

Linear Unmixing Methods for Spectral and Image Analysis

Sergei V. Kalinin

Linear Unmixing methods

1. Why linear unmixing?
 - Spectral images
 - Image analysis
2. Multiple linear regression
3. Principal component analysis (PCA)
 - Definition and implementation
 - PCA for scanning tunneling microscopy
 - Physical meaning of PCA: band excitation SPM
 - PCA on imaging data
4. Independent component analysis (ICA)
5. N-FINDR and Bayesian linear unmixing
 - Mapping phase transitions
 - Image segmentation

Physical constraints in linear models: **If solution exists and its unique, doesn't matter how you find it**

Spectroscopic Imaging

THE UNIVERSITY OF TENNESSEE  KNOXVILLE

Advancements in imaging led to a broad spectrum of the spectroscopic imaging techniques, in which response spectra are measured in each spatial location giving rise to 3- and higher dimensional data.

Scanning probe microscopy:

- Force-distance curve measurements
- Current-voltage measurements
- Piezoresponse force/electrochemical strain spectroscopy

Electron microscopy:

- Electron Energy Loss Spectroscopy

Optical microscopy:

- Hyperspectral imaging
- Time resolved measurements

Mass-spectrometry:

- Secondary ion MS imaging

In many cases, measured signal can be represented or approximated as a linear combination of signals. However, their functional forms are generally unknown

Very important: convolution with resolution function is also mixing

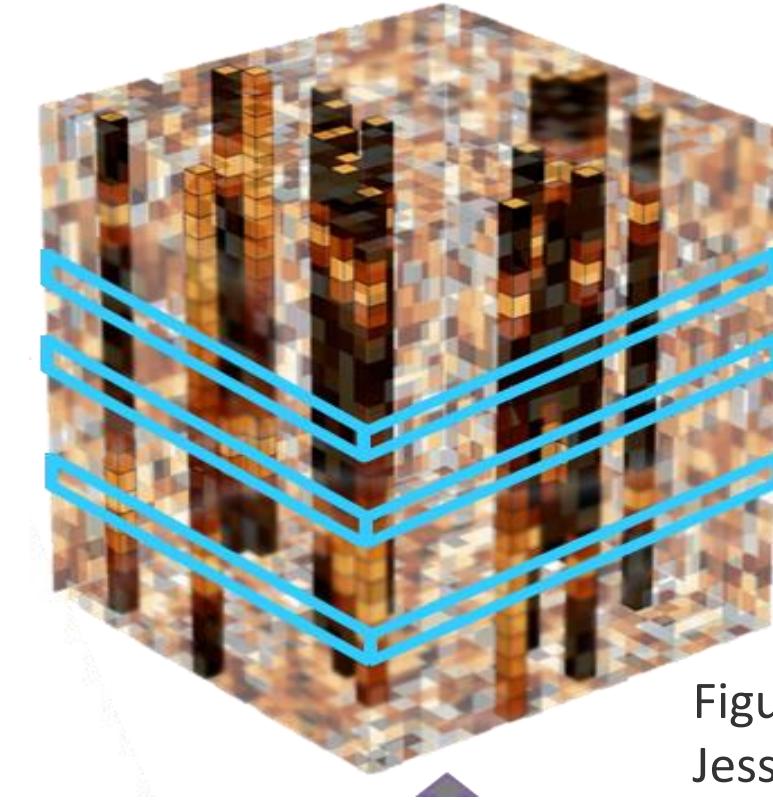
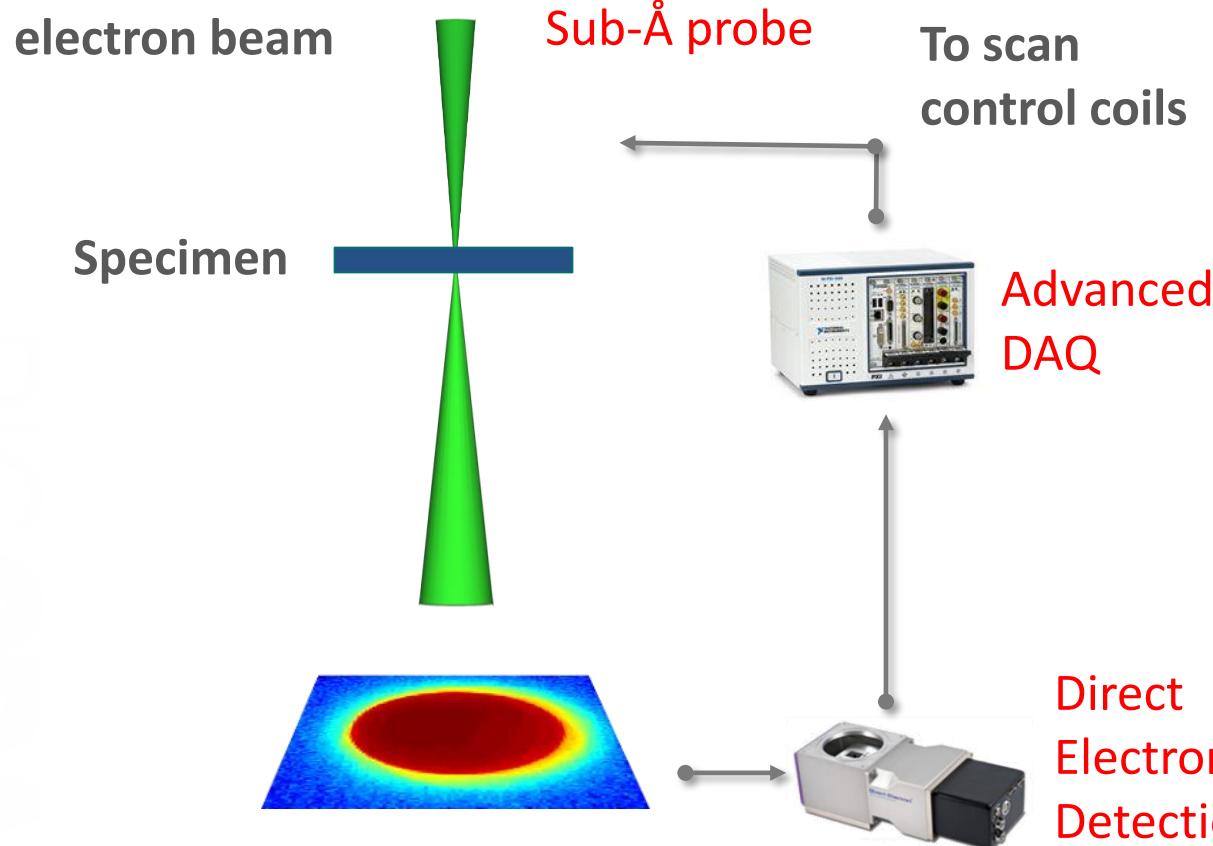


Figure by S.
Jesse

Less obvious cases

1. Ptychography in STEM



Collected is diffraction pattern (ronchigram) in each location

2. Focussed X-Ray

Collected is diffraction pattern in each spatial location in 2D or 3D

3. Image analytics

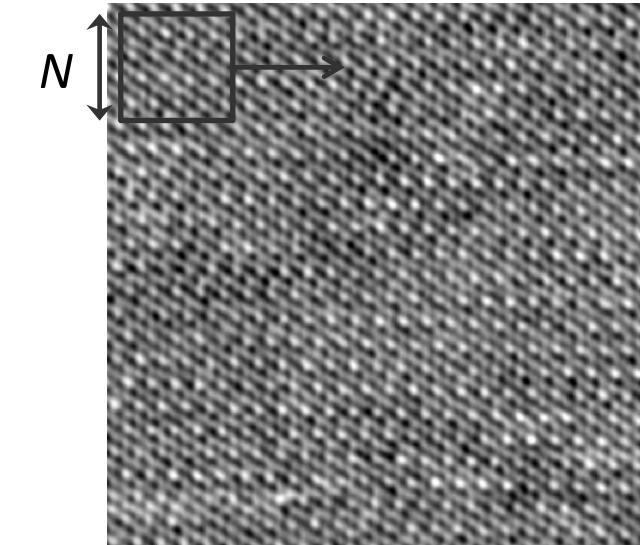


Figure by M. Ziatdinov

Sliding image transforms:

- Fast Fourier Transforms
- Correlation functions
- Intensity histograms
- Structural descriptors

The M pixel 2D image is transformed to M/N pixel image of more complex structure

General linear unmixing

$$S(\mathbf{x}, \mathbf{R}) = \sum_i a_i(\mathbf{x}) w_i(\mathbf{R}) + N$$

We start with:

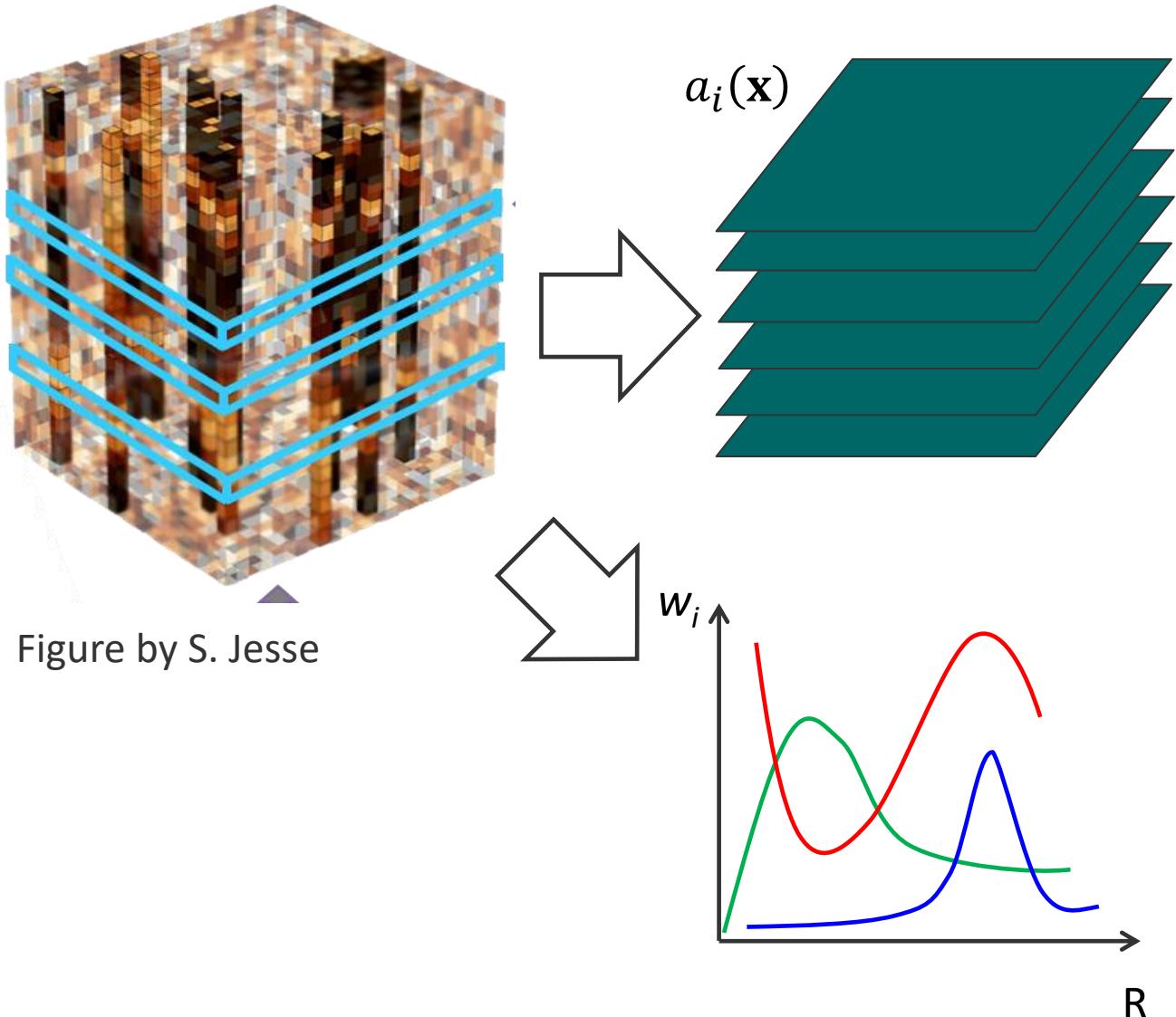
- \mathbf{x} is the spatial variable, $\mathbf{x} = (x, y)$
- \mathbf{R} is the (vector) parameter variable

Overall, for $M \times M$ image and P point in spectra, we have $M^2 P$ data points

We aim to get:

- $a_i(\mathbf{x})$ are loading maps
- $w_i(\mathbf{R})$ are endmembers/eigenvectors
- N is noise

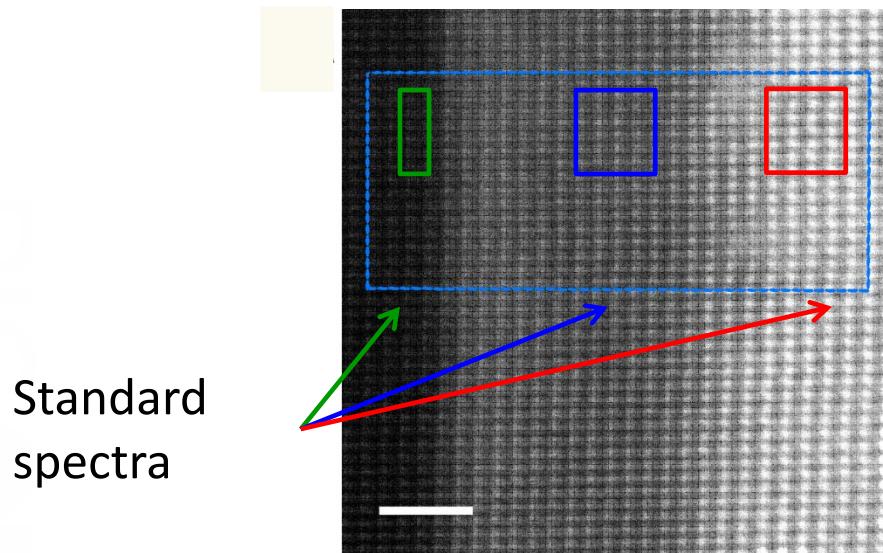
Overall, we can have (maximum) P loading maps of M^2 size. However, not all of them will have useful information



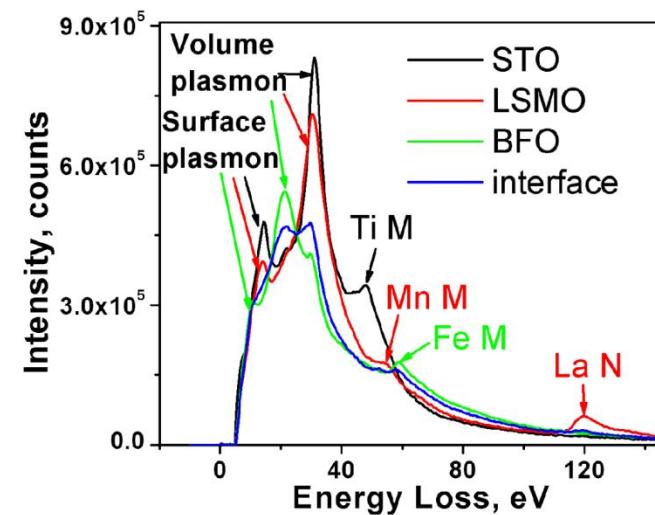
Multiple Linear Regression

Linear mixing $S(\mathbf{x}, \mathbf{R}) = \sum_i a_i(\mathbf{x}) w_i(\mathbf{R}) + N$ but $w_i(\mathbf{R})$ are known

STEM of STO/LSMO/BFO interface



Low-loss EELS spectra of three components



A.Y. BORISEVICH ET AL,
Suppression of Octahedral Tilts and Associated Changes in Electronic Properties at Epitaxial Oxide Heterostructure Interfaces, Phys. Rev. Lett. **105**, 087204 (2010).

Fit coefficient map



“Chemistry”:
35 to 125 eV

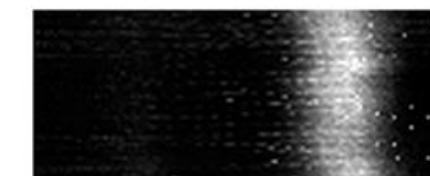
residuals map



χ^2 map



“Plasmons”:
5 to 35 eV



But what if endmembers are unknown?

At the first glance, the problem is impossible. We want to separate mixture in the components without knowing what the components are!

What we can do:

- Principal component analysis: how many components are there in the mixture
- Independent component analysis: going against the law of big numbers
- Bayesian linear unmixing: additivity to 1 and non-negativity constrains

What can be done:

- Bayesian linear unmixing: constraints on endmembers
- Sparse reconstructions: small number of components in each point
- Constraints on loading maps: smoothness or sharp boundaries
- Kernel transforms: data is simplest if physics is correct

Principal Component Analysis

$$S(\mathbf{x}, \mathbf{R}) = \sum_i a_i(\mathbf{x}) w_i(\mathbf{R})$$

- In PCA, the eigenvectors $w_i(\mathbf{R})$ are orthonormal and are arranged such that corresponding eigenvalues are placed in descending order by variance
- Can be used to separate “real data” from “noise” – but needs cut-off/selection criteria
- Can be performed by SVD decomposition (MatLab, Python, etc)
- PCA eigenvectors do not have defined physical meaning
- However, PCA is a starting point for many other unmixing methods

PCA Background

PCA: orthogonal transformation converting possibly correlated variables into linearly uncorrelated *principal components*

- PCA was invented by Karl Pearson in 1901, however the Singular Value Decomposition was independently derived some half a century earlier in Italy, Germany and France
- PCA transforms the data such that the greatest variance by any projection lies on the first coordinate
- Reveals internal structure of the data that best explains variance in the data set
- Since data often moves in clusters, PCA reveals those variables that drive the variance

Pearson, K. (1901). "On Lines and Planes of Closest Fit to Systems of Points in Space". *Philosophical Magazine Series 6* 2 (11): 559–572

PCA: Formal Definition

Principal component w_1 of a data set \mathbf{X} can be defined as:

$$\mathbf{w}_1 = \arg \max_{\|\mathbf{w}\|=1} \text{Var}\{\mathbf{w}^T \mathbf{X}\} = \arg \max_{\|\mathbf{w}\|=1} E \left\{ (\mathbf{w}^T \mathbf{X})^2 \right\}$$

Subsequent components k , can be found by simply subtracting $k-1$ components from the data

$$\hat{\mathbf{X}}_{k-1} = \mathbf{X} - \sum_{i=1}^{k-1} \mathbf{w}_i \mathbf{w}_i^T \mathbf{X}$$

And substituting as $\dot{\mathbf{X}}_{k-1}$ a new data set

$$\mathbf{w}_k = \arg \max_{\|\mathbf{w}\|=1} E \left\{ (\mathbf{w}^T \hat{\mathbf{X}}_{k-1})^2 \right\}$$

PCA in Python

```
# number of components
nc = 20

# PCA
U, S, V = jLA.svd(X_vec - X_vec.mean(0), full_matrices=False)
U, V = svd_flip(U, V)
X_vec_t = jnp.dot(U[:, :nc], jnp.diag(S[:nc]))
components = V

# Plot
rows = int(np.ceil(float(nc)/5))
cols = int(np.ceil(float(nc)/rows))
print('NUMBER OF COMPONENTS: ' + str(nc))
print('Components...')

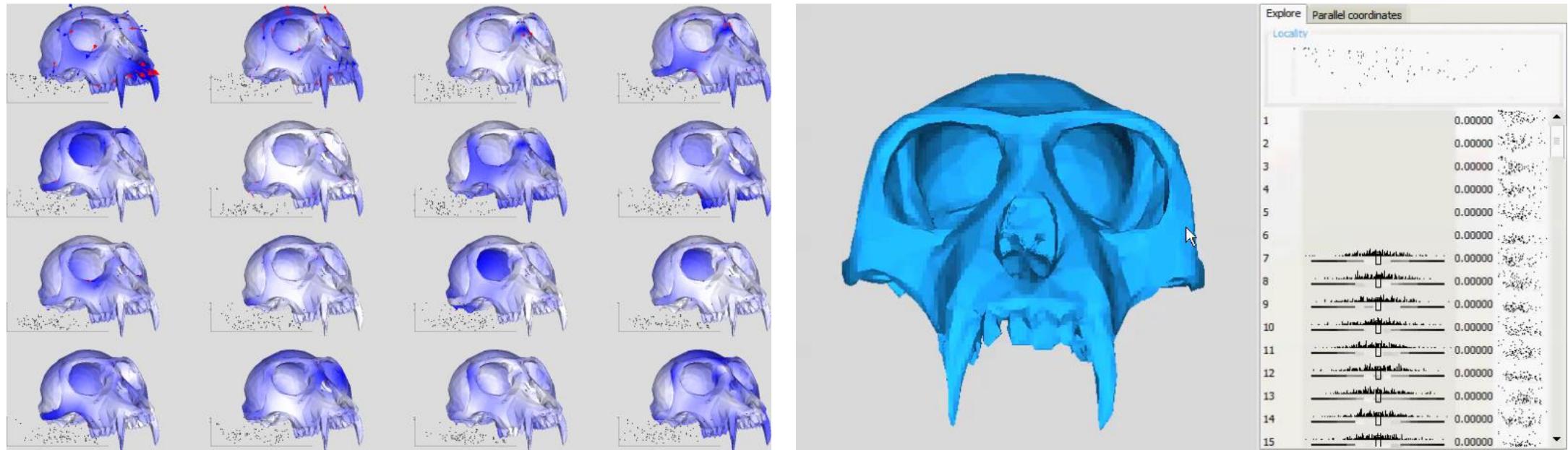
gs1 = gridspec.GridSpec(rows, cols)
fig1 = plt.figure(figsize = (4*cols, 3.5*(1+rows)//1.5))
for i in range(nc):
    ax1 = fig1.add_subplot(gs1[i])
    ax1.plot(components[i])
plt.show()

gs2 = gridspec.GridSpec(rows, cols)
fig2 = plt.figure(figsize = (4*cols, 4*(1+rows//1.5)))
for i in range(nc):
    ax2 = fig2.add_subplot(gs2[i])
    ax2.imshow(X_vec_t[:, i].reshape(d1, d2), cmap = 'jet')
    #ax2.set_title('Component ' + str(i + 1))
plt.show()
```

PCA: outside of imaging

Dan Alcantara, Localized Components Analysis,
<http://idav.ucdavis.edu/~dfalcant/research/loca.php>

Great, quick tool for looking at multichannel data



- Spectroscopic, or any type of series data becomes superposition of orthogonal eigenvectors with different weights
- First eigenvector contains the most information within spectral dataset
- Second eigenvector contains the most common response after subtraction of the 1st etc.

