Modern electron microscopy goes high dimensions: handling big data

102 YEARS 1917–2019

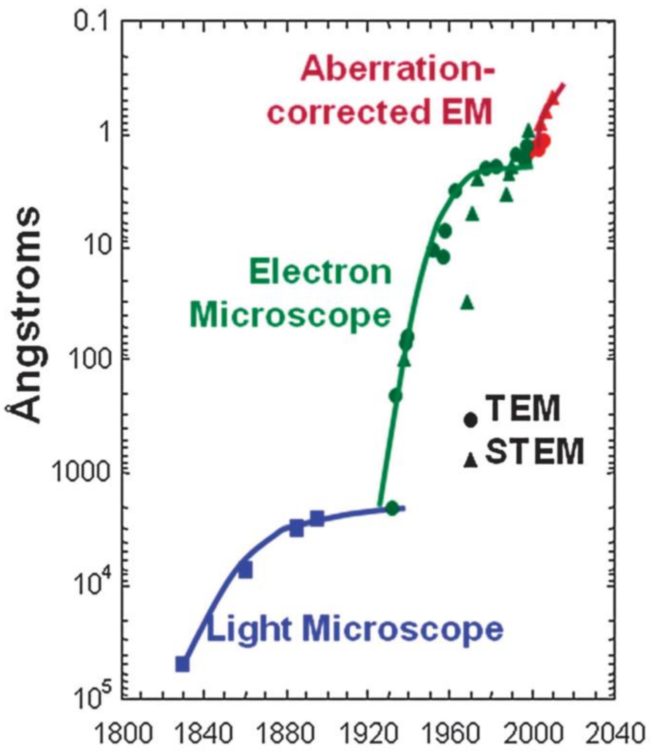
MAX-PLANCK-INSTITUT FÜR EISENFORSCHUNG

Spark (Siyuan) Zhang

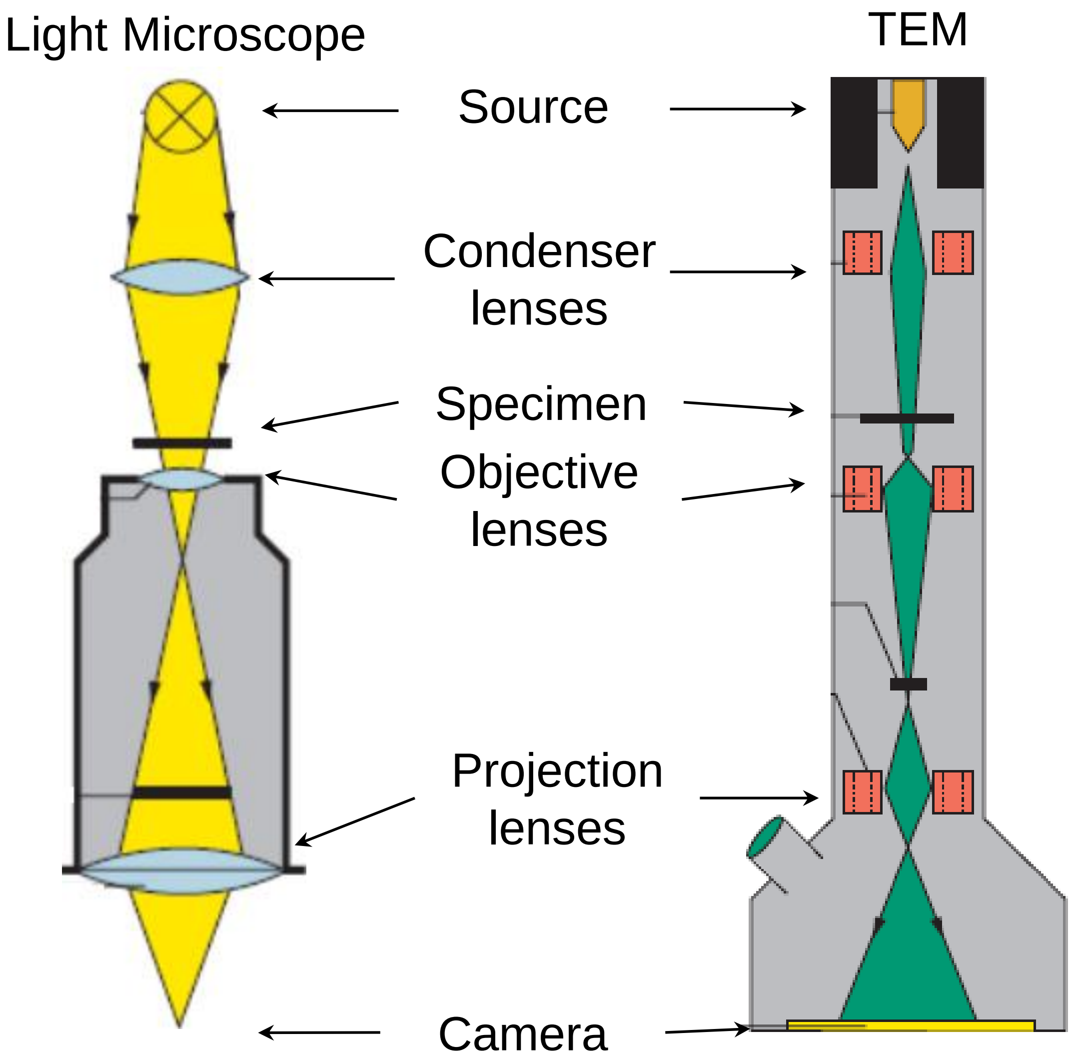
BIG DATA SUMMER – BiGmax Network, 10.09.2019, Platja d‘Aro, Spain

For the next 10 minutes

- **Electron microscopy and big data**
- Sparsify big data – dimension reduction
- Sparsify diffraction imaging data?
- Make use of sparsity in big data



Light & electron microscopy

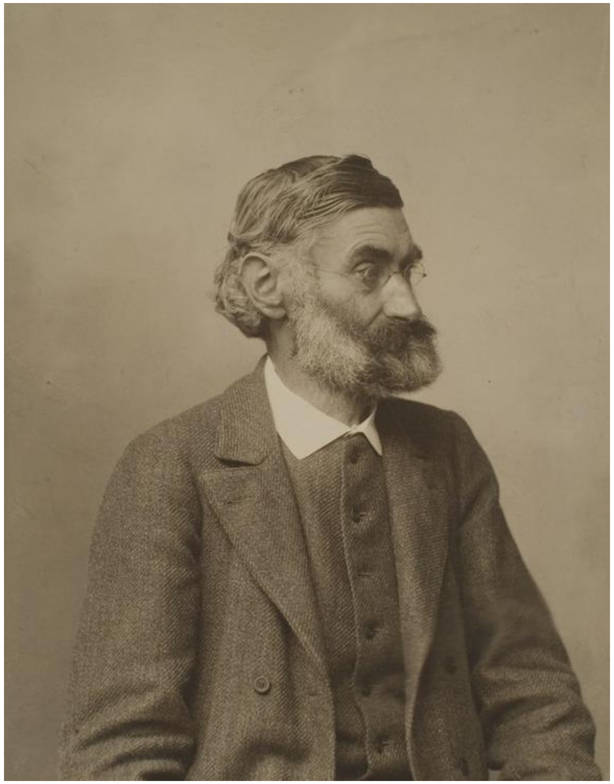


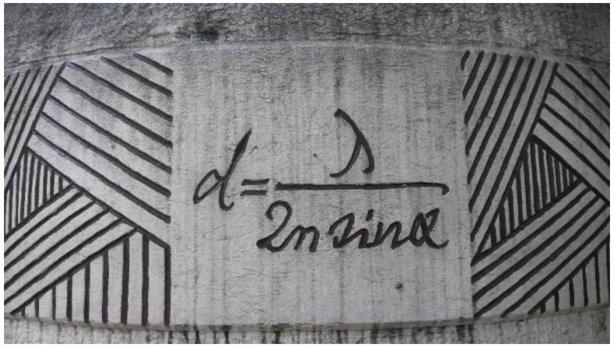
Ahmadian A.

Electron optics: continuous change of focal strengths

TEM/SEM are operated in vacuum (10^{-5} ~ 10^{-7} mbar)

Ernst Karl Abbe (1840 – 1905)





Ernst-Abbe-Denkmal, Jena Fürstengraben

Visible light microscopy:
λ = 380 ~ 770 nm
sinθ = 0 ~ 1
n = 1 ~ 2

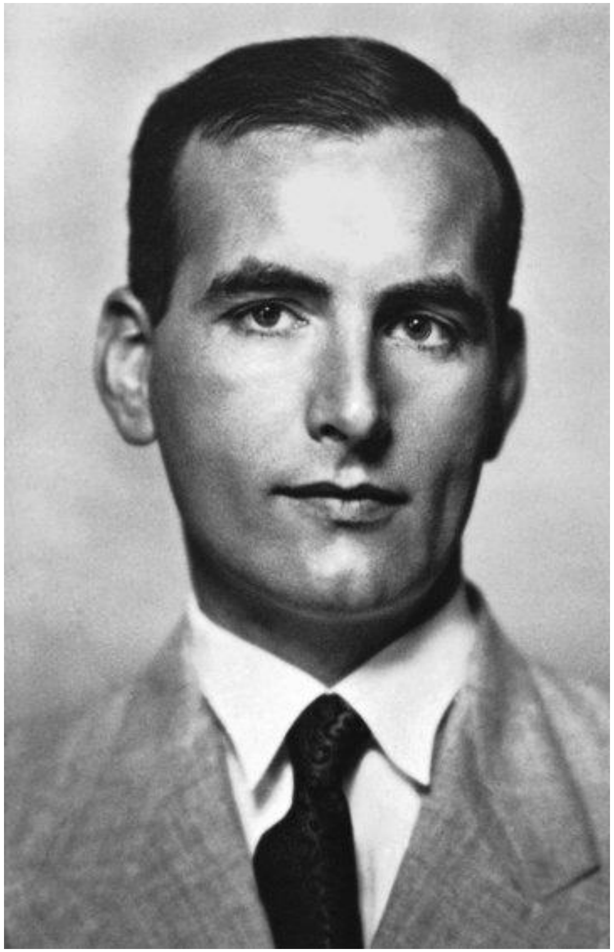
$$d = \frac{\lambda}{2n \sin\theta} > 100 \text{ nm}$$

The resolution of light microscopy
is diffraction limited, i.e., by λ.

X-ray microscopy: reduced λ, difficulty in lens

Super-resolution: 100 ~ 10 nm,
breaks Abbe theory of image formation.

