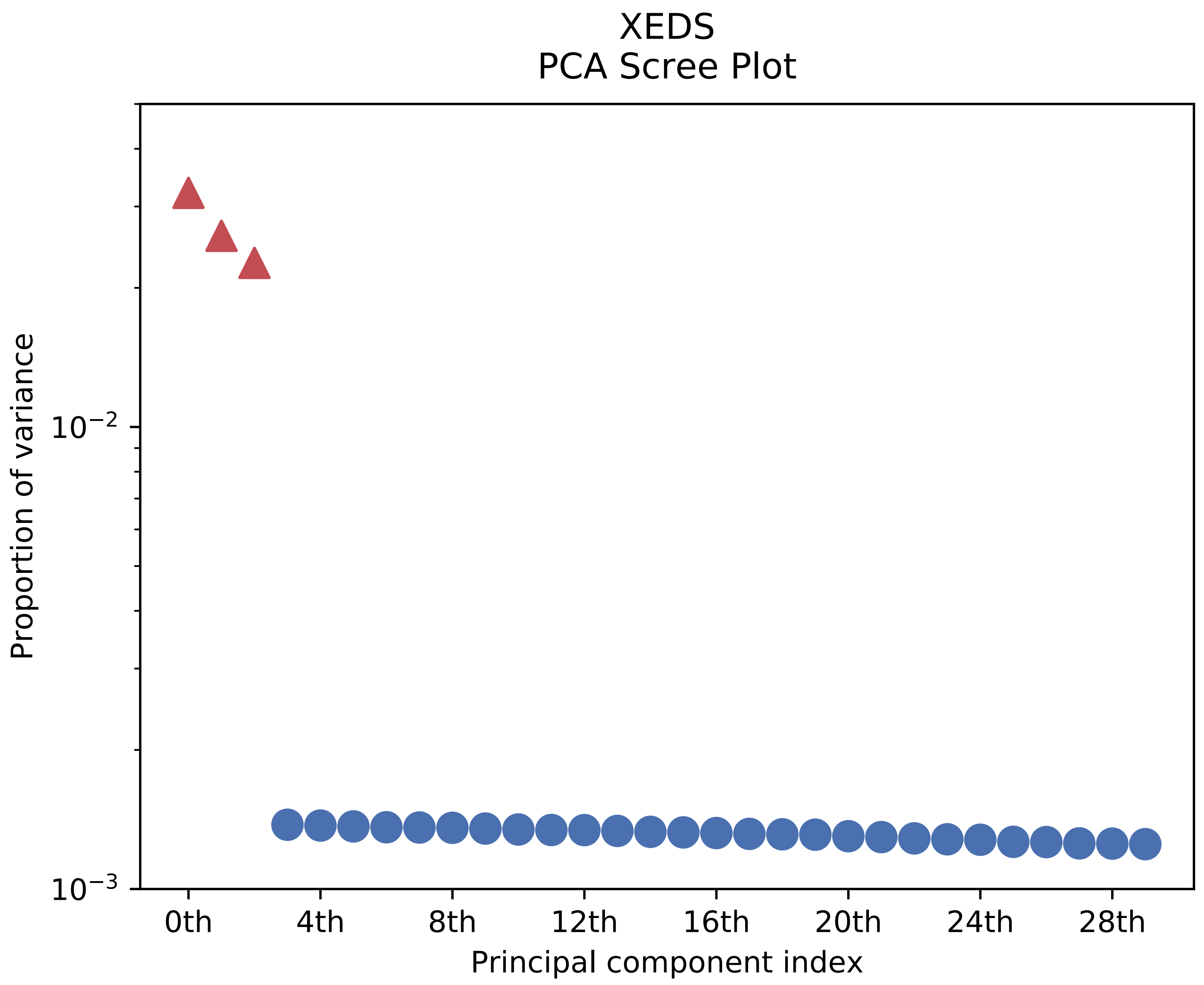
A simple example:



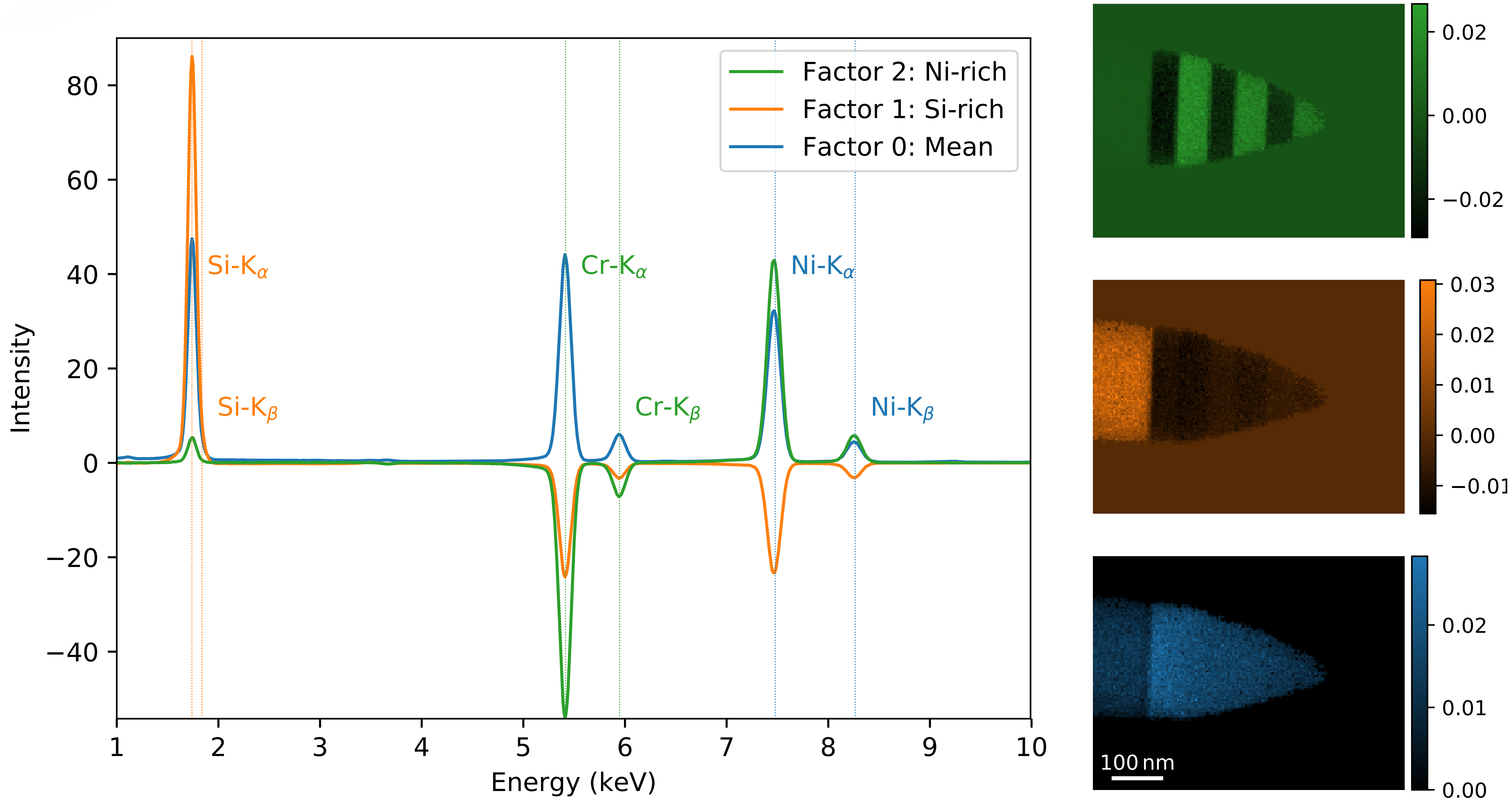
Single pixel counts in the single digits
Cr and Ni visible, but noisy

How many components to choose?