D. Alcantara, O. Carmichael, E. Delson, W. Harcourt-Smith, K. Sterner, S. Frost, R. Dutton, P. Thompson, H. Aizenstein, O. Lopez, J. Becker, and N. Amenta, "**Localized Components Analysis**", *Proceedings of IPMI*, 2007, pp. 519 - 531

Band excitation SPM

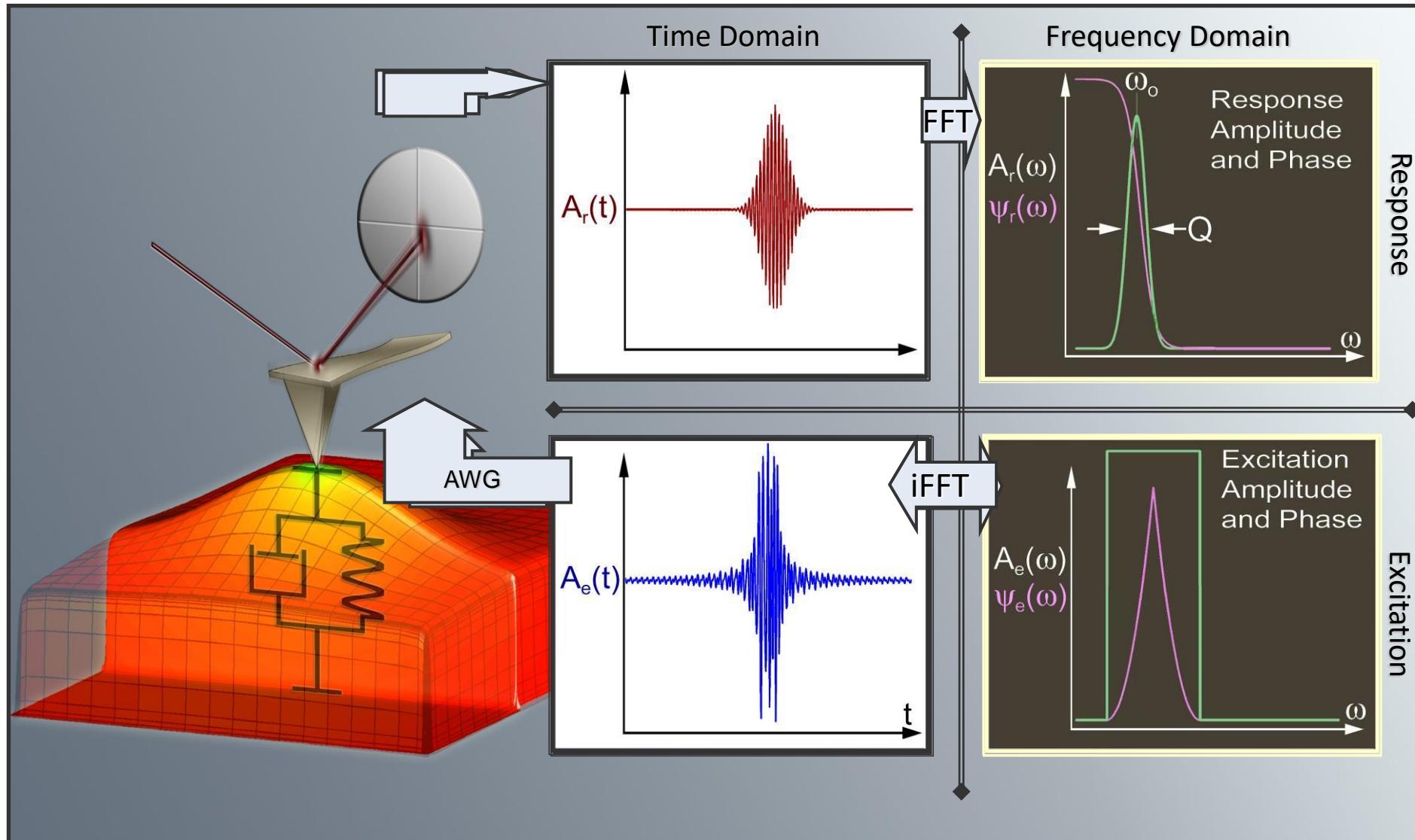
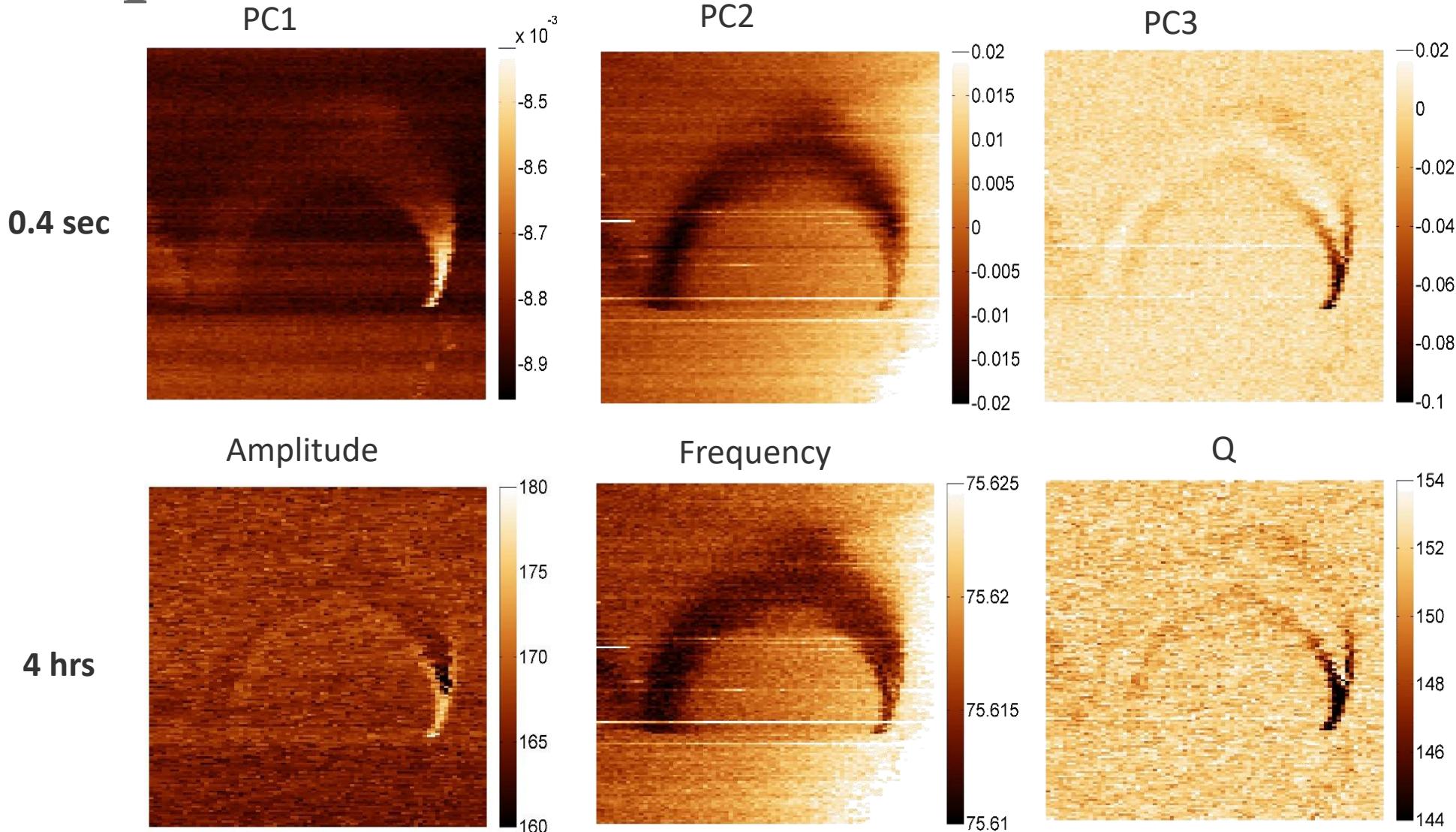


Figure by S. Jesse

Comparison: PCA vs. functional fit

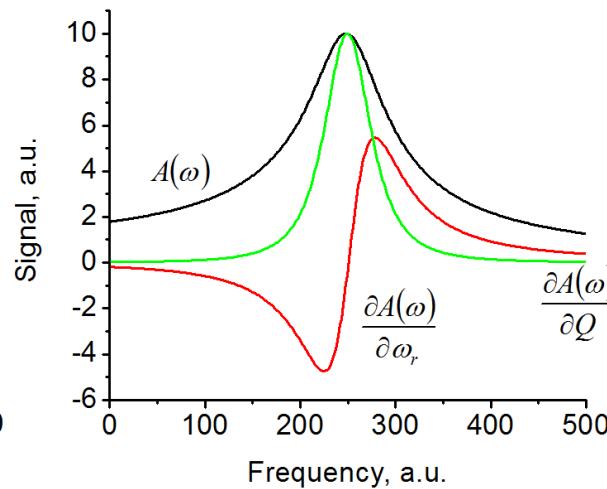
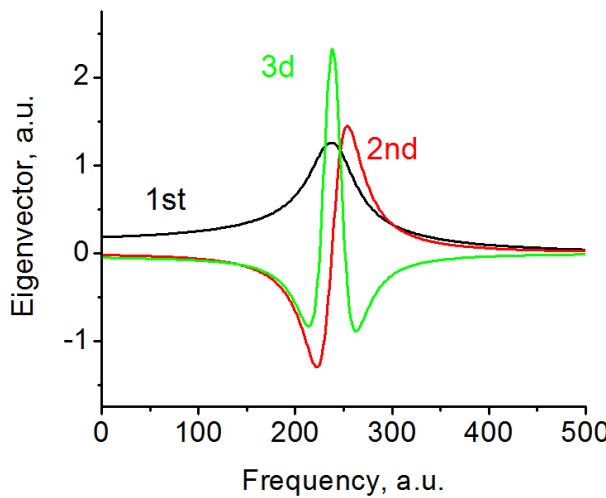
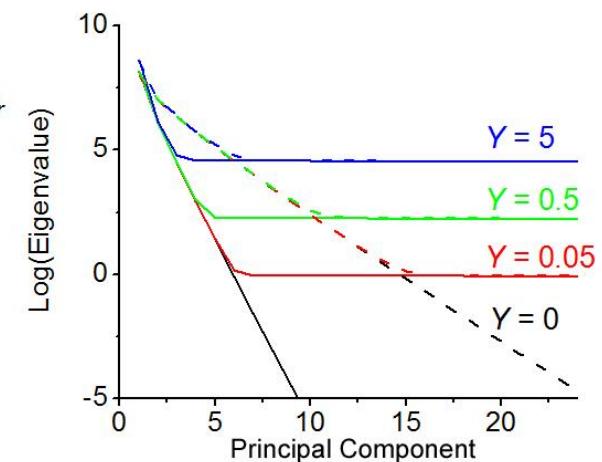
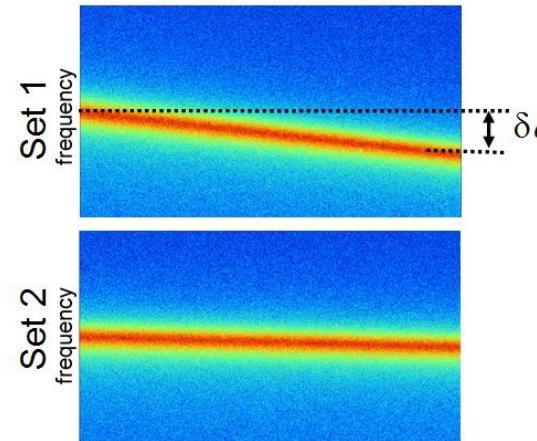


S. JESSE and S.V. KALININ, *Principal component and spatial correlation analysis of spectroscopic imaging data in scanning probe microscopy*, Nanotechnology **20**, 085714 (2009).

When does PCA match physics?

Simulate simple harmonic oscillator curves for different variations of resonance frequency and noise levels

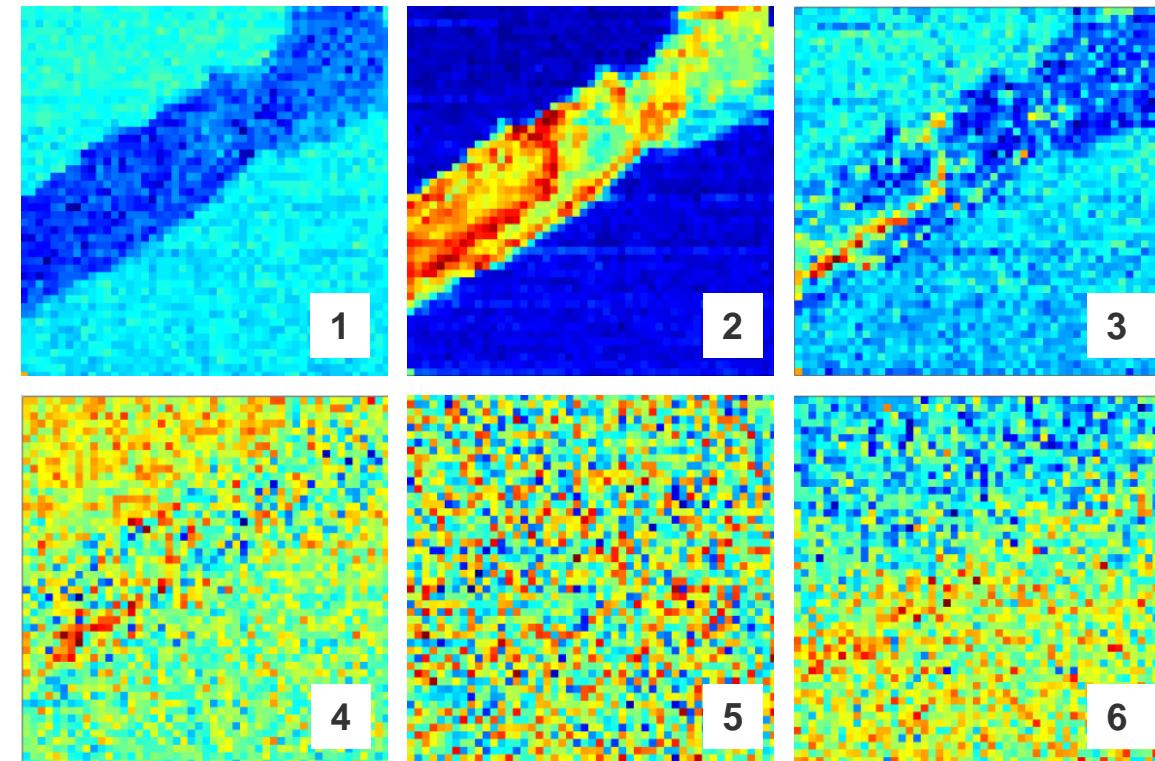
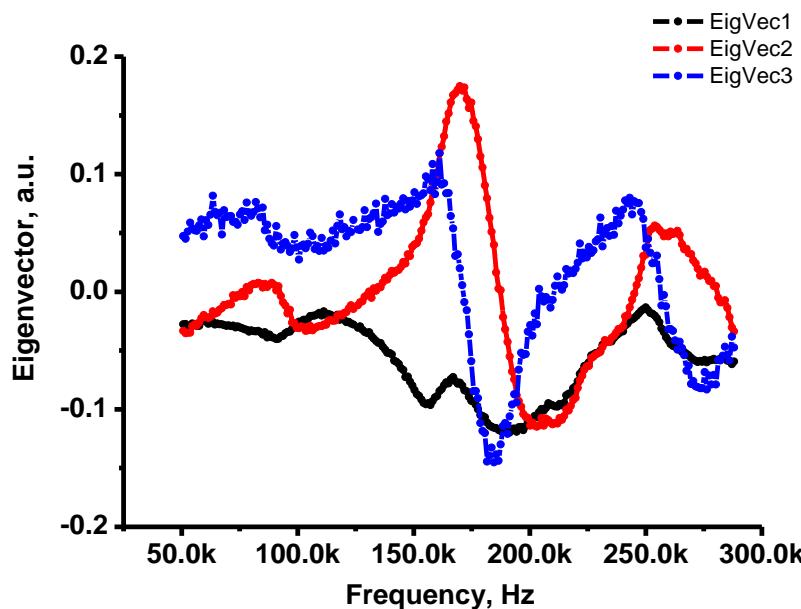
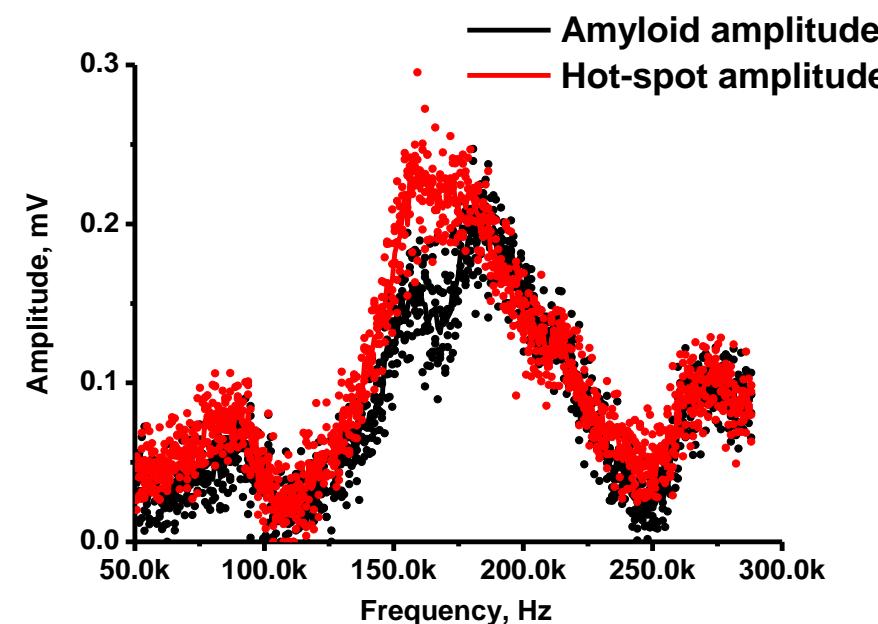
$$A(\omega) = \frac{F\omega\omega_r}{\sqrt{(\omega^2 - \omega_r^2)^2 + (\omega\omega_r/Q)^2}} + Y(\omega)$$



There is similarity between variational derivatives of SHO responses and PCA eigenvectors

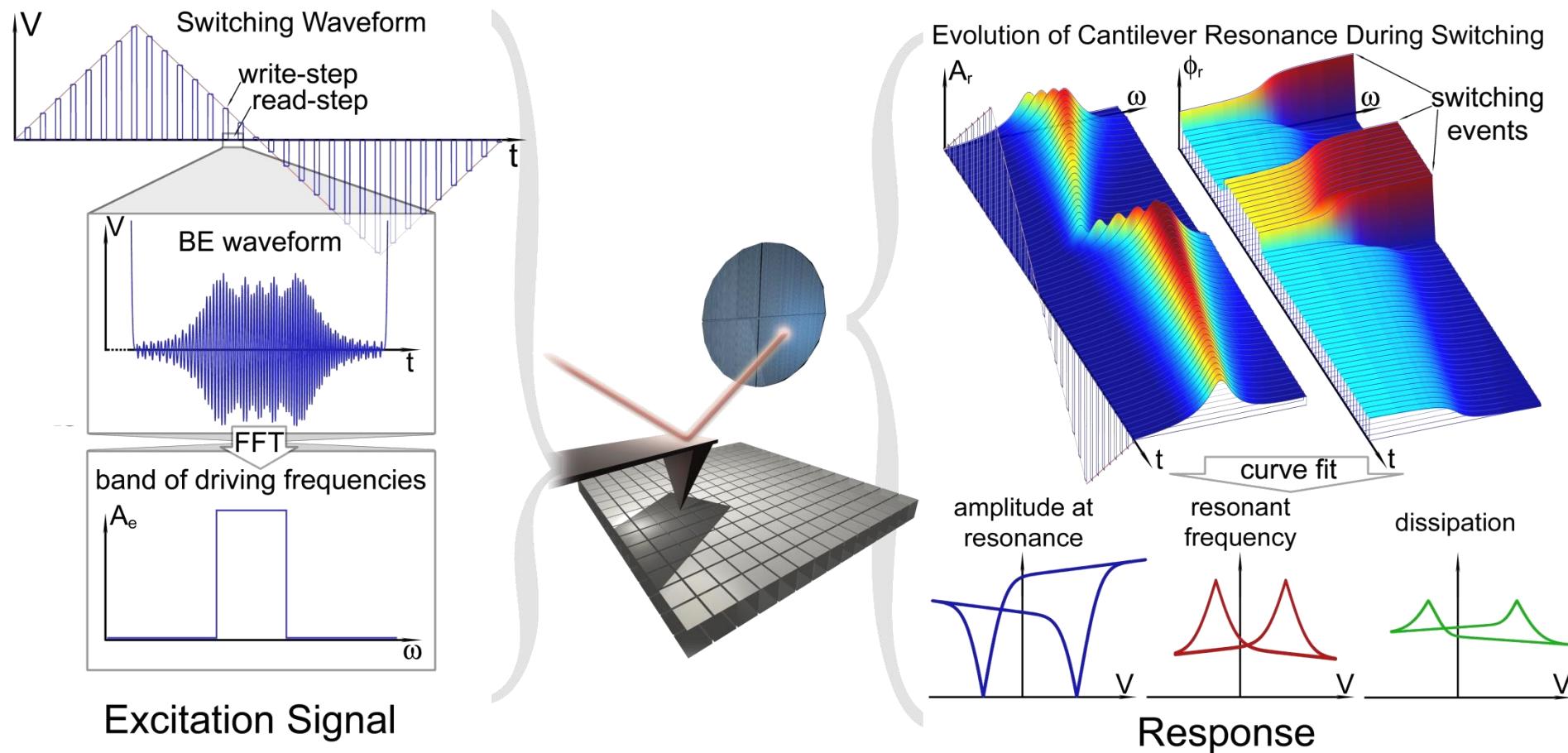
$$\delta A_i(\omega) = \frac{\partial A(\omega)}{\partial F} \delta F_i + \frac{\partial A(\omega)}{\partial \omega_r} \delta \omega_{r,i} + \frac{\partial A(\omega)}{\partial Q} \delta Q_i + Y(\omega)$$

PFM of amyloid fiber



M.P. NIKIFOROV, G.L. THOMPSON, V.V. REUKOV, S. JESSE, S. GUO, B.J. RODRIGUEZ, K. SEAL, A.A. VERTEGEL, and S.V. KALININ, *Double-layer Mediated Electromechanical Response of Amyloid Fibrils in Liquid Environment*, ACS Nano **4**, 689 (2010).

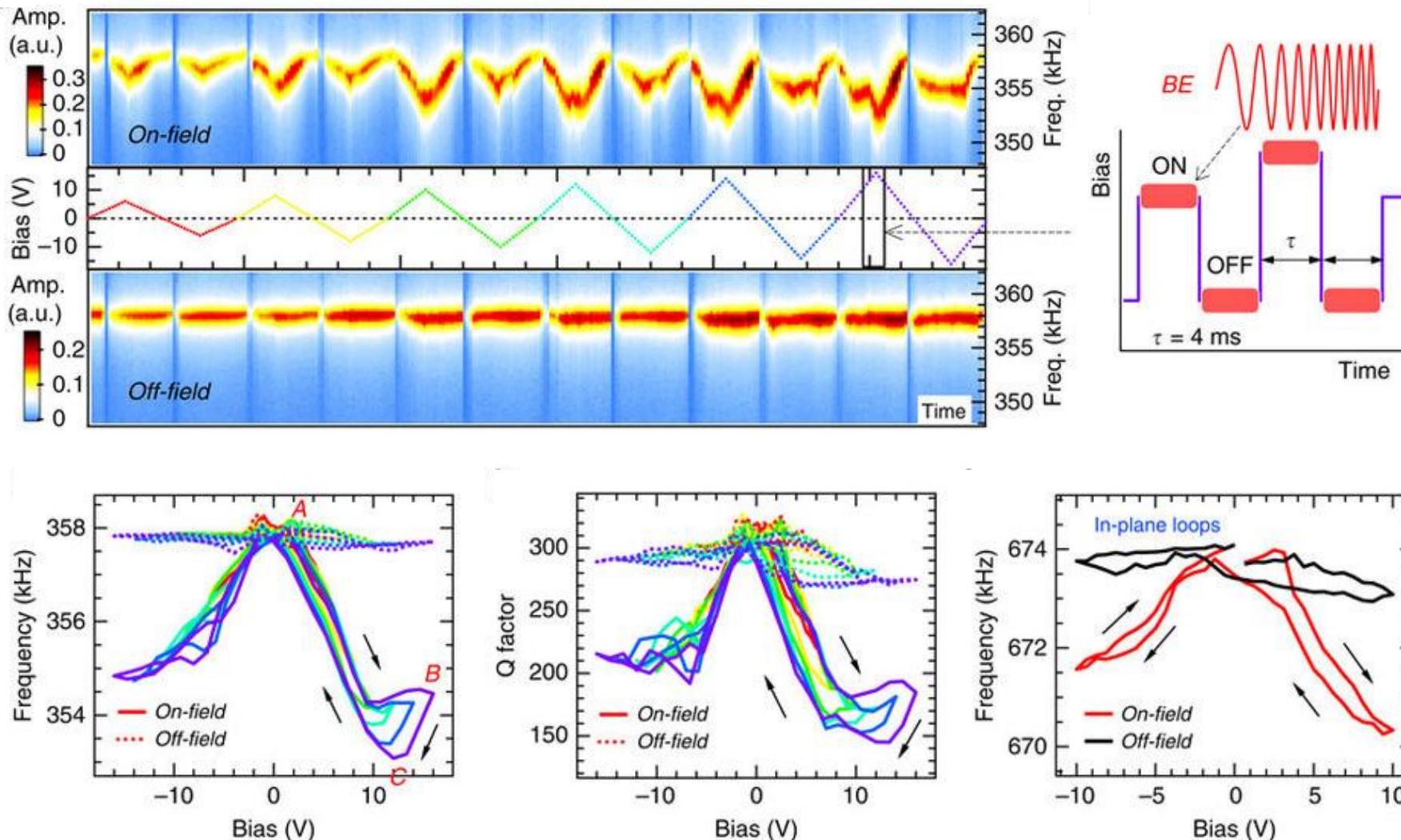
Band excitation SS-PFM (BEPS)



Typical 4D data array size: ~0.3-1 GB, Acquisition time: ~ 1 hour

Typical 5D data array size (Preisach, kinetics): ~3-30 GB, Acquisition time: ~ 12 hours

5D PFM: First order reversal curves

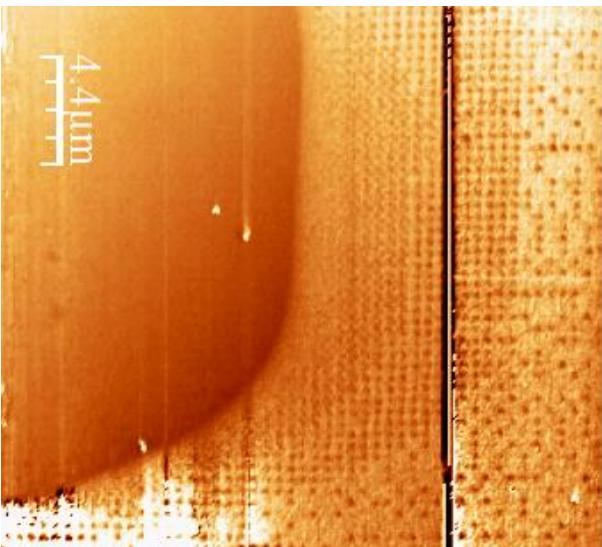


In BFO, changes in elastic properties is found *during* field application (not remnant).