Ernst Ruska (1906 – 1988)



First TEM, Berlin 1933

Louis de Broglie
1924 Electron wave

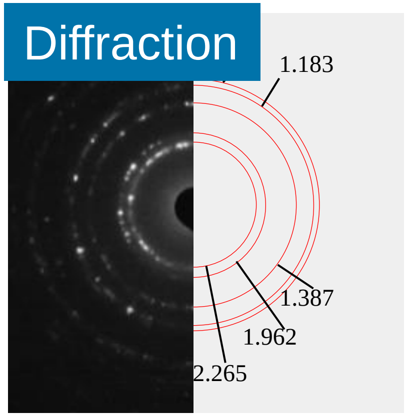
Ernst Ruska
1931 Electron optics
1933 TEM prototype
PhD
1939 Commercial
TEM, Siemens
1986 Nobel prize
in physics

λ = 2 ~ 10 pm
$\sin\theta$ = 0 ~ 0.01
0.05
(aberration correction)

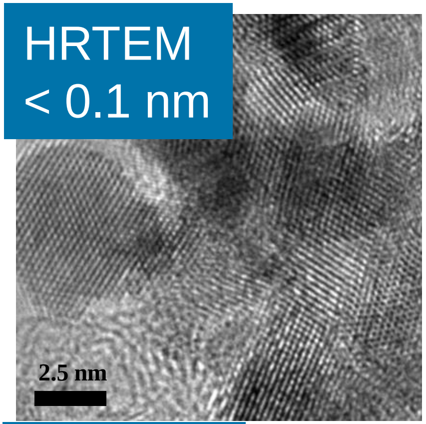
$d = \frac{\lambda}{2n\sin\theta}$ > 50 pm

High resolution analytical EM @ MPIE

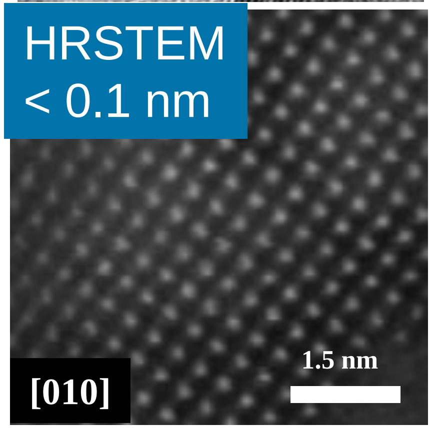
Diffraction

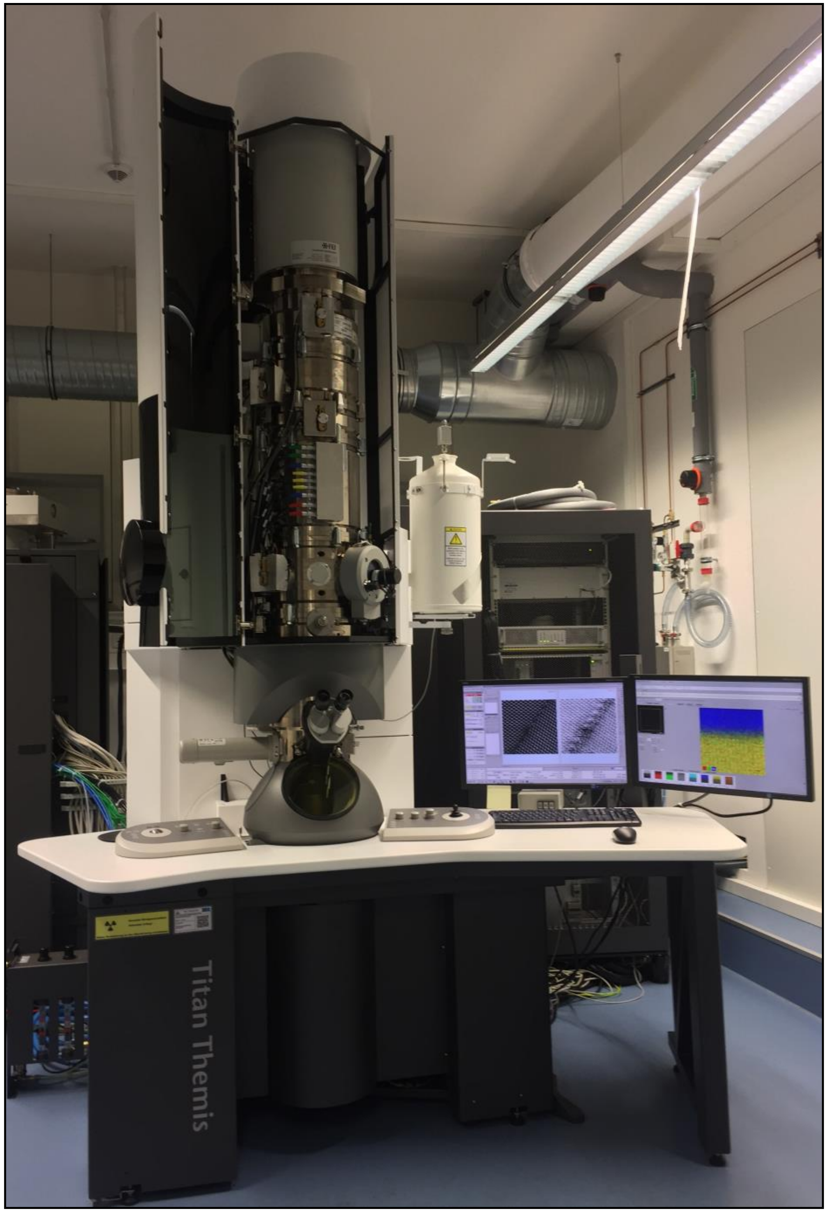


HRTEM
< 0.1 nm

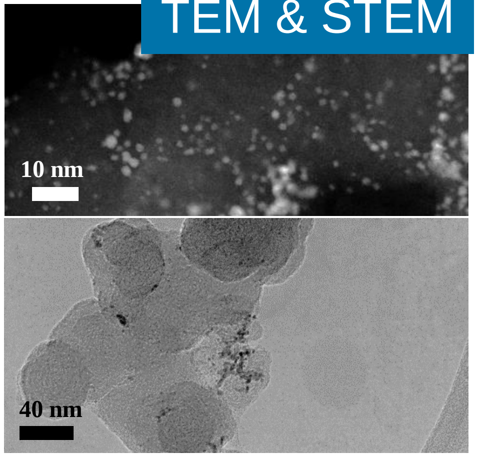


HRSTEM
< 0.1 nm

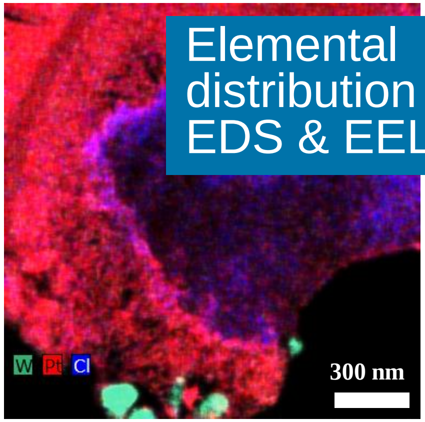


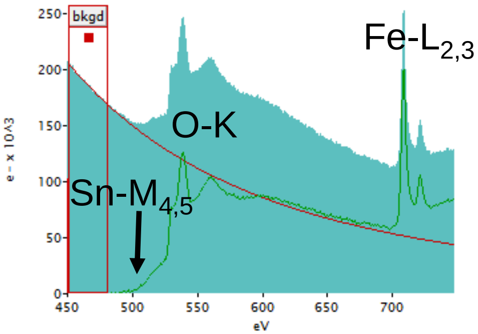


TEM & STEM

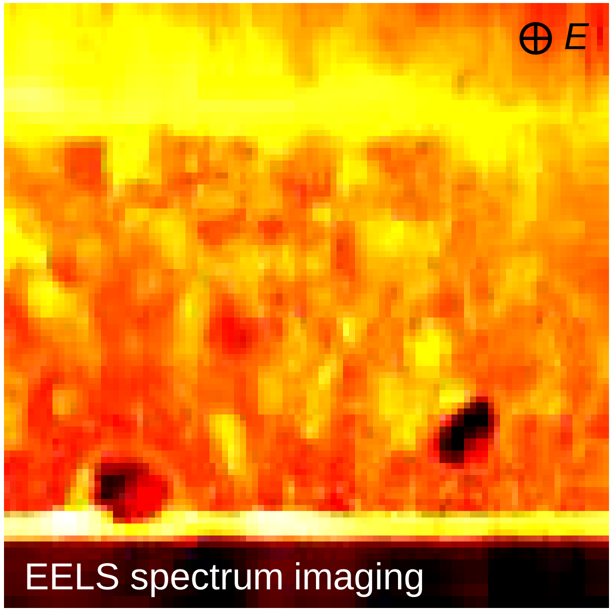


Elemental distribution
EDS & EELS



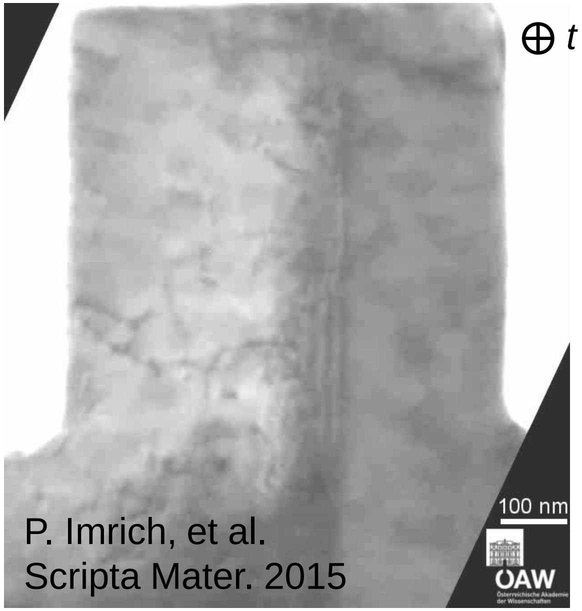


High dimensional TEM data



tilt series

⊕ *θ (z)*



⊕ *t (F)*

For the next 10 minutes

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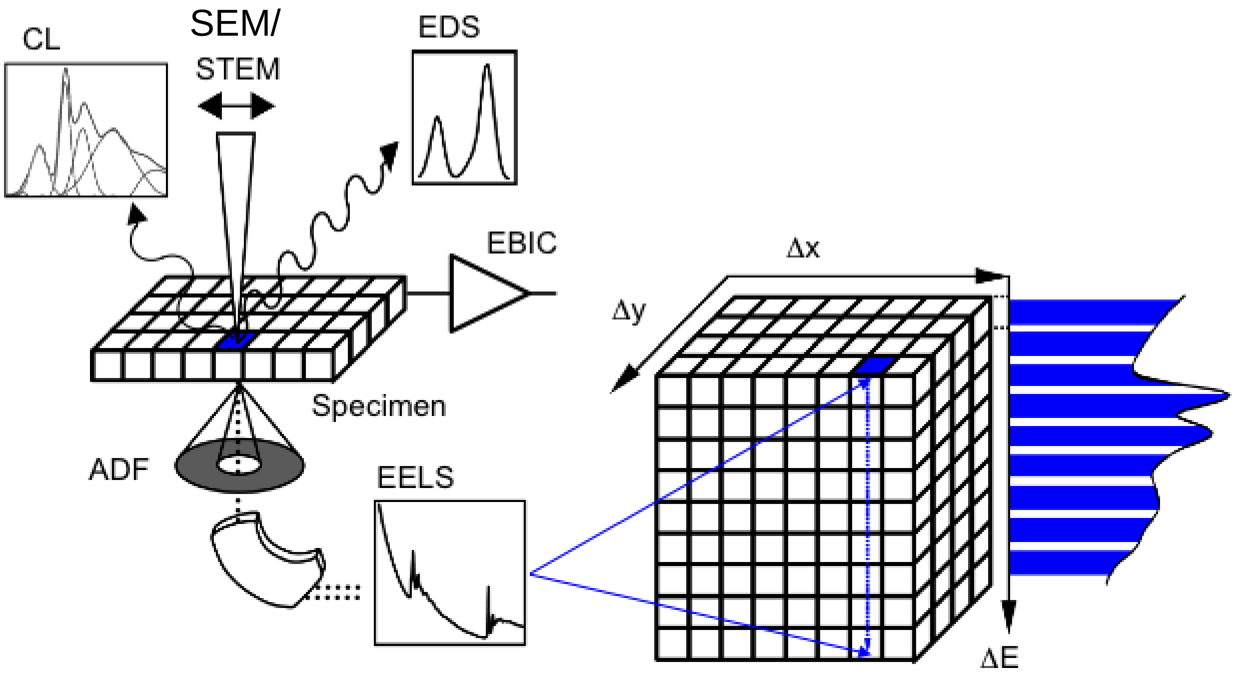
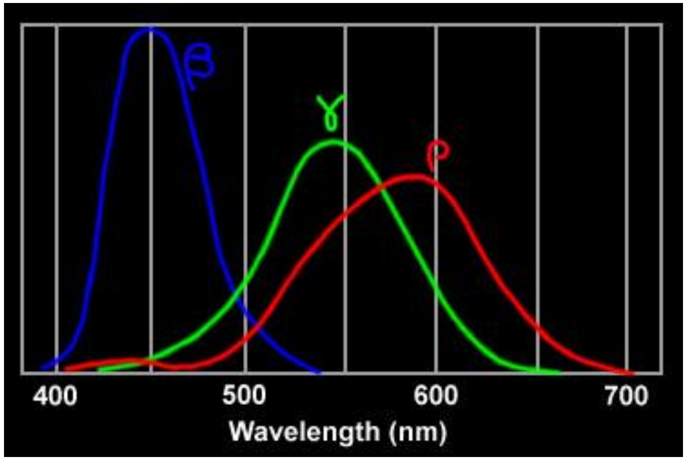
- **Sparsify big data – dimension reduction**
- Sparsify diffraction imaging data?
- Make use of sparsity in big data



