


# Welcome to the 2021 M&M Short Course X-15

## Data Analysis in Materials Science with



Presented by (a selection of) the HyperSpy developers:

- Håkon Wiik Ånes
- Carter Francis
- Eric Prestat
- Joshua Taillon

A decorative header featuring a repeating pattern of light blue and white hexagons, resembling a molecular or crystalline structure.

# **Session 3:**

# **An Introduction to Machine Learning in Electron Microscopy**

***Electron Microscopy in the age of "Big Data"***

**Josh Taillon**

*August 1, 2021*

A decorative header featuring a repeating pattern of light blue and white hexagons, some of which are slightly offset to create a 3D effect.

# 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?

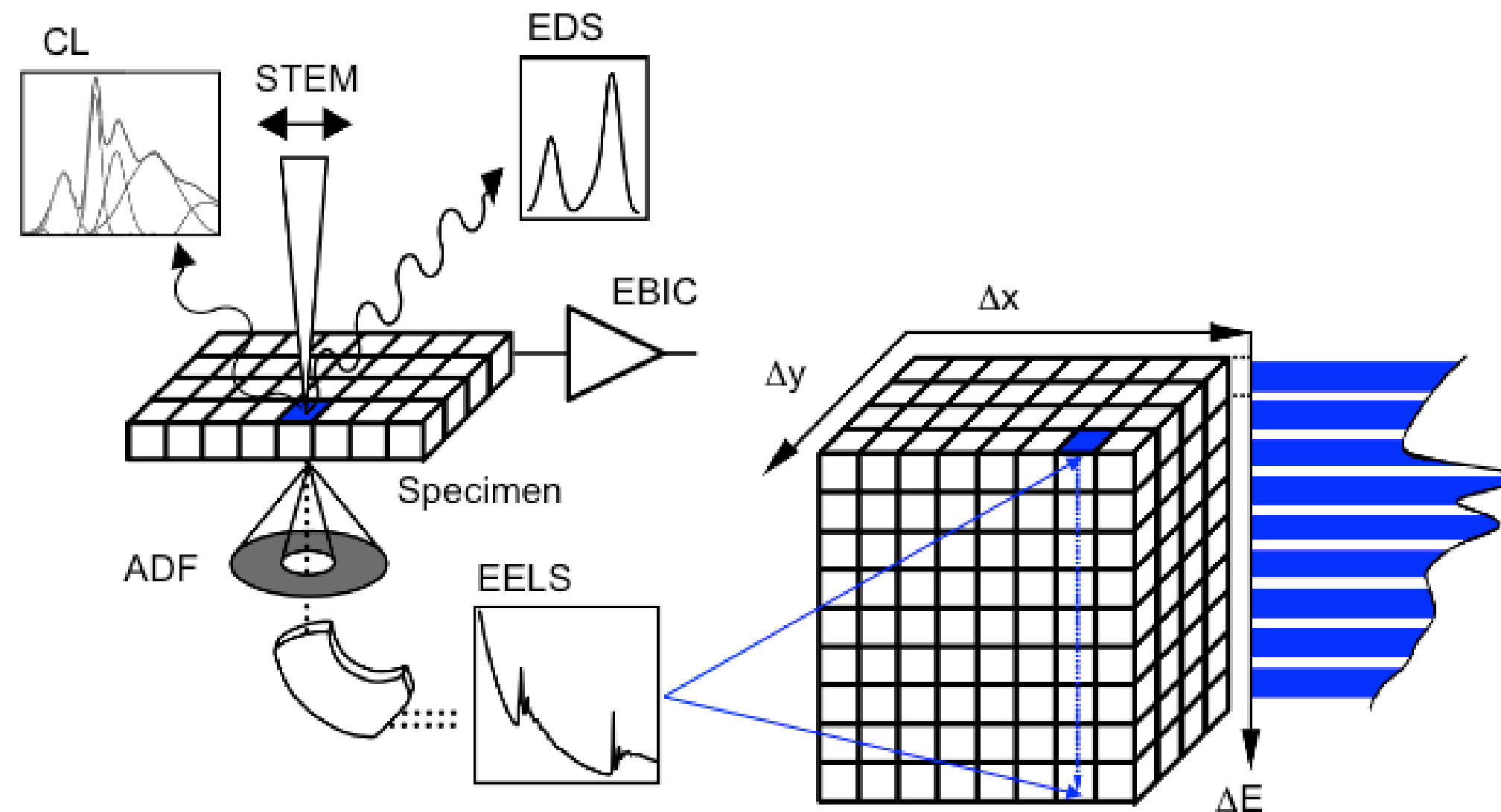
- The primary use for unsupervised learning is in *signal separation*
  - Sometimes called *hyperspectral unmixing* as well
- Ideally, we can automatically determine what signals are present in the data, and where they are located
  - This is the basis of most vendors' *phase mapping* offerings
- Can 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
  - ( $\mu$ -)XRF mapping
  - FTIR mapping
  - Cathodoluminescence mapping
- Otherwise, these techniques can be used on any type of data:
  - Images, time series, etc.

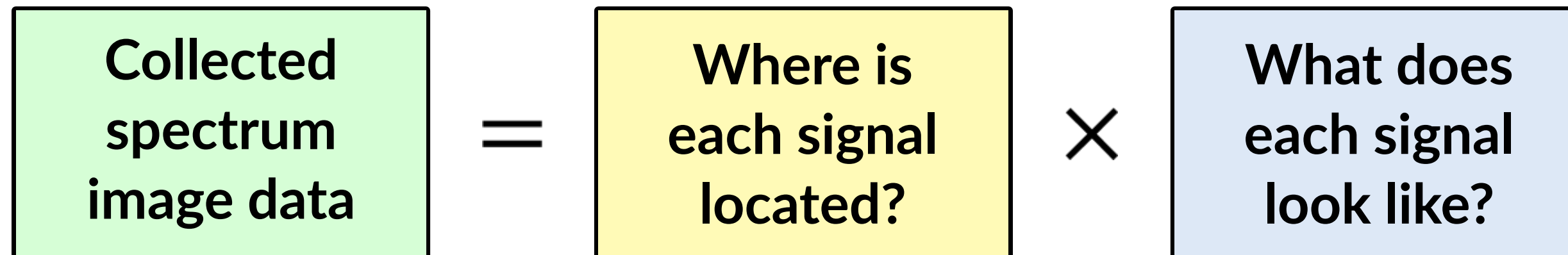
# What *is* hyperspectral unmixing?