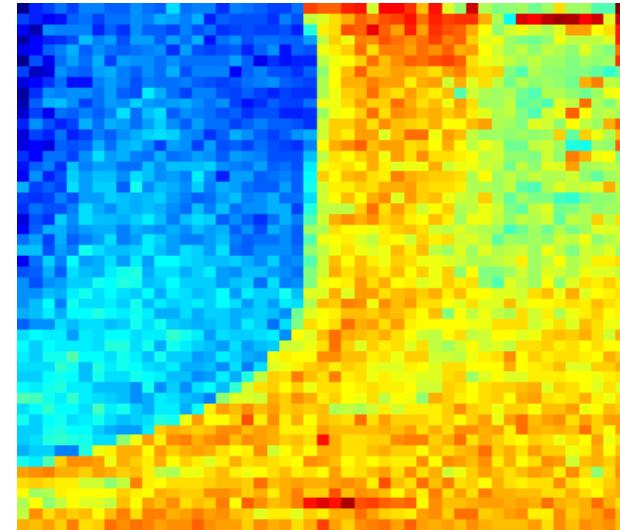
FORC BE PFM in H-exchanged LiNbO₃

Data by
A. Kumar

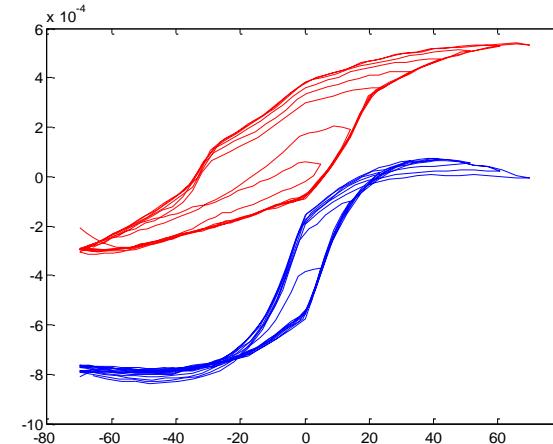
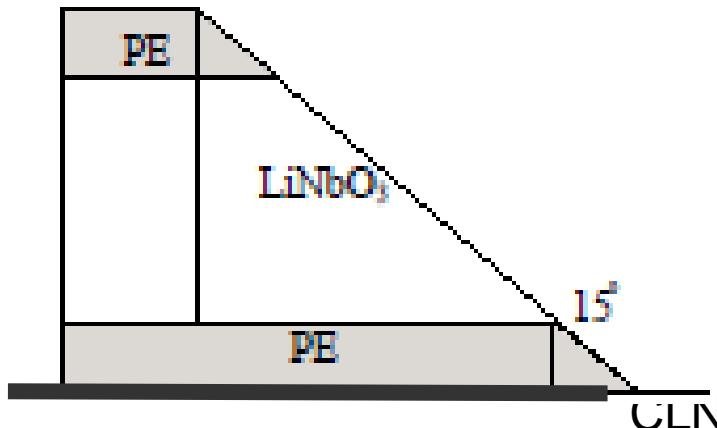
PFM after measurements



Hysteresis loop area map



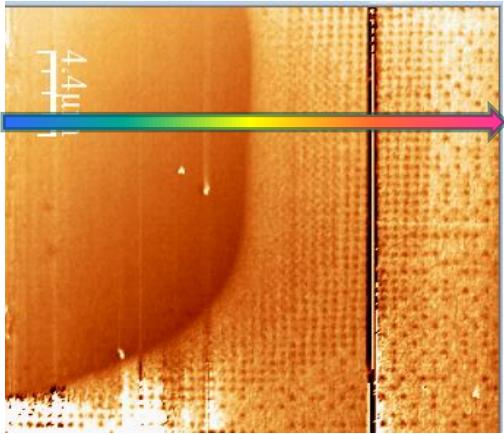
FORC loops from selected locations



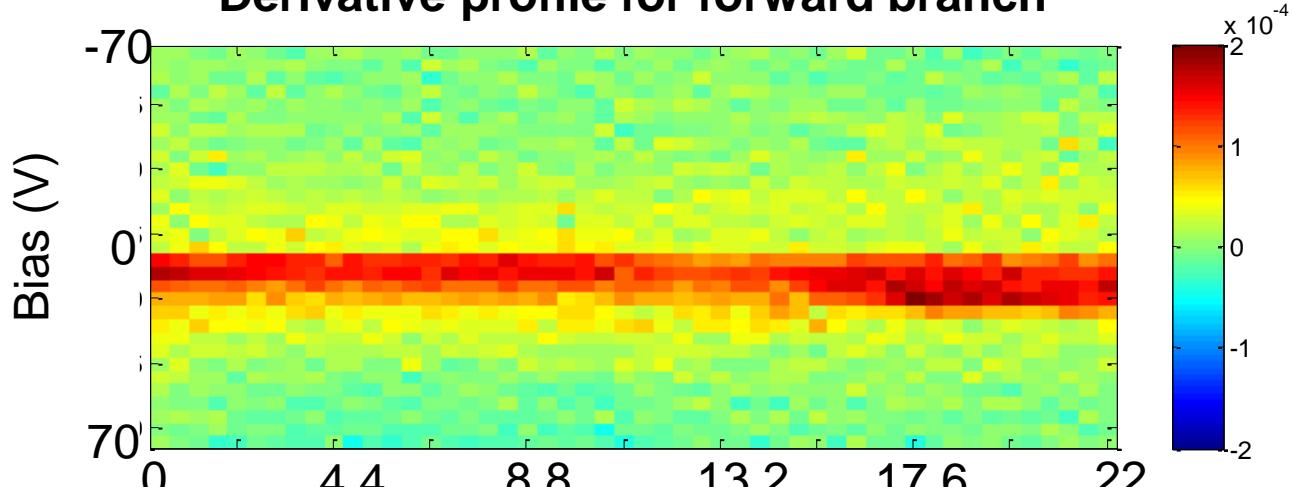
Strong variability of switching behavior and spectra from H-LNO to LNO

Spatial evolution of switching

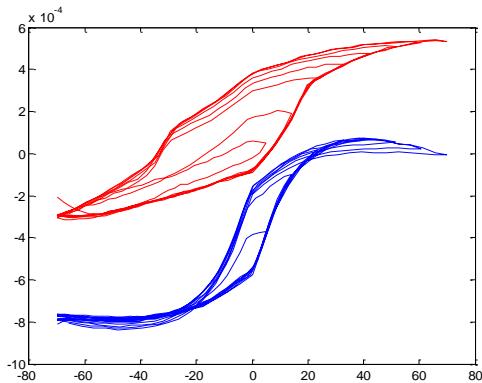
PFM after measurements



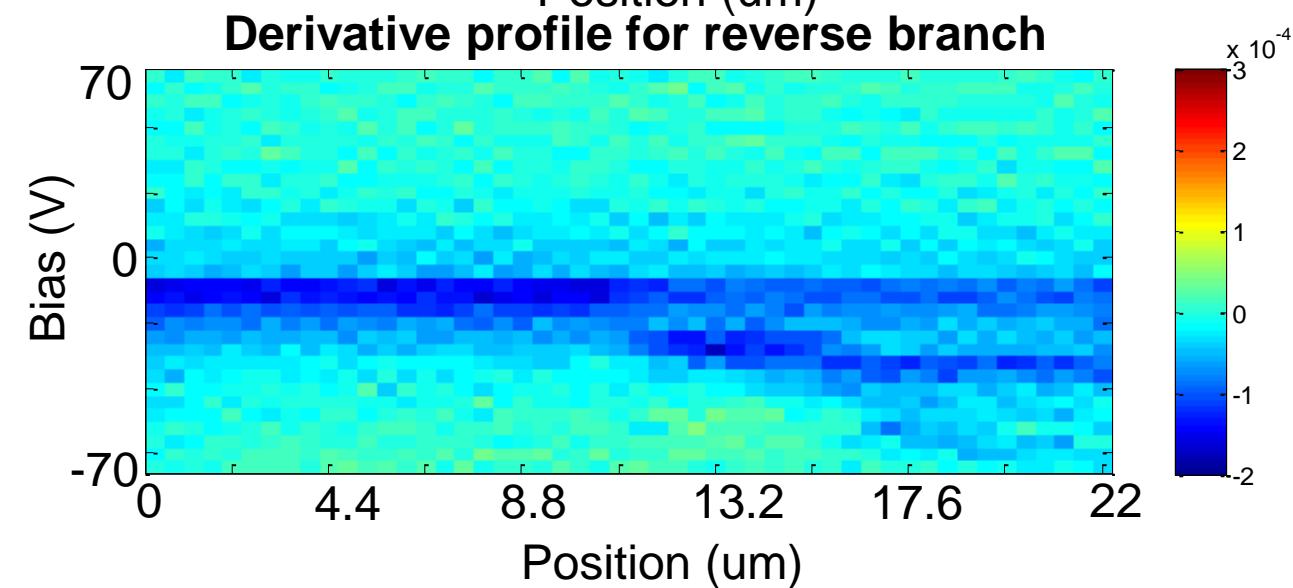
Derivative profile for forward branch



FORC loops

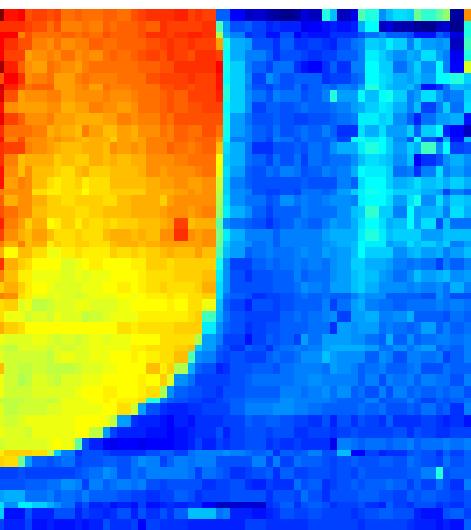


Derivative profile for reverse branch

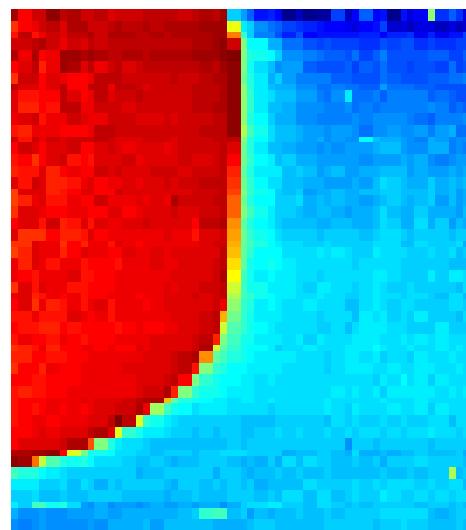


Principal component analysis

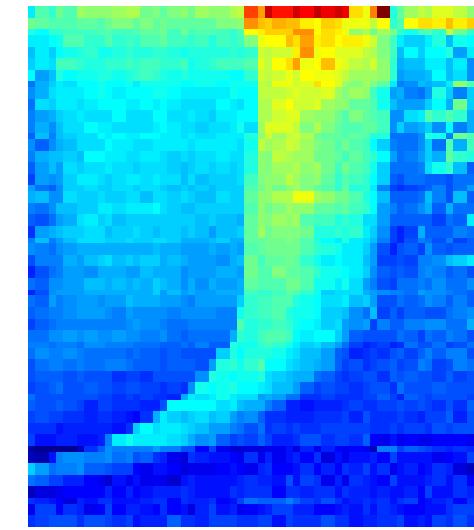
1st Component



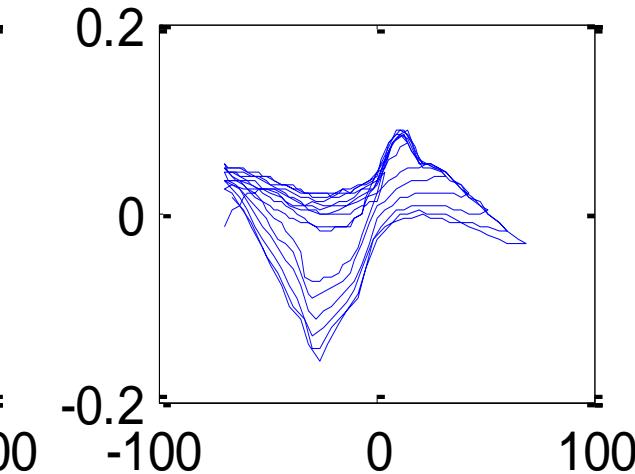
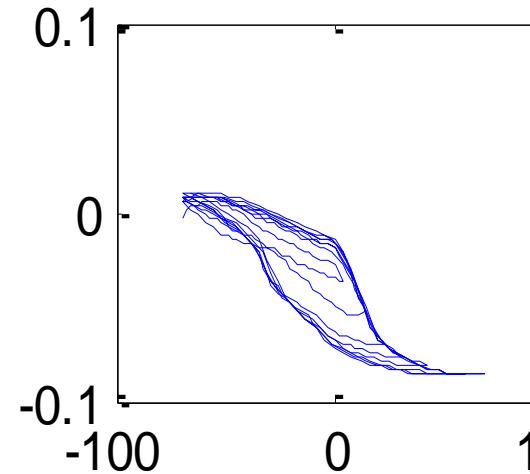
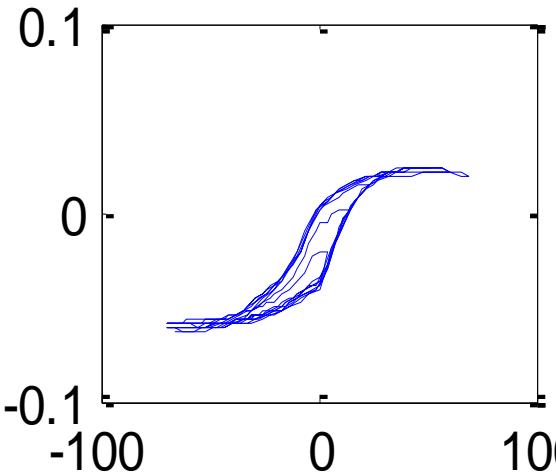
2nd Component



3^d Component

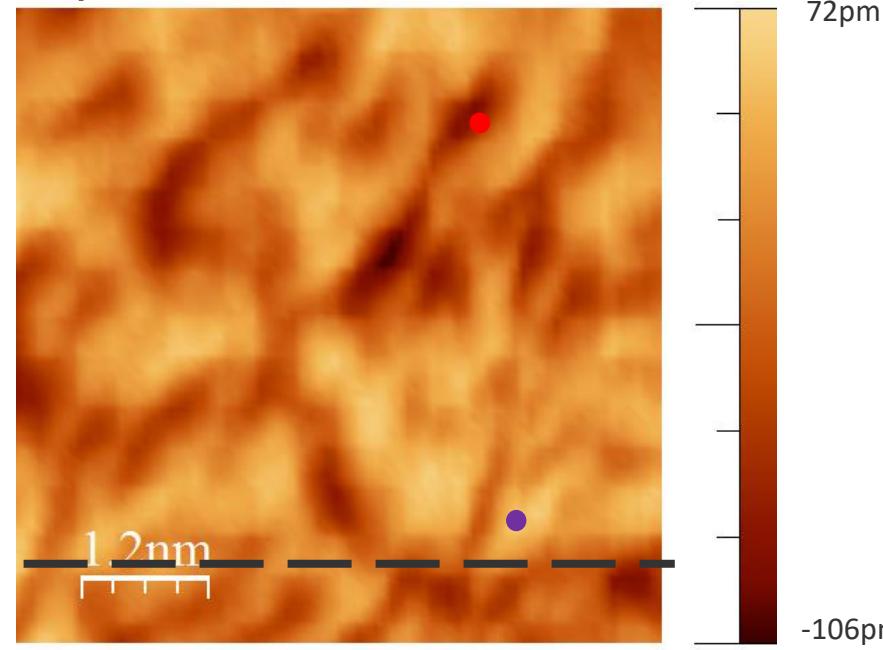
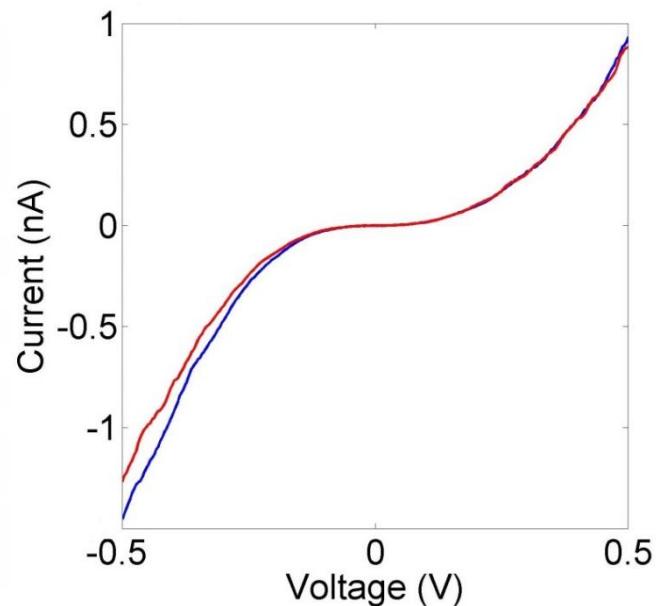
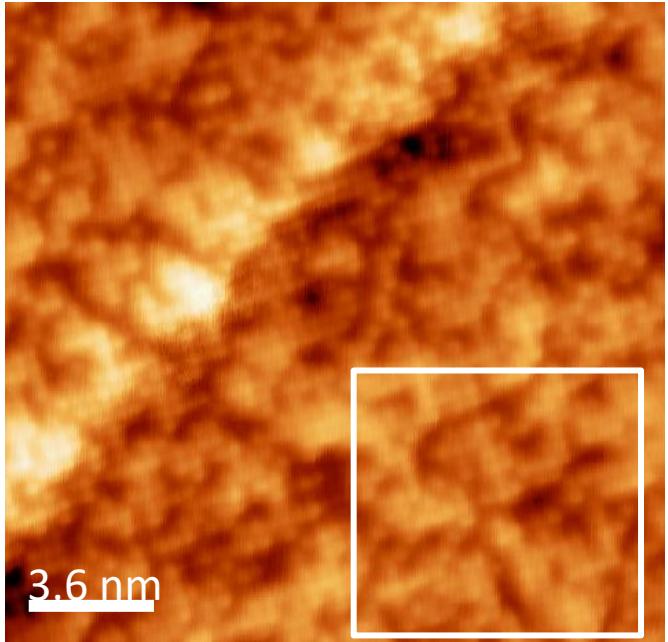


Data by
A. Kumar

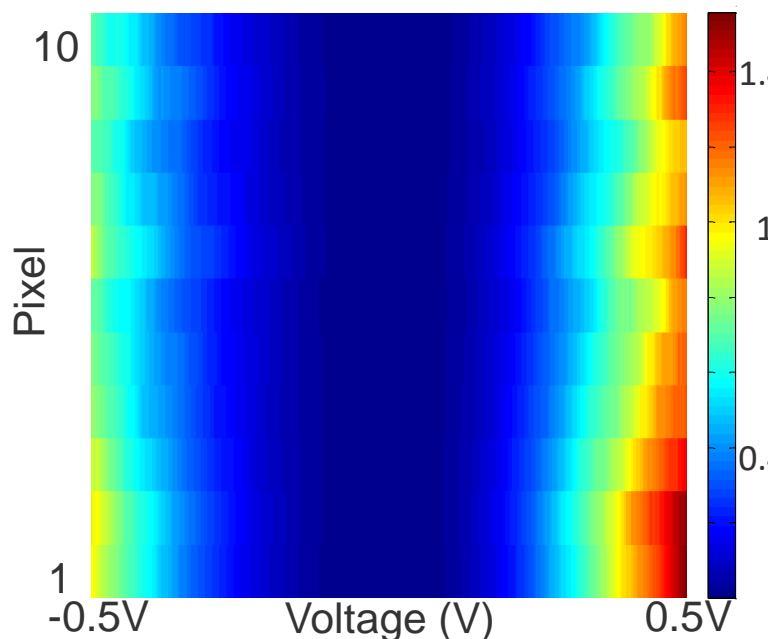


- Loops shape is clearly a superposition of a small number of significant component
- The regions with dissimilar behavior are now correlated to microstructure

Grain boundary by STM



Topographical STM of FeSeTe, $T = 82\text{K}$ $15 \times 15\text{nm}^2$, 50mV, 100pA, white rectangle represents area where CITS was performed; (b) CITS 80×80 pixel graphical average of the spectrographic data.



M. ZIATDINOV, A. MAKSOV,
L. LI, A. SEFAT, P.
MAKSYMOVYCH, and S.V.
KALININ, *Deep data mining in
a real space: Separation of
intertwined electronic
responses in a lightly-doped
BaFe₂As₂*, Nanotechnology
27, 475706 (2016).

Eigenvectors and loadings

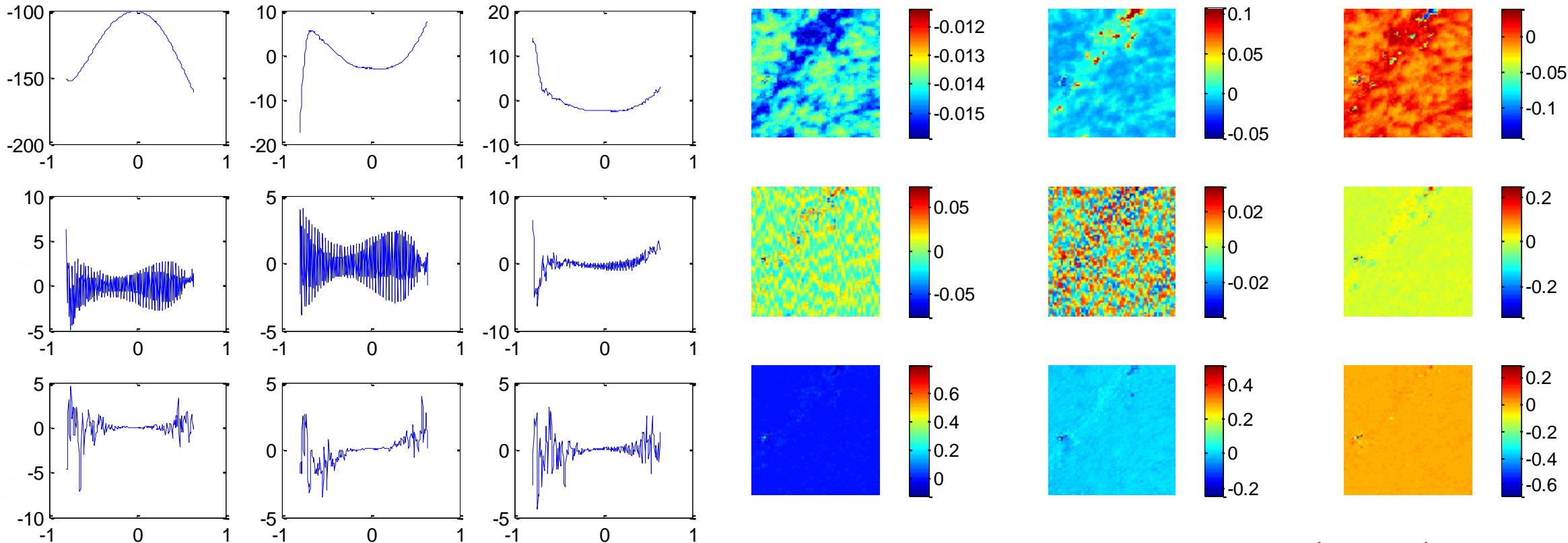


Figure by A. Belianinov

Scree plot and correlations

- Semi log plot indicating the “weight” of each component as a function of all components
- Only the first few components contain useful info, while others are dominated by noise

