Artificial neural network for automatic alignment of electron optical devices

Enzo Rotunno

Summary

Introduction to Artificial Intelligence

- What is AI and why to use it
- What is machine learning
- What is an artificial neural network

State of the art in electron microscopy

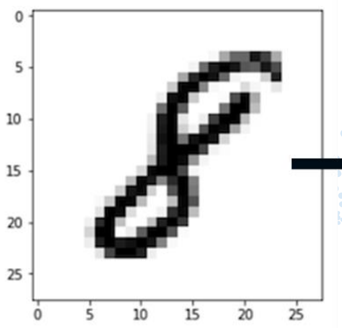
- Key role in automatic alignment
- Electron beam shaping

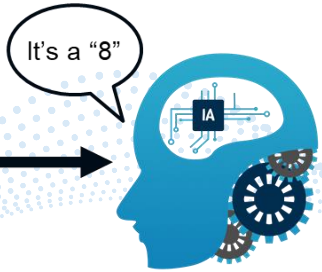
AI automation examples:

- Automatic tuning of optical systems within the microscope
- Real-time optimisation of experiments
- Workflow: from sample to model

Machine learning and neural networks

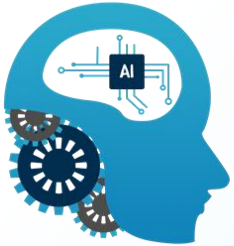
Artificial intelligence (AI) is **the ability of a computer to do tasks** that are usually done by humans because they require human intelligence and discernment.





Canonical example: reading hand-written digits

AIs perform seemingly impossible tasks with speed exceeding conventional algorithms.

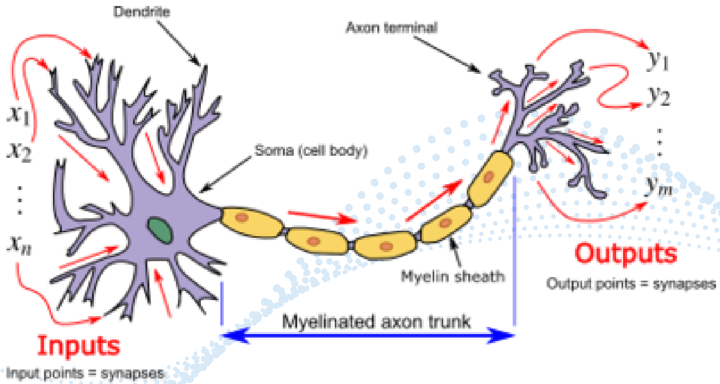


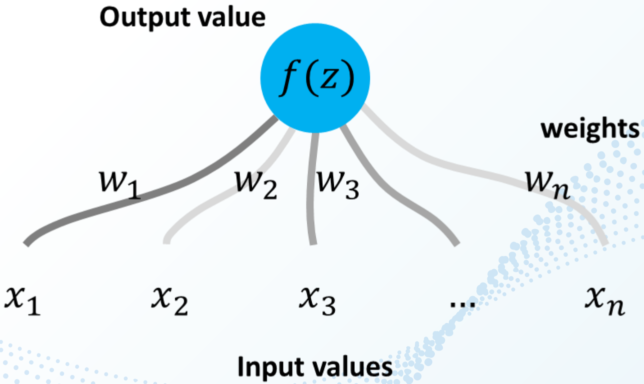
Machine learning is a method of data analysis that automates model building. It is based on the idea that systems can learn from data

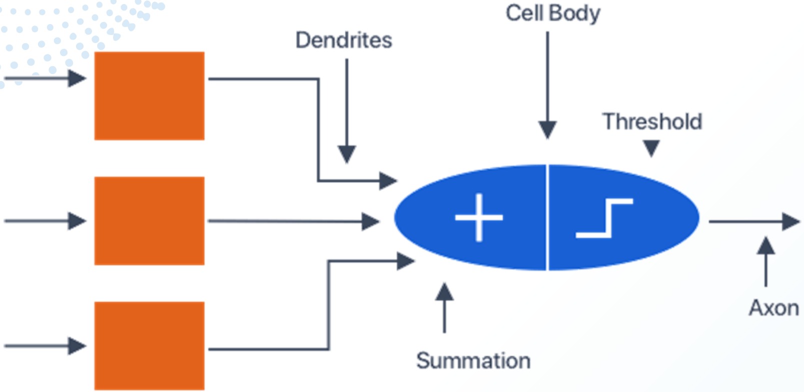
Artificial neural networks (ANNs) are **computing systems inspired animal brains**.

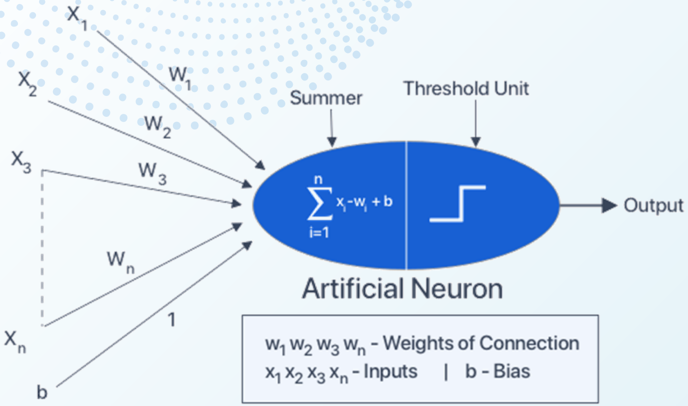
Artificial Neural Network

Artificial Neural Networks are biologically inspired network of artificial neurons configured to perform specific tasks.



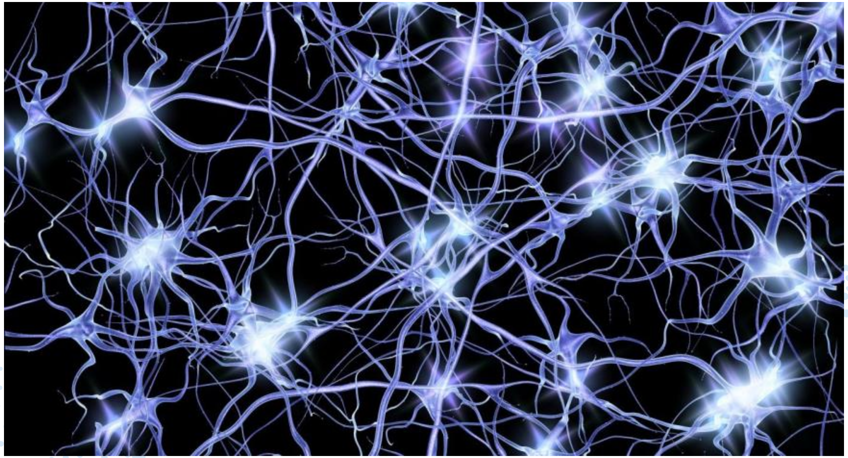






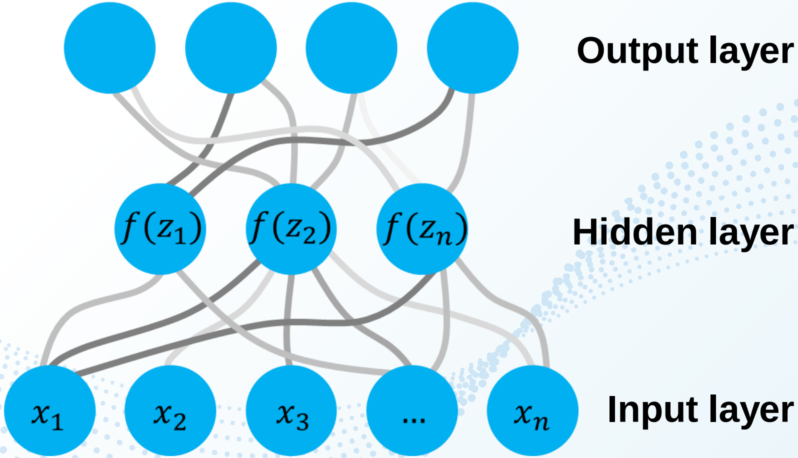
Artificial Neural Network

Brain



The human brain is a **network** composed of more than 100 billion neurons.