=

+

+



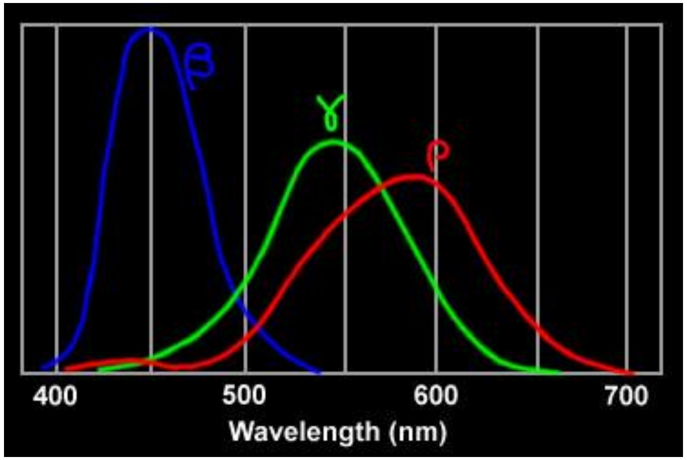
Reflectogram:
300 channels × 1 M pixels

RGB:
3 channels × 1 M pixels

Sparsity in colour

$=$

300 channels × 1 M pixels



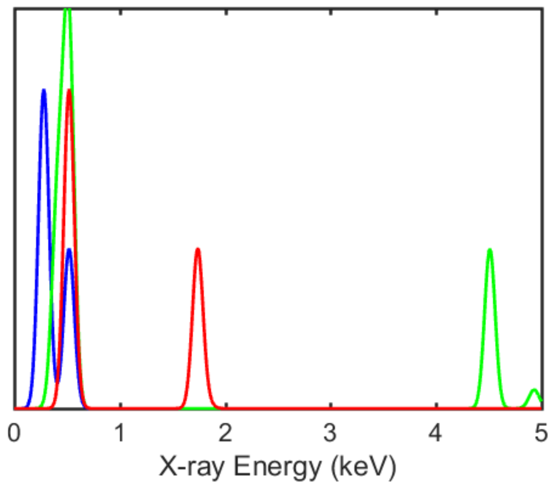
$\times$

300 channels × 3 channels

3 channels × 1 M pixels

Sparsity in composition

1 k channels × 1 M pixels



1 k channels × 3 channels

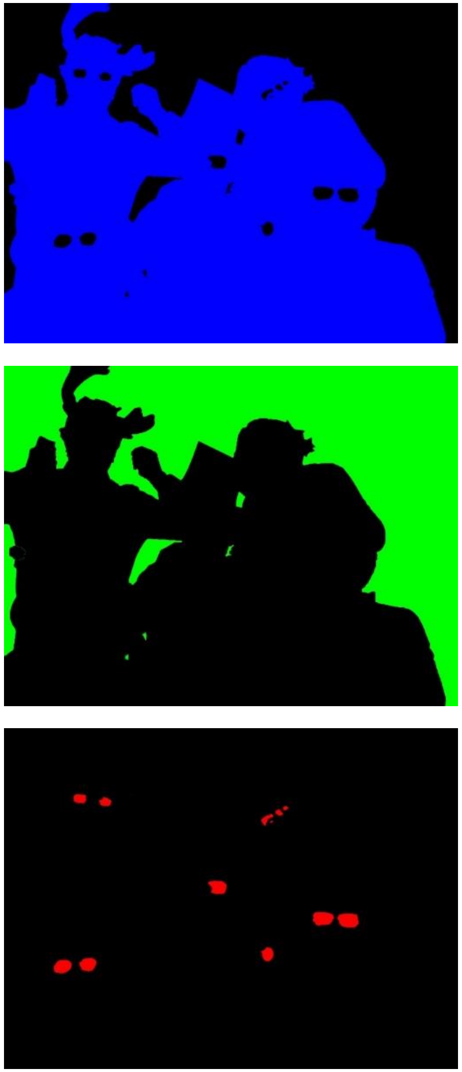
=

skin/fabrics

paint

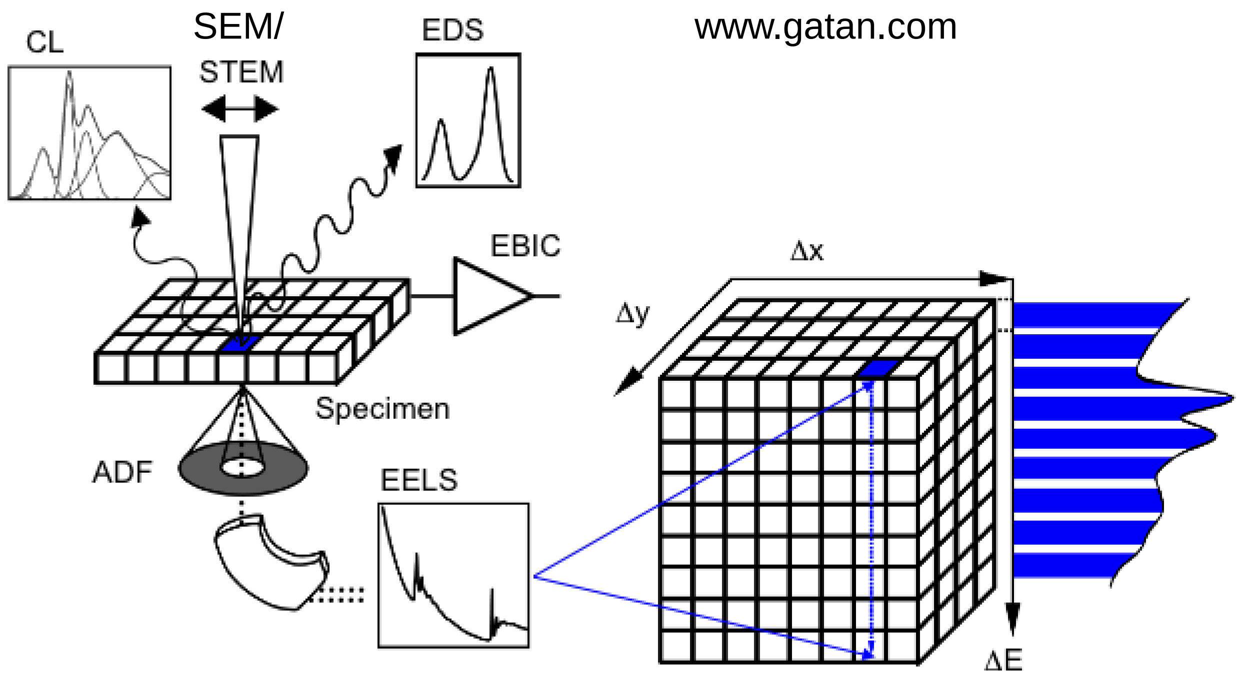
glass

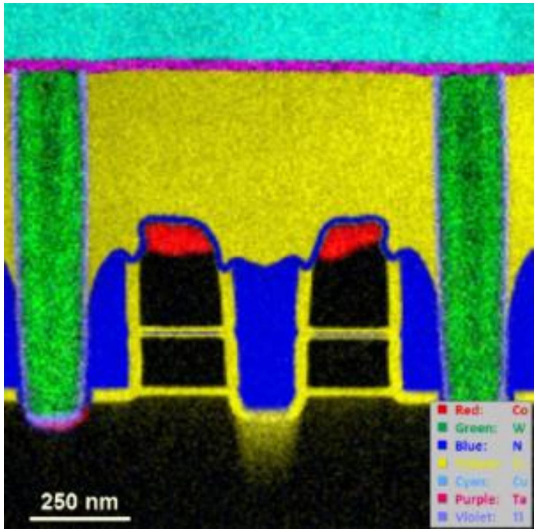
×

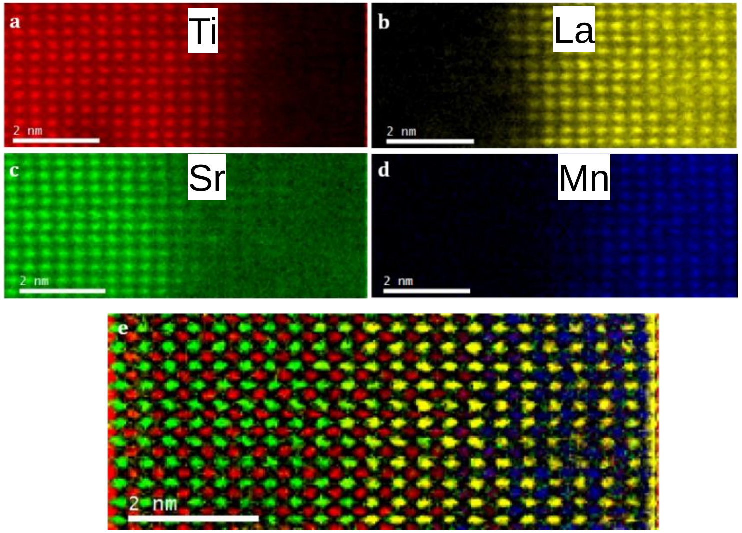


3 channels × 1 M pixels

Spectrum imaging







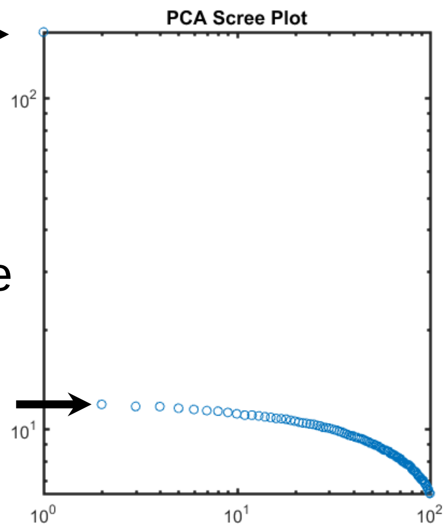
Principal component analysis

100 × 1000 random numbers

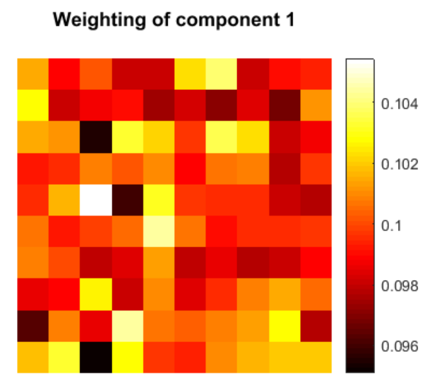
mean →

Variance

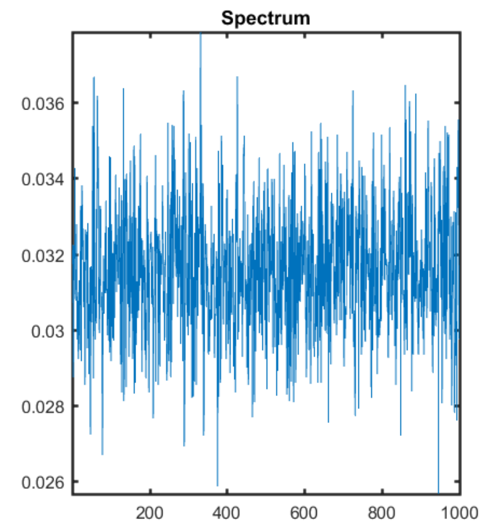
noise →



Component #



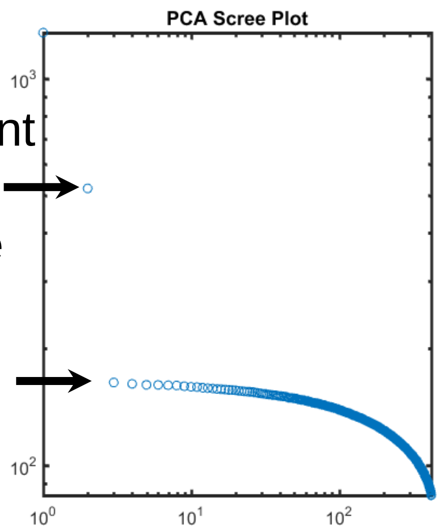