- Start with some hyperspectral data:



*Image courtesy of Gatan, Inc.*

# What is hyperspectral unmixing?

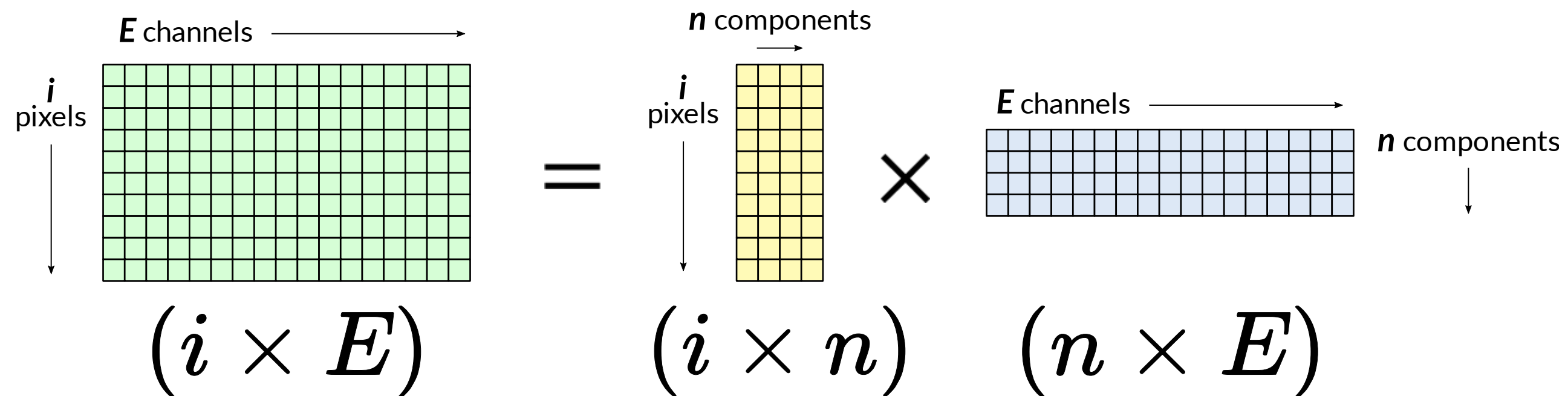


$$\mathbf{D}_{(x,y),E} = \mathbf{W}_{(x,y),n} \times \mathbf{S}_{n,E} + \epsilon_{(x,y),E}$$

$$\mathbf{D}_{i,E} = \mathbf{W}_{i,n} \times \mathbf{S}_{n,E} + \epsilon_{i,E}$$



# What is hyperspectral unmixing?



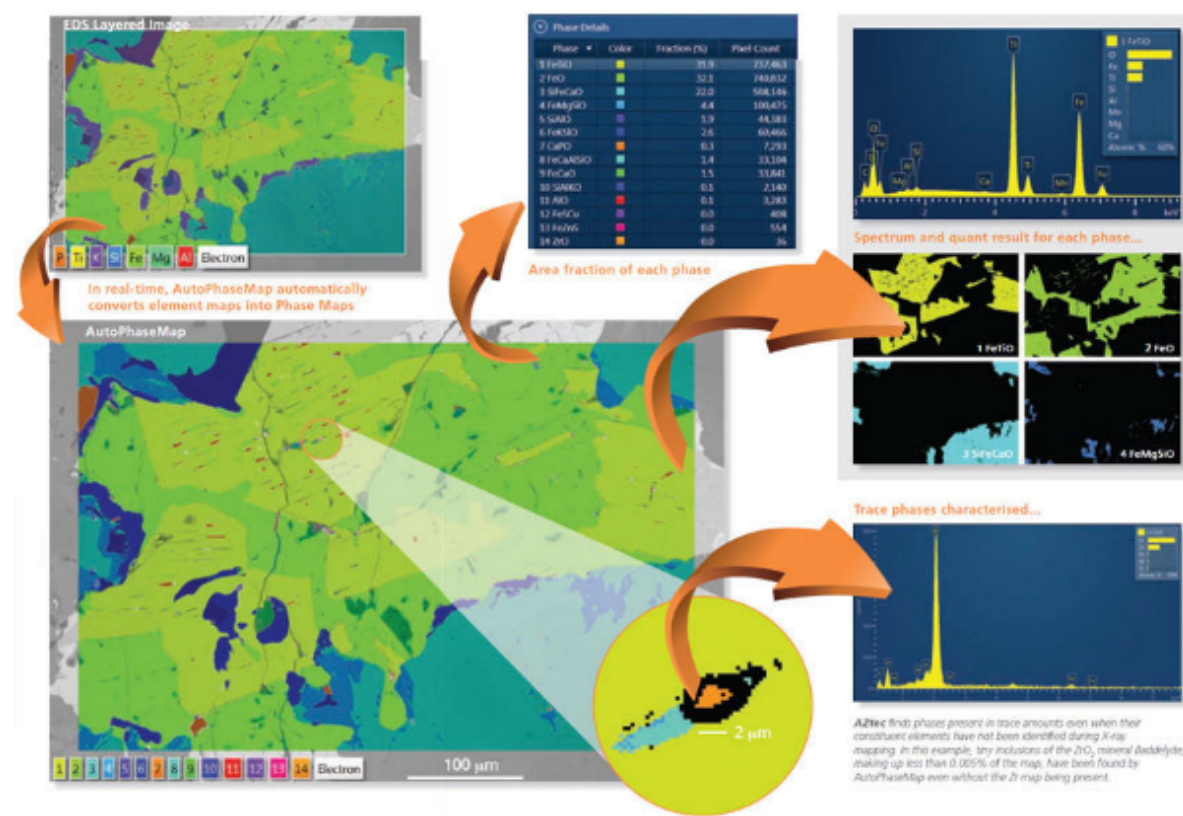
The diagram illustrates the hyperspectral unmixing equation using matrix notation and grid representations:

- Left Matrix (Green Grid):** A grid with  $i$  pixels (rows) and  $E$  channels (columns). It is labeled  $(i \times E)$ .
- Equality:** An equals sign ( $=$ ) follows the green grid.
- First Matrix (Yellow Grid):** A grid with  $i$  pixels (rows) and  $n$  components (columns). It is labeled  $(i \times n)$ .
- Multiplication:** A multiplication symbol ( $\times$ ) follows the yellow grid.
- Second Matrix (Blue Grid):** A grid with  $n$  components (rows) and  $E$  channels (columns). It is labeled  $(n \times E)$ .