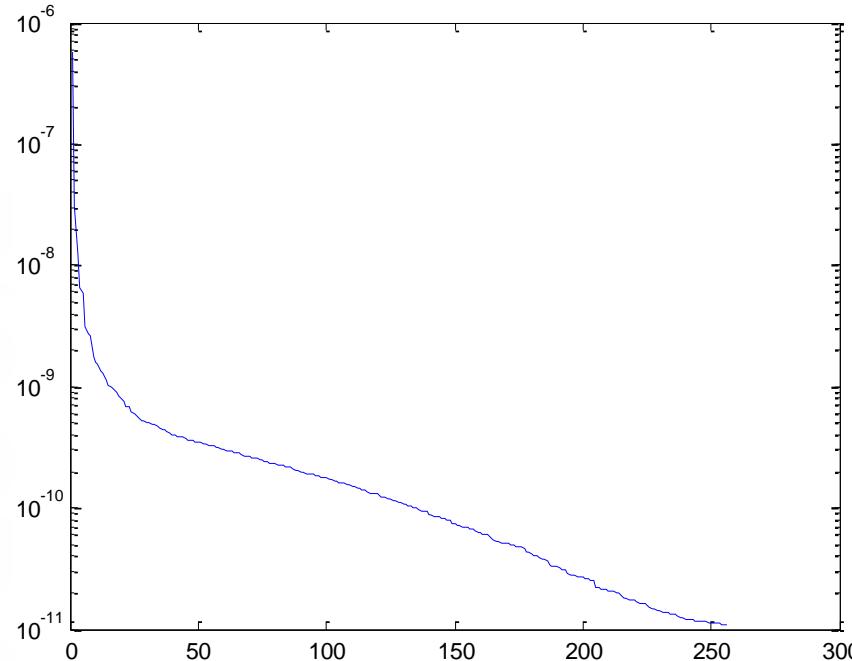
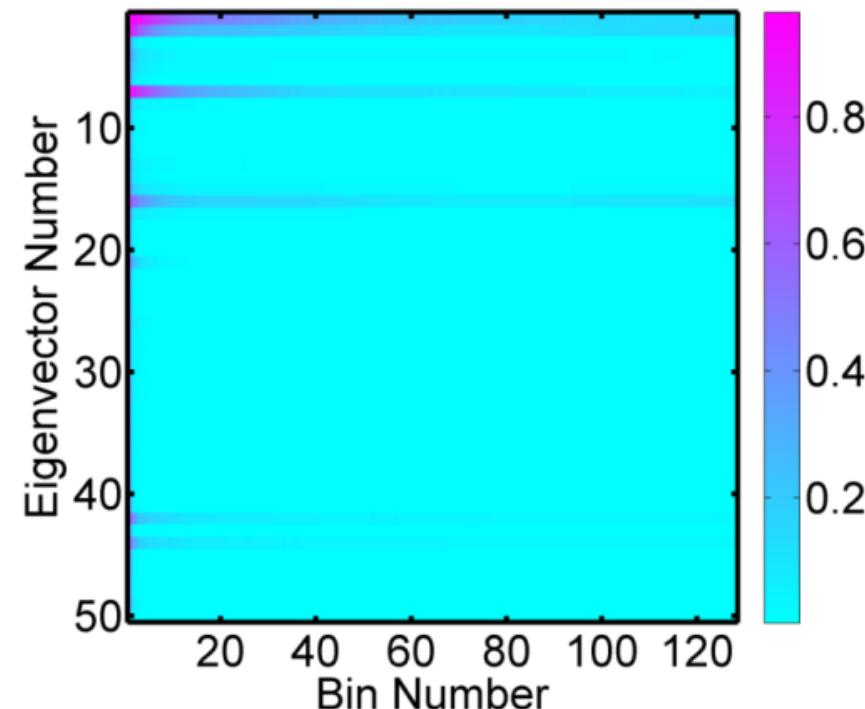


Figure by A. Belianinov

- We can also analyze correlations in images

For AFM data

PCA Eigenvectors



Spatial correlations

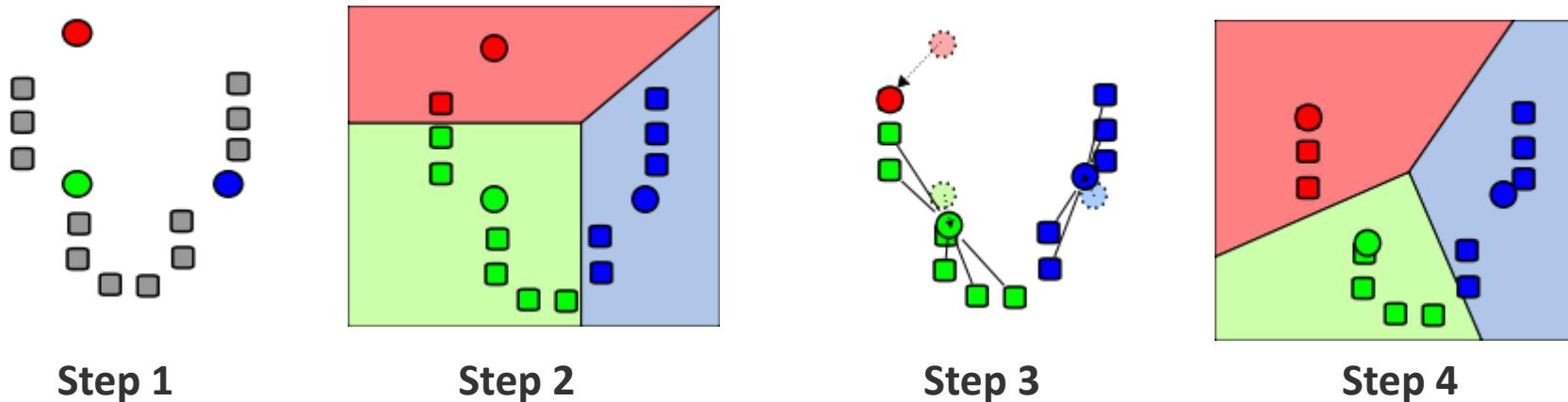
K-mean clustering

- PCA is decomposition. But sometimes, we don't want to decompose our signal, but just group them in 'alike' sets.
- This is termed 'clustering'. The easiest and most widely used method is the k-means algorithm

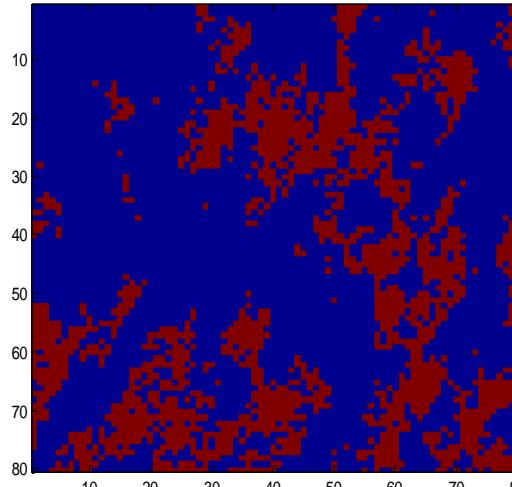
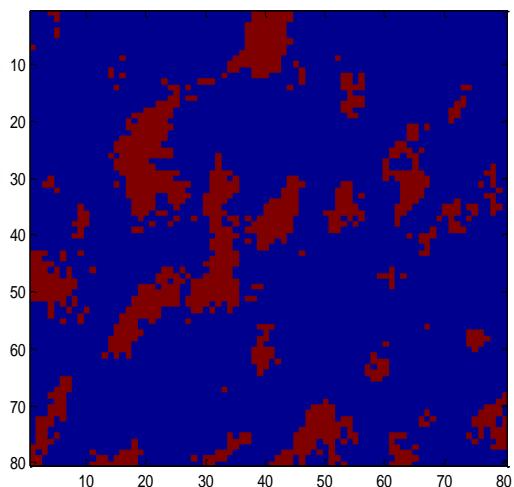
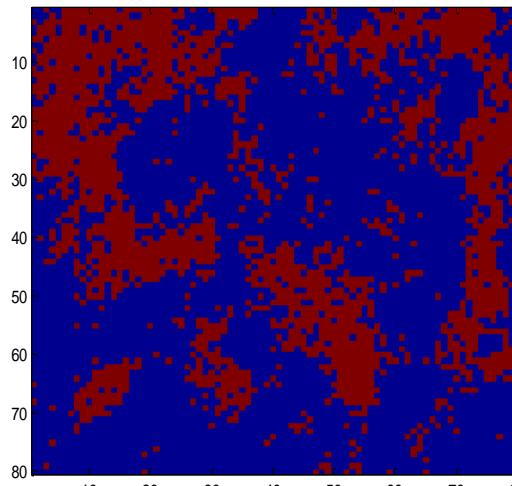
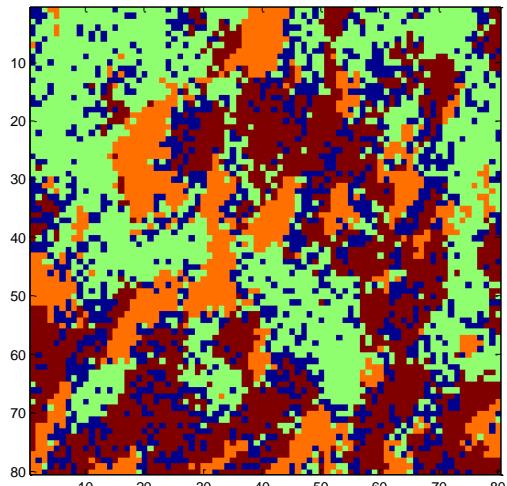
K-means Clustering algorithm, to separate data (x_1, x_2, \dots, x_n) into k clusters

$$\arg \min_s \sum_{i=1}^k \sum_{x \in S_i} \|x - \mu_i\|^2 \quad \text{where } \mu_i \text{ is the mean of points in } S_i$$

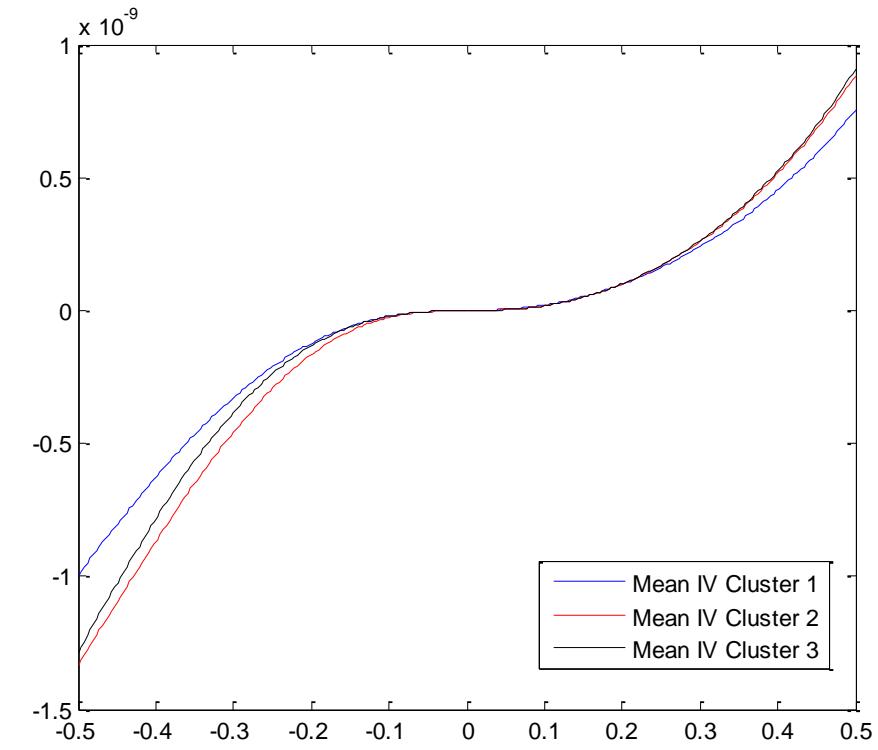
(Determine $S = \{S_1, S_2, \dots, S_k\}$, such that within cluster sum of squares is minimized)



K-means clustering



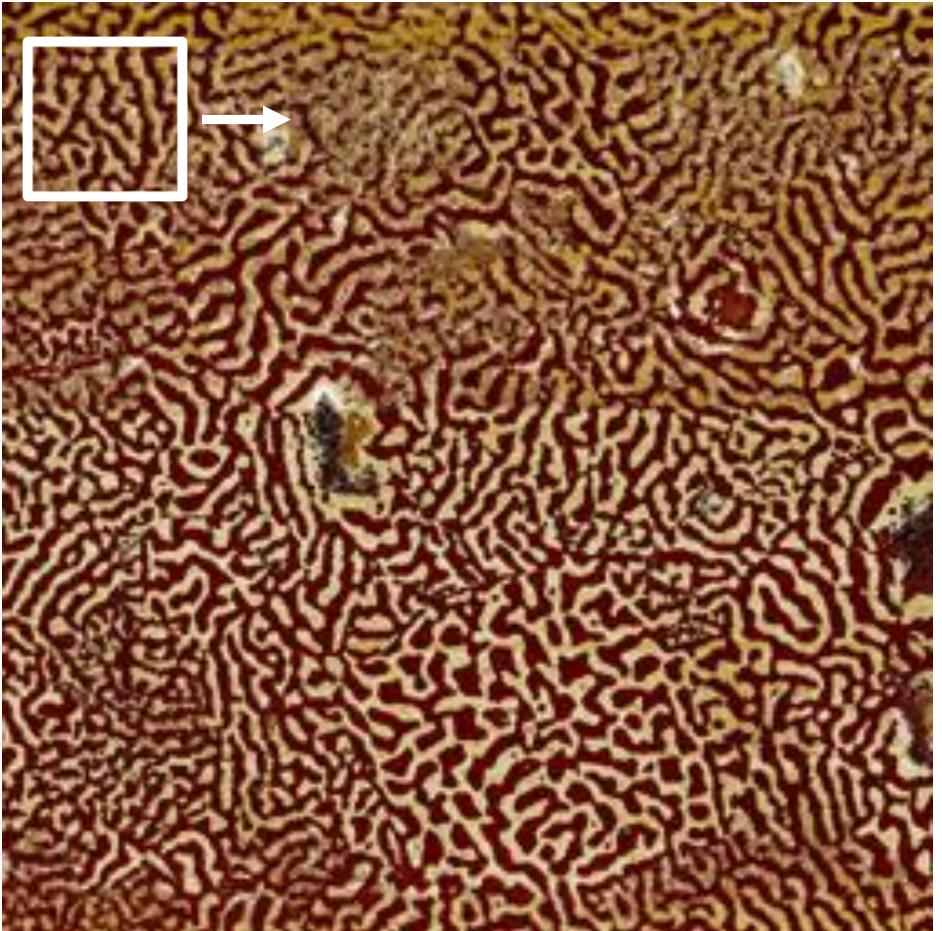
K-means result of the CITS map broken into three distinct clusters: CITS map of all three clusters combined vs. individual cluster distribution in the map



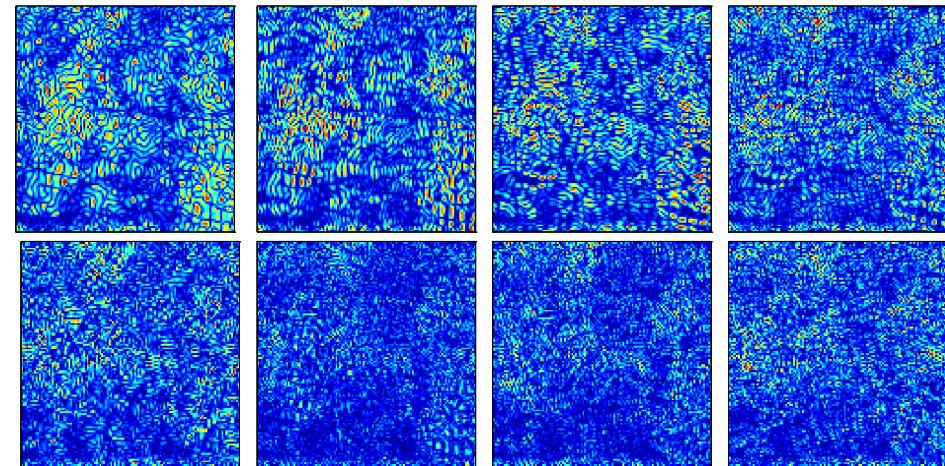
M. ZIATDINOV, A. MAKSOV, L. LI, A. SEFAT, P. MAKSYMOVYCH, and S.V. KALININ, *Deep data mining in a real space: Separation of intertwined electronic responses in a lightly-doped BaFe₂As₂*, Nanotechnology **27**, 475706 (2016).

Sliding PCA-FFT

Can we use PCA of FFT transform in sliding windows to find periodicity?



First 8 maps



First 16 eigenvectors

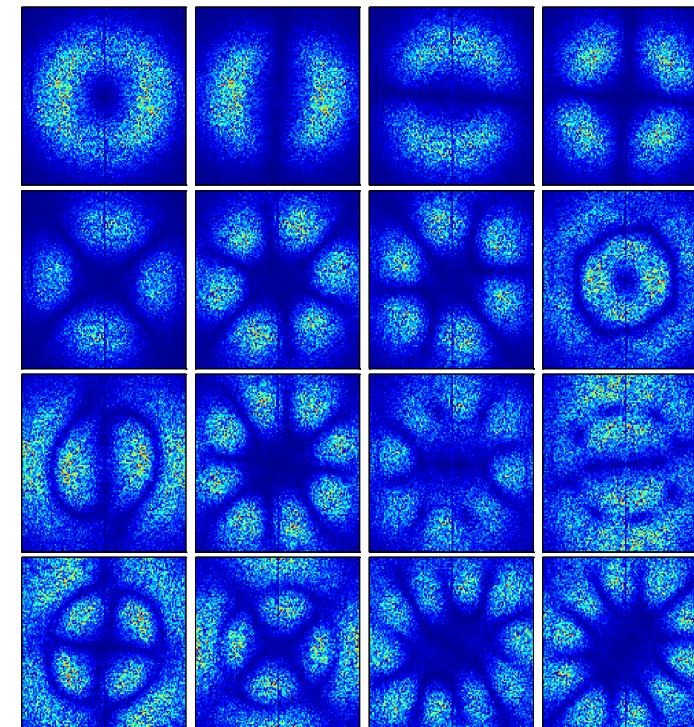


Figure by S. Jesse, data D. Gobelic

Independent Component Analysis

- **PCA:** orthogonal transformation of possibly correlated variable into a set of linearly uncorrelated variables
 - Analyzes data representing observations described by dependent variables which are inter-correlated
 - Main goal is to find true variables assuming that corrupting noise is Gaussian
- **ICA”** method for separating multivariate signal into additive subcomponents assuming statistical independence of source signals
 - Finds components that are maximally independent and non-Gaussian
 - Blind source separation – cocktail party problem

Compared to PCA, ICA can produce statistically independent non-Gaussian components by decorrelating the higher-order moments in addition to the first- and second-order moments of the statistical distribution

Mathematics of ICA

The Goal is to transform observed data into maximally independent components measured through some function $F(s_1, \dots, s_n)$ of independence.

- Data as a set of vectors $\longrightarrow x = (x_1, \dots, x_m)^T$
 - Components of the data $\longrightarrow s = (s_1, \dots, s_n)^T$.
- $$s = Wx$$

An observed data vector x can then be represented as a sum of independent components s weighted by some mixing weight a :

$$x_i = a_{i,1}s_1 + \dots + a_{i,k}s_k + \dots + a_{i,n}s_n$$

or

$$x = \sum_{k=1}^n s_k a_k$$

In other words, our data vector x is represented by basis vectors $a_k = (a_{1,k}, \dots, a_{m,k})^T$ that can form columns of a mixing matrix such that: $x = As$

Mathematics of ICA - 2

$$x = As$$

Given that our data is set of vectors x , we want to find both, the mixing matrix A and sources s

This can be done by calculating w vectors and a cost function that can maximize the Non-Gaussianity, or minimize mutual information of

$$s_k = (w^T * x)$$

Original sources can then be recovered by multiplying observed data vectors x with the inverse of the mixing matrix:

$$W = A^{-1}$$

- Not as easy to utilize as PCA, but excellent premade algorithms are readily available:

Aapo Hyvärinen – FastICA*

RIKEN developed – ICALAB Toolbox

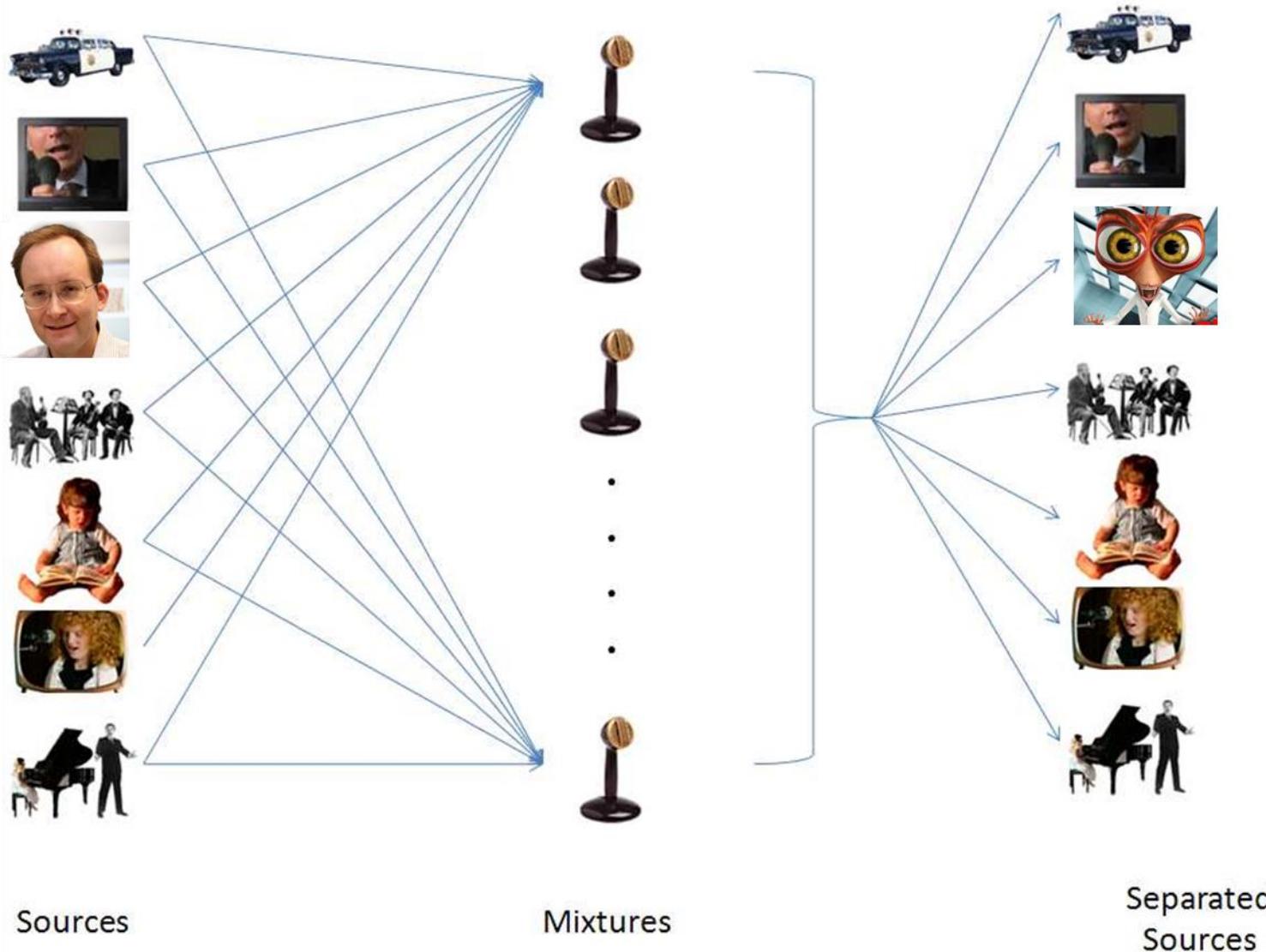
Bell-Sejnowski, Molgedey-Schuster – ICA Toolbox

http://cis.legacy.ics.tkk.fi/aapo/papers/IJCNN99_tutorialweb/IJCNN99_tutorial3.html

<http://research.ics.aalto.fi/ica/fastica/>

Cocktail Party Problem

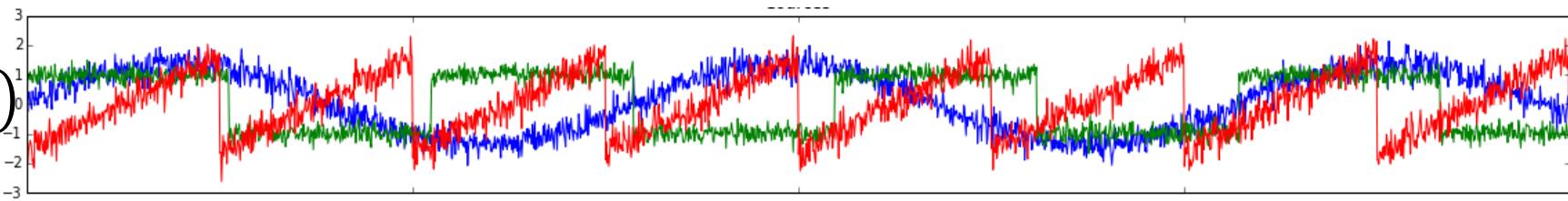
Number of signals are being produced simultaneously; with the objective of separating and following each source separately