100 pixels

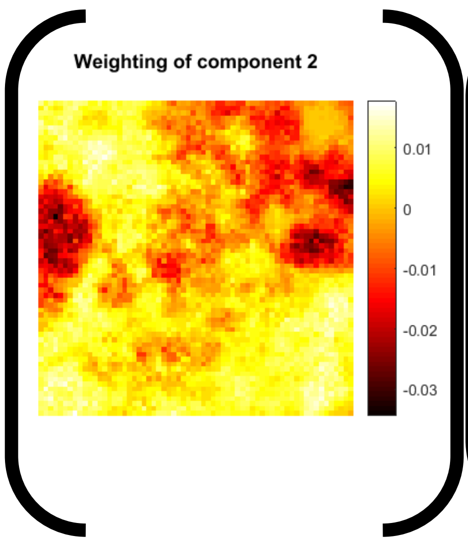


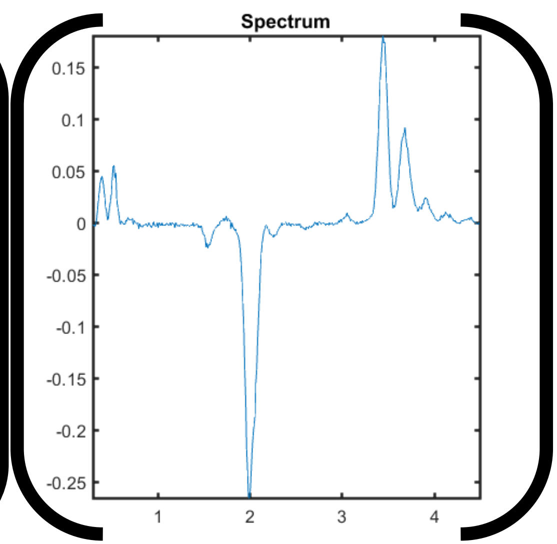
1000 channels

significant spatial variance →

noise →







10 000 pixels × 2 components   2 × 1 000 channels

For the next 20 minutes

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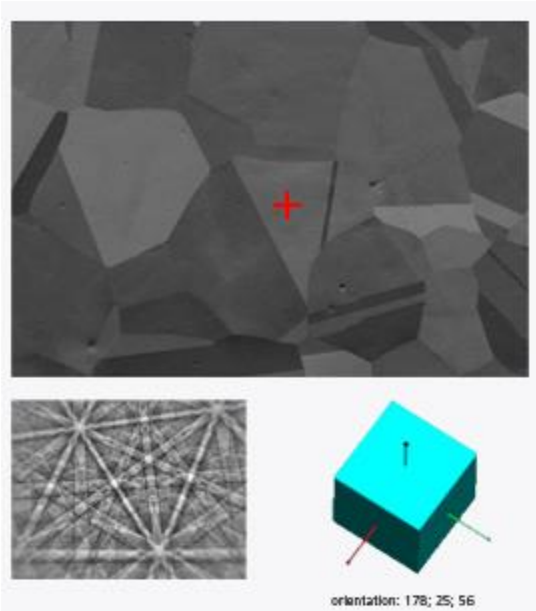
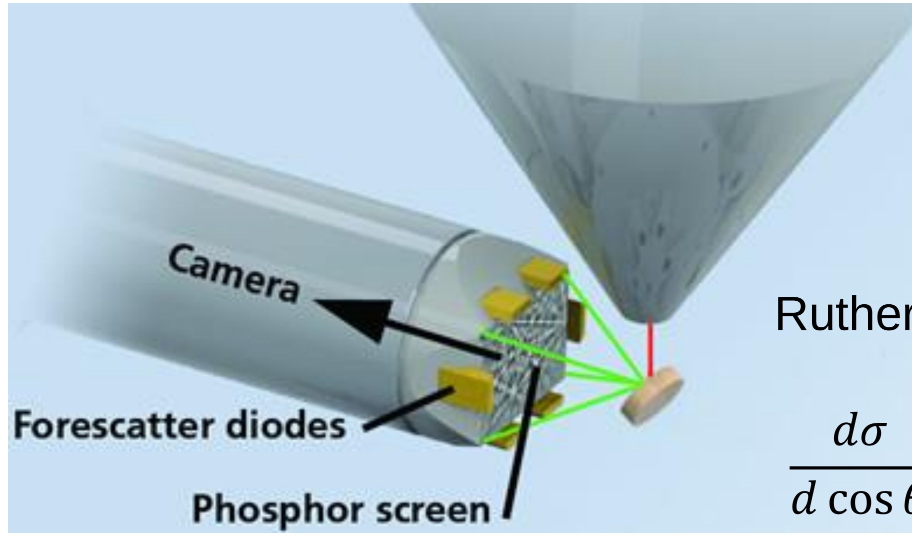
- **Sparsify diffraction imaging data?**
- Make use of sparsity in big data

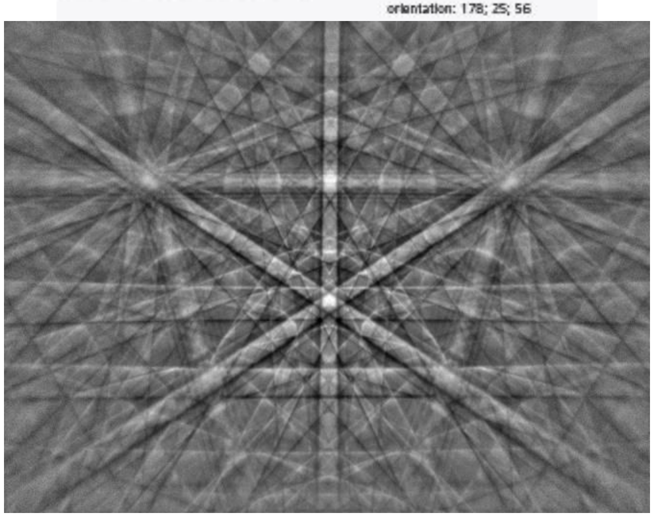
Electron backscattered diffraction





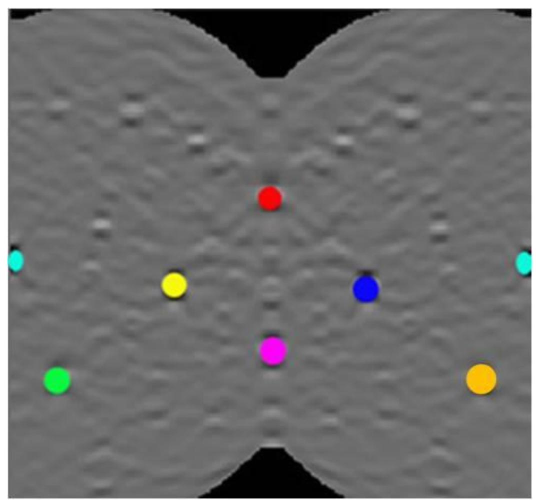
Rutherford scattering:

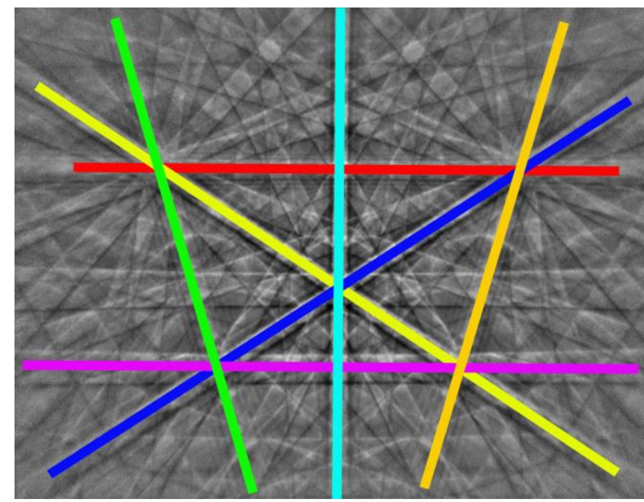
$$\frac{d\sigma}{d\cos\theta} \propto \frac{NZ^2}{(1-\cos\theta)^2}$$



20 keV EBSD of a Si grain

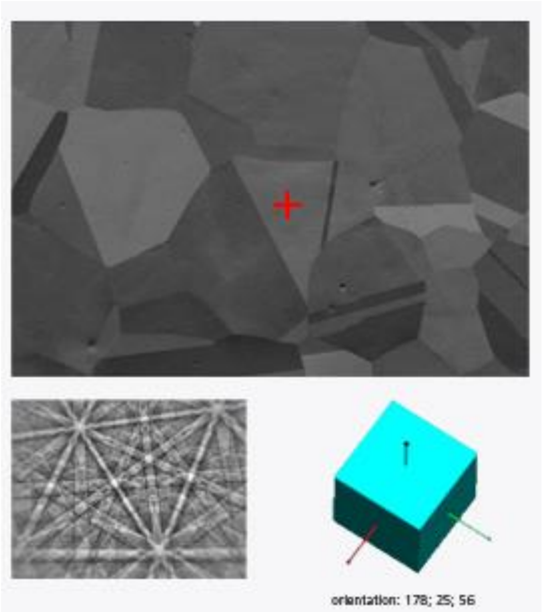
www.ebsd.com

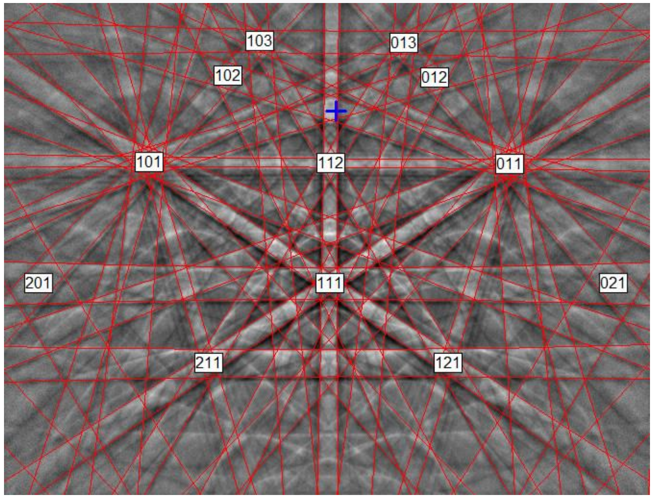




- Hough transform Kikuchi bands to points.