ANN

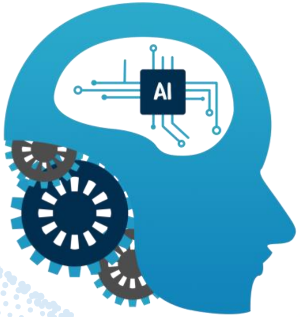


$$z_j = \sum_i w_{ij} x_i + b_j$$

Learning is a minimisation problem

Universal approximation theorem: Any function f(x) can be approximated

General application



Speech

- Speech recognition
- Text to speech
- Speech to text

Computer vision

- Image recognition
- Classification
- Anomaly detection

Robotics

- Industrial automatization
- self driving vehicles

Language

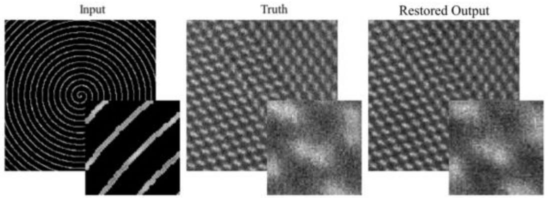
- Translation
- Information extraction

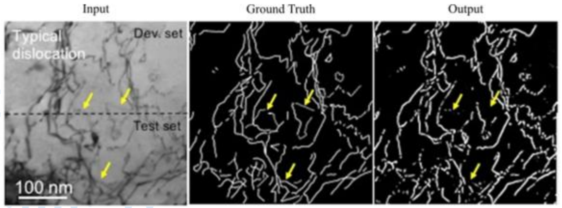
Other

- Predictive analytics
- Decision making
- consumer behaviour
- social media recommendation engines

Electron microscopy applications

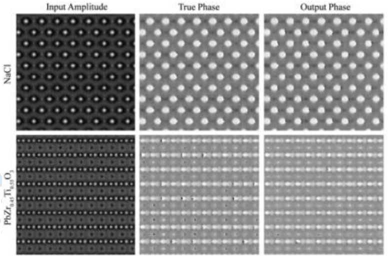
Image processing

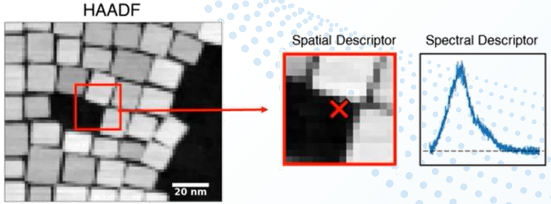




De-noising, restoration, segmentation, compressed sensing

Data analysis





Exit wave reconstruction, holography and ptycography

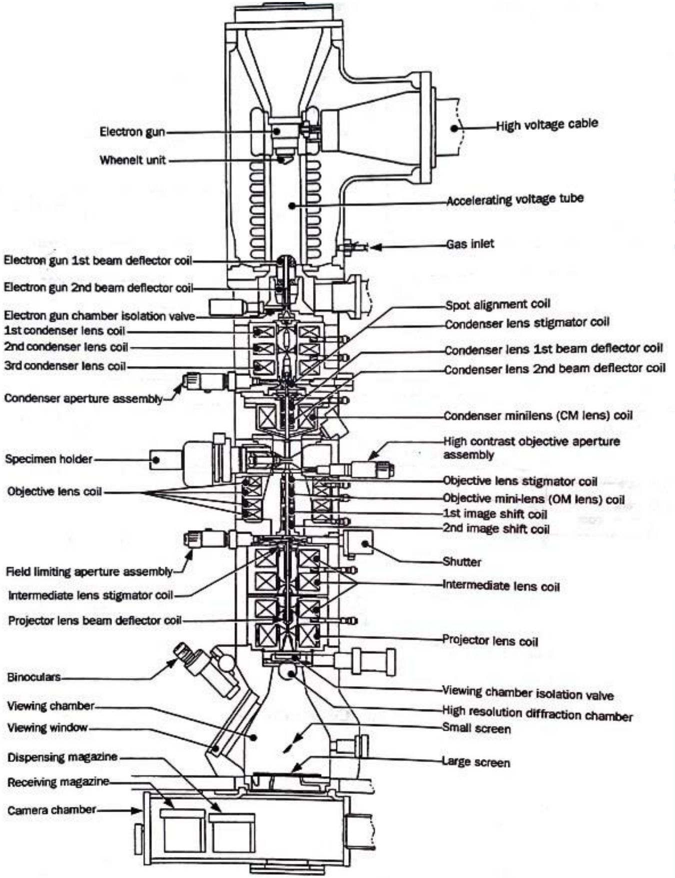
Automation

Only a few timid approaches to automatic alignment.

J.M. Ede, *Mach. Learn.: Sci. Technol.* **2** (2021) 011004

TEM automation

Automation is not a new idea in electron microscopy



In its basic configuration, a TEM is a fairly complicated machine.

Modern microscopes are equipped with a:

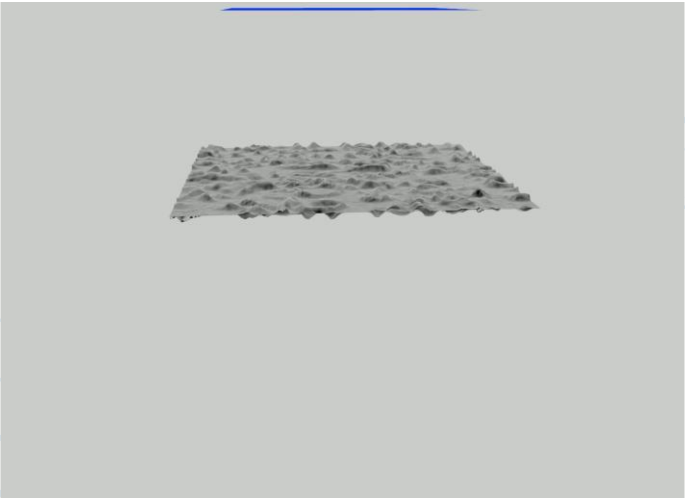
- A number of cameras
- Detectors
- Energy filters
- Spectrometers
- Aberration correctors

Coming very soon a variety of beam shaping devices

As research progresses this complexity is becoming the true bottleneck of further instrumental development

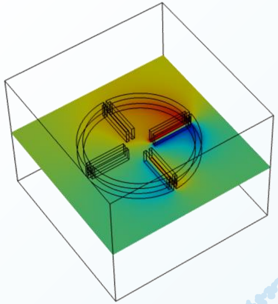
Beam Shaping: the next frontier

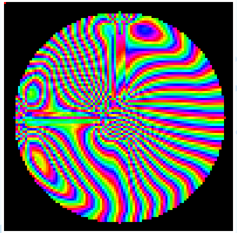
Ensemble of techniques used to control the shape of the electron wave function



A. Tavabi et al. Phys. Rev. Lett. **126** (2021), 09480
Bechè et al. Nat. Phys. **10** (2016) 26
A.M. Blackburn Ultramic. **136** (2014) 127–143
Vanacore et al Nat. Mat. **18**, (2019) 573–579
G. Pozzi et al., Ultramicroscopy **181**, 191 (2017)
Verbeeck, et al., Nature **467** (2010) 301–304
A.M. Blackburn et a. Ultramicroscopy **136** (2014)
A. Tavabi, et al. Scientific reports **8** (1), 5592

We exploits MEMS technology to put electrodes directly along the electron beam path





We use fields

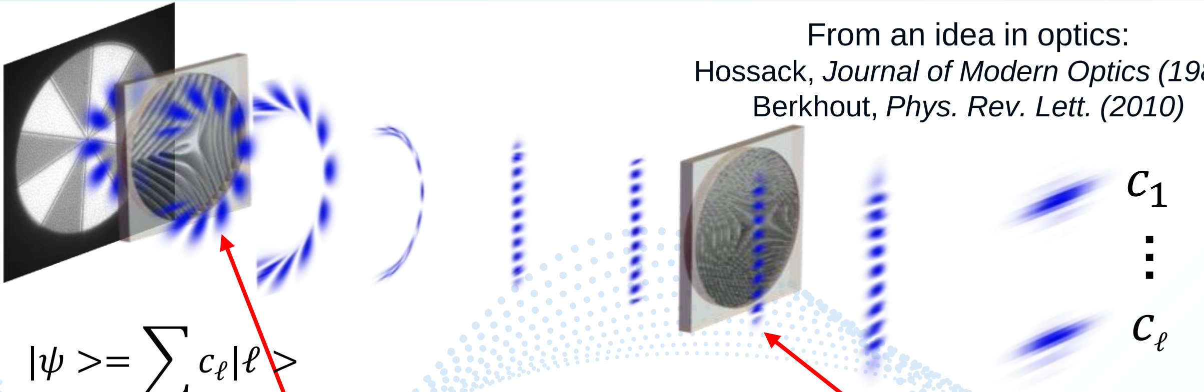
$$\varphi' = C_E \int_{-\infty}^{\infty} V dz + \frac{e}{h} \int_{-\infty}^{\infty} A_z dz$$

The phase shift depends on the electric and magnetic fields

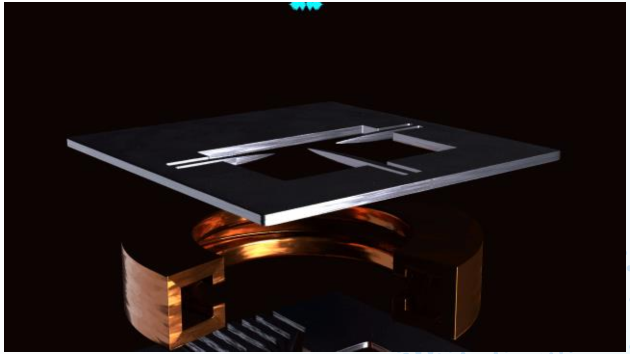
We can arbitrarily tune the phase:
programmable phase plate!