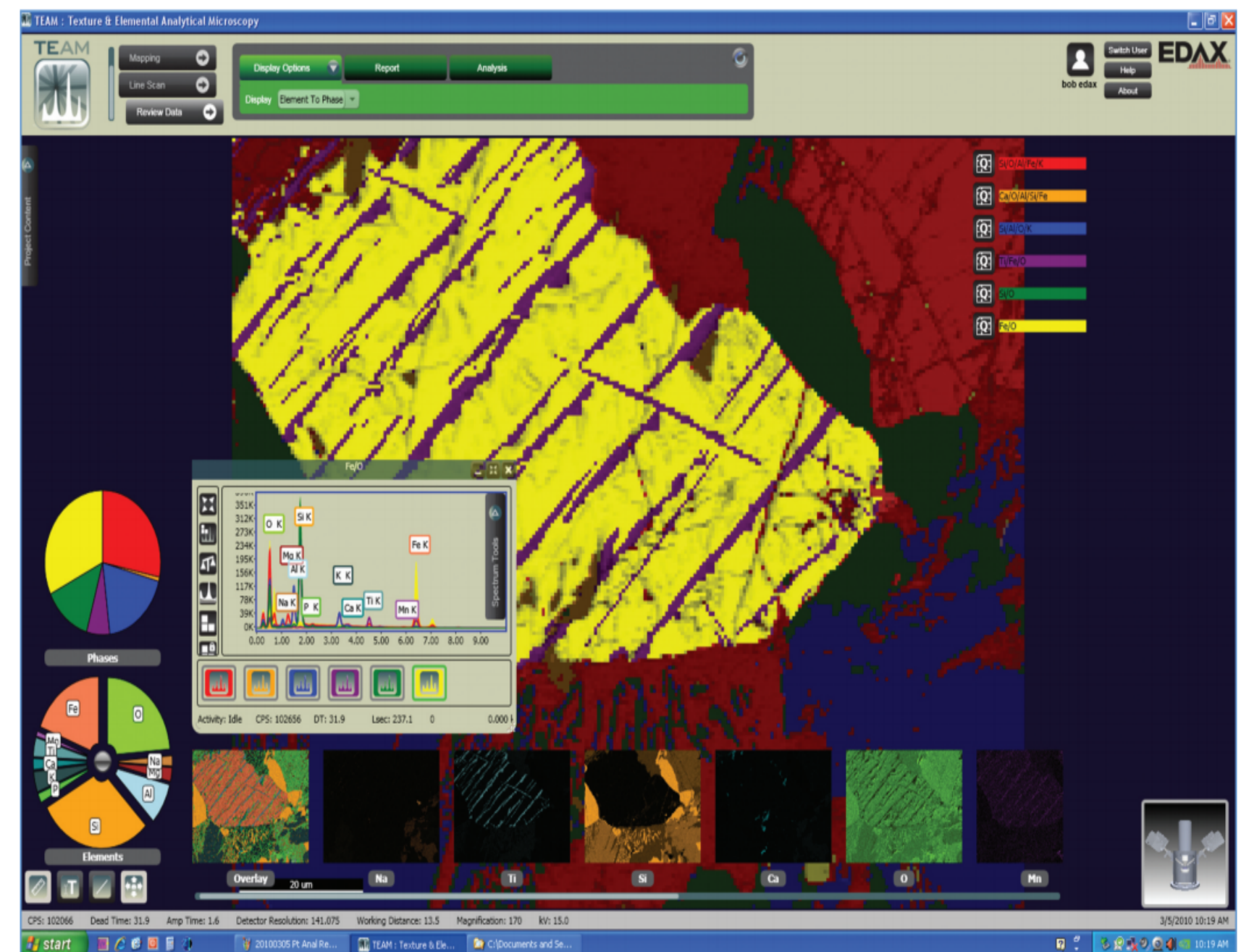
A linear algebra problem!