Analysis of EBSD patterns





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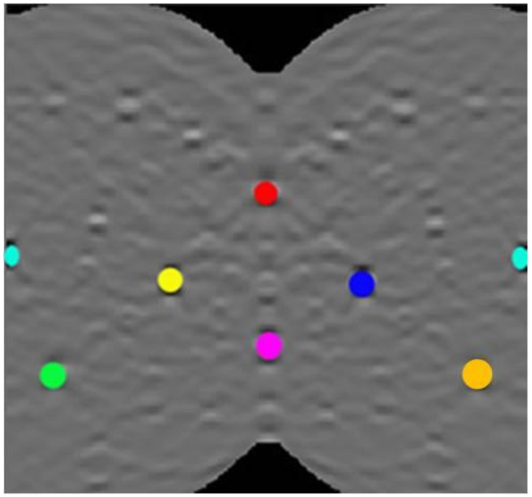


Unit cell U_{ij}
Rotation (φ, θ, ψ)

Best match

Simulated databank

Image correlation

Common procedures:

- Known crystal U_{ij}
  - → orientation (φ, θ, ψ)
  - → phase (best match U_{ij})
  - → strain (optimize U_{ij})
- Unknown crystal?

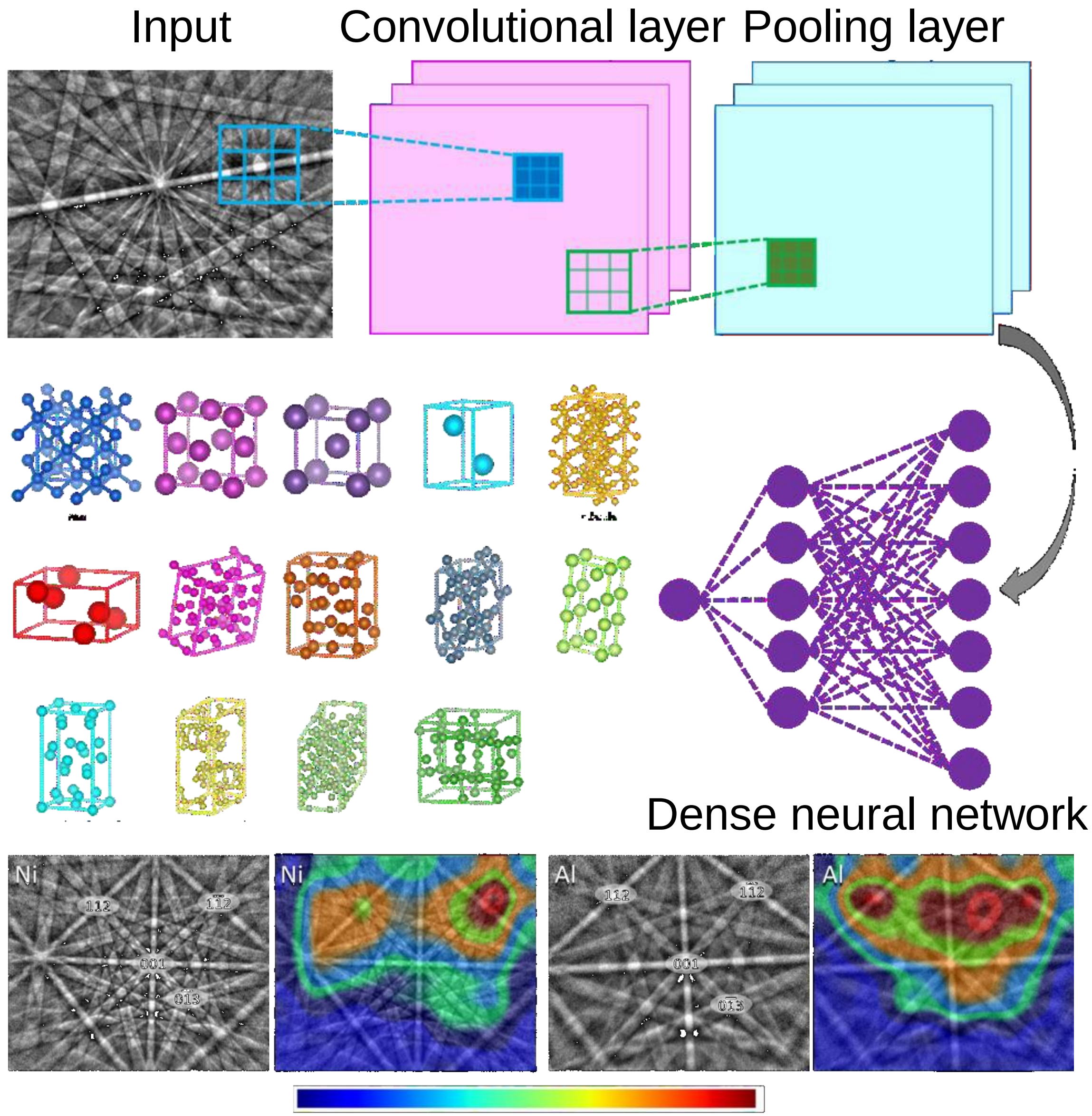
EBSD: symmetry of unknown phases

Training:
40 crystals, each 640 patterns
- Each pattern covers limited range of reciprocal space
- Redundancy sampled over multiple grain orientations

Validation:
1 of 14 Bravais lattices

300 000 patterns (3 TB)
same 40 crystals
- ResNet50: 89~100%

50 000 patterns
different 9 crystals
- ResNet50: 93.5%
- Xception: 91.2%

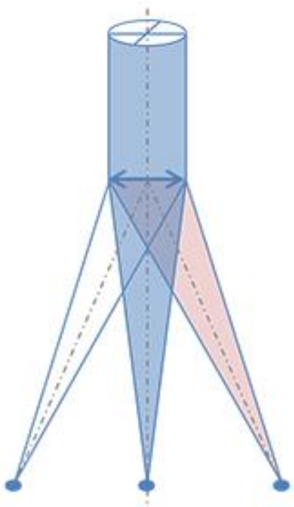


Forward electron diffraction

Parallel beam | Convergent beam | Large angle convergent beam

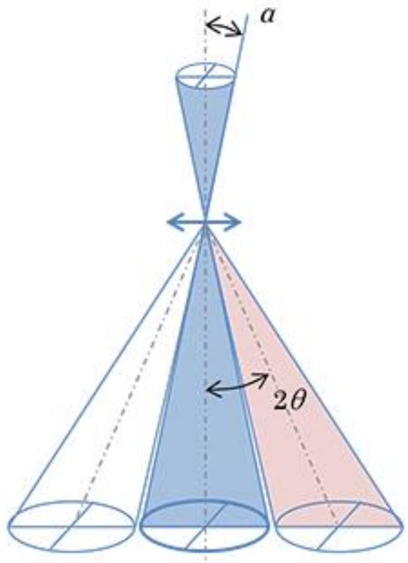
$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

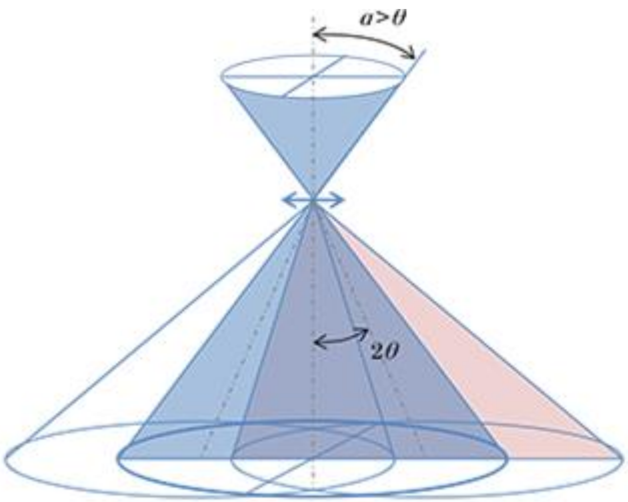
$$\Delta x \cdot \Delta \theta \geq \frac{\lambda}{2}$$



Sample

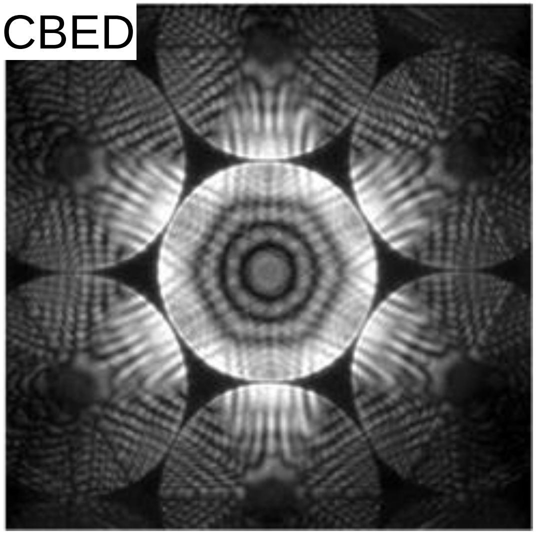
Back focal plane



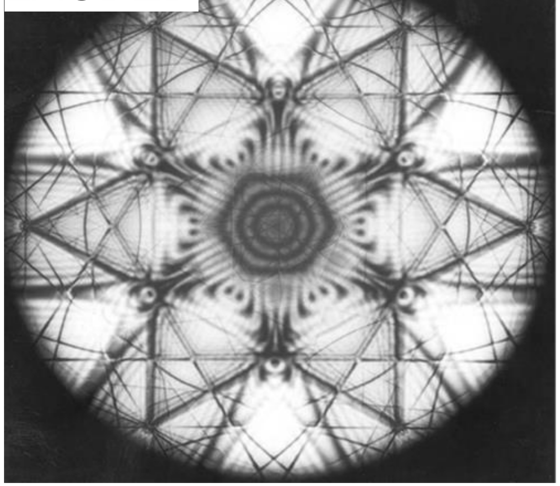


SAED

CBED



LACBED



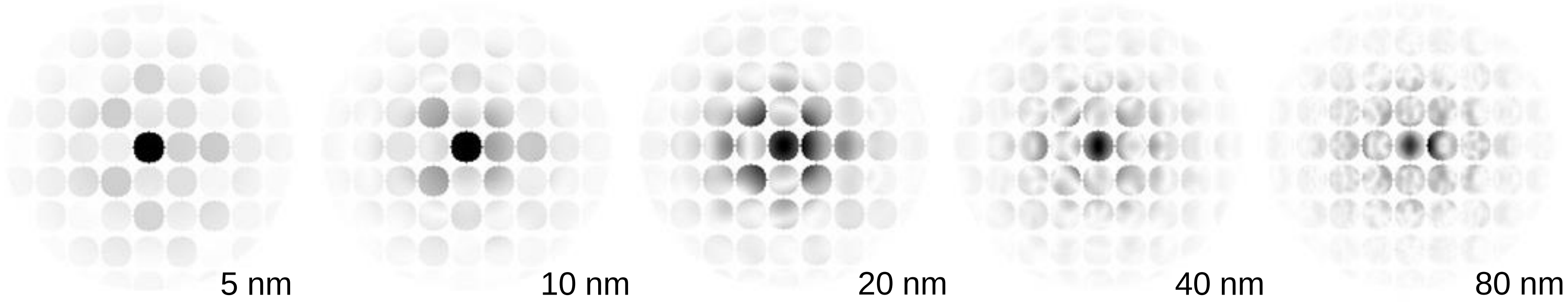
Diffraction patterns of Si [111] (200 keV). www.jeol.co.jp

Coherency in electron diffraction

- Diffraction depends on
  Unit cell U_{ij}
  Rotation (φ, θ, ψ)
  Thickness (oscillitary!)