The OAM sorter

From an idea in optics:
Hossack, *Journal of Modern Optics (1987)*
Berkhout, *Phys. Rev. Lett. (2010)*

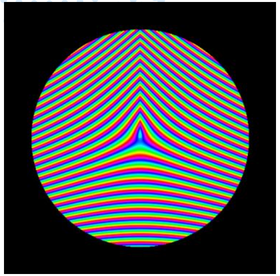


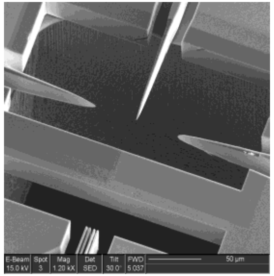
$$|\psi> = \sum c_\ell |\ell>$$



A spectrometer able to measure the orbital momentum of electrons

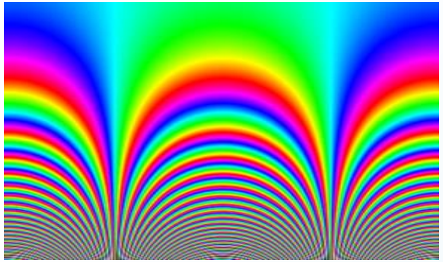
Unwrapper (S1)

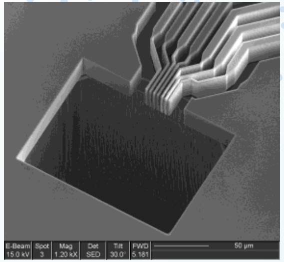




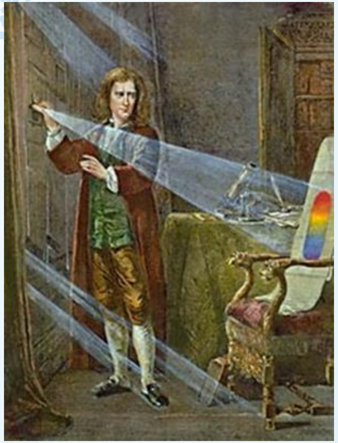
$$W_{12}(x,y) = \frac{ka}{f_1}\left(y\tan^{-1}\frac{y}{x} - x\log\left(\frac{\sqrt{x^2+y^2}}{b}\right) + x\right)$$

Corrector (S2)





$$W_{21}(u,v) = -\frac{kab}{f_1} e^{-\frac{u}{a}} \cos\left(\frac{v}{a}\right)$$



Sorter alignment: crucial point

Electron wavefunction | S2 element phase | PSF

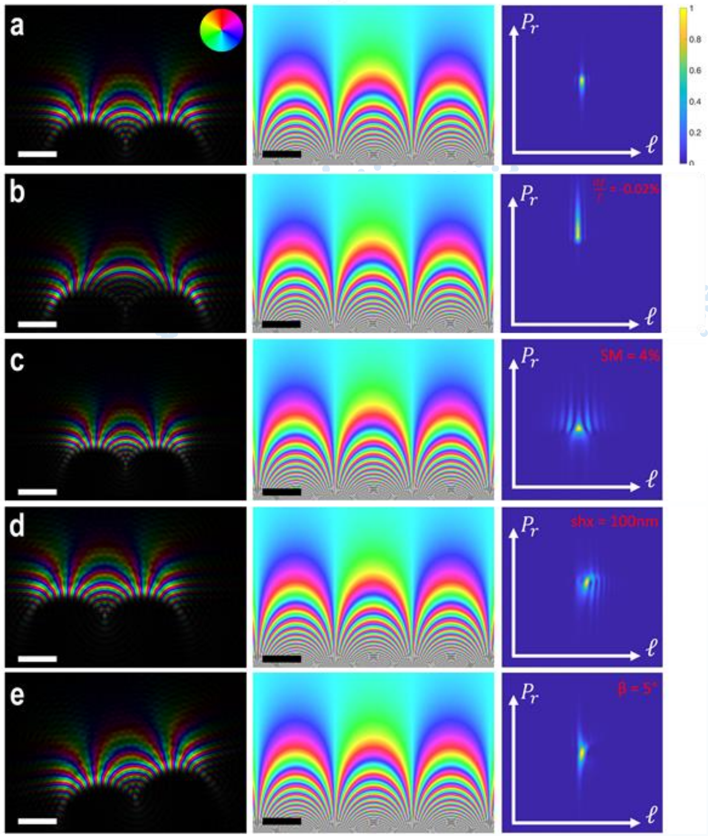
Perfect Match

Defocus (df)

Size mismatch (SM)

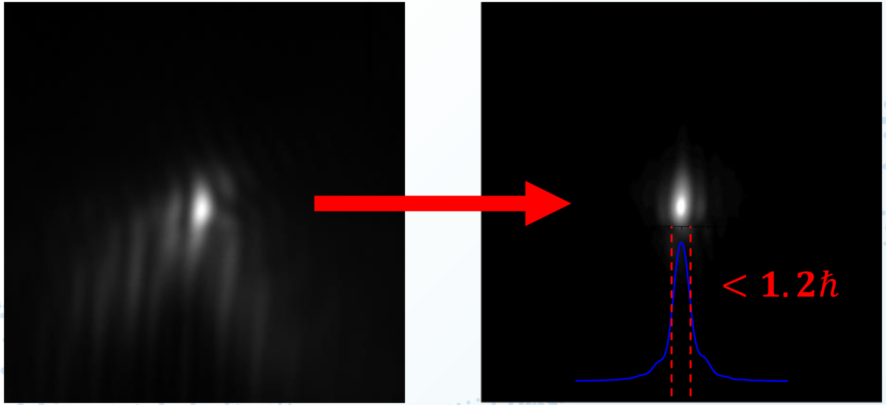
Position (shx and shy)

Rotation (β)



marker is 5 μm

Typical situation | Perfect alignment



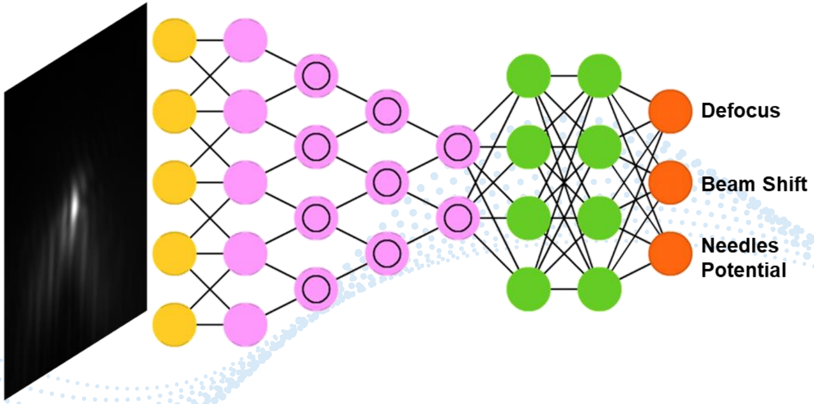
Manual alignment of the sorter is possible but takes several minutes and a certain degree of skills.

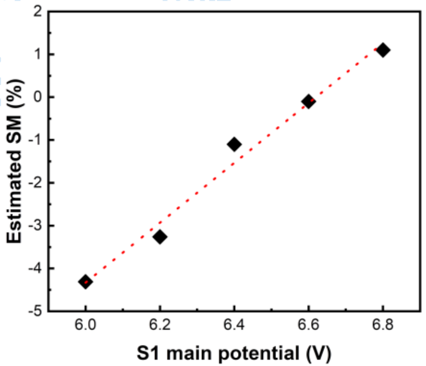
We want to move the focus from the alignment of the sorter to the actual material investigation

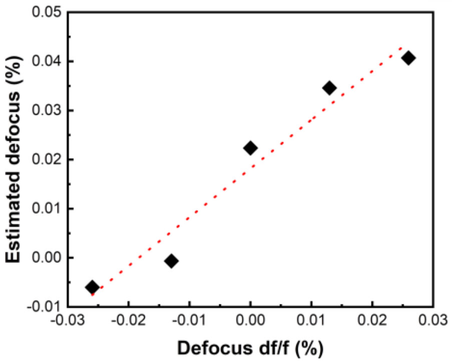
We need a fast and reliable alignment tool

Fitting aberrations with an ANN

Convolutional neural network is a class of deep neural networks most commonly applied to analysing visual imagery

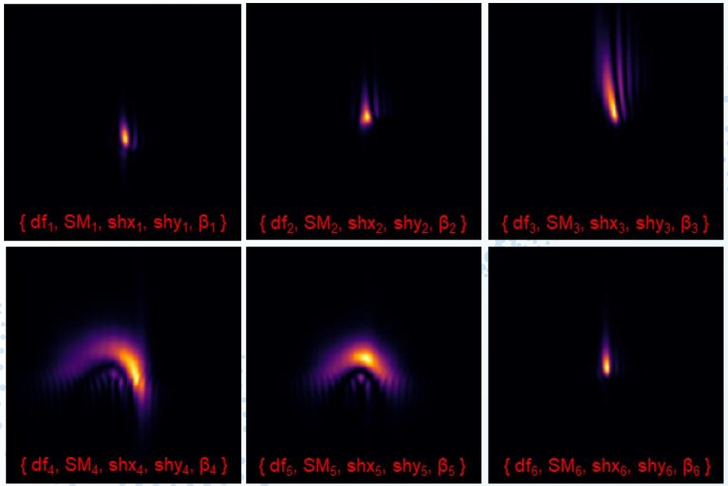






We can still improve through an iterative process.