- PCA orders components by "described variance"
- *a priori* we know there should be three components
- Three important components confirmed



Result of PCA - Factors and Loadings



Signals are non-physical; Elements mixed between factors
Drastically enhances S/N ratio in "loading" maps

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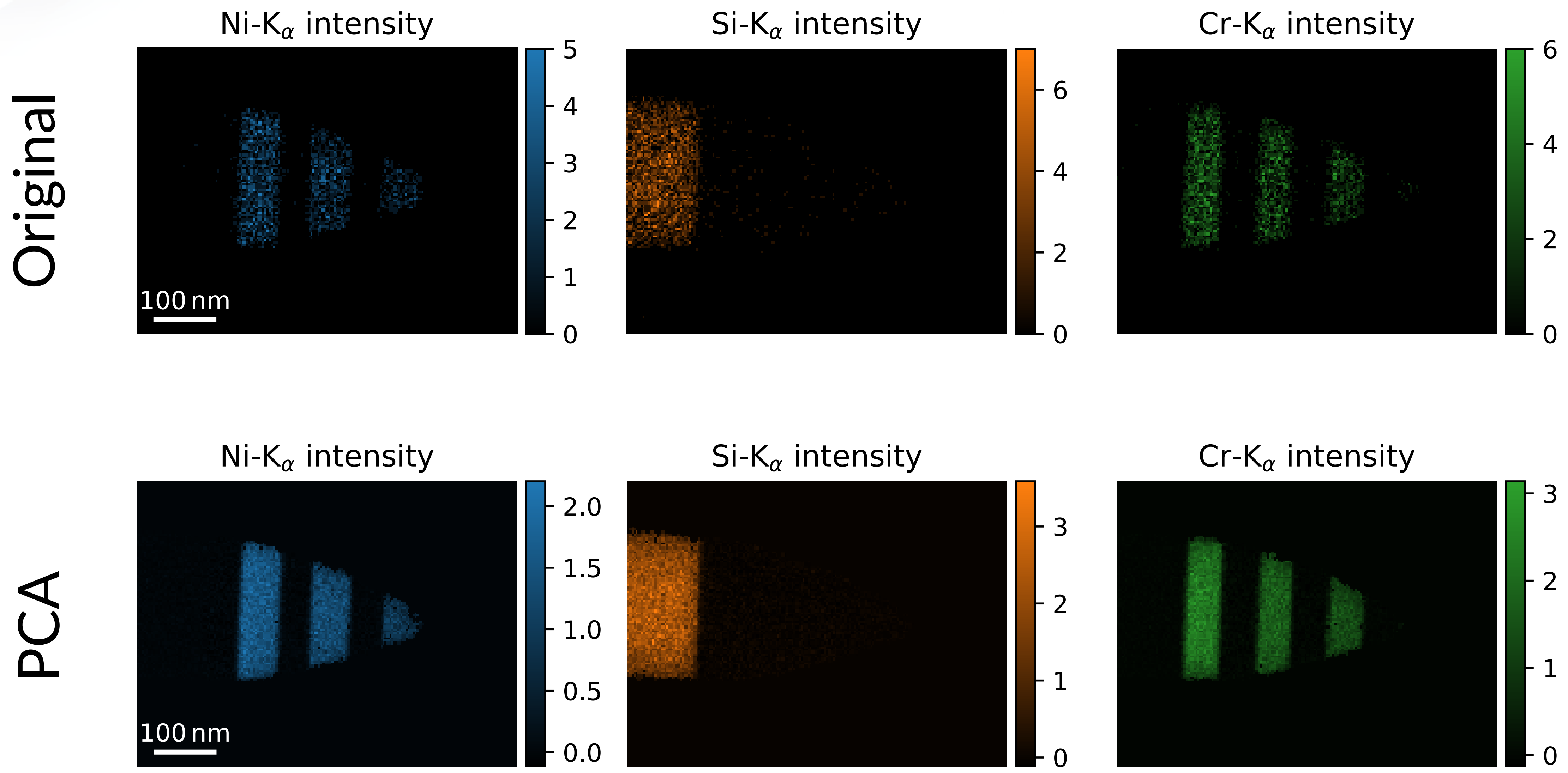