# 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



EDAX — Smart Phase Mapping

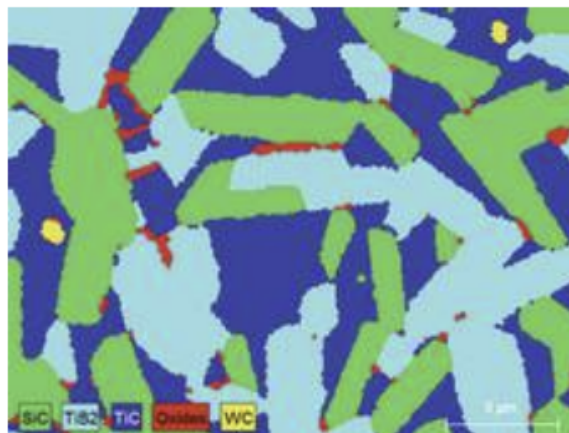


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## ESPRIT AutoPhase

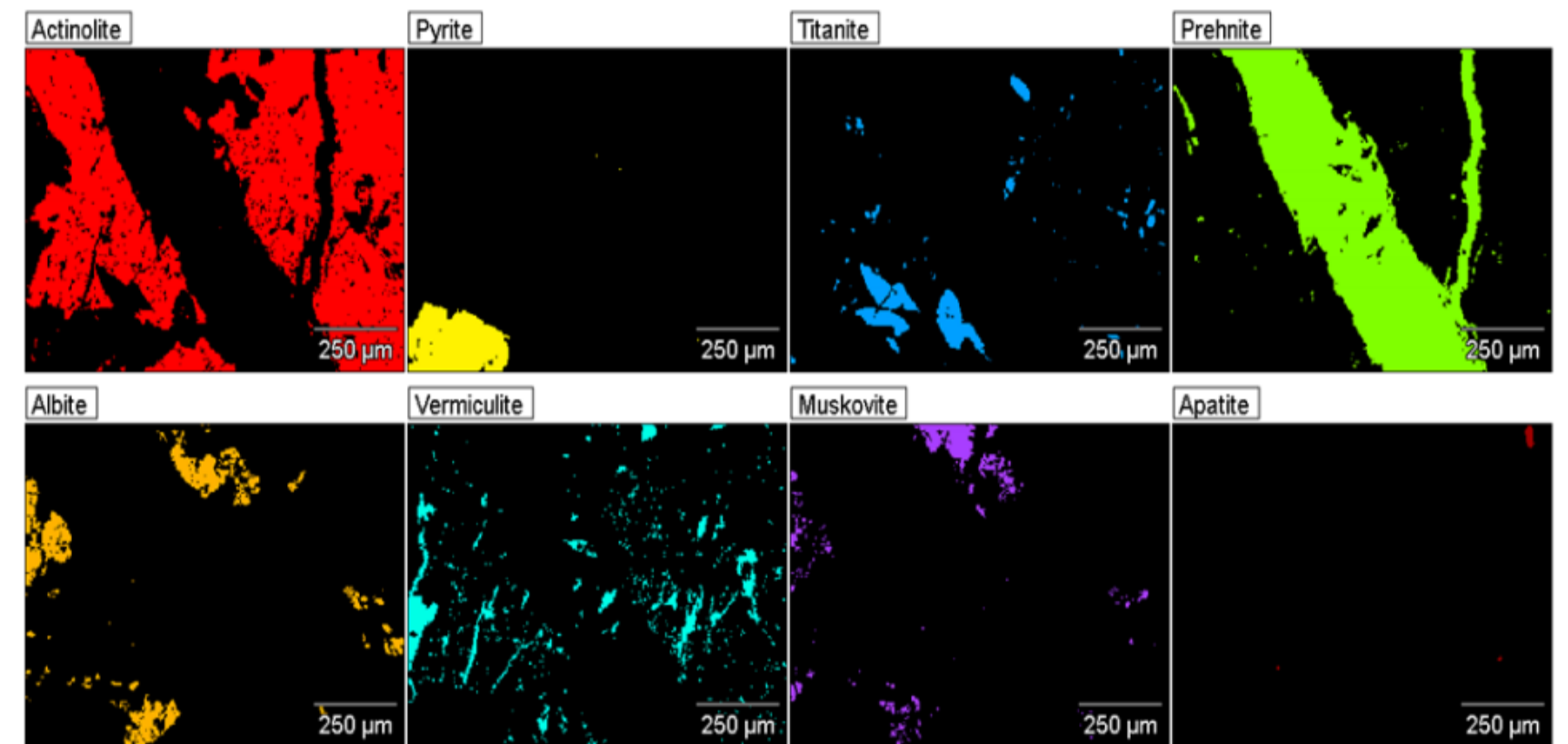
The Automatic Phase Analysis Tool



Chemical phase map of a hard ceramic material

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

Bruker — *AutoPhase*



COMPASS

ThermoFisher  
SCIENTIFIC

Thermo Fisher — *COMPASS*

# Strengths/challenges 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/challenges 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:  $\mathbf{D}_{(x,y),E} = \mathbf{W}_{(x,y)} \times \mathbf{S}_E$ 
  - This is a highly underdetermined problem, with an infinite number of solutions
  - Assumptions implicit in each algorithm 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

# Principle component analysis + blind source separation

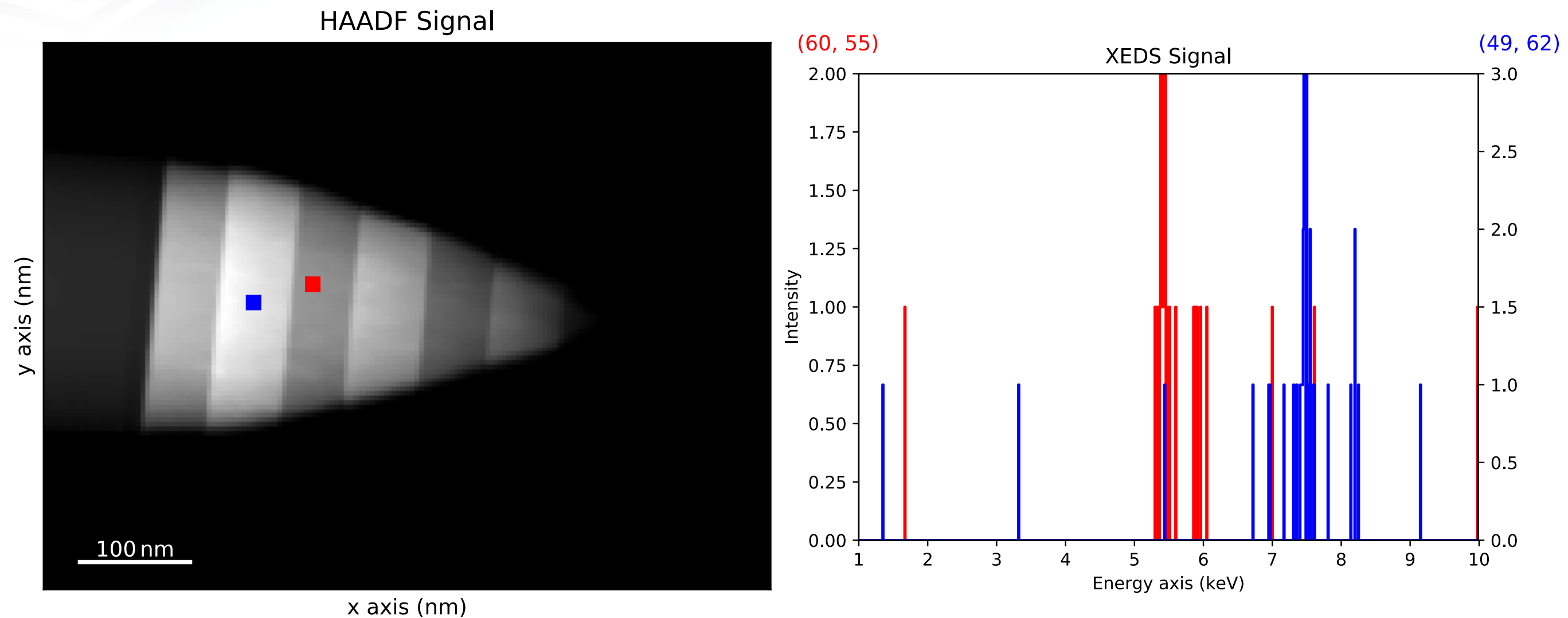
- PCA will find the spectra that describe the maximum amount of variance within the data set
  - These principle components (PCs) will contain the most "information" – but not information relevant to a microscopist
  - The results will look like vaguely spectral, but almost guaranteed to be non-physical
- [Blind source separation](#) often gives more interpretable results:
  - Independent component analysis (ICA):
    - Operates on the PCs to maximize independence between spectral results
  - Non-negative matrix factorization (NMF):
    - Decompose the matrix with constraints that match physical expectations

# 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 (73 spectrum images)
  - Dataset is  $(x, y, \theta, E) : (165, 124, 73, 900)$ – 12.2GB
- HAADF and XEDS SI data collected simultaneously