We prepared a database of **20000** simulated spectra. Plus a second database of **2000** images for validation.



We used a free space propagation algorithm based

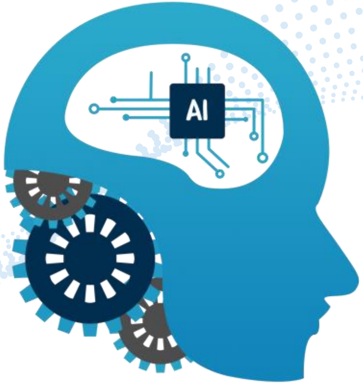
$$U_z(u,v) = \frac{e^{ikz}}{i\lambda z} \iint U_0(x,y)\, e^{-ik\frac{xu+yv}{z}} dxdy$$

And a simple quadratic phase term for the lenses:

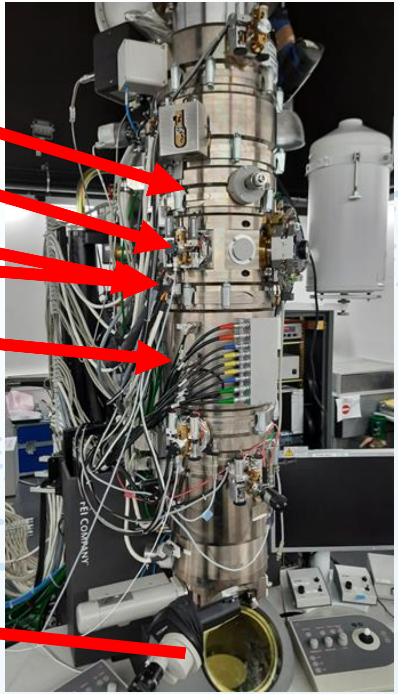
$$\Psi_L = e^{i\frac{\pi r^2}{f\lambda}}$$

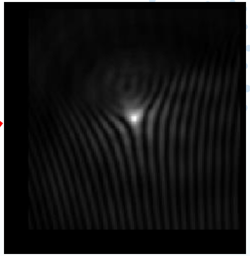
Automatic Alignment

We only applied 1/5 of the correction to get rid of fitting error and make the CNN more stable.



df
SM
shx
shy
β



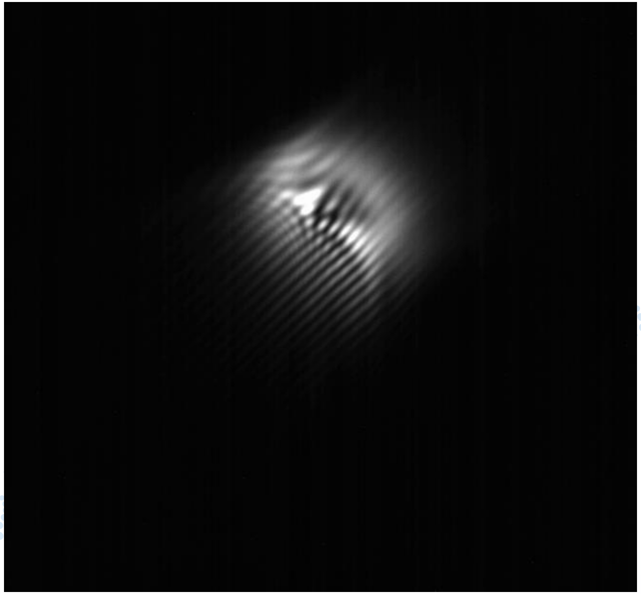


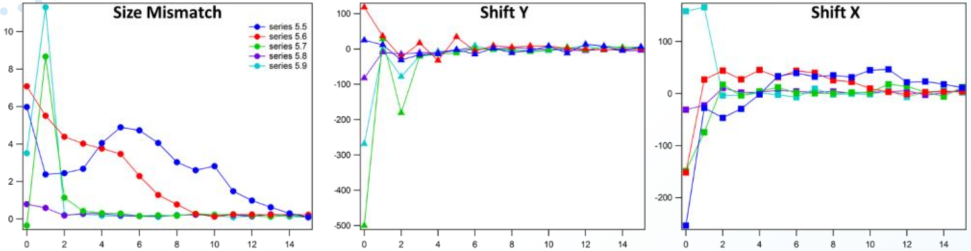
Direct readout from camera

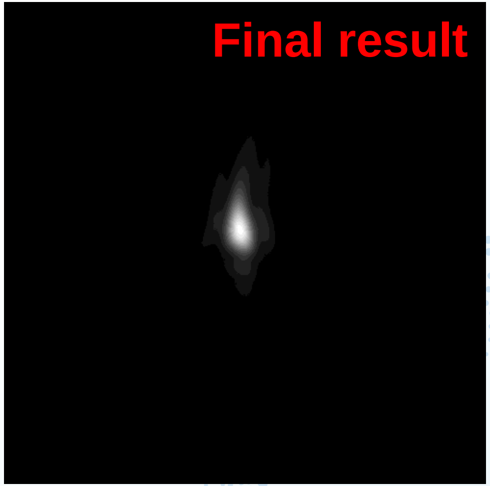
The CNN is connected to the microscope throughout a python based interface

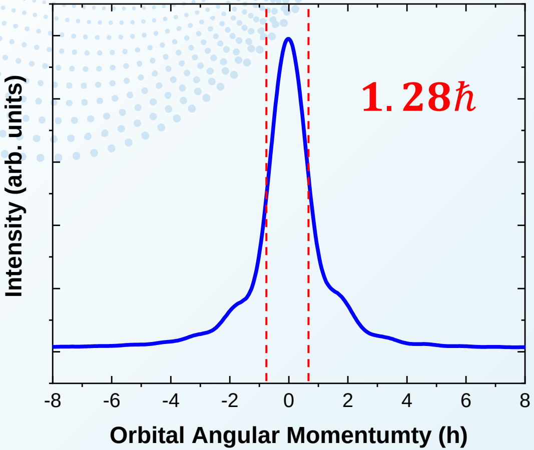
Credit: Dieter Weber
Alexander Clausen

Automatic Alignment





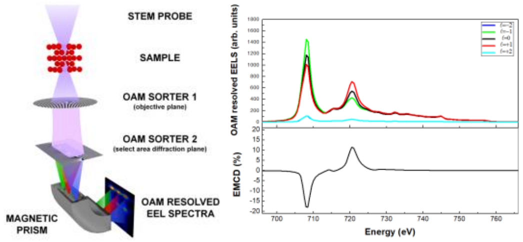




Credit: Paolo Rosi

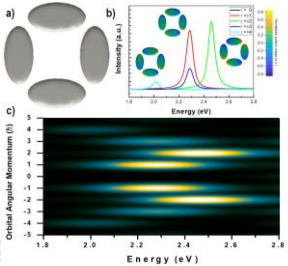
OAM sorter applications

Electron magnetic chiral dichroism



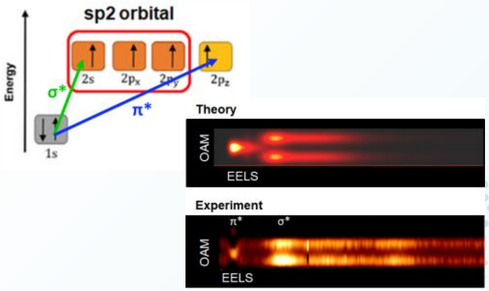
E. Rotunno *et al.* Phys. Rev. B **100** (2019), 224409.

Study of plasmon symmetry



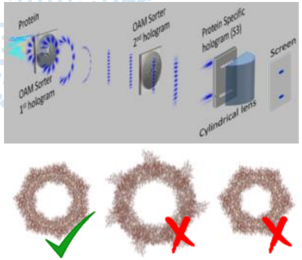
M. Zanfrognini *et al.* ACS Photonics, **6** (2019), 620-627.

Orbital mapping



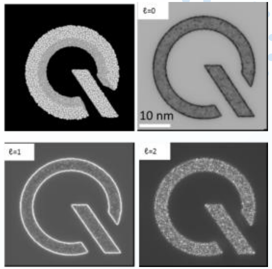
G. Bertoni *et al.* Microsc. Microanal, *26* (2020), 1752-1753

Identification of molecular structures



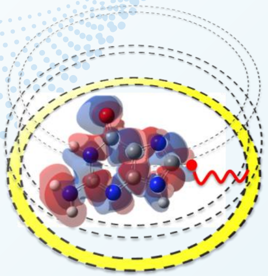
F. Troiani et al. Phys. Rev. A **102** (2020), 043510.