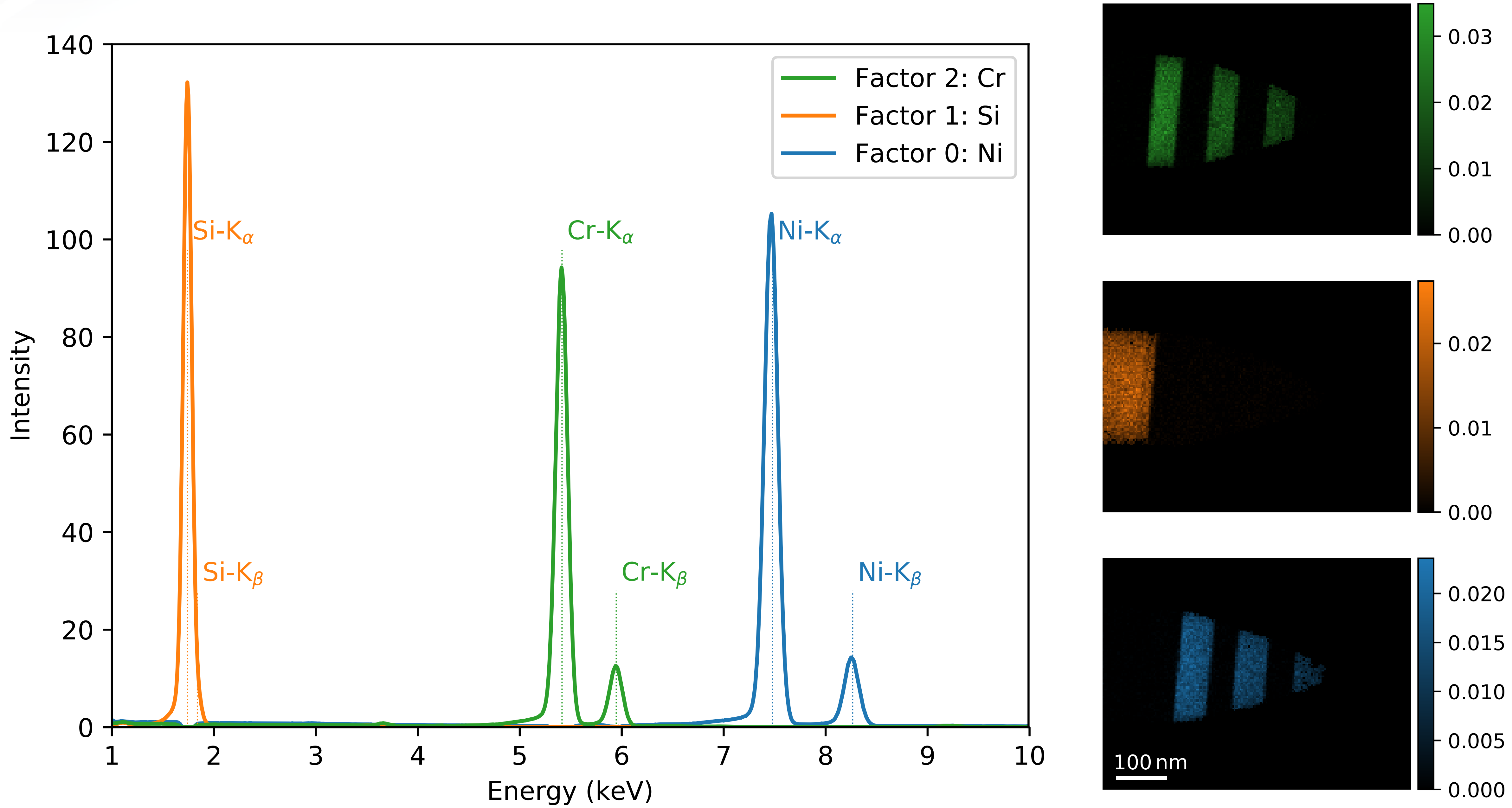
Result of PCA - Denoising

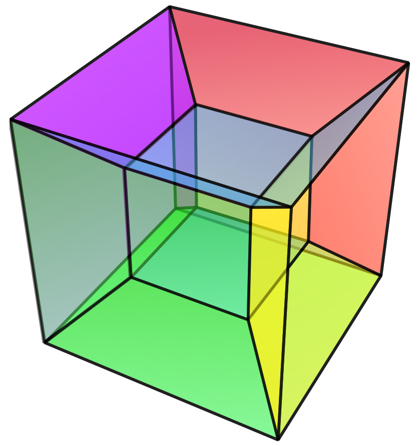


Line intensities extracted from model with top 3 PCA elements;
Drastically enhances S/N ratio in "loading" maps

Result of NMF



One component for each element (phase)
Drastically enhances S/N ratio in "loading" maps



Thank you!

Onto the demo...