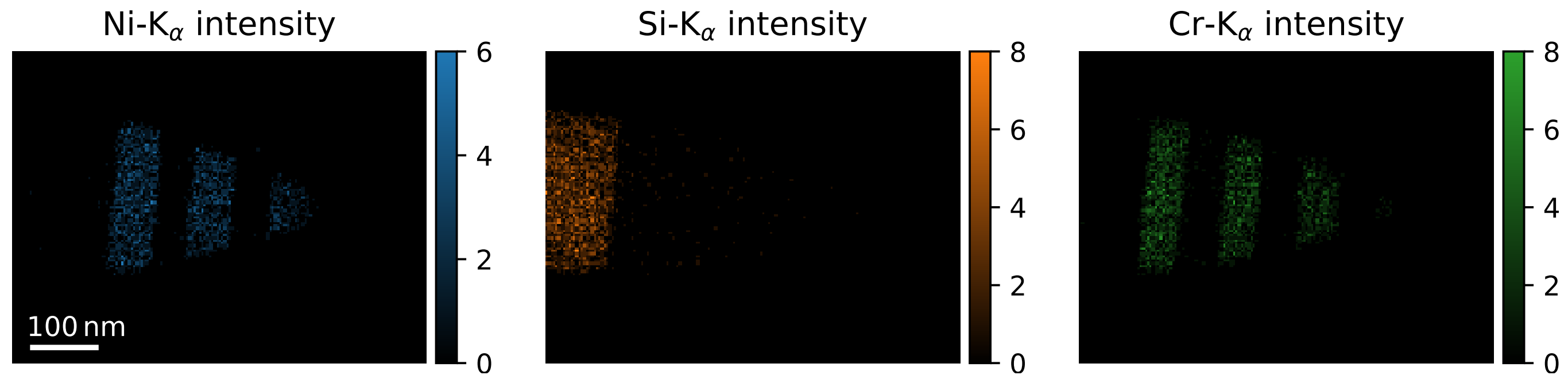


# A simple example:



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

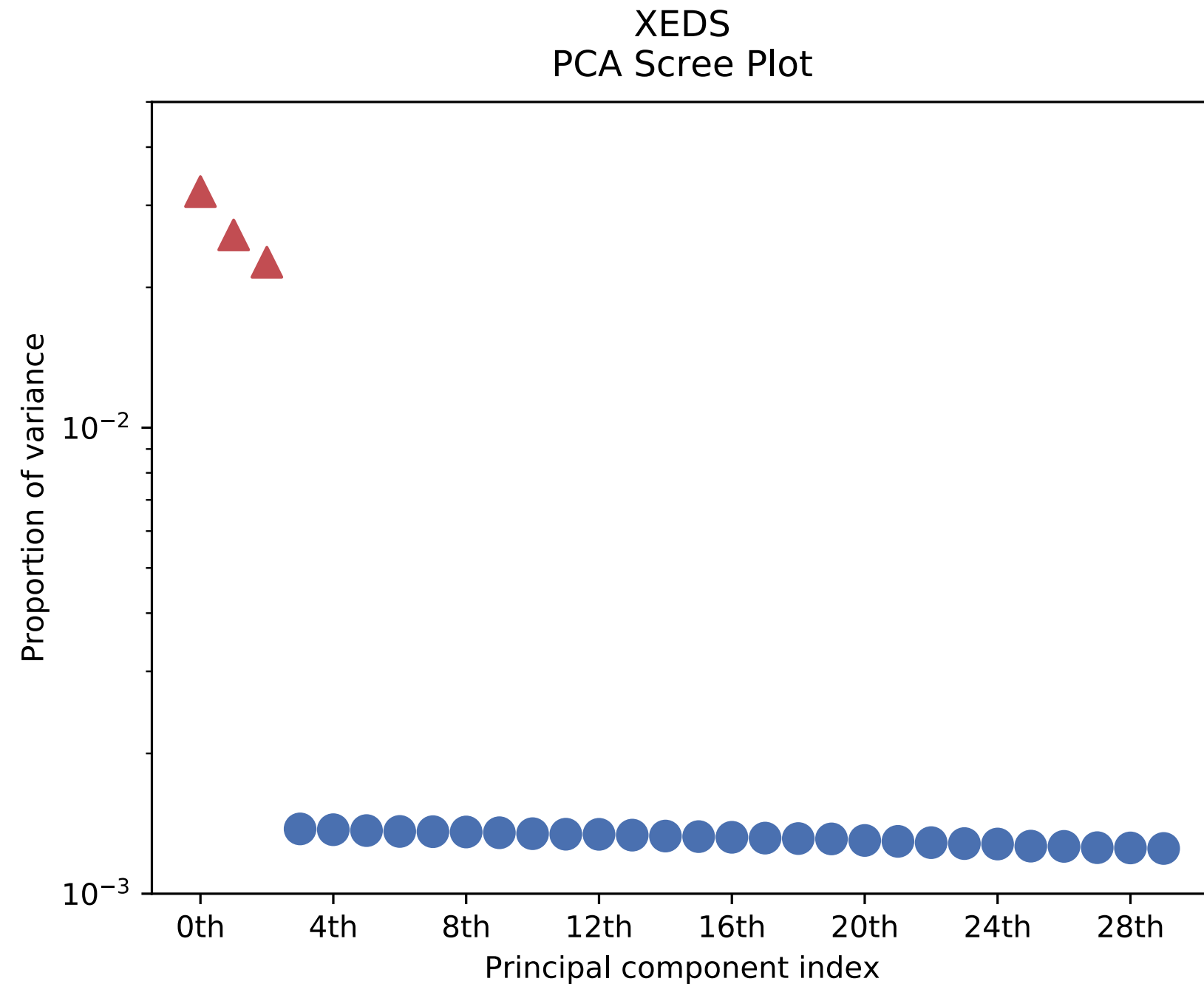
# A simple example:



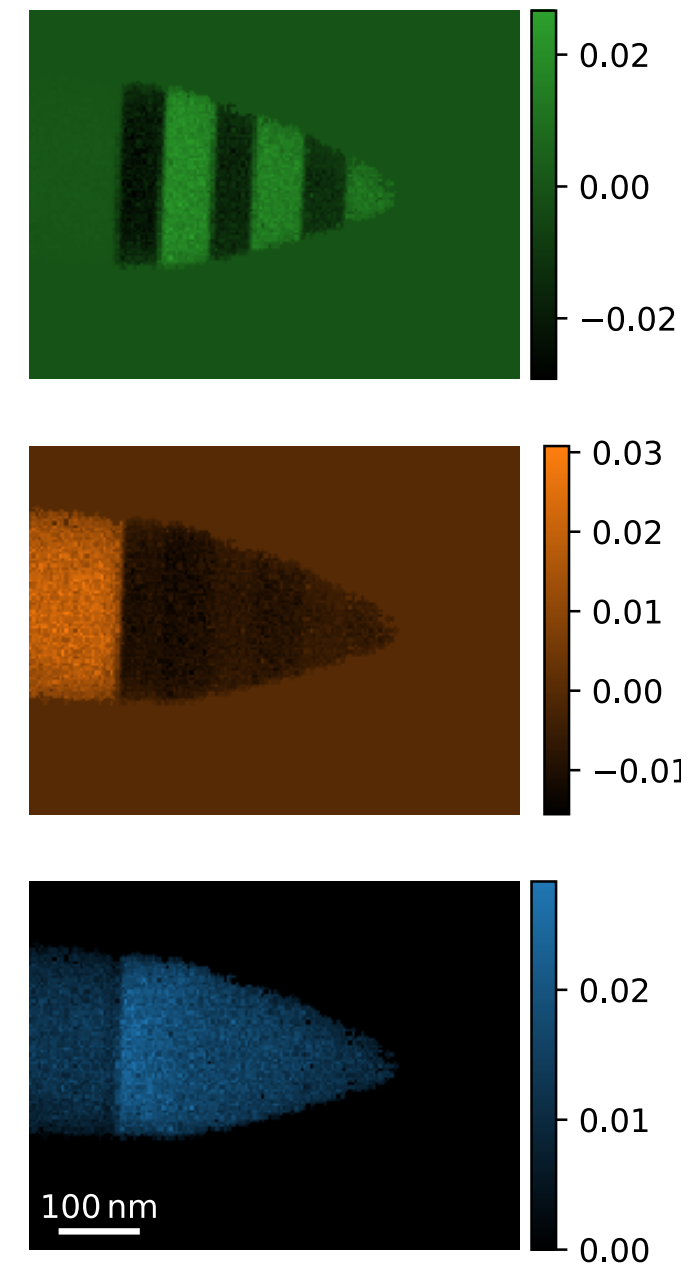
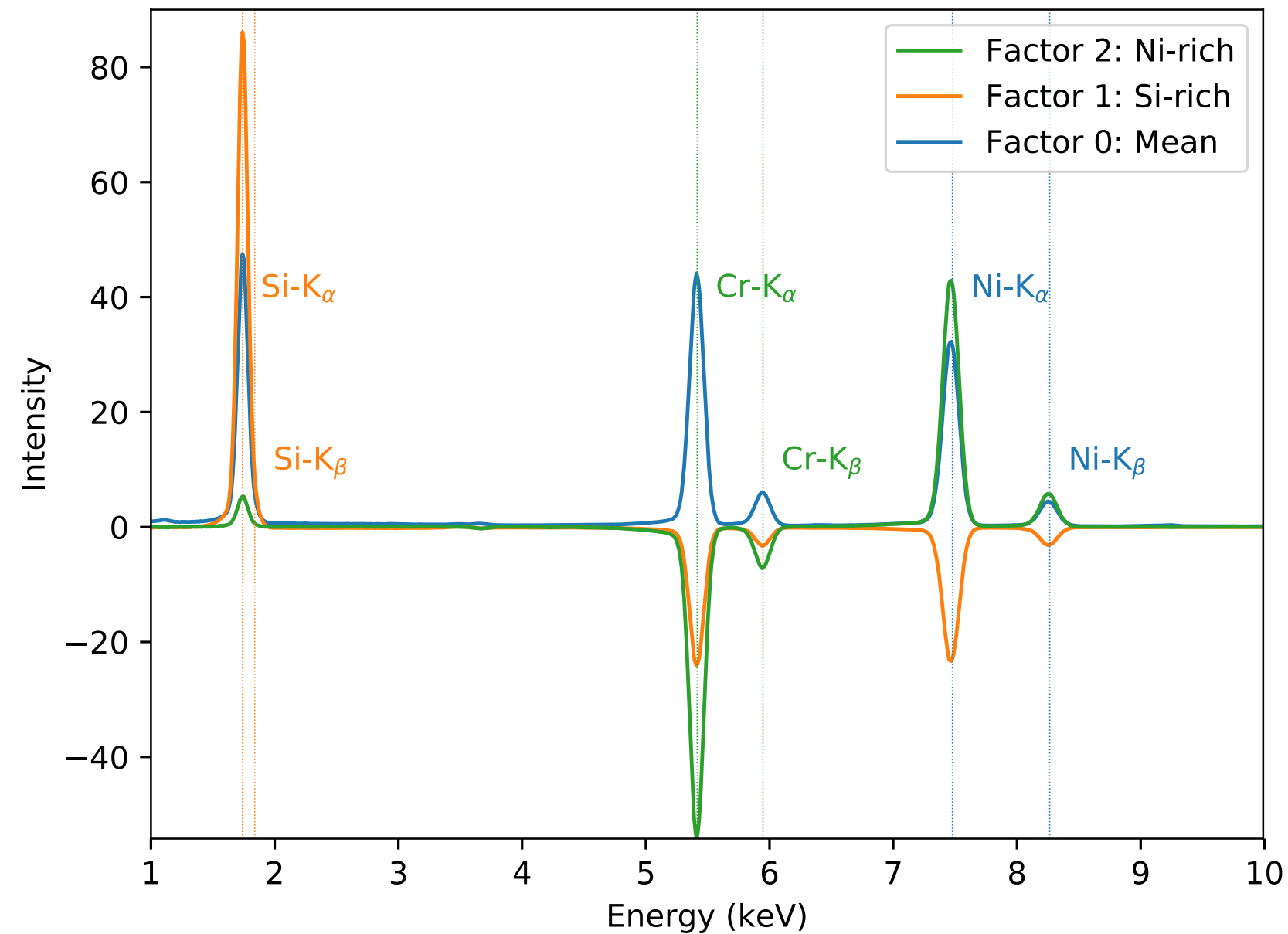
*Single pixel counts in the single digits  
Cr and Ni visible, but noisy*