Edge enhancement in STEM



E. Rotunno *et al.* Microsc. Microanal, *26* (2020), 236-238

Molecular electronic transitions

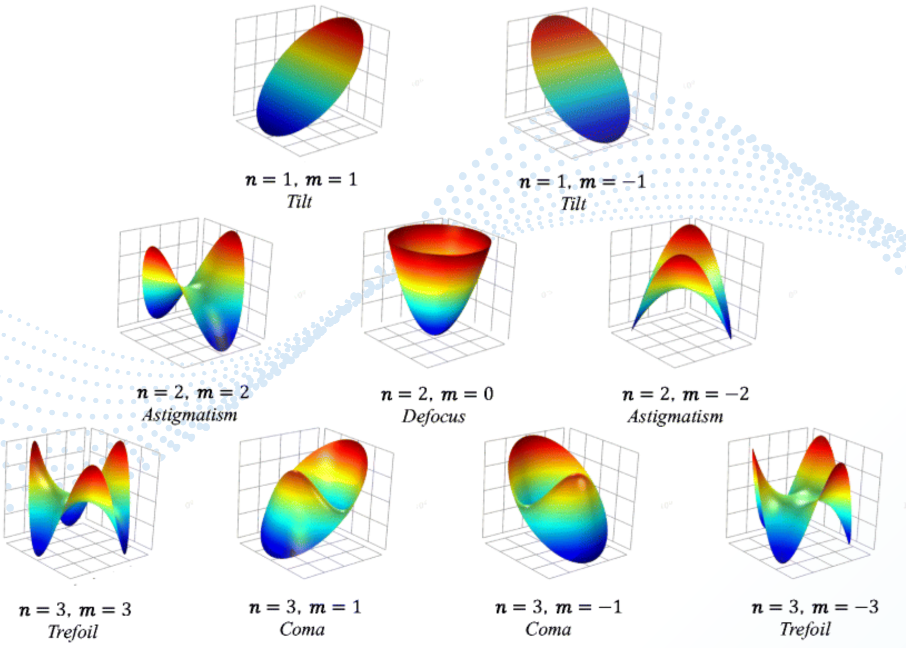


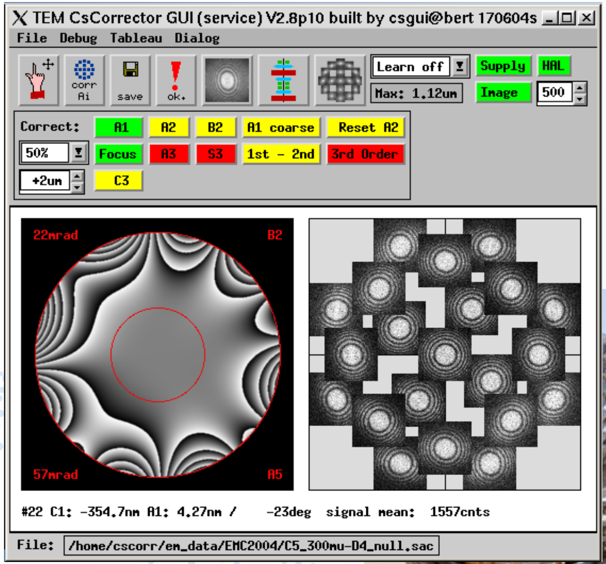
C. Guido, *et al.* J. Chem. Theory Comput. (2021) 17, 2364–2373

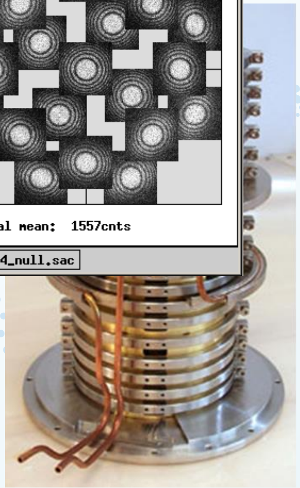
Most of the practical applications of the sorter require a resolution of 1ħ

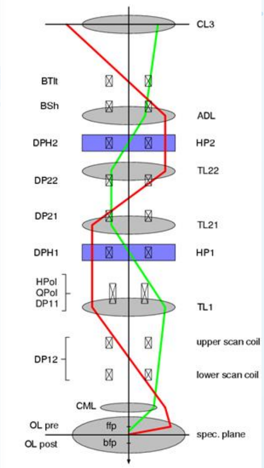
Measuring lens aberrations

Phase profile of axial aberrations



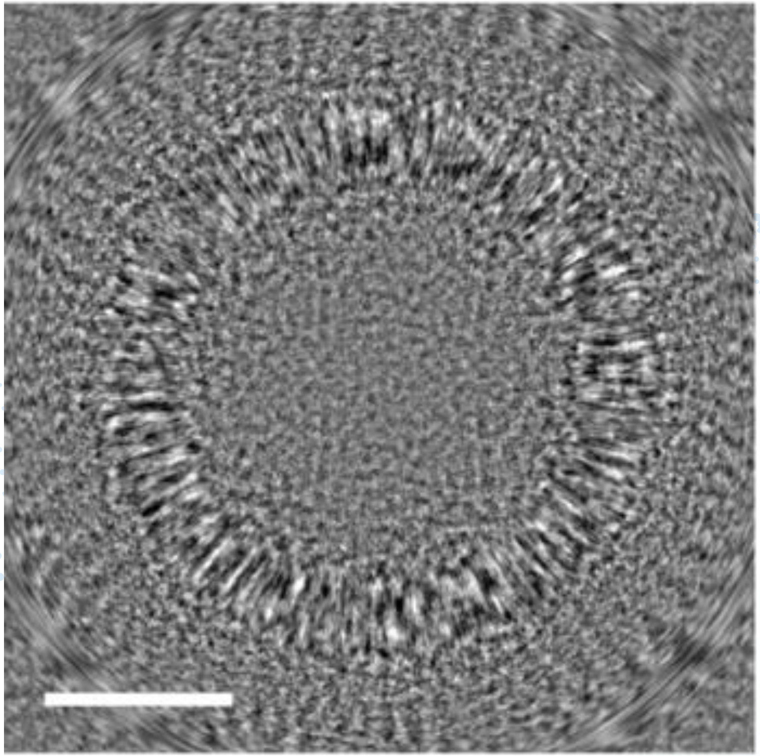






Larger numerical aperture → higher resolutions
Can an ANN do better?

The Ronchigram



Ronchigram is the convergent beam diffraction pattern of an amorphous materials.

The structure of the Ronchigram encodes information about the aberration phase field across the objective aperture.

We build a database of simulated 20000 images

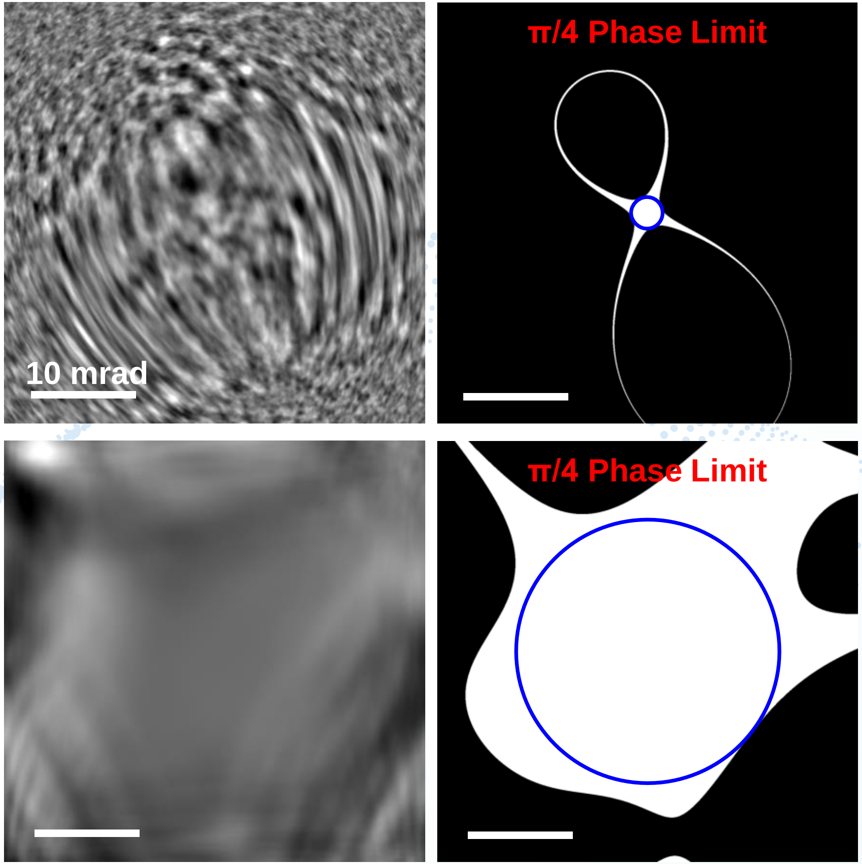
Aberrations range:	ANN fitting error:
C1 (defocus) = [-2000nm, -1000nm]	**MAE = 23 nm**
A1 (2-fold ast.) = [-100nm, +100nm]	**MAE = 5 nm**
B2 (coma) = [-1um, +1um]	**MAE = 49 nm**
A2 (3-fold ast.) = [-1um, +1um]	**MAE = 38 nm**
C3 = [-100um, +100um]	**MAE = 4 μm**