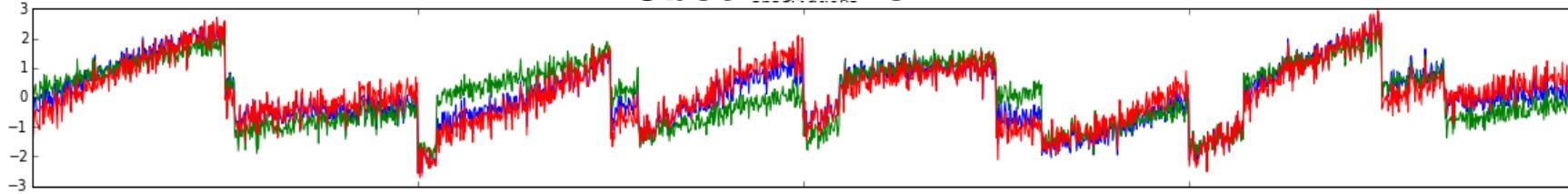
ICA Example

$$(R_1(t), R_2(t), \dots, R_n(t))$$

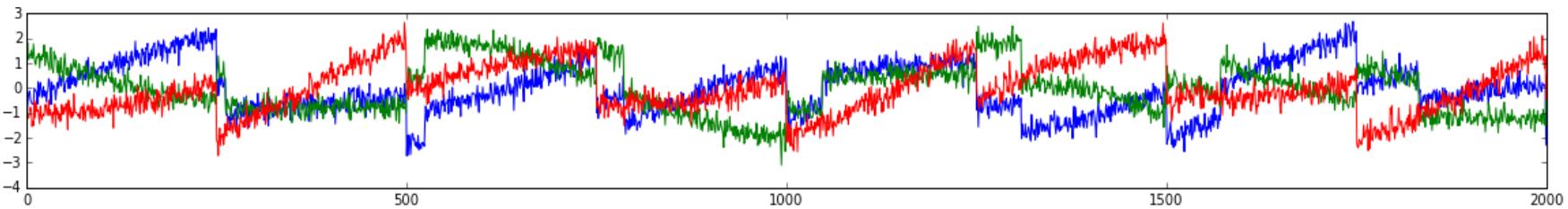
Sources



Observations



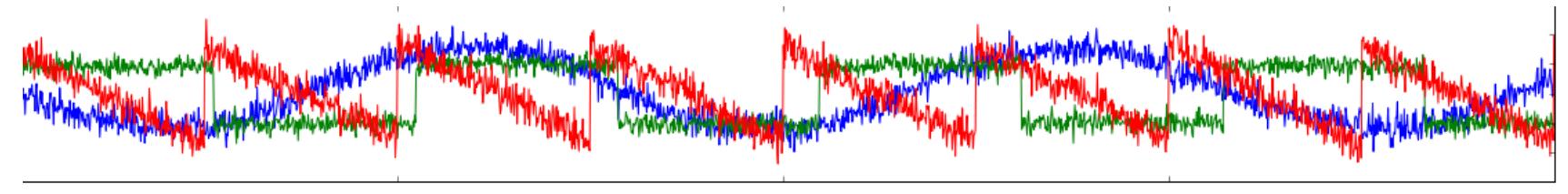
PCA Components



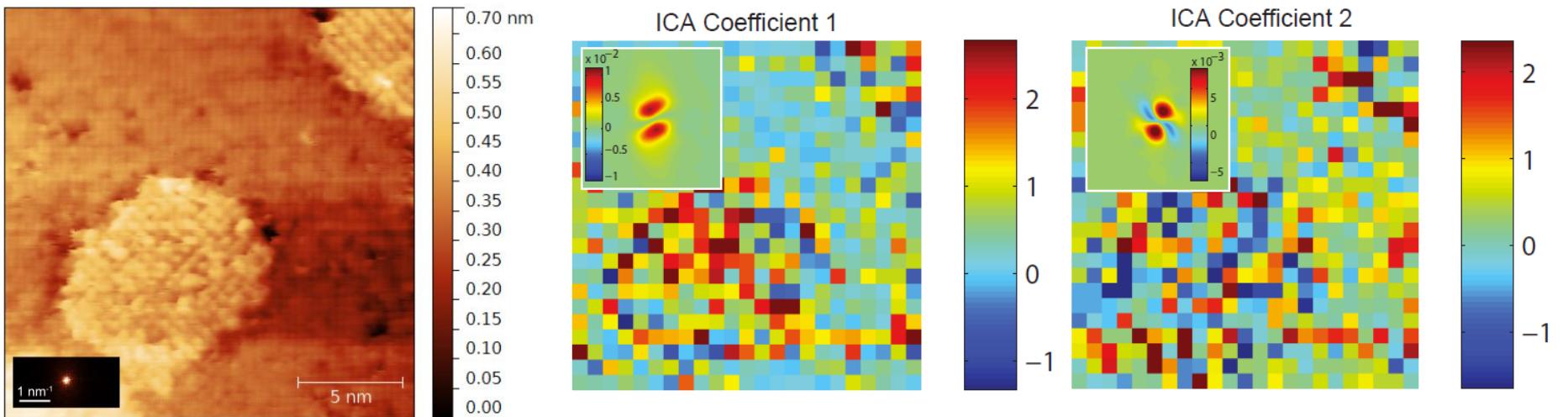
Components are
maximally independent

$$\begin{pmatrix} R_1(t) \\ \dots \\ R_n(t) \end{pmatrix} = A \begin{pmatrix} s_1(t) \\ \dots \\ s_n(t) \end{pmatrix}$$

ICA Components



ICA on Sliding FFT



- Appears to separate into pairs of components
- Unsuitable to the physics of the problem

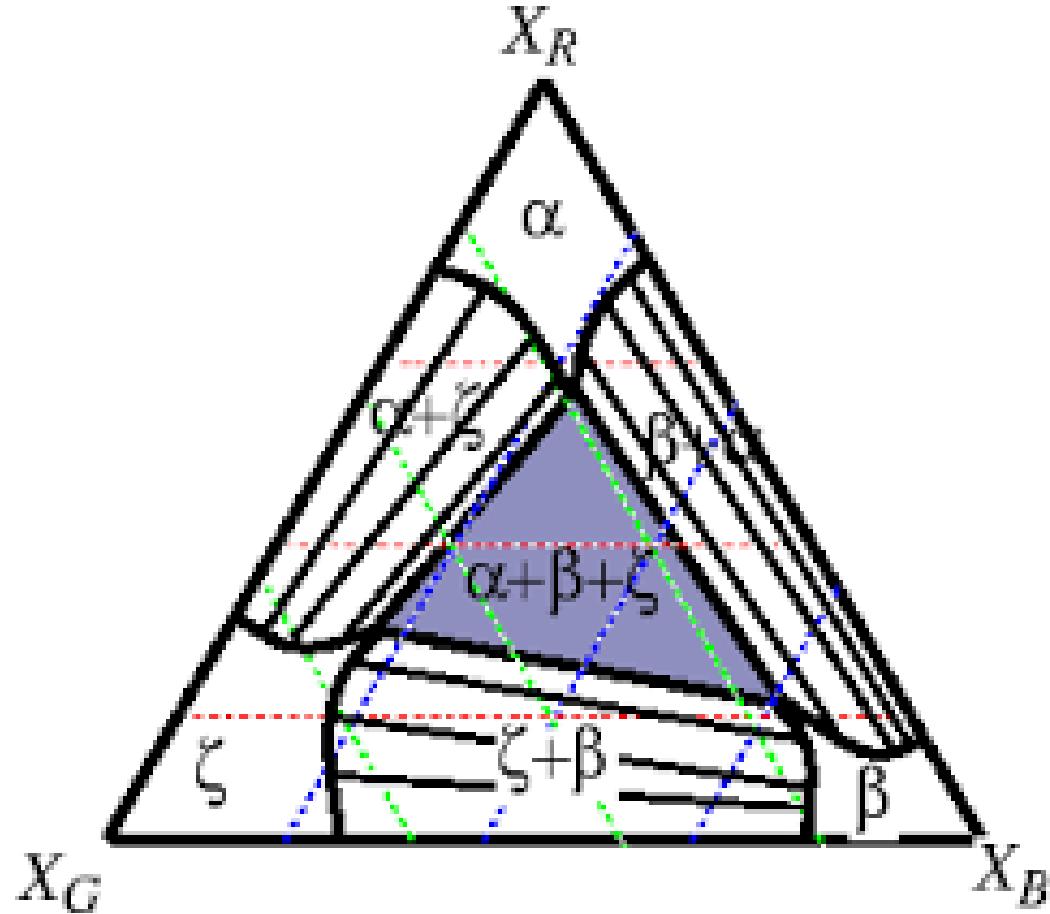
Figure by R. Vasudevan

Bayesian Linear Unmixing

$$S(\mathbf{x}, \mathbf{R}) = \sum_{i=1}^K a_i(\mathbf{x}) w_i(\mathbf{R}) + N$$

$$\sum_{i=1}^K a_i(\mathbf{x}) = 1$$

- The eigenvectors $w_i(\mathbf{R})$ are non-negative, $w_i(\mathbf{R}) \geq 0$
- The loading coefficients sum to 1
- The number of eigenvectors, K , is a priori unknown



BLU is ideally suited for certain classes of problems, e.g. conduction through parallel channels, optical or electronic spectra of mixtures, etc

Dobigeon BLU

- Dobigeon presents a Bayesian with a MCMC Gibbs sampler for estimating endmember spectra and its relative abundance in a spectral image

$$\mathbf{Y} = \mathbf{MA} + \mathbf{N}$$

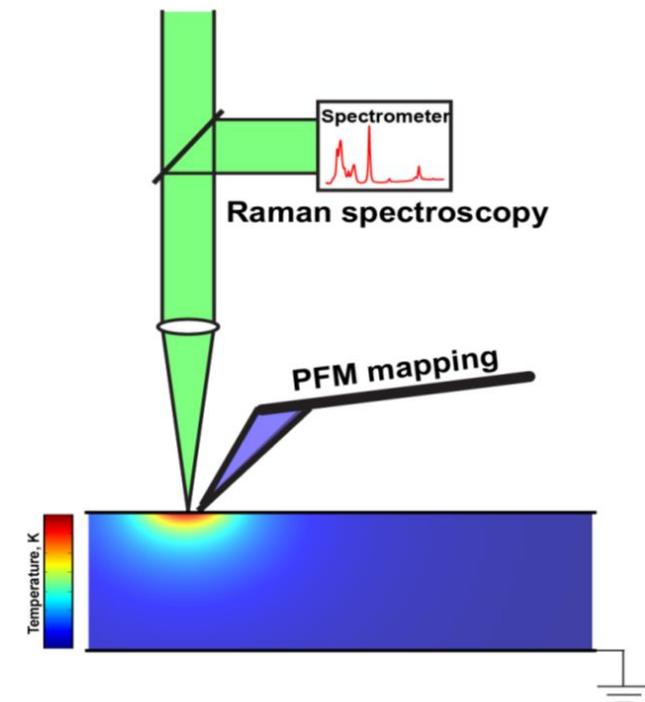
Where Y is the noisy observation comprised of endMembers with corresponding Abundances corrupted by additive Gaussian Noise

- This algorithm proposes to estimate the initial projection of endmembers in a dimensionality reduced subspace (PCA) via N-FINDR that finds simplex of maximum volume that can be inscribed within the hyperspectral data set using a simple non-linear inversion
- Endmember Abundance priors as well as Noise variance priors are chosen by a multivariate Gaussian distribution (this is a nontrivial assumption that rests in computational implementation)
- Posterior Distribution is calculated based on endmember independence using Markov Chain Monte Carlo that generates asymptotically distributed samples probed by Gibbs sampling strategy

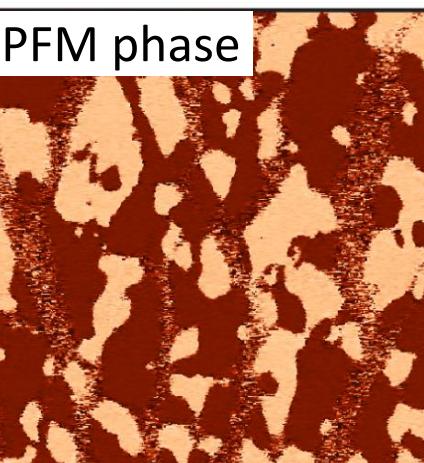
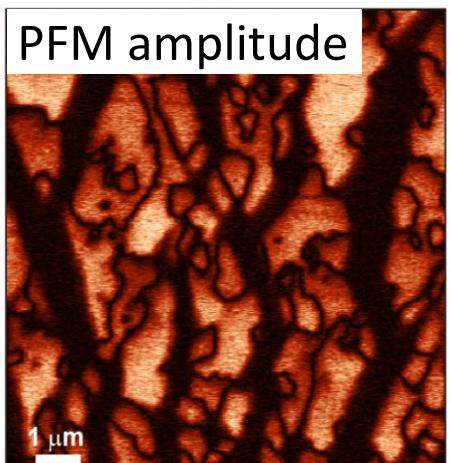
Laser heating induced phase transitions

- Copper indium thiophosphate ($\text{Cu}_{0.77}\text{In}_{1.12}\text{P}_2\text{S}_6$) layered ferroelectric
 - Ferroelectric state at room temperature
 - Curie temperature $T_c = 320$ K
 - Non-polar $\text{In}_{4/3}\text{P}_2\text{S}_6$ inclusions
- Combined Atomic Force Microscopy (AFM) and confocal Raman spectroscopy investigative approach
 - AFM – topography measurements
 - Piezoresponse force microscopy (PFM) – static ferroelectric domain structure
 - Raman – crystallographic structure via Raman spectra

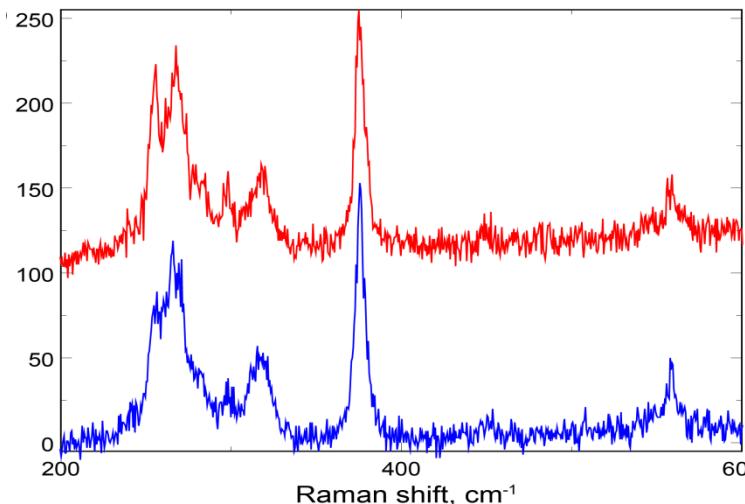
Experimental scheme



Ferroelectric domain structure



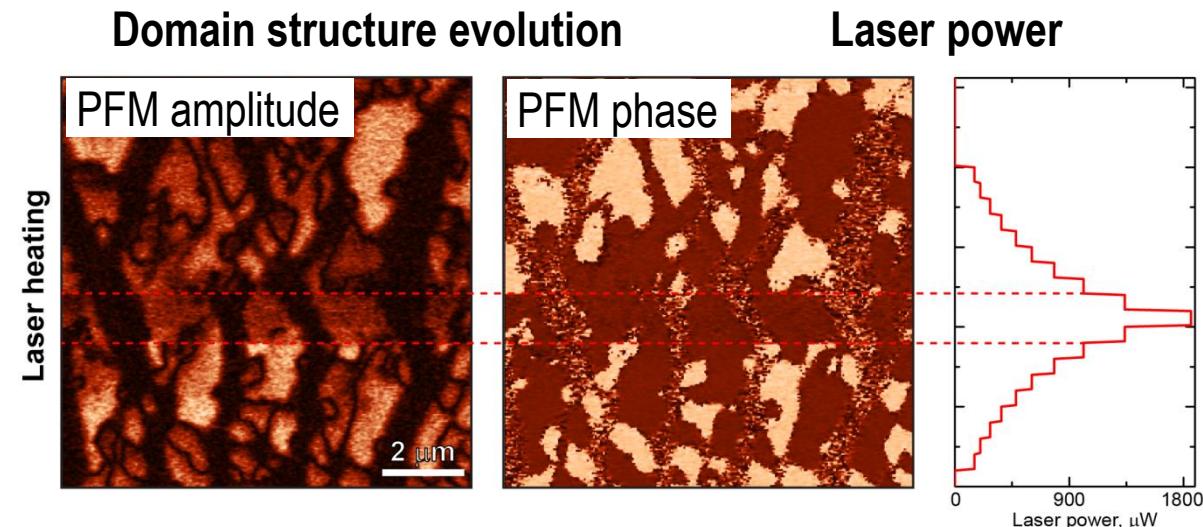
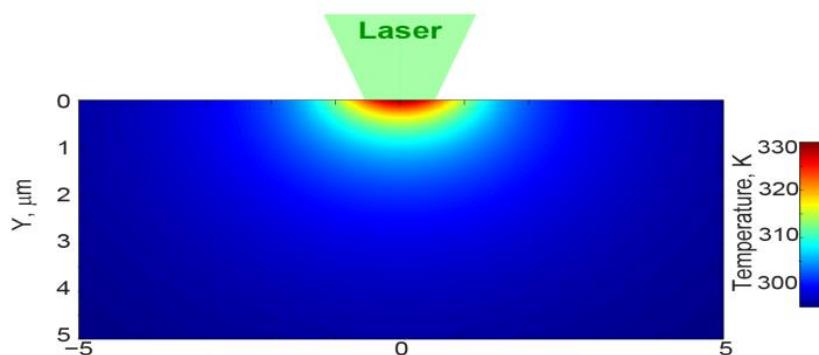
Single point Raman spectra



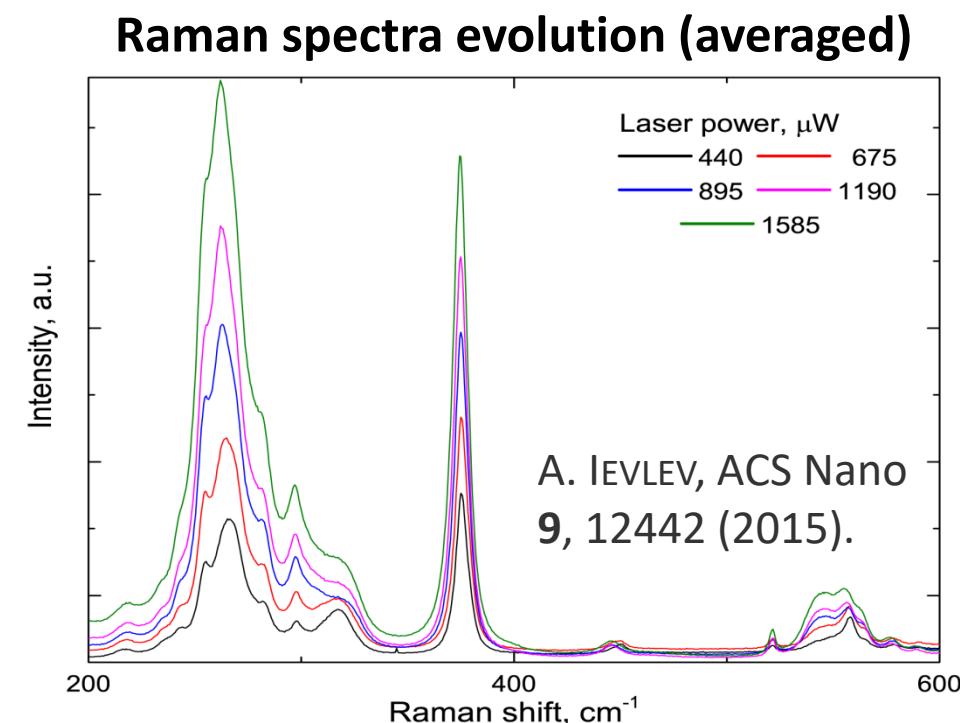
A. ILEV, ACS Nano
9, 12442 (2015).

Laser heating induced phase transition

Laser can be used for local heating to induce ferroelectric- paraelectric phase transition

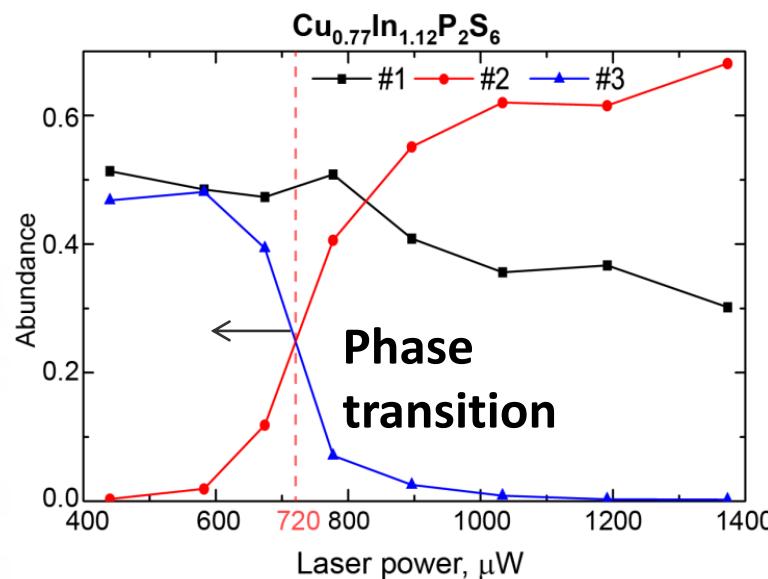


- Measurements with variation of the laser power
 - PFM – *in-situ* change in the domain structure above T_c
 - Raman – evolution of the Raman spectra through the phase transition
- Comprehensive analysis of Raman spectra is complicated by inhomogeneous chemical composition and high noise level
- Bayesian Linear Unmixing can be used for automated identification of spectra evolution