# How many components to choose?

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

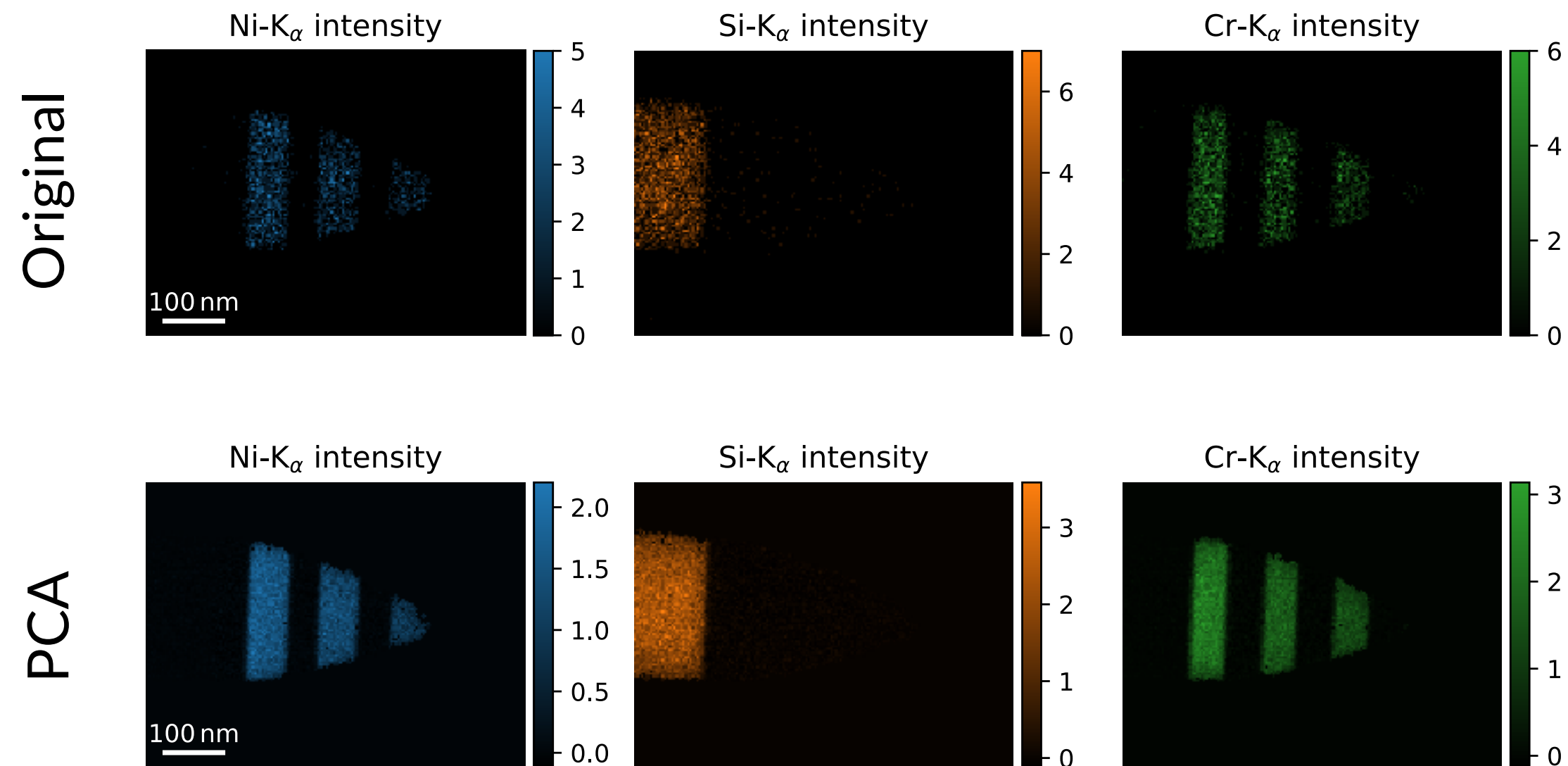


# Result of PCA - Factors and Loadings



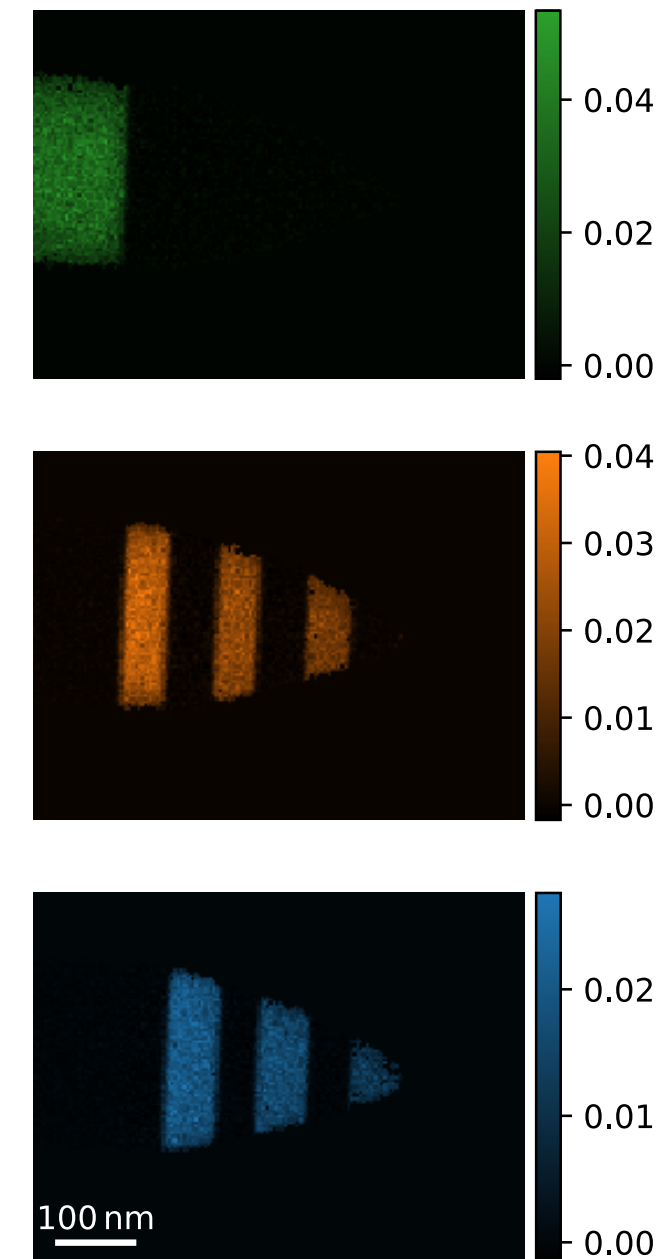
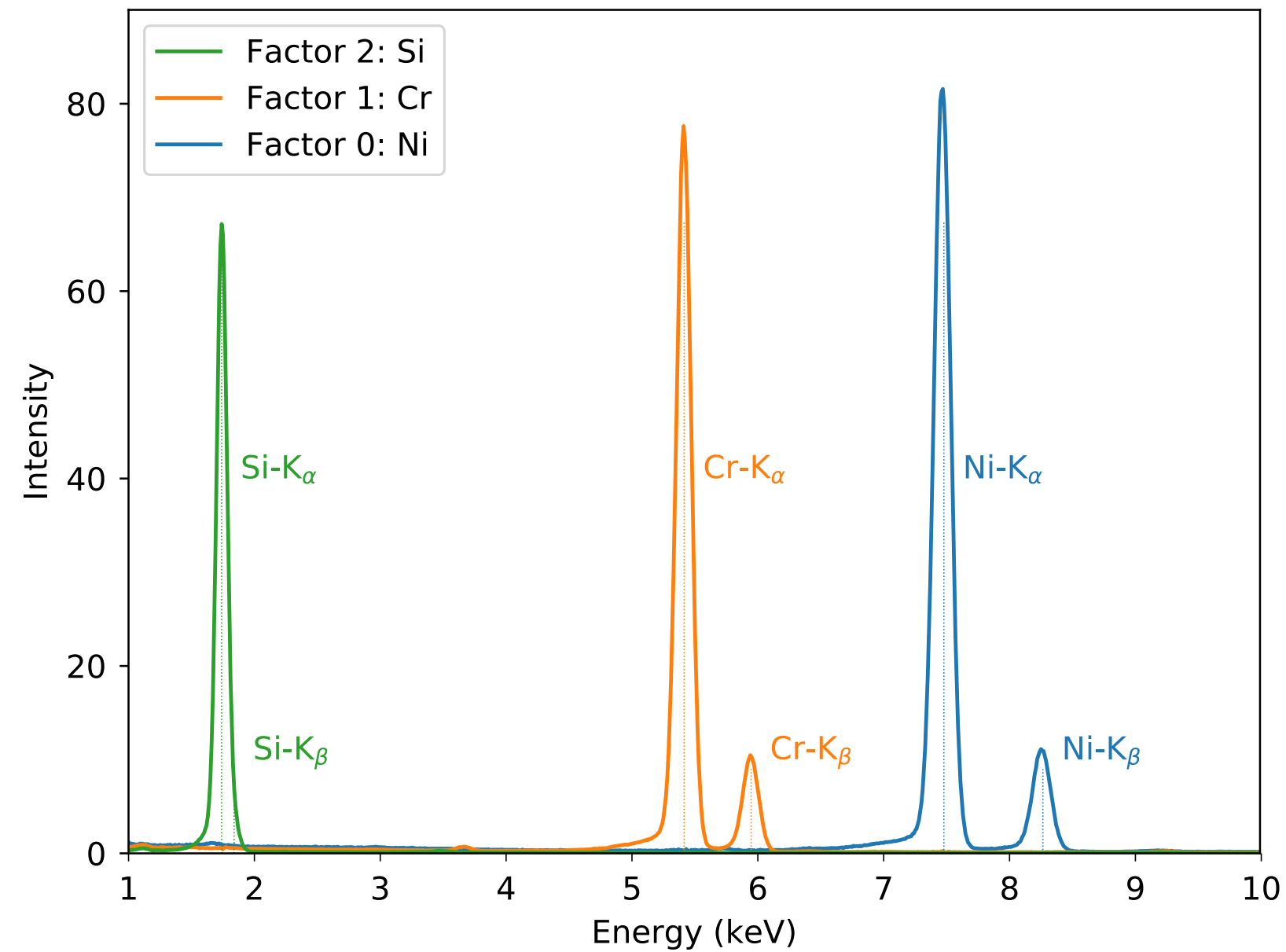
*Signals are non-physical; Elements mixed between factors  
Drastically enhances S/N ratio in "loading" maps*