Credit: Giovanni Bertoni

Fitting aberrations with an ANN

before correction

after correction



Quarter wave criterion: we want aberration phase to be below $\frac{\pi}{4}$

$$\alpha = \min\left(|\chi(q)| < \frac{\pi}{4}\right) = 2.8 \text{ mrad}$$

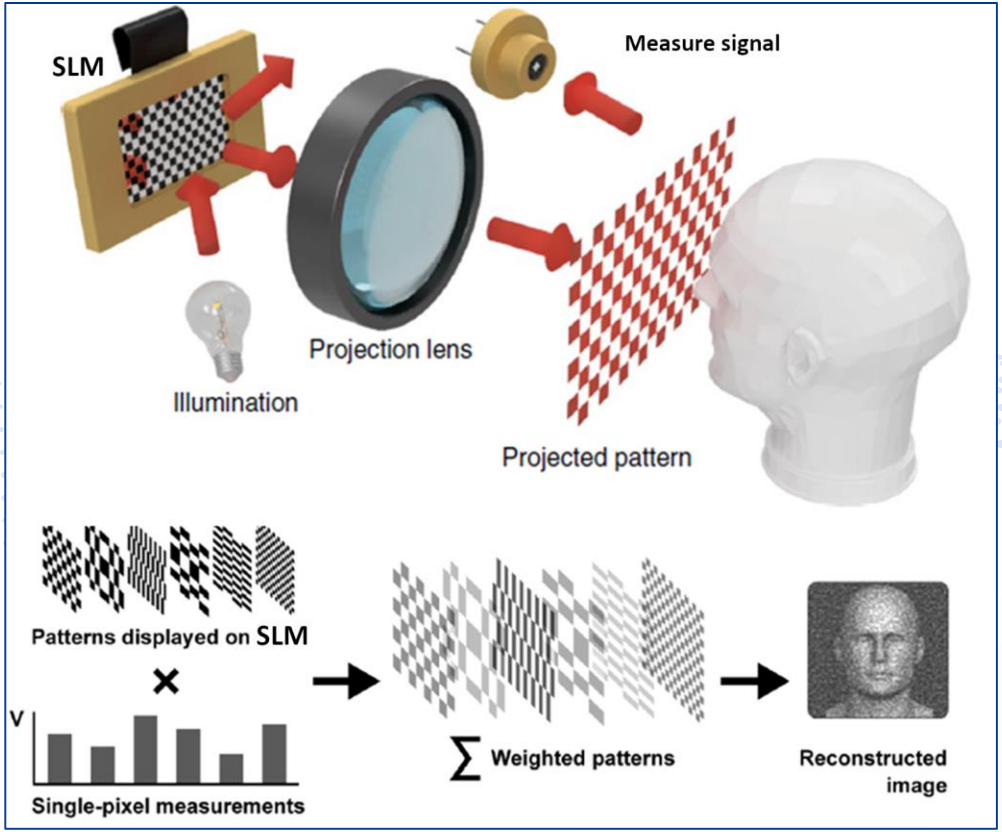
$$d = 0.61\frac{\lambda}{\alpha} = \underline{\underline{4.3\ \text{Å}}}$$

$$\alpha = \min\left(|\chi(q)| < \frac{\pi}{4}\right) = 25.1 \text{ mrad}$$

$$d = 0.61\frac{\lambda}{\alpha} = \underline{\underline{0.5\ \text{Å}}}$$

Comparable with conventional means but probably faster.

Real-time optimisation of experiments



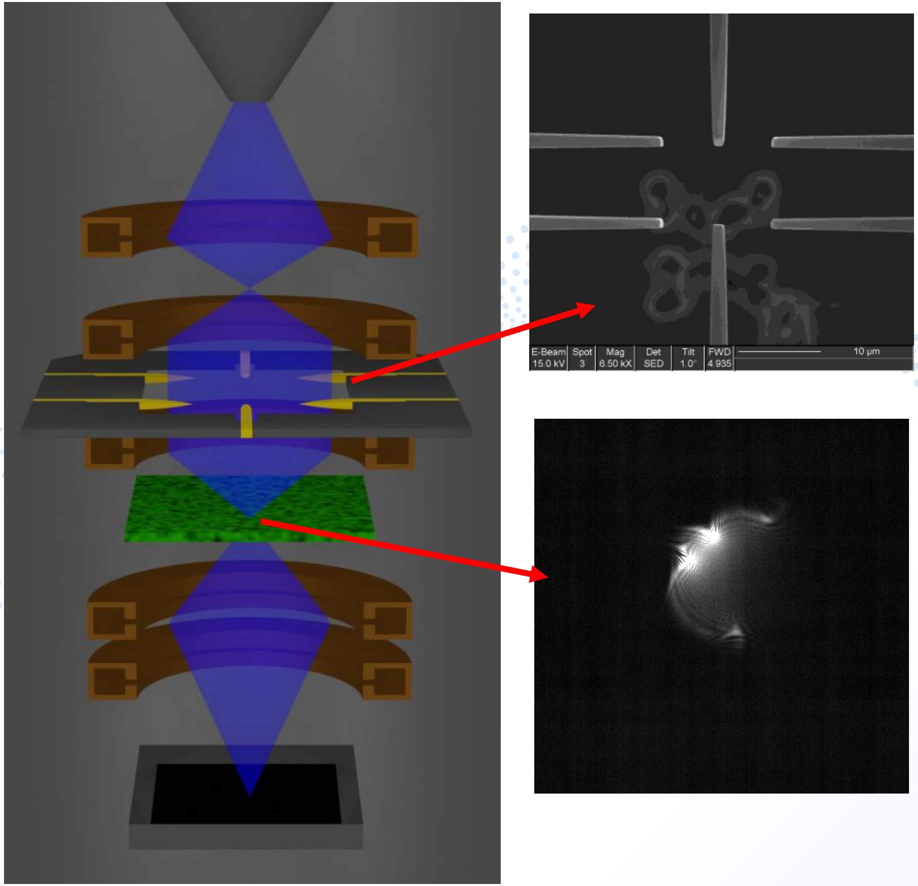
Single Pixel Imaging is a weighted sum of illumination patterns with their respective total transmitted intensity

Benefit: reconstruct the image with less measurements than the number of pixels. Easy implementation of compressed sensing algorithm.

Useful for beam sensitive materials

We need a spatial light modulator for electron beams

Electron Single Pixel Imaging



We can use our custom electron-optics as an illumination pattern generator.

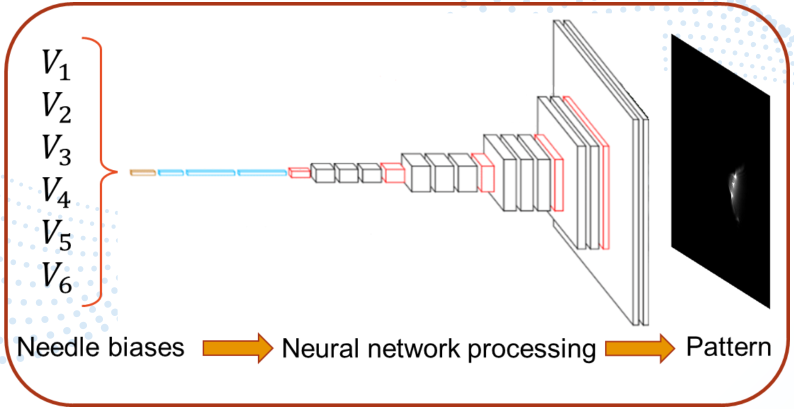
Controlling caustic pattern is a rather challenging problem.

Minor changes of the electric field will significantly affect the quality of the patterns in term of shape and position.

Prediction of caustic patterns with ANN

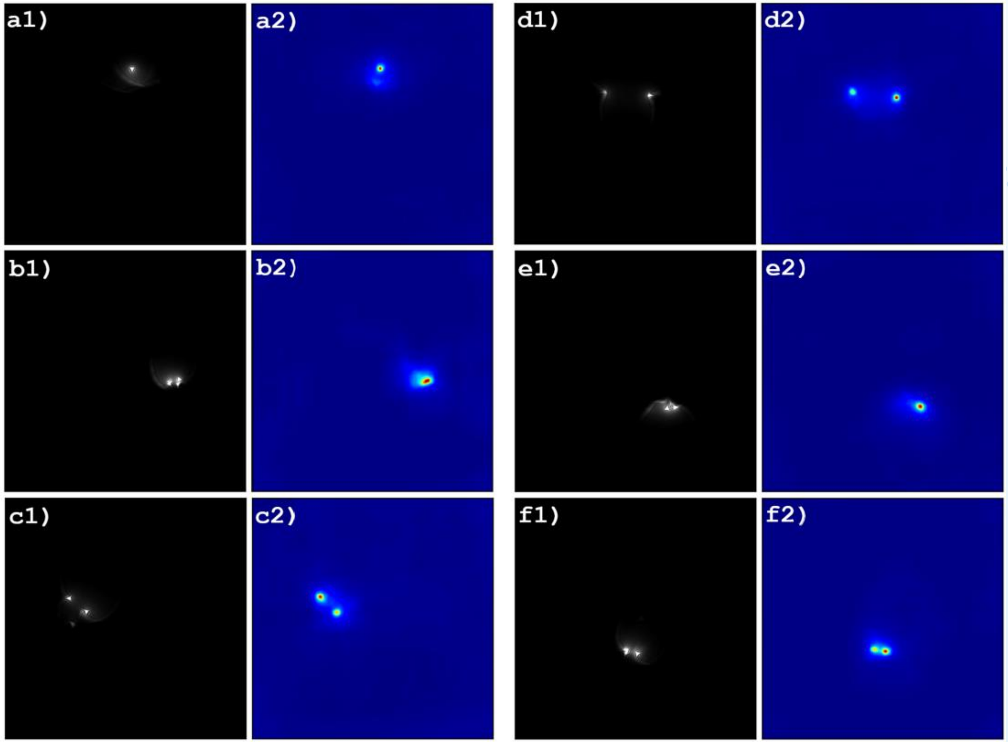
AI can offer two advantages:

1) Improve control over pattern generation
2) Optimize the measurement process



We trained a ANN to return the illumination patterns from the nominal applied biases

Training on experimental data!!!