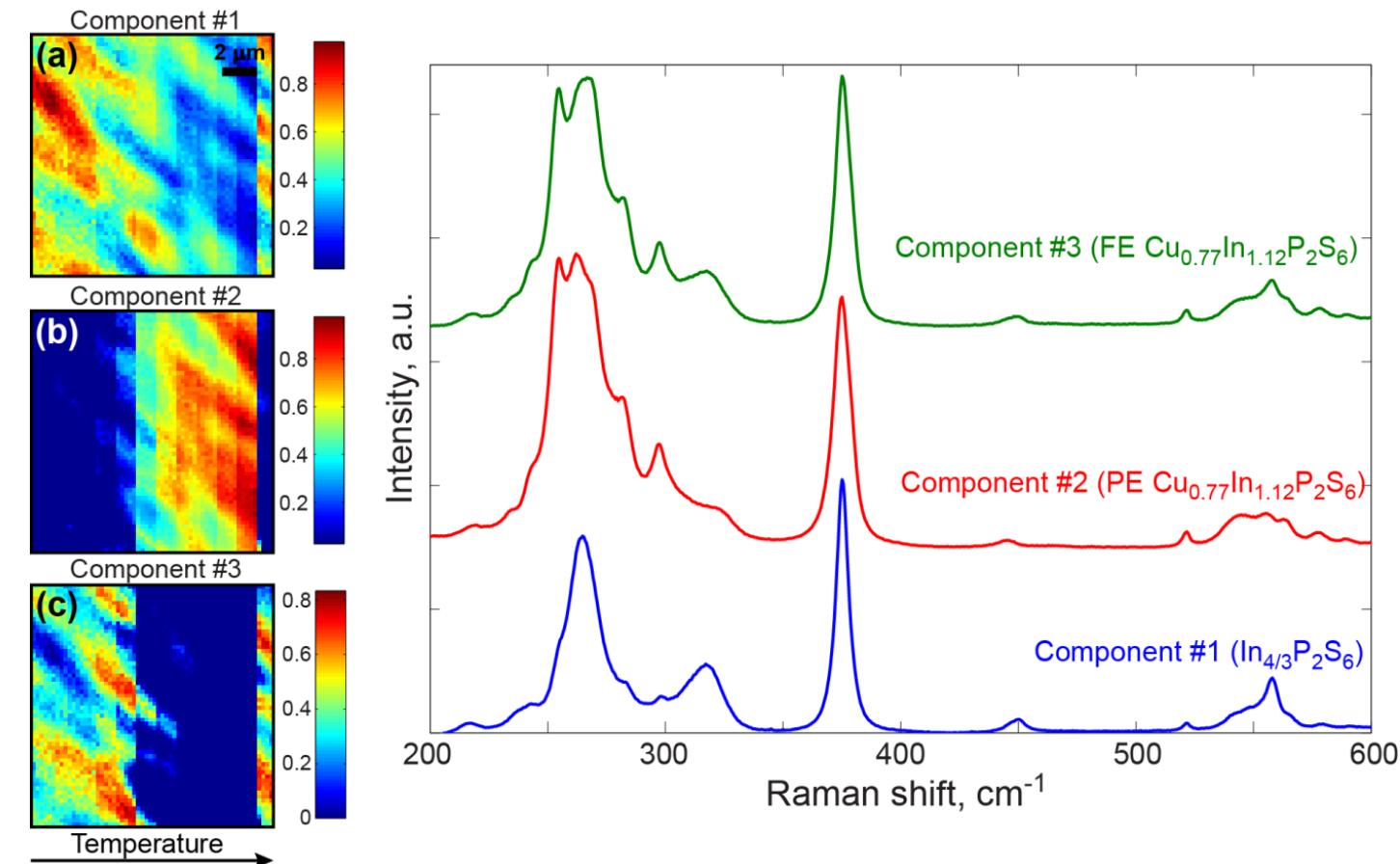
BLU separation of components

Spatial concentration of components



A. Ievlev, ACS Nano 9, 12442 (2015).

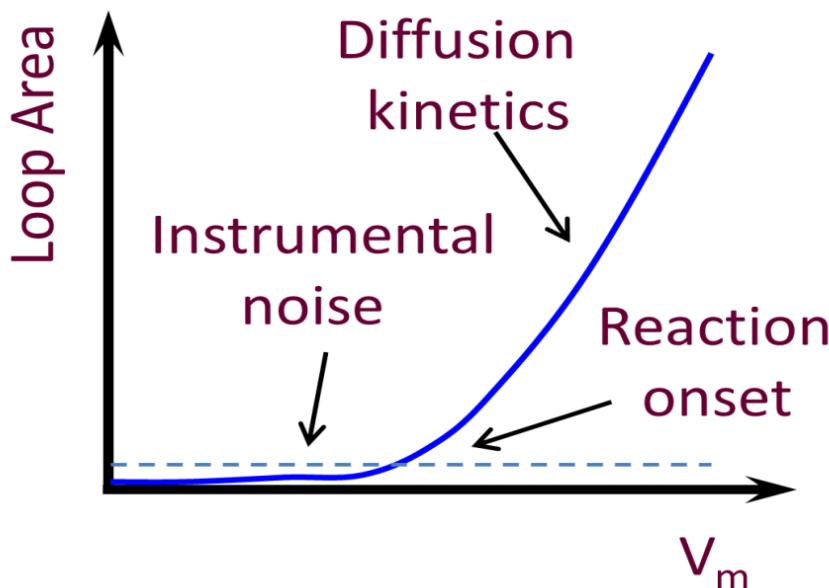
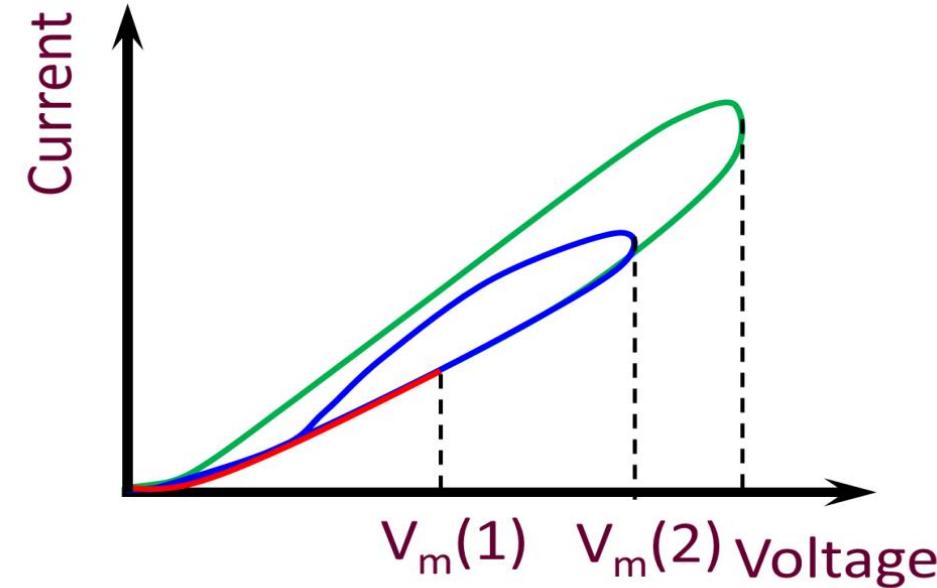
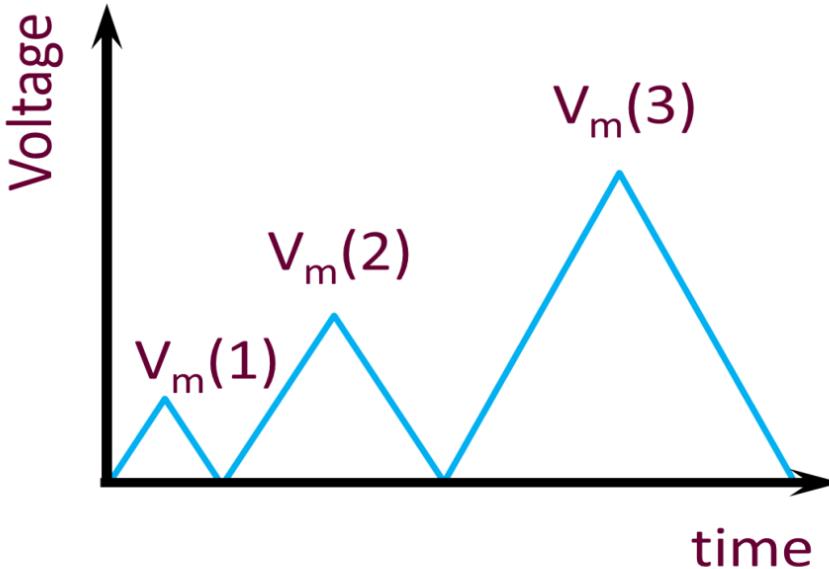
Results of BLU: components and loading maps



Unmixing showed presence of three independent components (contributions into Raman spectra):

1. Non-polar In_{4/3}P₂S₆ – weak changes in intensity with temperature
2. Paraelectric CuInP₂S₆ above T_c – appears at higher laser powers
3. Ferroelectric CuInP₂S₆ below T_c – disappears at higher temperatures

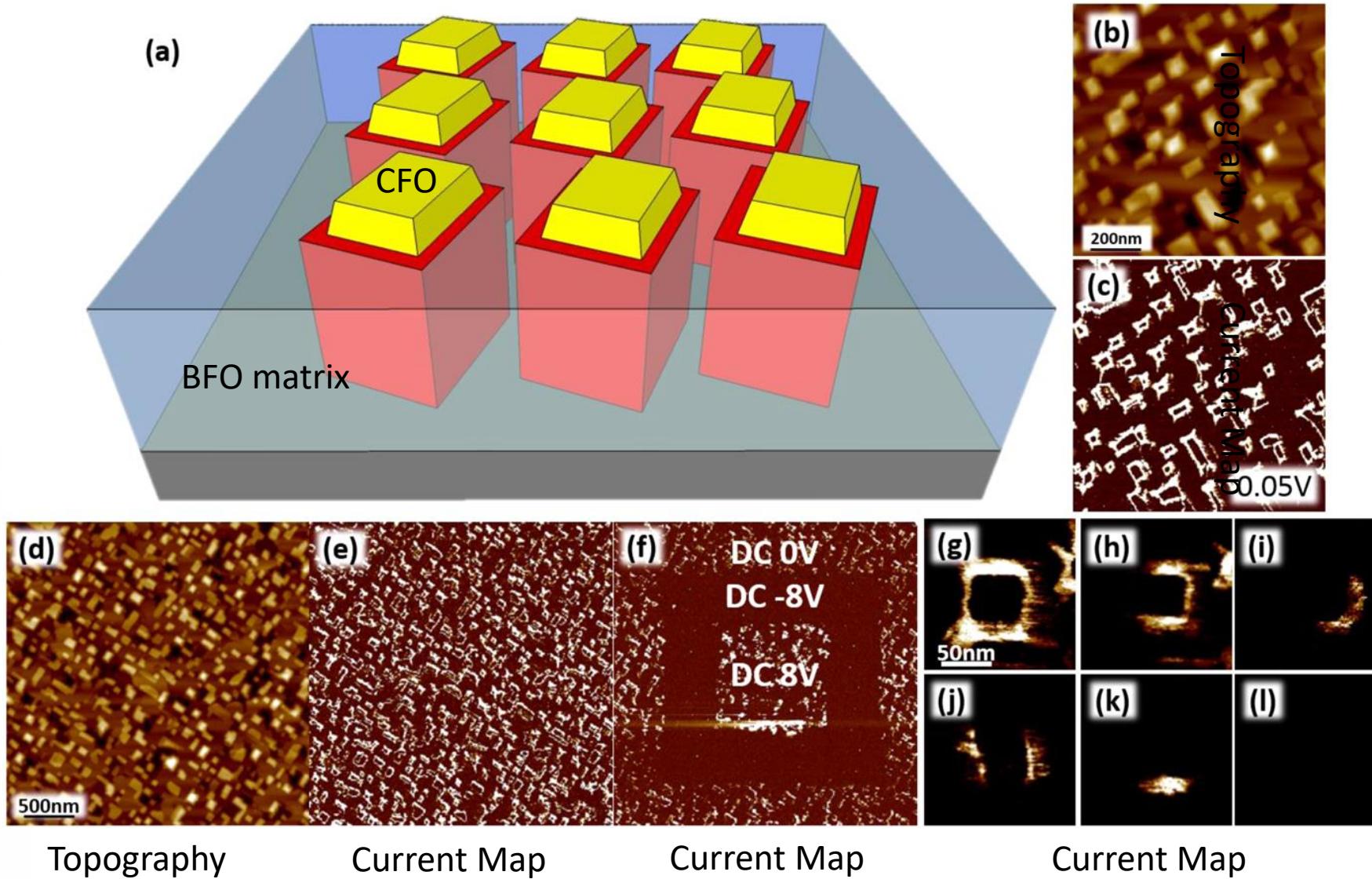
First order reversal curve IV measurements



- First order reversal curves in IV measurements
- Opening of hysteresis loops indicates onset of slow-bias-induced changes
- These can be explored as a function of rate and bias

Conductance in nanotubular structures

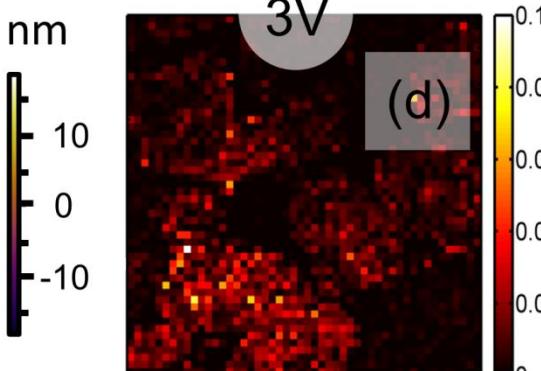
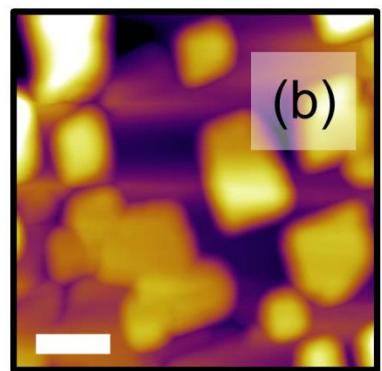
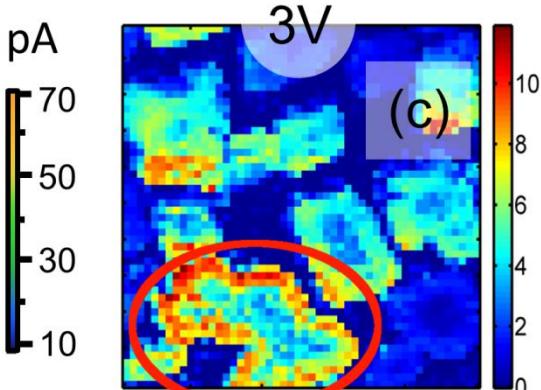
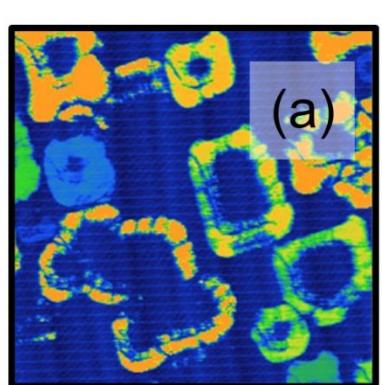
Probing electrochemistry through electronic degrees of freedom



Y.H. HSIEH, E. STRELCOV, J.M. LIOU, C.Y. SHEN, Y.C. CHEN, S.V. KALININ, and Y.H. CHU, *Electrical Modulation of the Local Conduction at Oxide Tubular Interfaces*, ACS Nano 7, 8627 (2013).

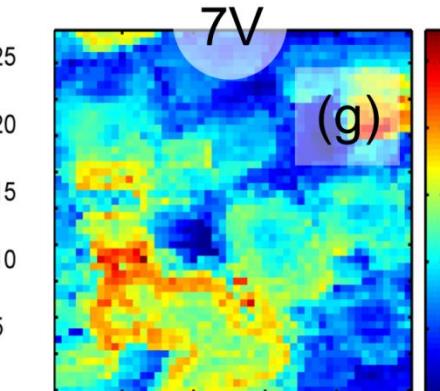
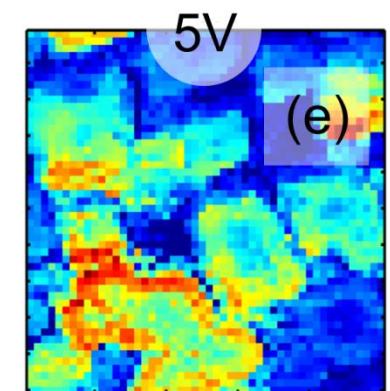
FORC IV of BFO-CFO

Current map @ 0.1 V

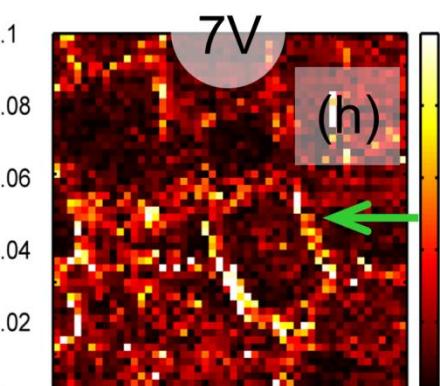
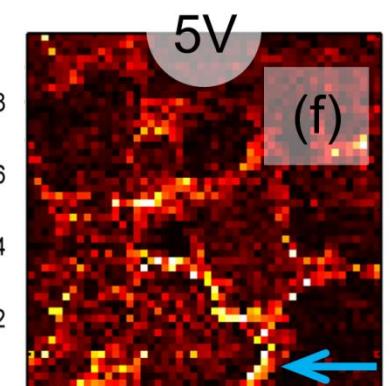
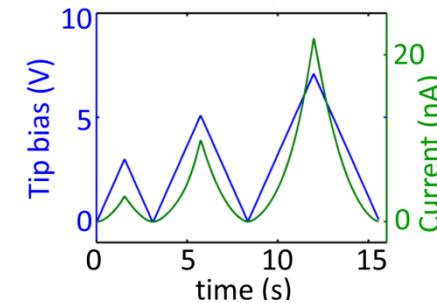


Topography

Current maps



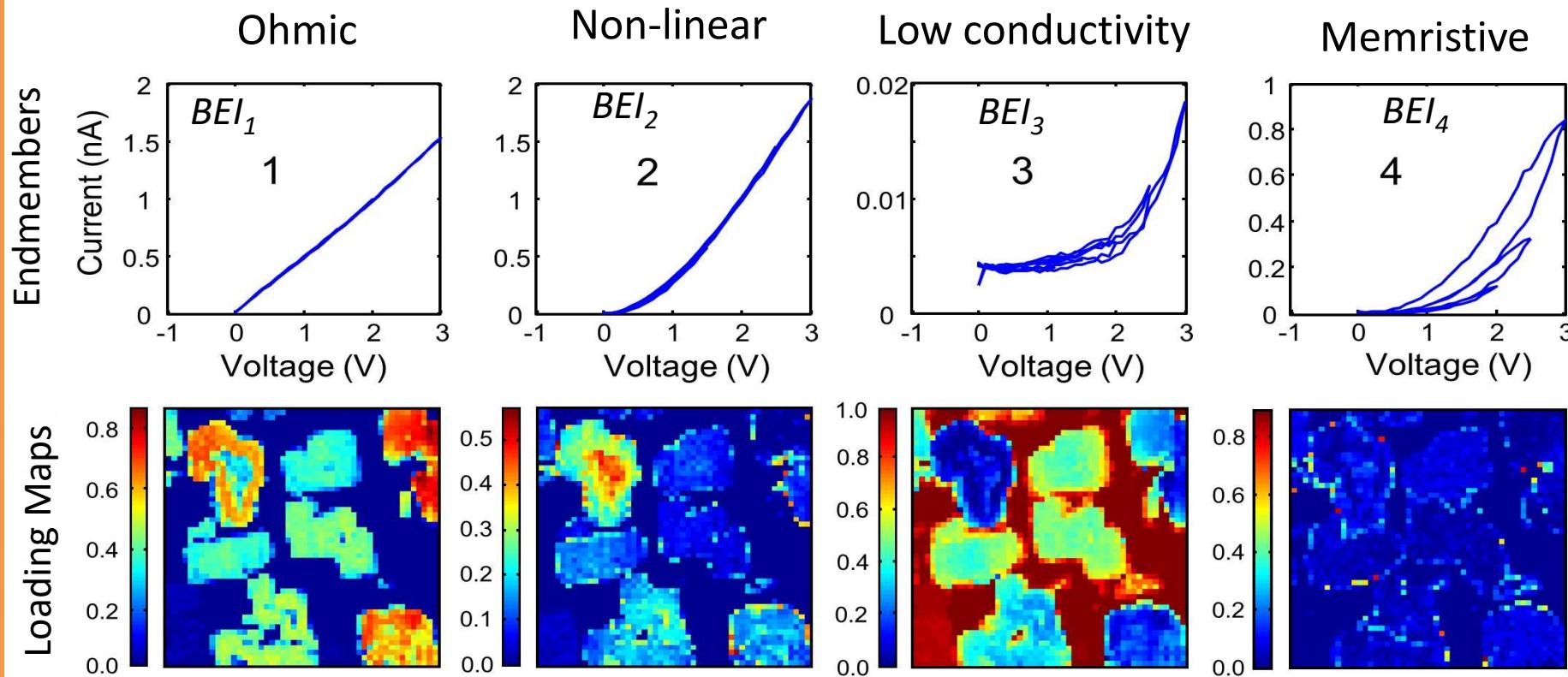
Averaged IV's



FORC-IV Loop area maps

- Clear variability of conductance and loop opening behavior
- “Too much data” – FORC IV loops that can be reduced to multiple current and loop opening maps as a function of peak voltage

Bayesian linear unmixing



Separates 4 different types of behavior, all making physical sense. Loading maps normalized to unity.

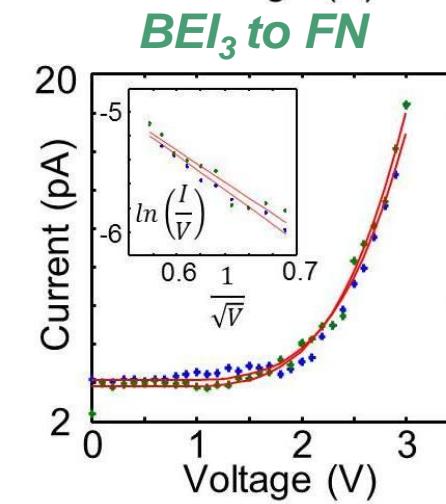
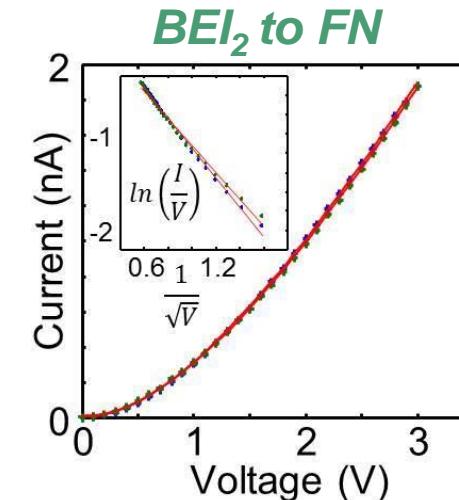
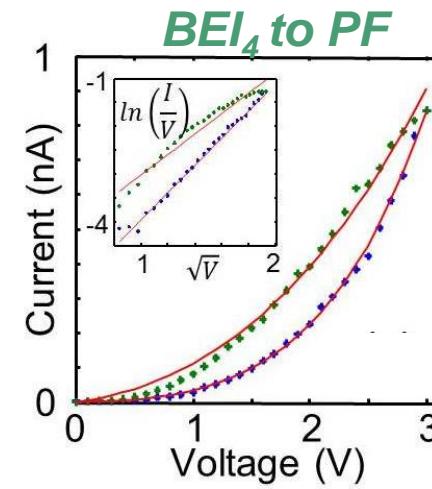
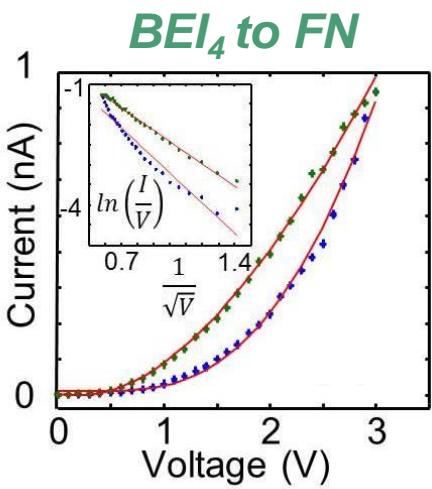
$$I_{xy} = \sum_j^n I_{xyj} = \sum_j^n \alpha_{xyj} BEI_j \quad \sum_j^n \alpha_{xyj} = 1$$

E. STRELCOV, A. BELIANINOV, Y.H. HSIEH, S. JESSE, A.P. BADDORF, Y.H. CHU, and S.V. KALININ,
Deep Data Analysis of Conductive Phenomena on Complex Oxide Interfaces: Physics from Data Mining, ACS Nano **8**, 6449 (2014).