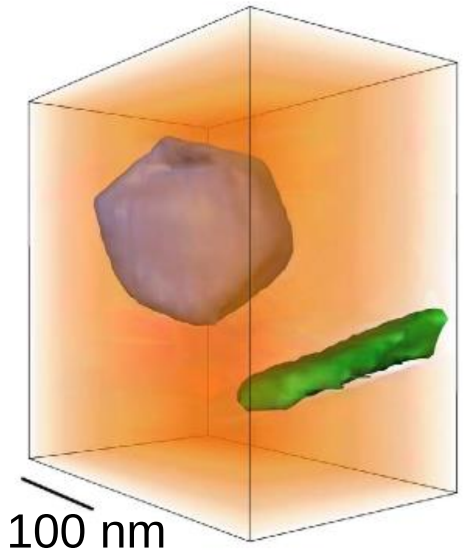
- Kinematic approximation rarely applies
  mean free path a few tens of nm,
  especially small at Bragg conditions.

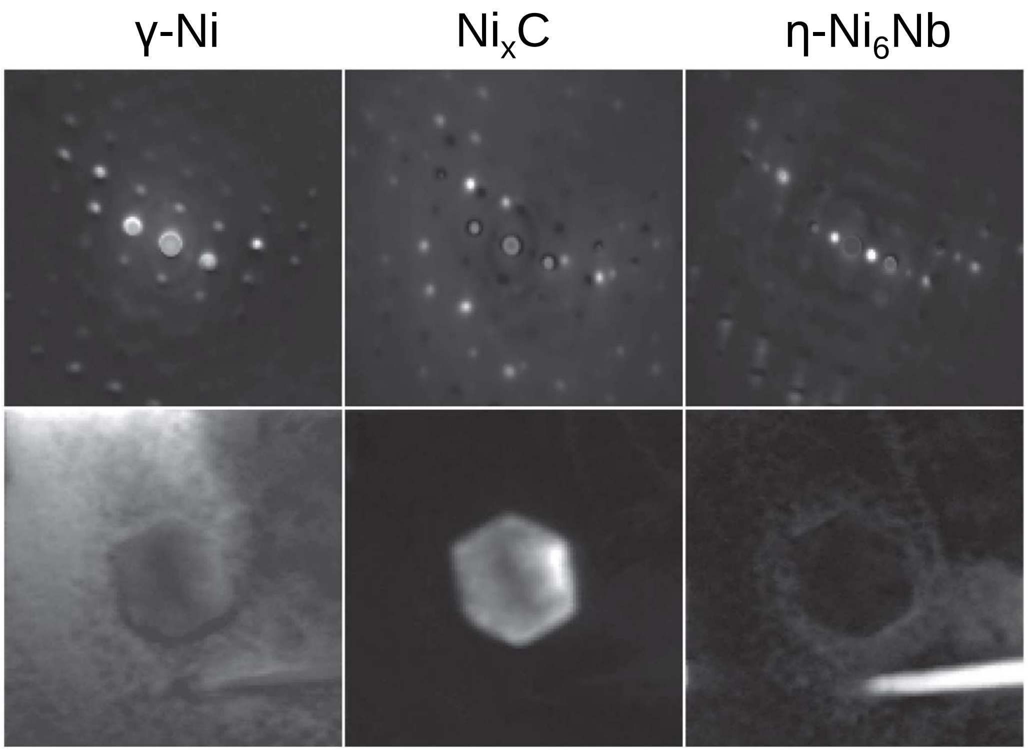
- Simulation with wave propagation
  through multiple thin slices.



Convergent beam diffraction pattern of $BiFeO_3$
I. Maclaren, *et al.* Ultramicroscopy 154, 57 (2015)

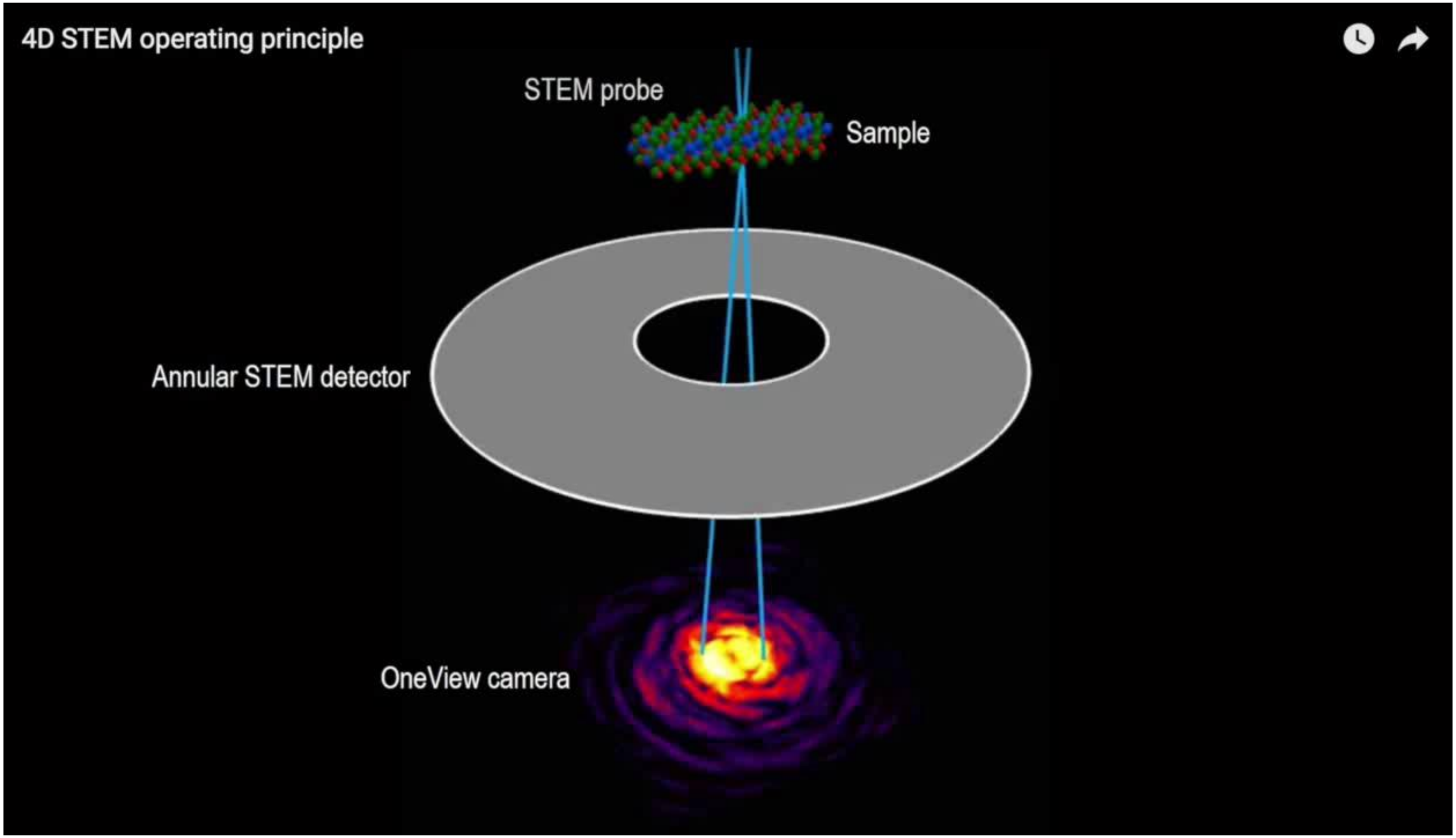
Diffraction imaging: orientation

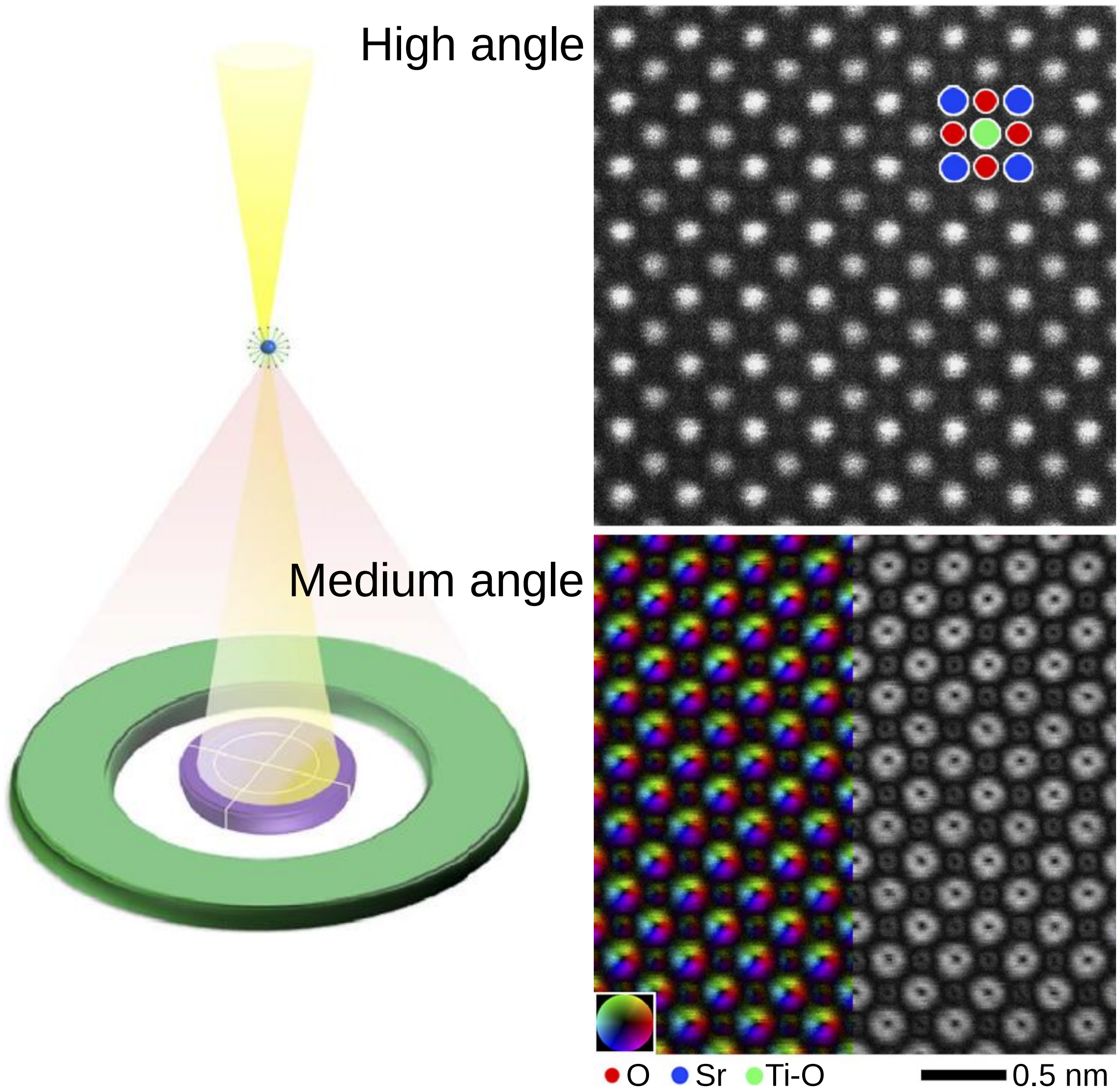




- 20 NMF components to capture all 3 phases.
- Need further sparsification:
most components account for intensity variation due to changes in strain/thickness

4D-STEM goes atomic resolution



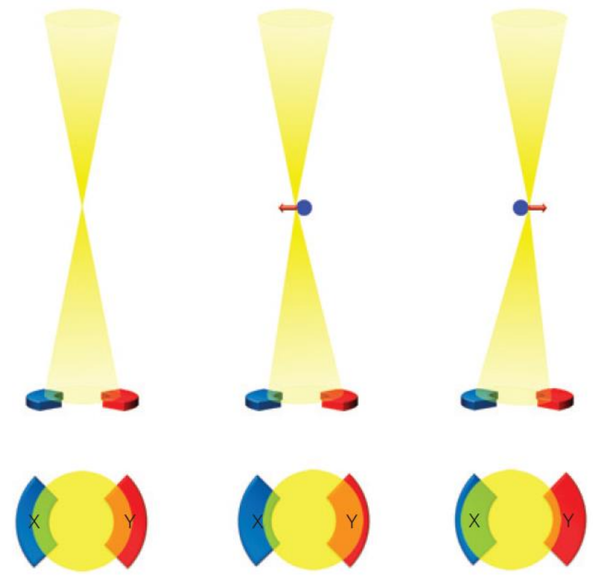


High-angle annular dark field (**HAADF**)