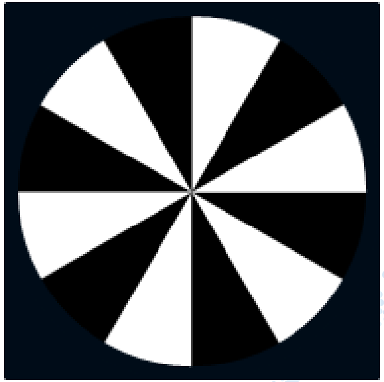


Credit: Lorenzo Viani

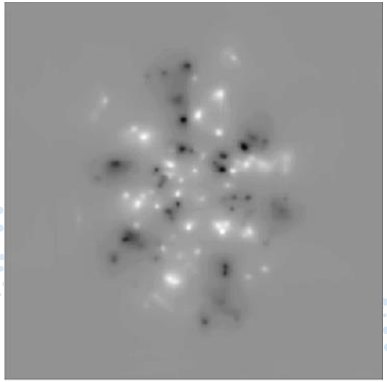
Thanks' to the speed of ANN, patterns can be computed in real time

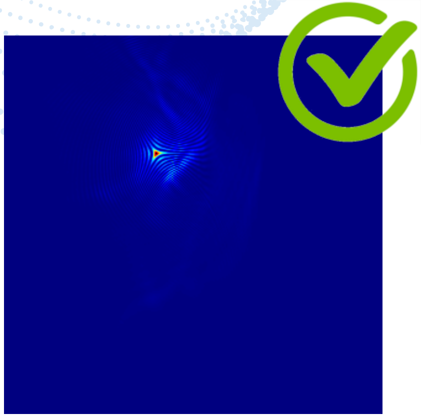
Adaptive pattern generation

Target image

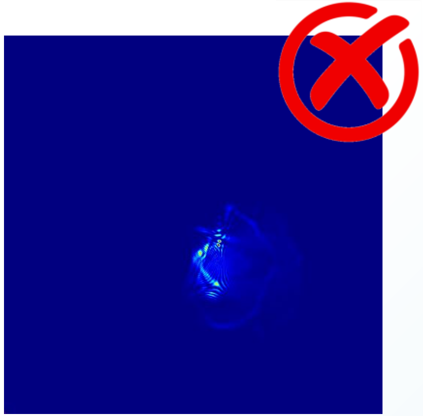


Partial measurement





Good pattern



Bad pattern

Bayesian approach: the partial measurement results are used in real-time to optimise the experiment

Kullback-Leibler divergence

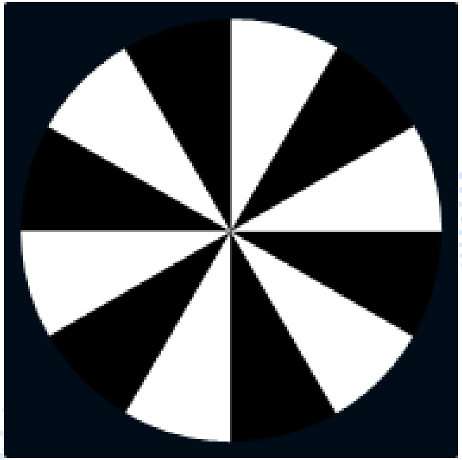
$$D_{KL}(P||Q) = \sum_x P(x) \log\left(\frac{P(x)}{Q(x)}\right)$$

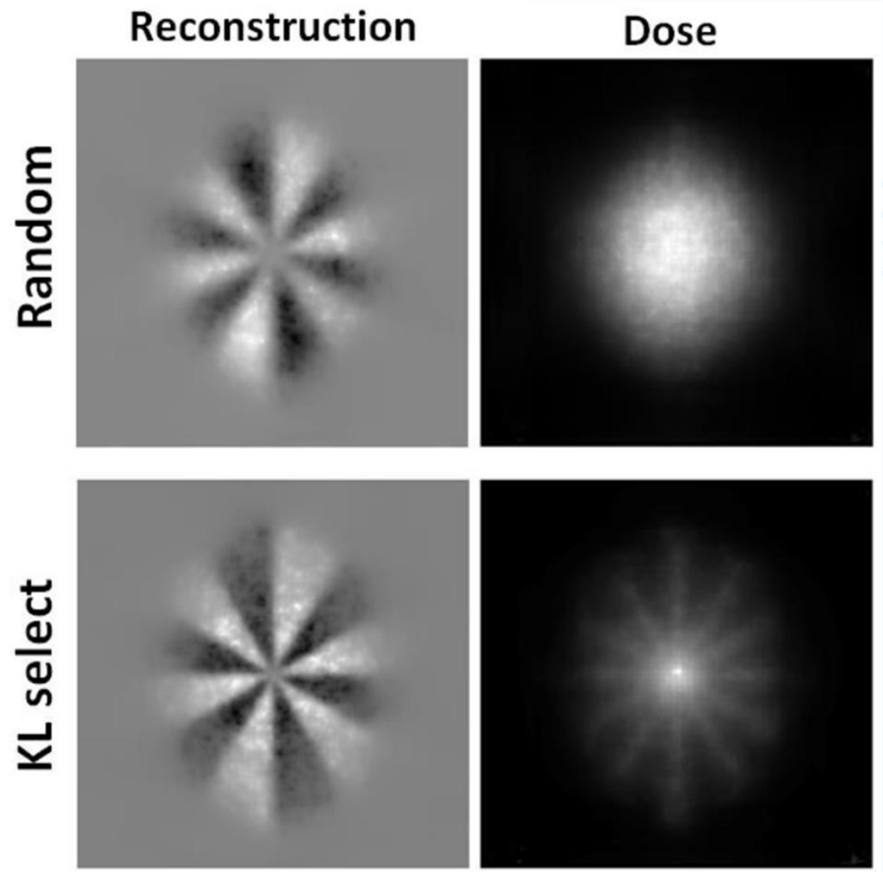
P(x): observed data

Q(x): model used to approximate P(x)

Optimal ESPI conditions

Target image





Two reconstructions obtained with the same number of patterns (5000).

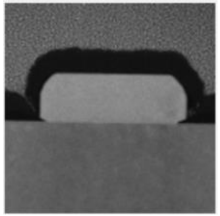
The algorithm implementing KL divergence produces sharper images by distributing the dose where it is most needed.

Workflow automation

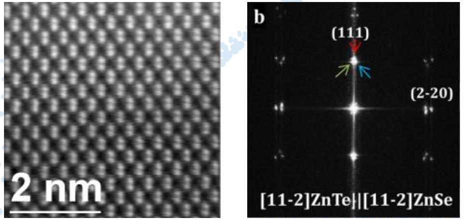
In collaboration with J. Arbiol @ ICN2

Credit: Marc Botifoil
Ivan Pinto

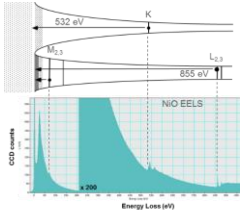
Low magnification (Morphology)

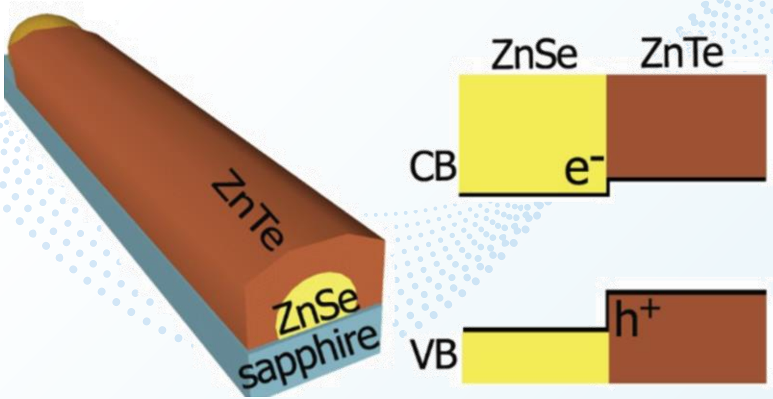


High magnification (Crystallography)



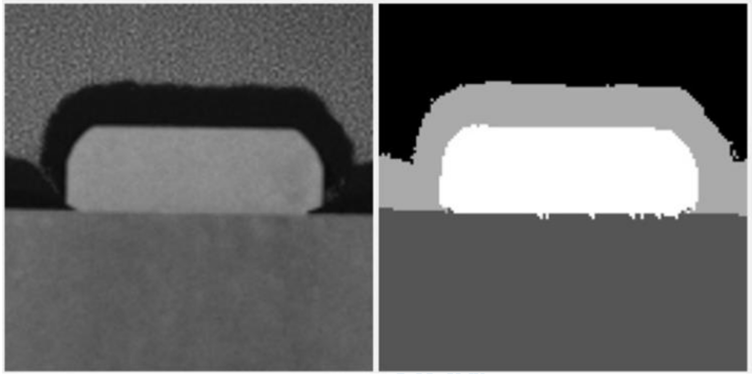
Spectroscopy (Properties)





Can we use AI to automatically create a model of the sample?