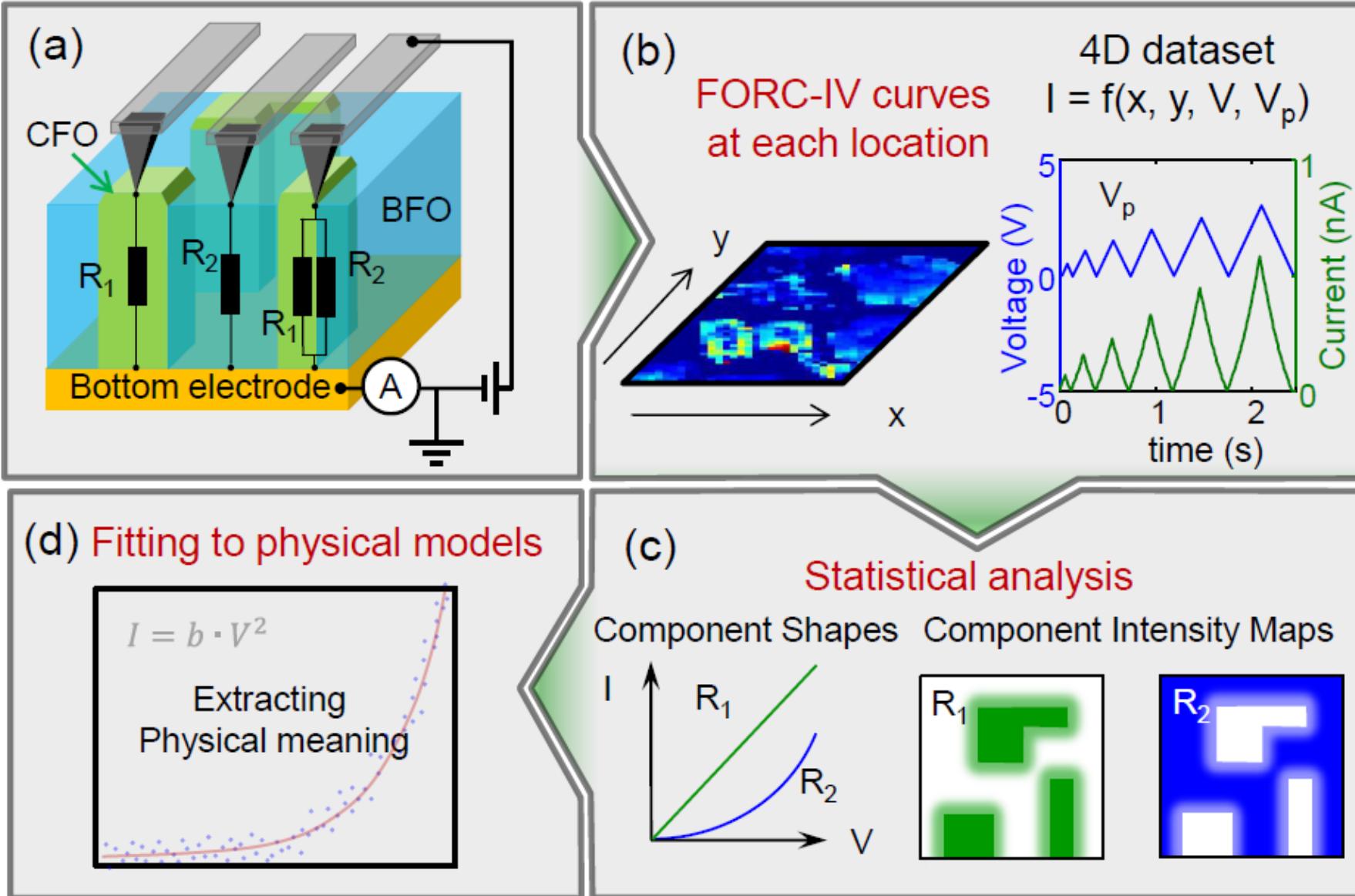
Fit to physical models

Mechanism\Endmember	Fowler-Nordheim	Poole-Frenkel	Schottky	Mott-Gurney	Child's Law
1 st	-	-	-	-	-
2 nd	good [†]	bad	bad	good	good
3 rd	fair [†]	bad	bad	bad	bad
4 th forward	bad	good [†]	bad	bad	bad
4 th reverse	good [†]	bad	fair	bad	bad

†The values of the fitting coefficients are physically meaningful



FORC IV workflow



Spectral Unmixing: N-FINDR

- Spectra for a given pixel is assumed to be a linear combination of the end-member spectra (+ Gaussian noise). The mixing proportions sum to 1

Physics constraint

$$p_{ij} = \sum_k e_{ik} c_{kj} + \varepsilon \quad \sum_k c_{kj} = 1$$

- Let E be the matrix of end-members (here, 3).

$$E = \left[\frac{1}{\vec{e}_1} \quad \frac{1}{\vec{e}_2} \quad \frac{1}{\vec{e}_3} \right] \quad V \left(\frac{\mathbf{1}}{(l-1)!} \right) |\det(E)|$$

- Iteratively select endmembers, accepting the new selection if the volume increases

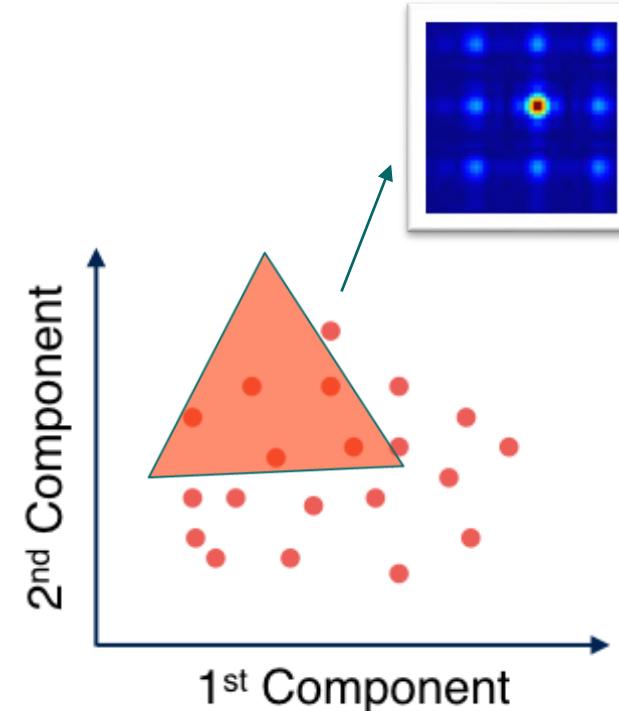


Figure by R. Vasudevan

Ideal test case

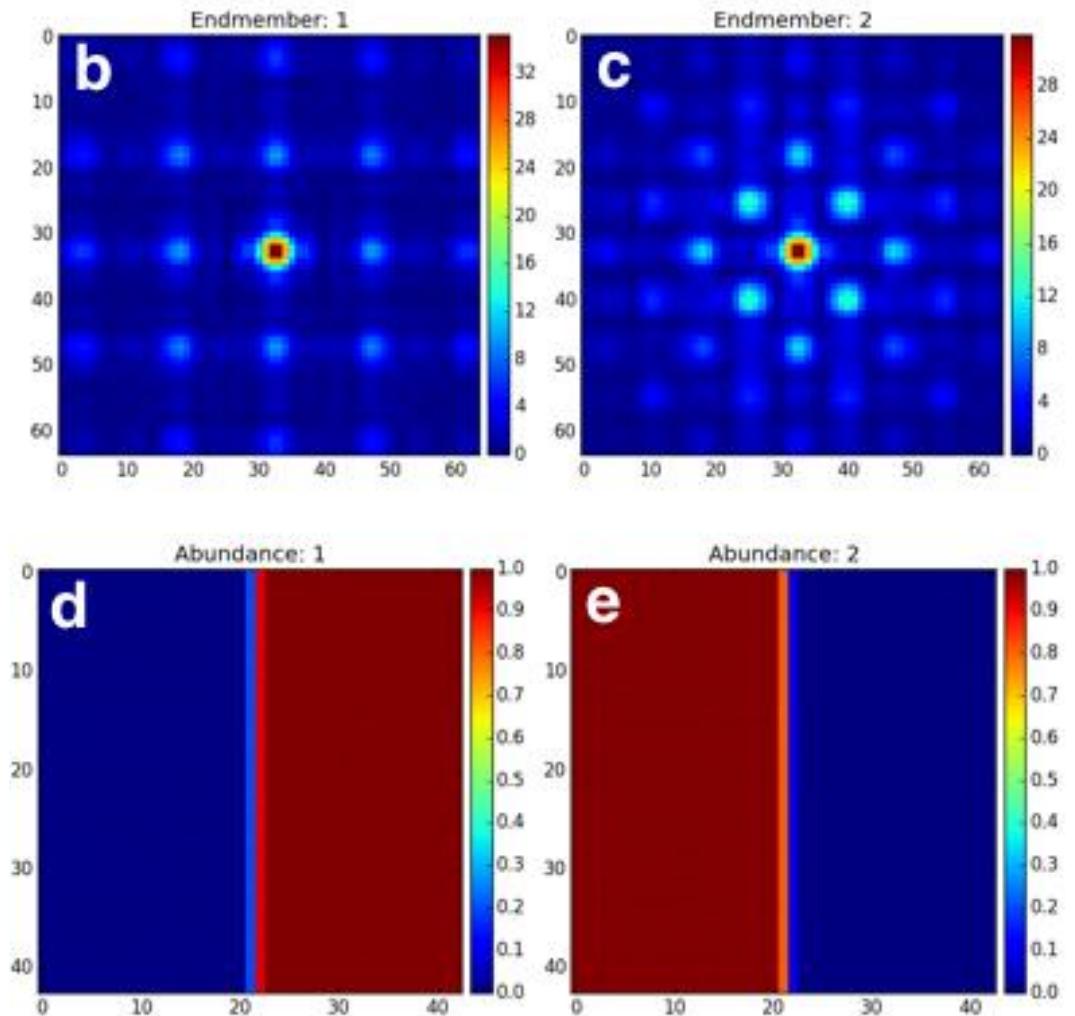
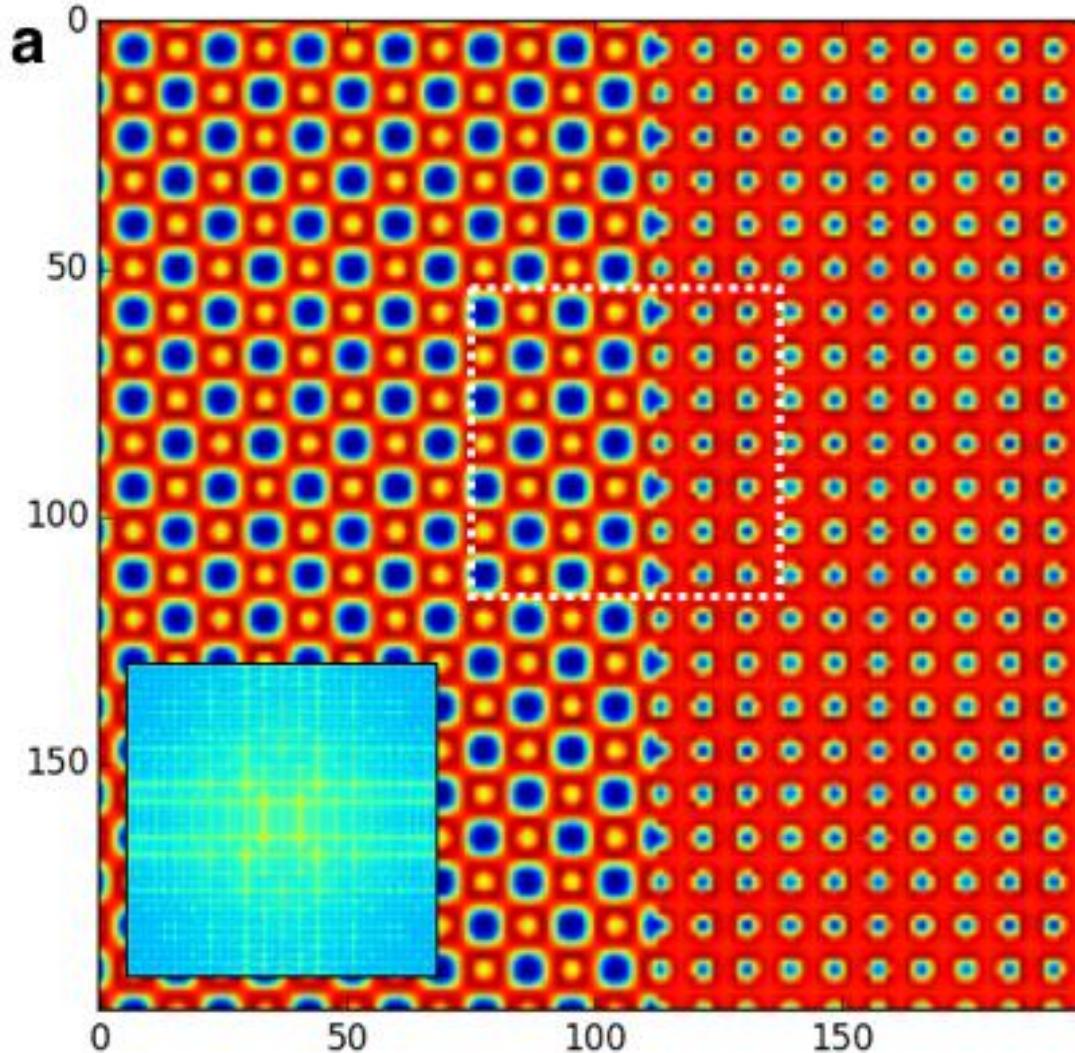
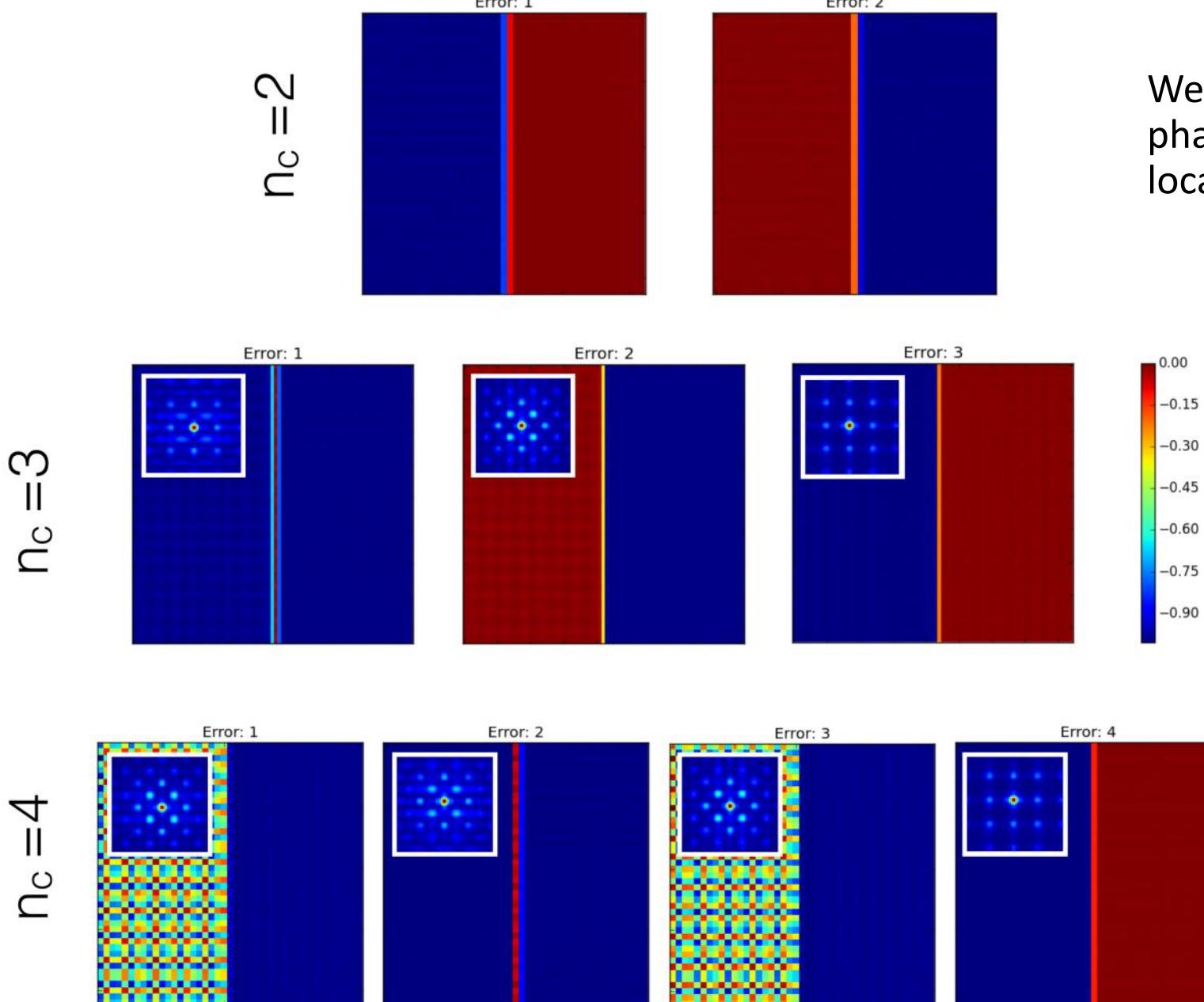


Figure by R. Vasudevan

Main idea:

- FFT amplitudes are non-negative;
- FFT removes translation

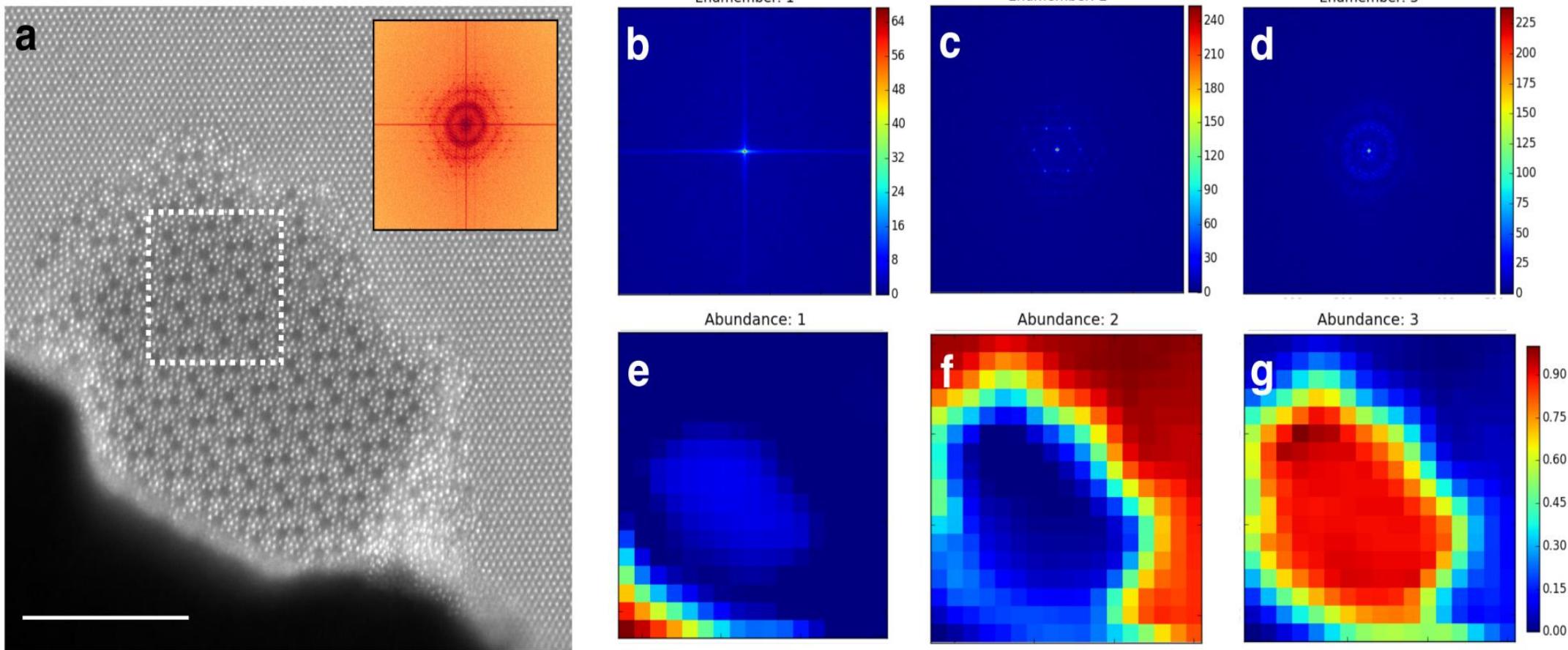
N-FINDR for image segmentation



We can determine number of phases based on spatial localization and geometry

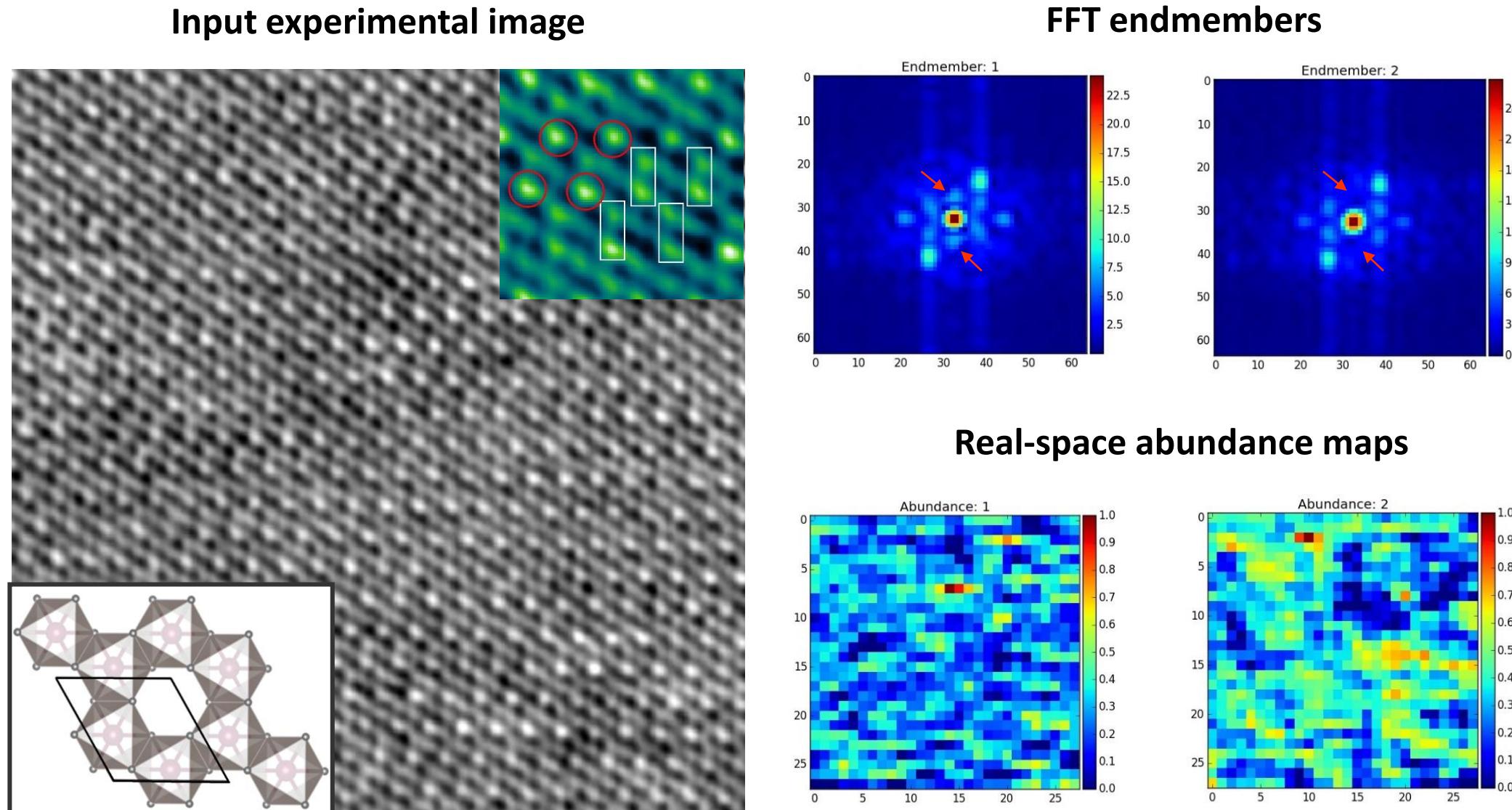
Figure by R. Vasudevan

N-FINDR for chemically separated images



Q. He, J. Woo, A. Belianinov, V.V. Gulians, A.Y. Borisevich, Better catalysts through microscopy: mesoscale M1/M2 intergrowth in Molybdenum–Vanadium based complex oxide catalysts for propane ammoxidation
ACS Nano 9, 3470-3478

NFINDR for coexisting order parameters



In a good agreement with test case, 2 spots in the “inner hexagon” are strongly suppressed in the 2nd component reflecting a fine structure of charge ordered pattern

Figure by M. Zlatdinov

NFIND-R for coexisting order parameters

FFT endmembers

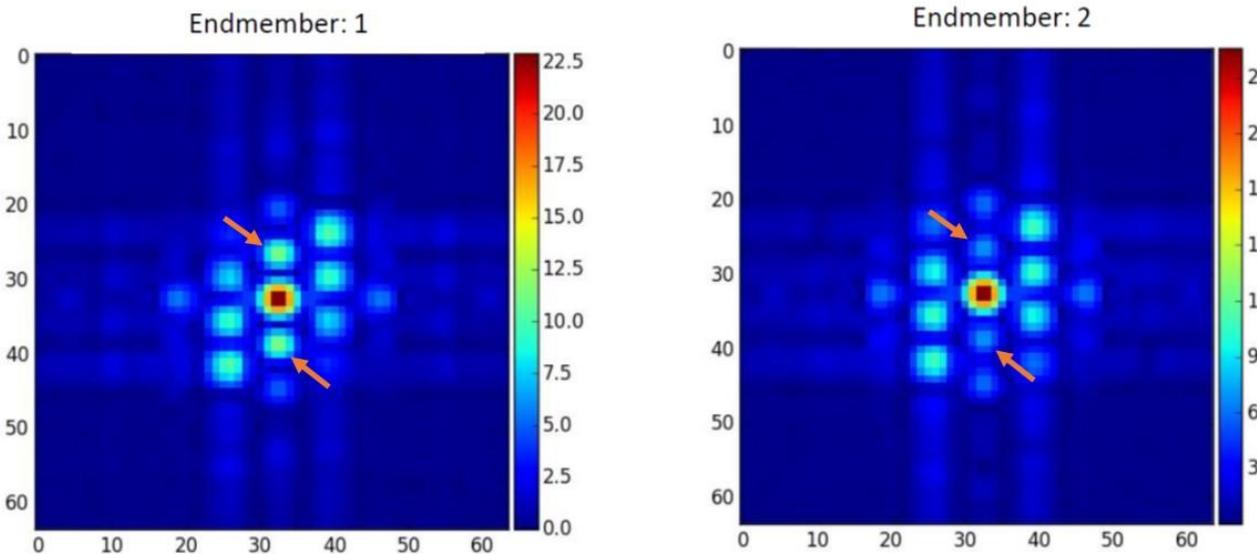
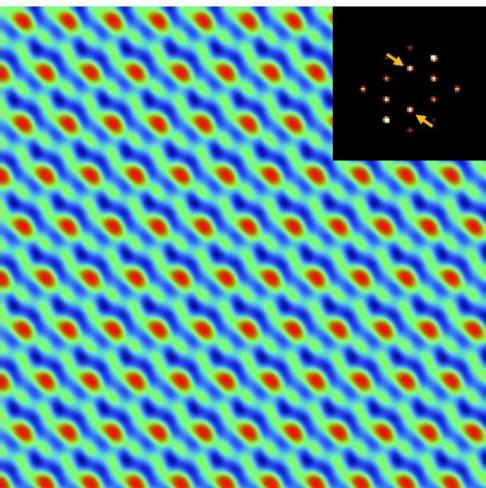
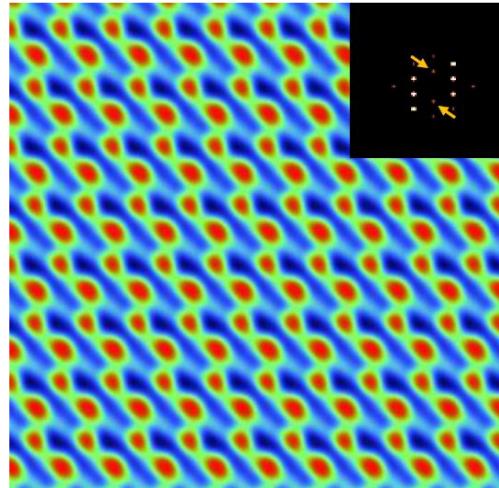