# Result of PCA - Denoising



*Line intensities extracted from model with top 3 PCA elements;  
Drastically enhances S/N ratio in line intensity maps*

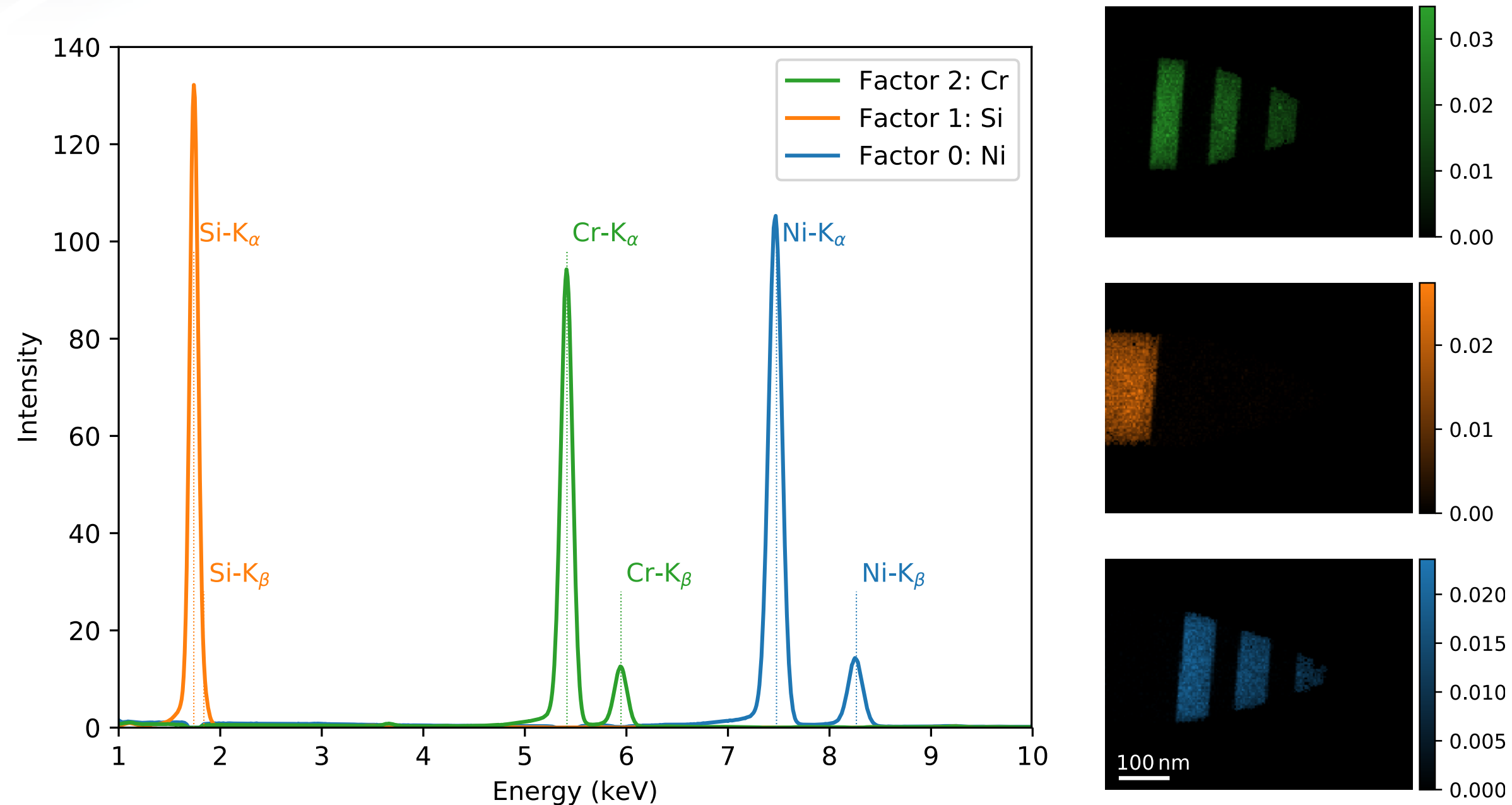
# Result of PCA + BSS



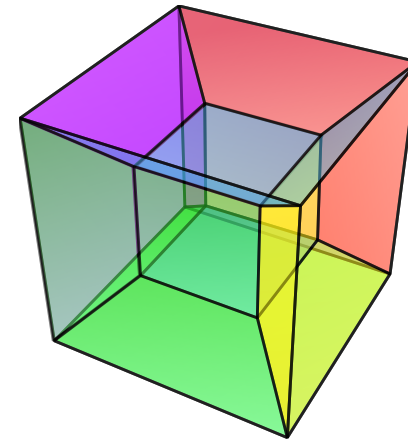
*One component for each element (phase)  
Much more interpretable results*



# Result of NMF



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



# Thank you!

Onto the demo...

Any questions?

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