Automatic data analysis



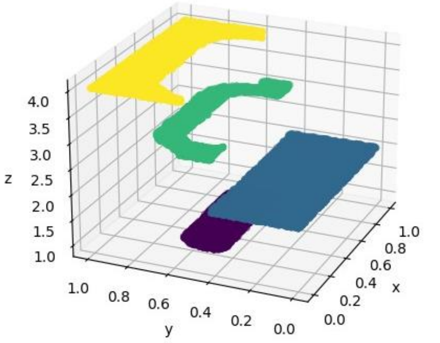
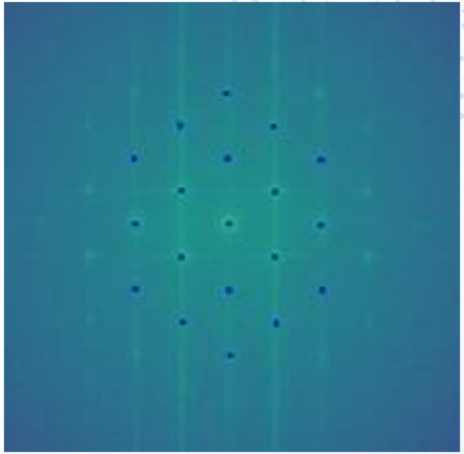


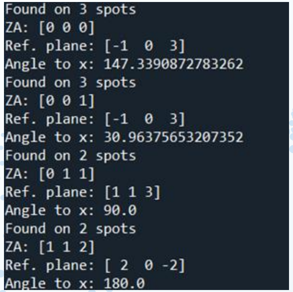
Image segmentation

We use the segmented image to drive the acquisition of a series of atomically resolved images and chemical maps.

Automatic Indexing

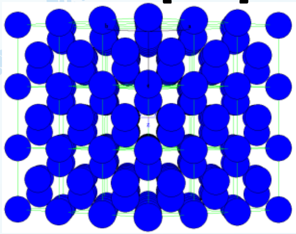
AI able to accurately find diffraction spots to know the phase and orientation of every crystalline domain, or to automate the production of strain field maps.

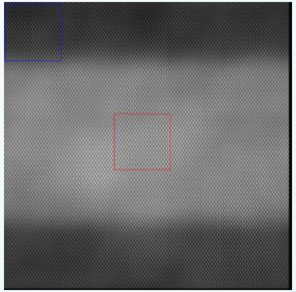


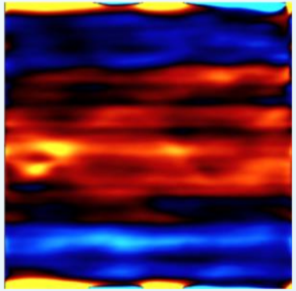


```
Found on 3 spots
ZA: [0 0 0]
Ref. plane: [-1  0  3]
Angle to x: 147.3390872783262
Found on 3 spots
ZA: [0 0 1]
Ref. plane: [-1  0  3]
Angle to x: 30.96375653207352
Found on 2 spots
ZA: [0 1 1]
Ref. plane: [1 1 3]
Angle to x: 90.0
Found on 2 spots
ZA: [1 1 2]
Ref. plane: [ 2  0 -2]
Angle to x: 180.0
```

ZB Ge [011]

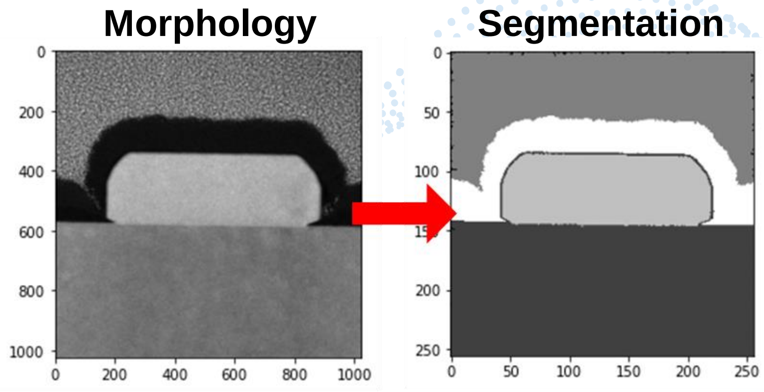


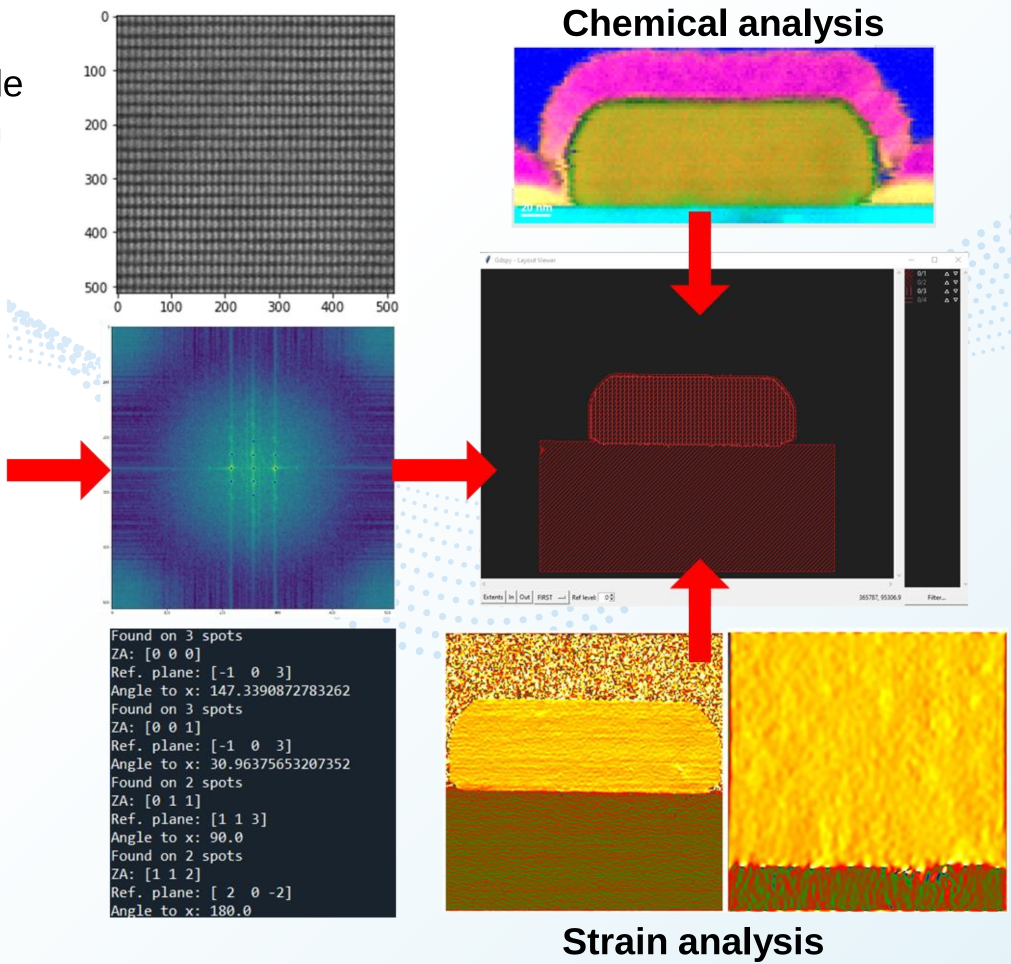




From sample to model

Combining all those tools together it is passible to automate the entire characterization chain





Conclusive remarks

AI can:

- Improve data quality
- Speed up data analysis
- Take care of the alignment
  - Custom optics
  - Conventional lenses
- Optimize in real time experiments
- Drive full workflows

AI will:

- Make TEM more accessible (in compliance with FAIR principles)
- Increase the TEM throughput
  - Availability of TEM data for AI application
- Enable new experiments

Acknowledgement

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Thank you for your kind attention!

Any questions?