Figure by M. Ziatdinov

Real-space images of corresponding phases



Hexagonal superlattice



Dimer superlattice

In the 2nd component, 2 spots in the “inner hexagon” are strongly suppressed reflecting a fine structure of charge ordered pattern

NFIND-R vs. ICA

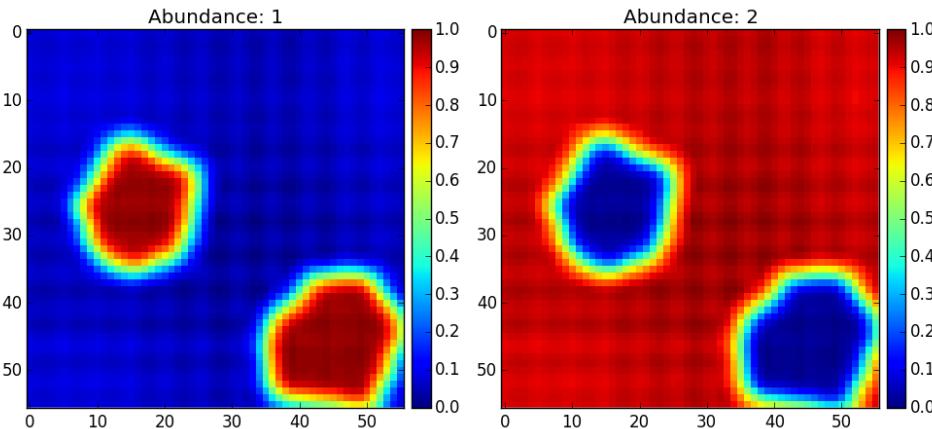
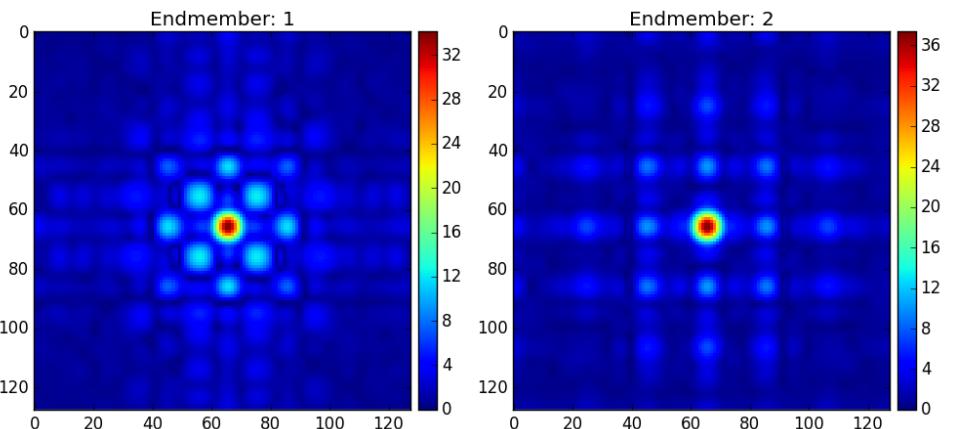
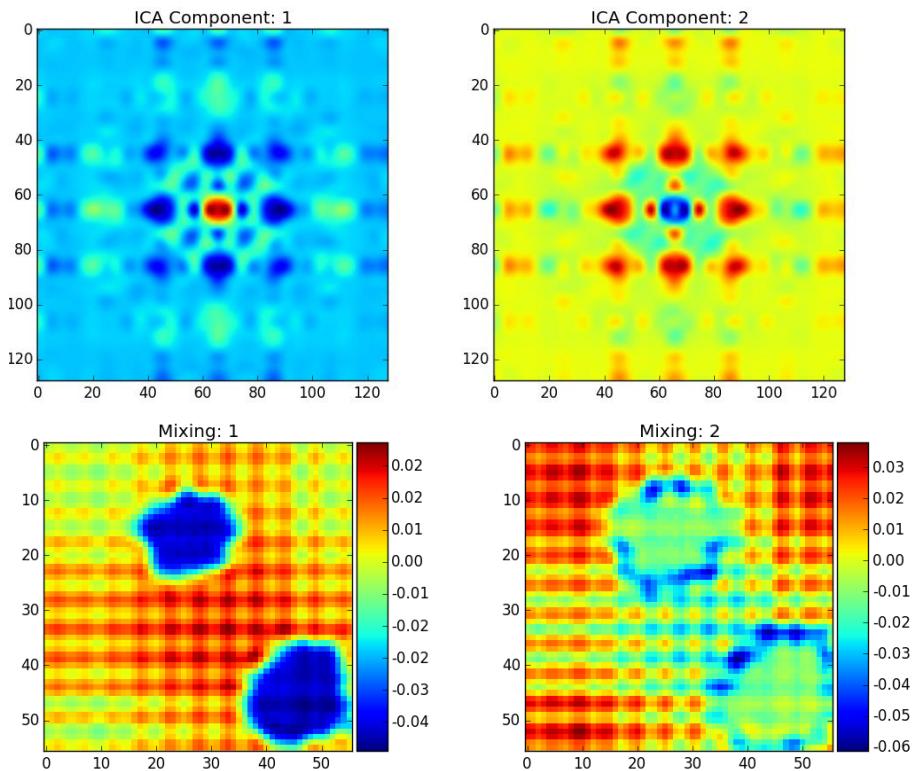
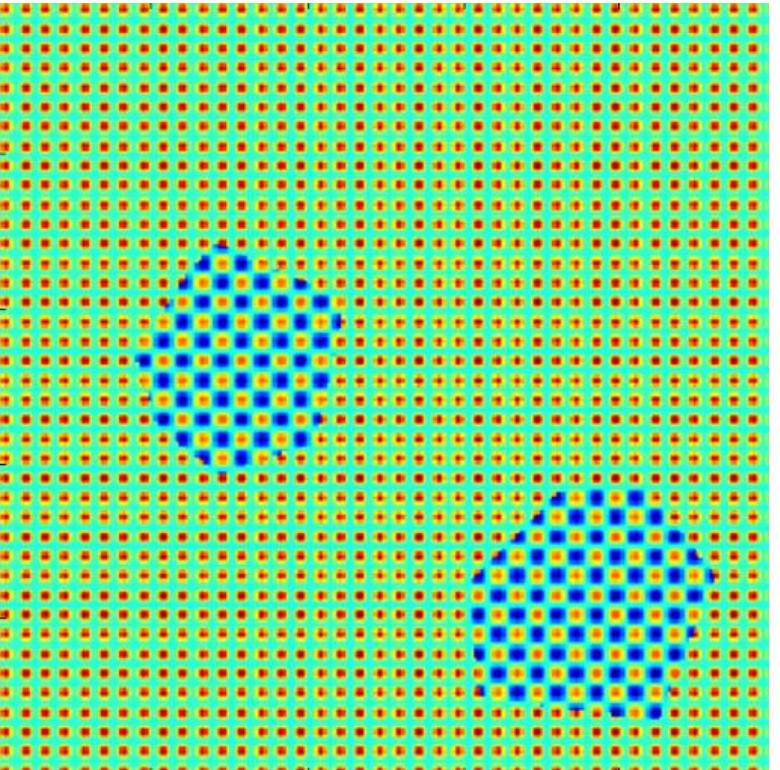
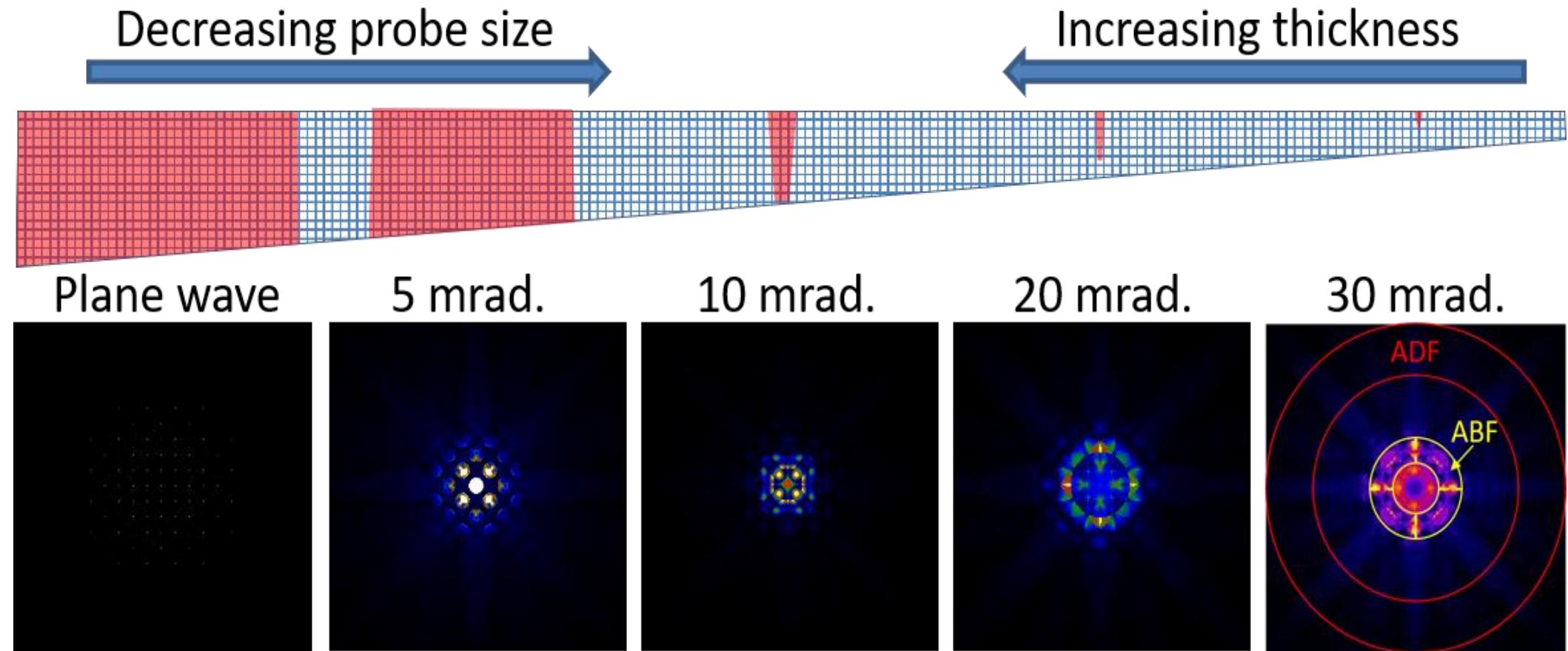
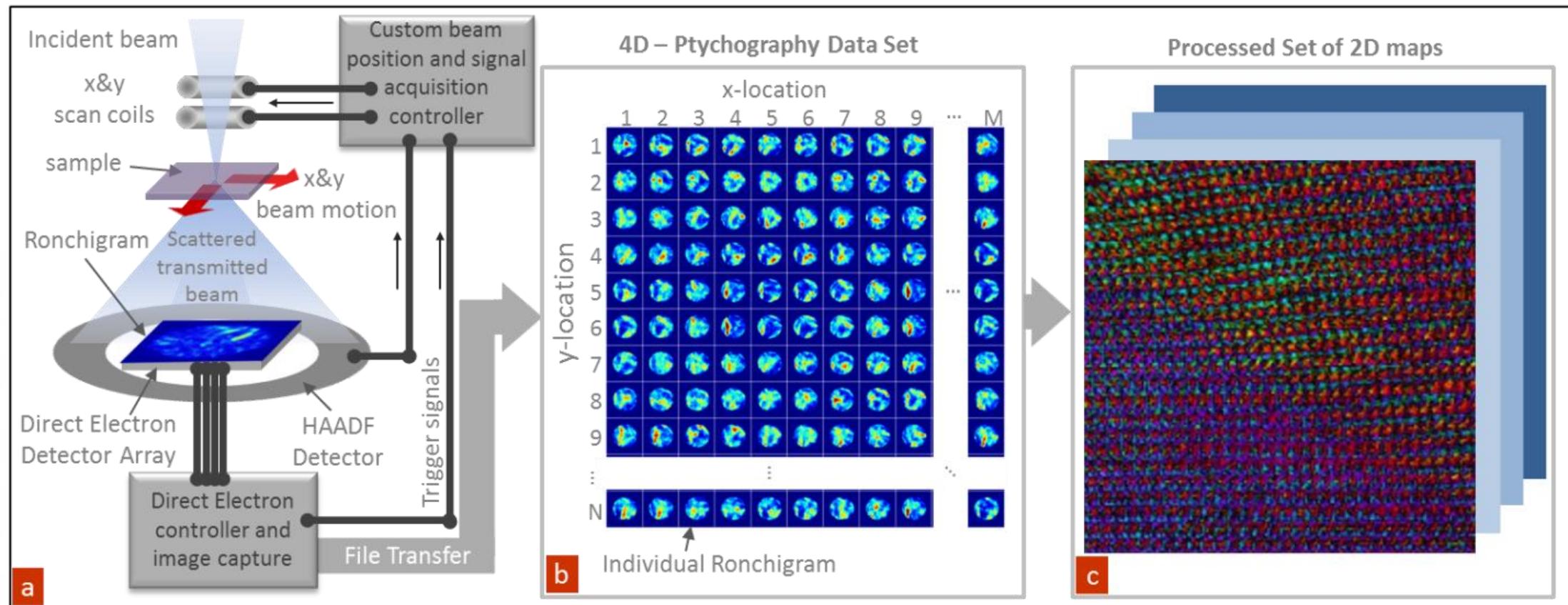


Figure by
R. Vasudevan

PCA on 4D STEM

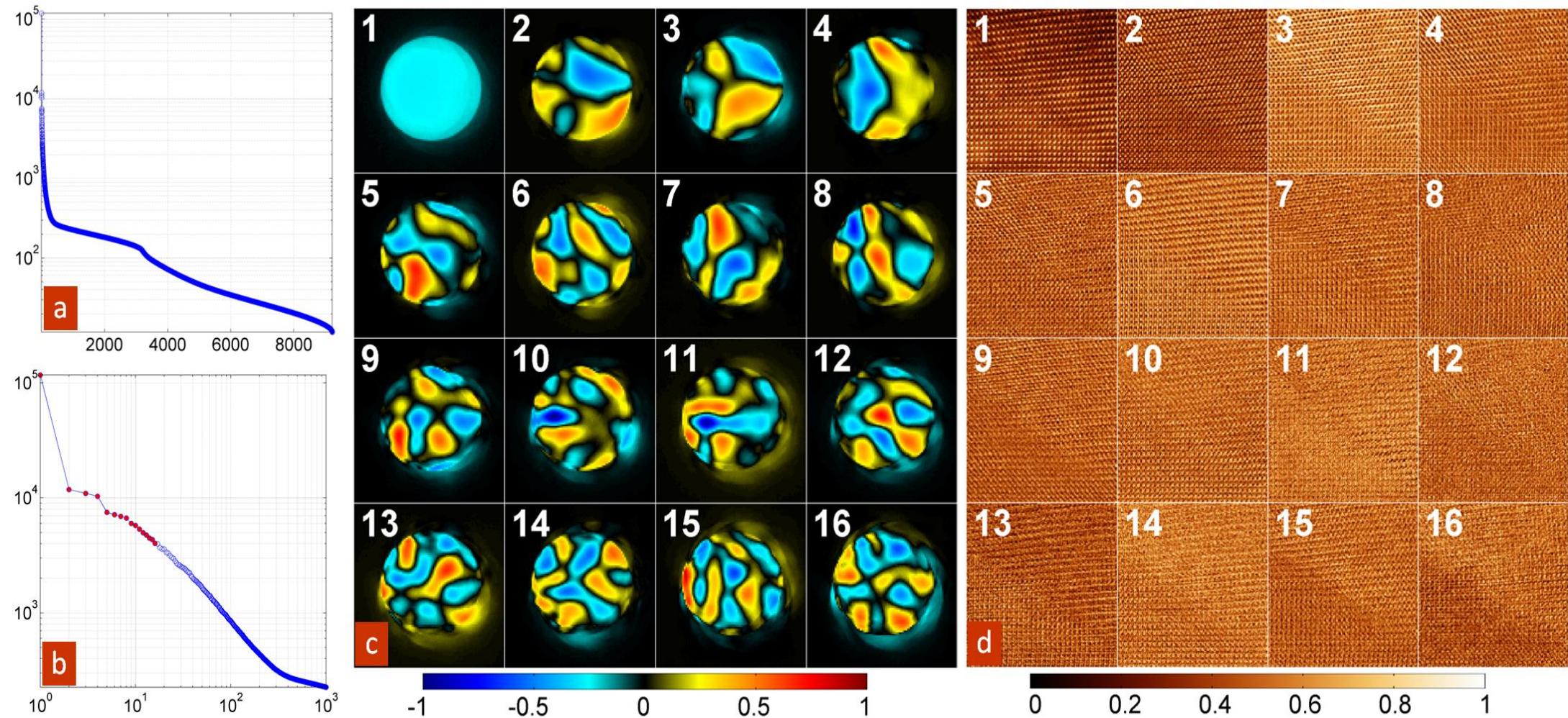


4D STEM Data



S. JESSE, M. CHI, A. BELIANINOV, C. BEEKMAN, S.V. KALININ, A.Y. BORISEVICH, and A.R. LUPINI, *Big Data Analytics for Scanning Transmission Electron Microscopy Ptychography*, Sci. Rep. **6**, 26348 (2016).

PCA on 4D STEM Data

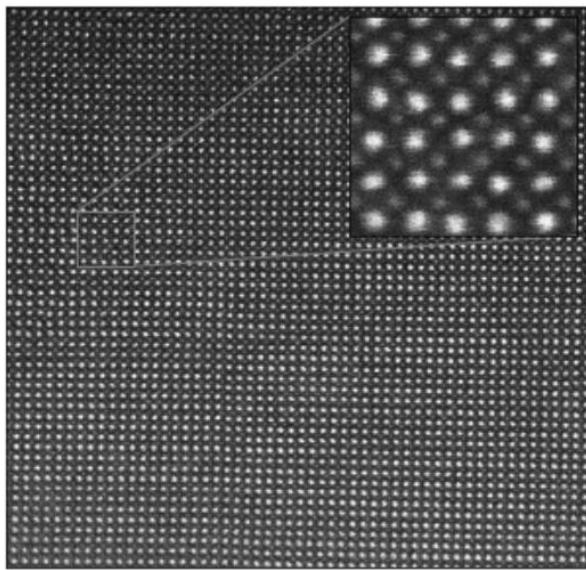


S. JESSE, M. CHI, A. BELIANINOV, C. BEEKMAN, S.V. KALININ, A.Y. BORISEVICH, and A.R. LUPINI, *Big Data Analytics for Scanning Transmission Electron Microscopy Ptychography*, Sci. Rep. **6**, 26348 (2016).

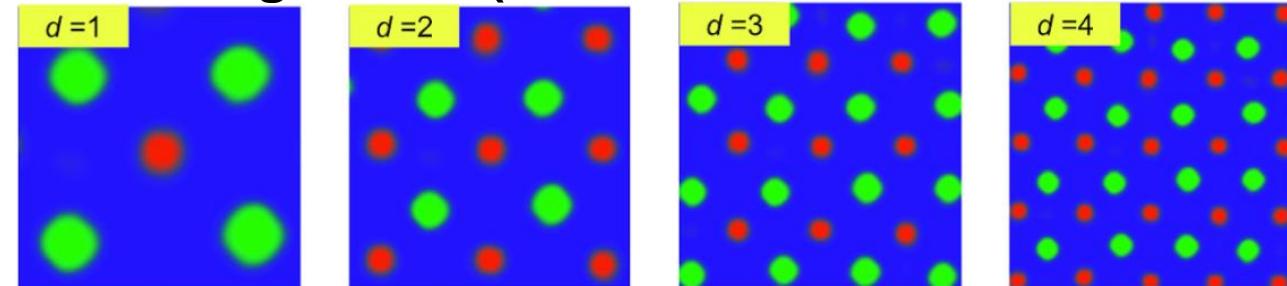
FerroNet: Finding Descriptors

THE UNIVERSITY OF TENNESSEE  KNOXVILLE

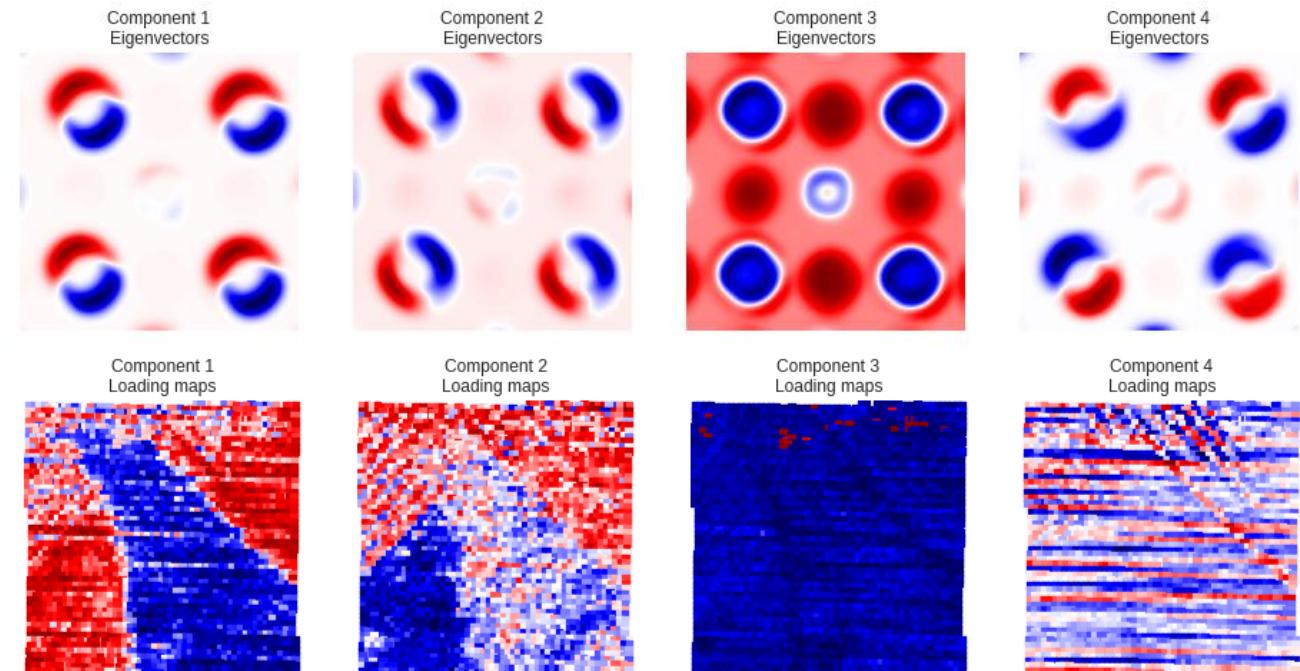
Experimental (LBFO film)



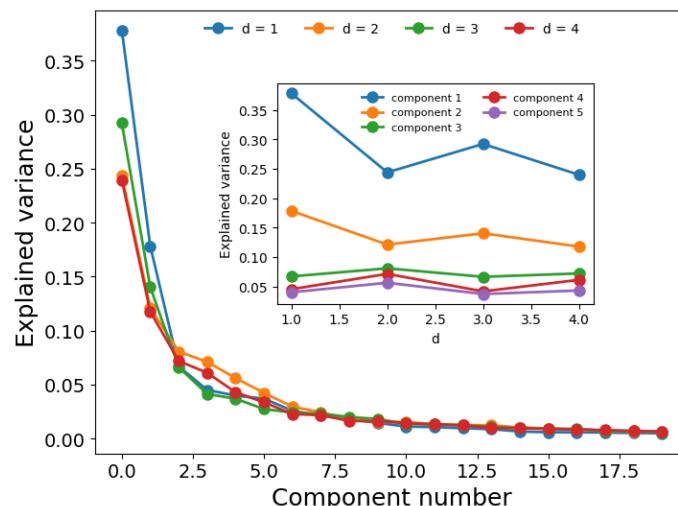
Building blocks (from neural network output)



PCA eigenvectors and loading maps



Information Content



GitHub: PyCroscopy and AICrystallographer

Wait, there is more!

We need un-mixing/decomposition that are infused in some universal manner with a priori physical information (trivial example is constraints, a less trivial one is a simulation of some expected components) so that the resultant components can be directly interpreted in physical terms.

For example:

- Bayesian linear unmixing: constraints on endmembers
- Sparse reconstructions: small number of components in each point
- Constraints on loading maps: smoothness or sharp boundaries
- Kernel transforms: data is simplest if physics is correct