Rutherford scattering:

$$\frac{d\sigma}{d\cos\theta} \propto \frac{N(Z - f(\theta))^2}{(1-\cos\theta)^2}$$

- ➢ **Z (mass-thickness) contrast**



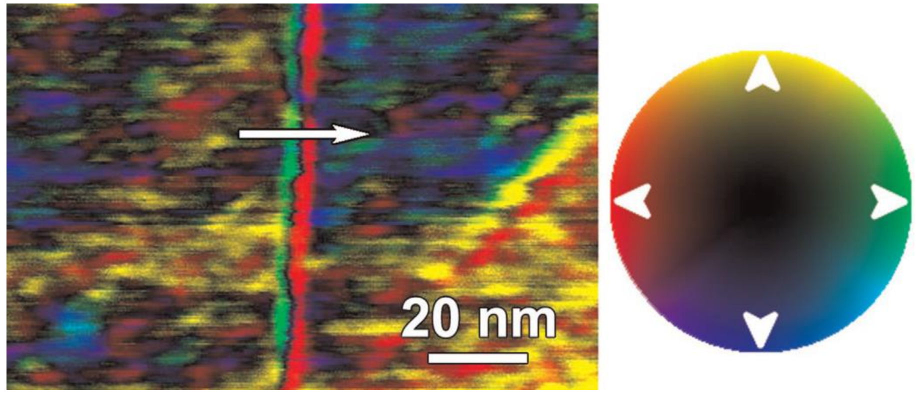
- ➢ **Differential phase contrast**

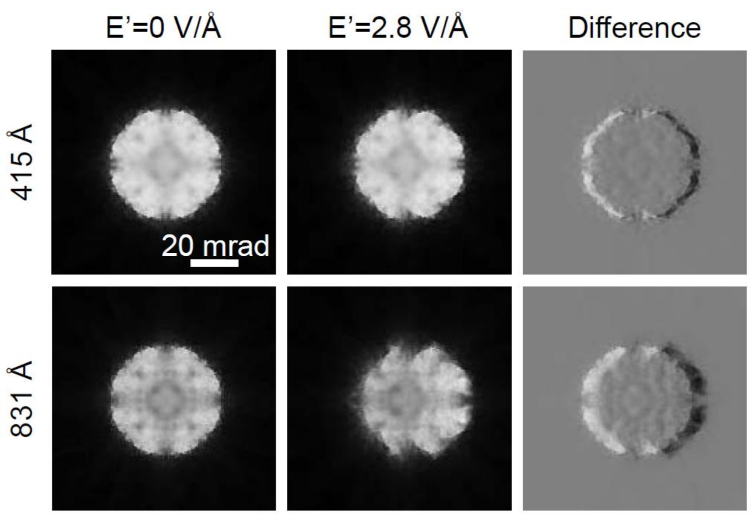
Shibata *et al.*, Nat. Phys. 8, 611 (2012); Nat. Commun. 8, 15631 (2017)

Interpretate differential phase contrast

Ferroelectric phase boundary $BiFeO_3$

I. Maclaren, *et al.* Ultramicroscopy 154, 57 (2015)

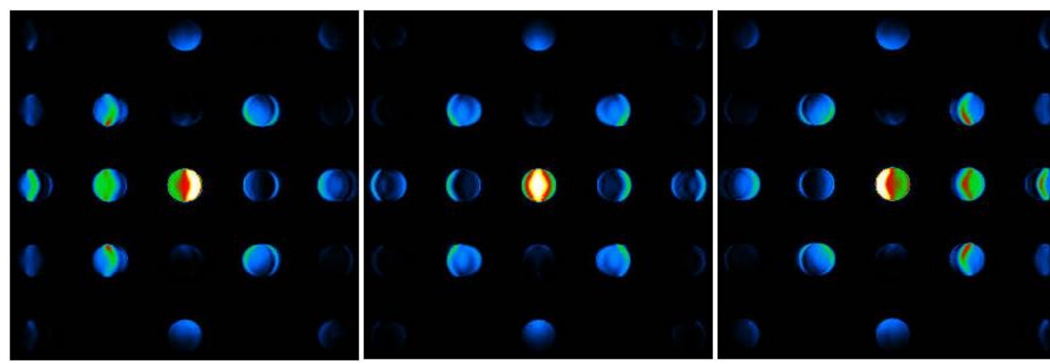




Shift of diffraction disc in free electric field

Shibata *et al.*, Nat. Phys. 8, 611 (2012)

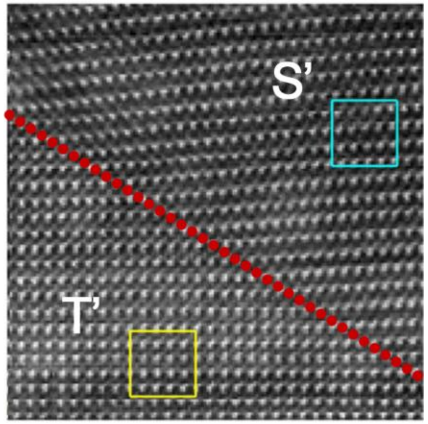
20 nm thickness



Shift of disc intensity centroid at the phase boundary

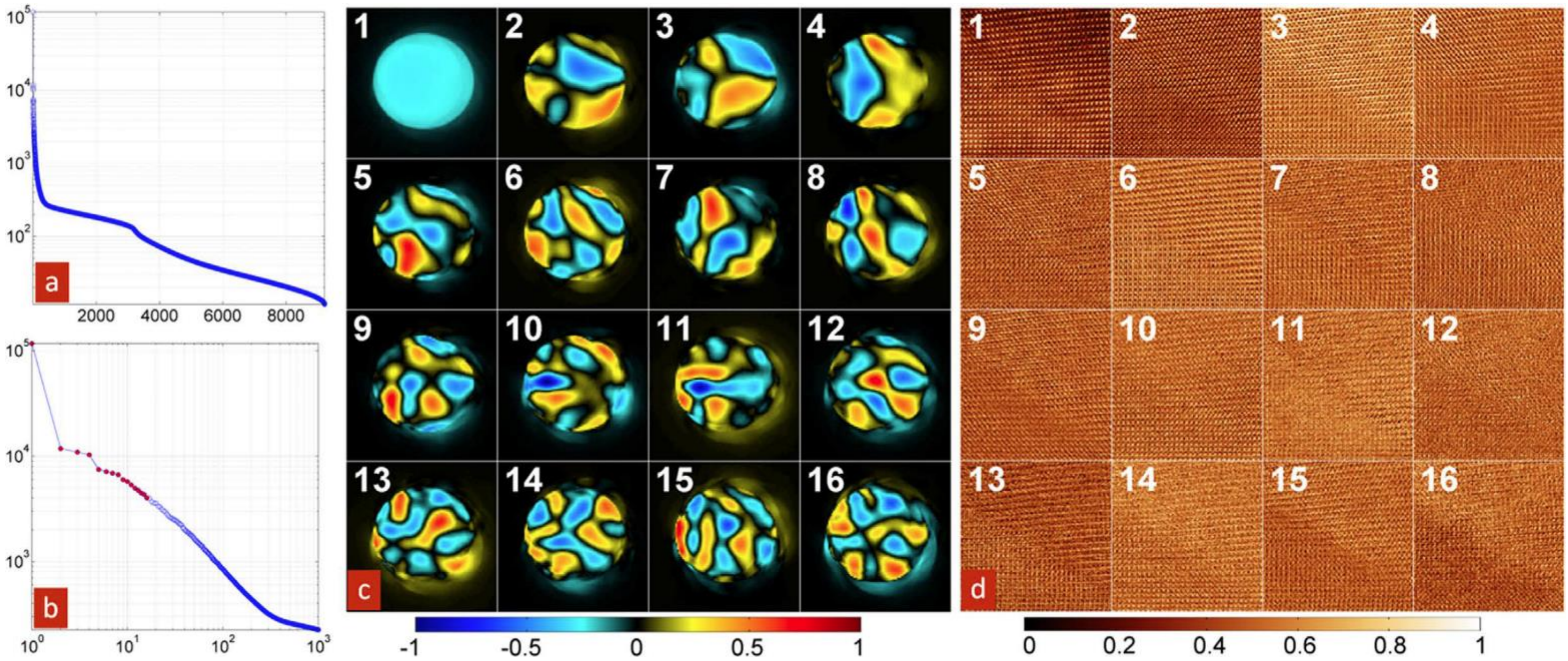
Sparsify atomic resolution 4D-STEM

BiFeO_3 domain boundary



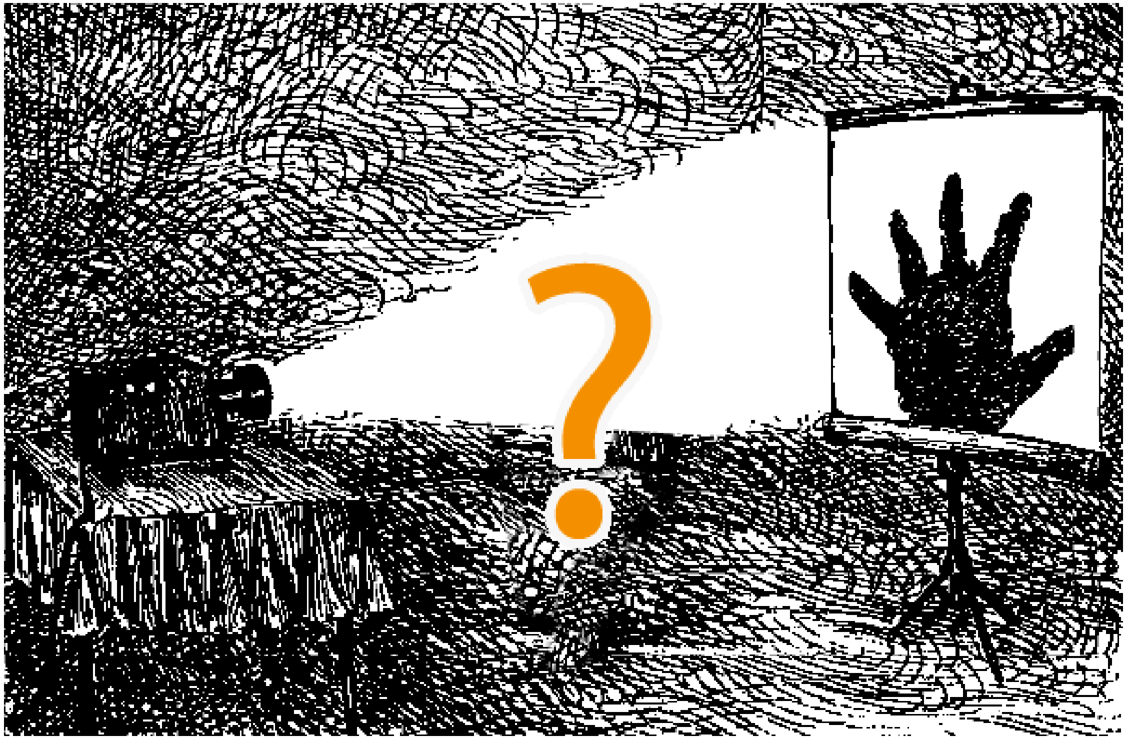
Data not sparse despite only 2 grains:

- CBED pattern varies on the relative position of the electron probe in the unit cell.
- High dynamic range of intensity within the CBED pattern, sensitive to the thickness;

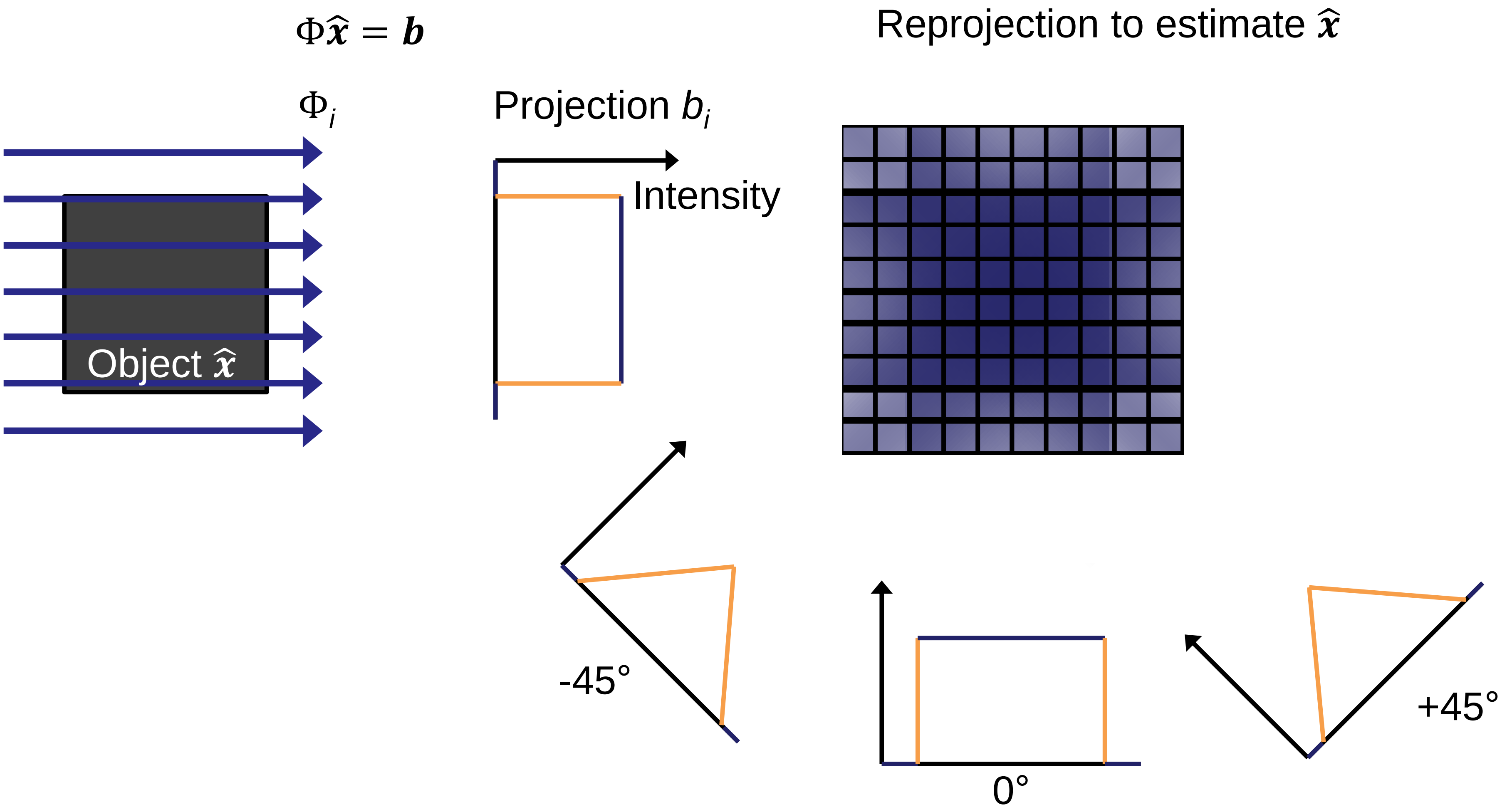


For the last 10 minutes

- Electron microscopy and big data
- Sparsify big data
- **Make use of sparsity in big data**
  Compressed sensing in electron tomography

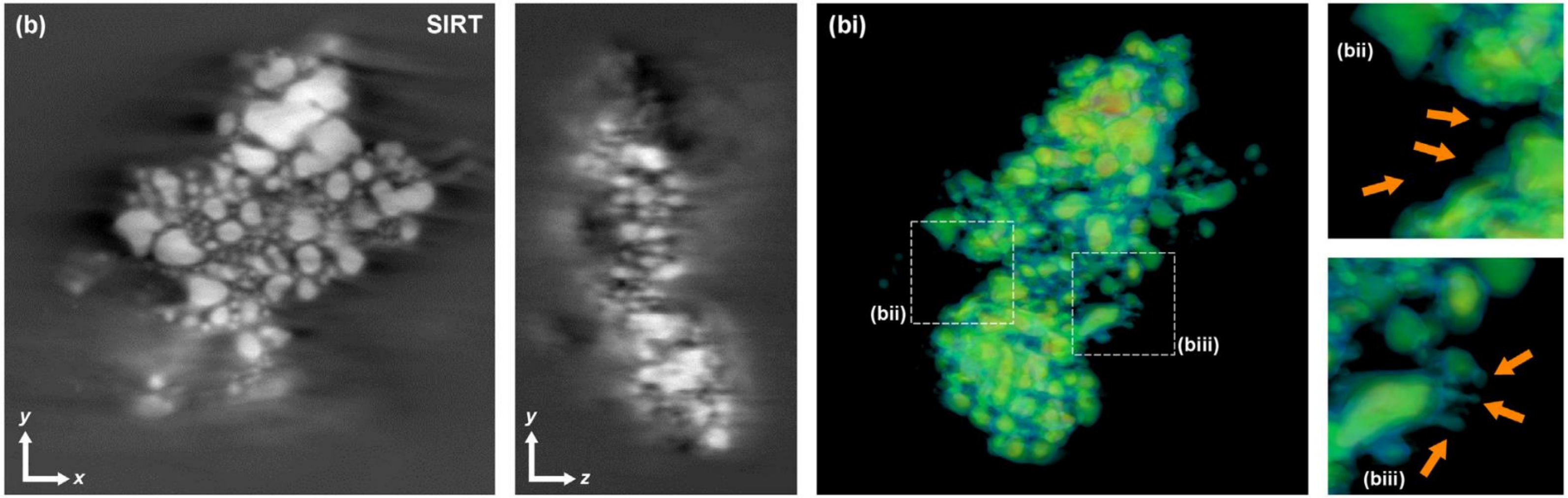


Tomogram reconstruction

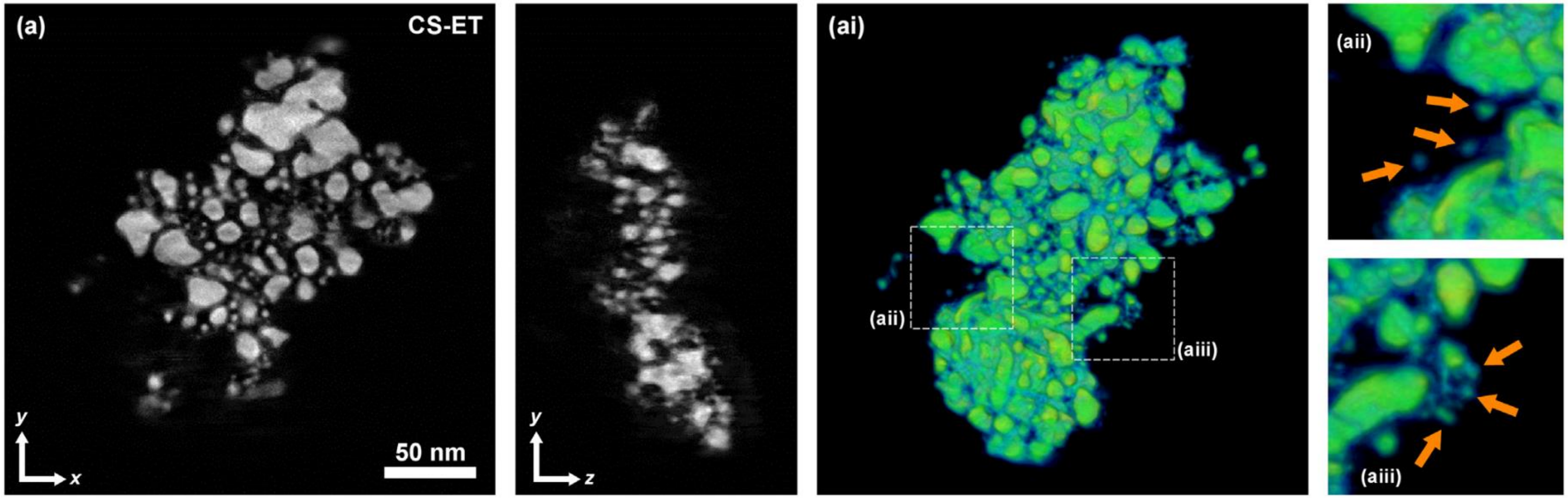


Application of compressed sensing

$$\hat{\boldsymbol{x}} = \arg\min\{\|\Phi\hat{\boldsymbol{x}} - \boldsymbol{b}\|_{l_2}^2\}$$



$$\hat{\boldsymbol{x}}_\lambda = \arg\min\{\|\Phi\hat{\boldsymbol{x}} - \boldsymbol{b}\|_{l_2}^2 + \lambda\|\Psi\hat{\boldsymbol{x}}\|_{l_1}\}$$, e.g., Ψ = I, or $\Psi = \nabla$



R. Leary, *et al.*, Ultramicroscopy **131**, 70 (2013).

Summary

- Electron microscopy and big data

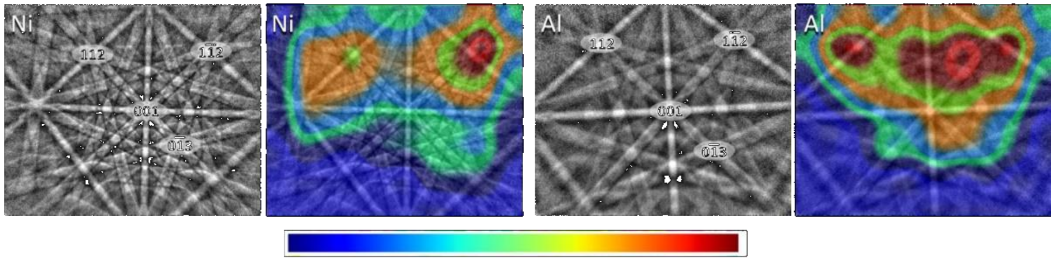
- Sparsify big data

  Multivariate analysis
  Clustering

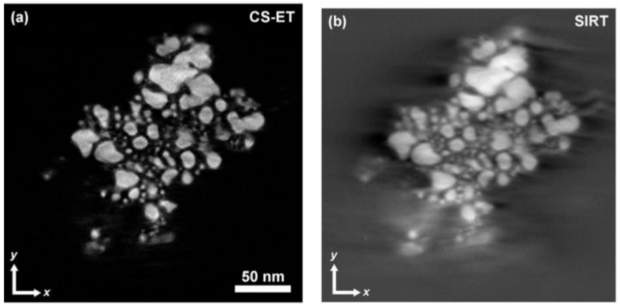
- Sparsify diffraction imaging data?

  Machine-learning driven

  opportunities in 4D-STEM
  challenges in coherent data



- Make use of sparsity in big data
  Compressed sensing in
  tomogram reconstruction



Thanks for your attention!

Christina Scheu, Ruben Bueno Villoro, Raquel Aymerich Armengol, Gerhard Dehm, Christian Liebscher, Silas Wolff-Goodrich, Ali Ahmadian, Ye Wei, Michael Beetz

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