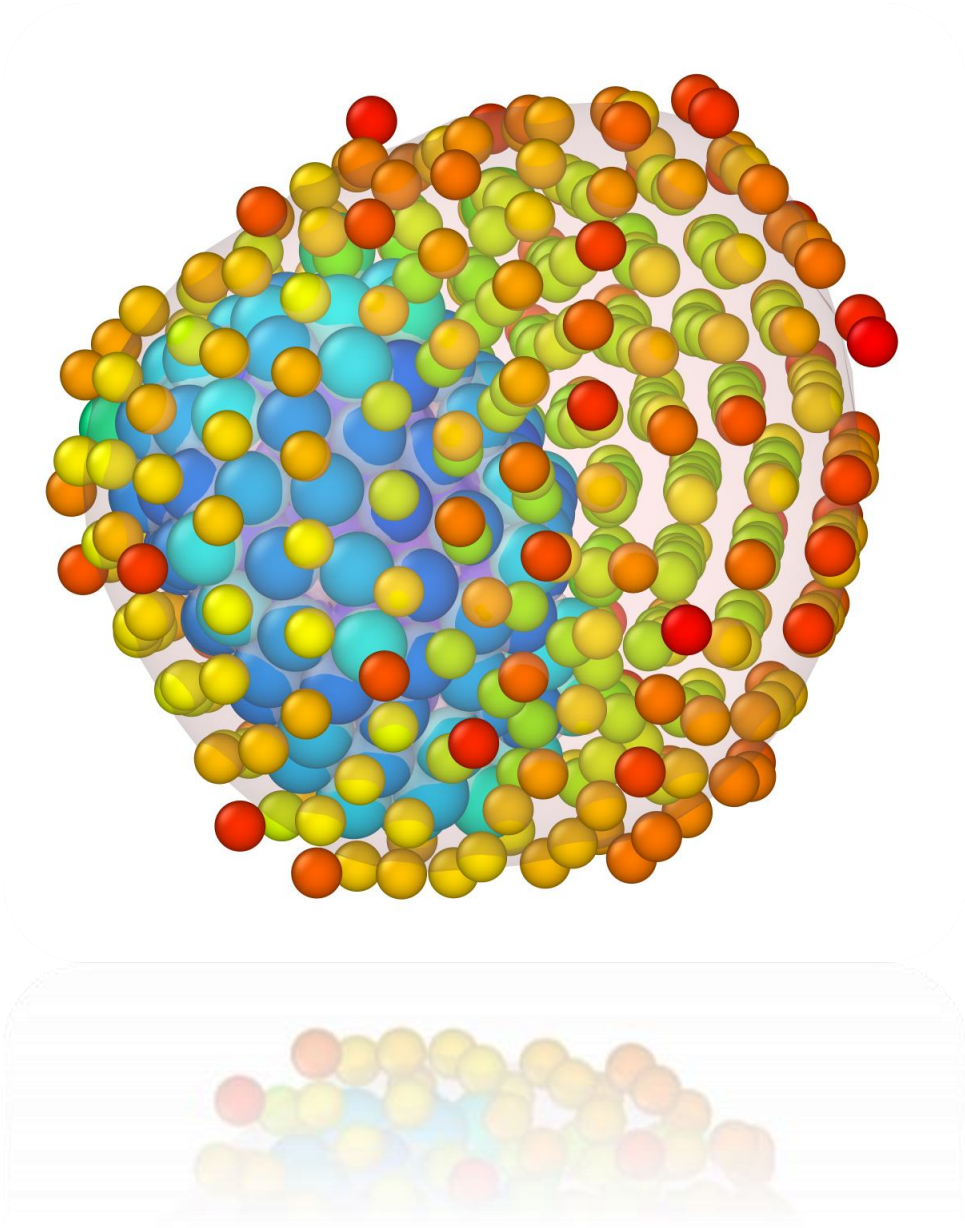
Value of deep learning for HRTEM image analysis

Co/Ag nanoalloys, carbon nanotubes and amorphous carbon

- Atomistic simulation & HRTEM image generation
- Deep learning
- Application to images from experiments

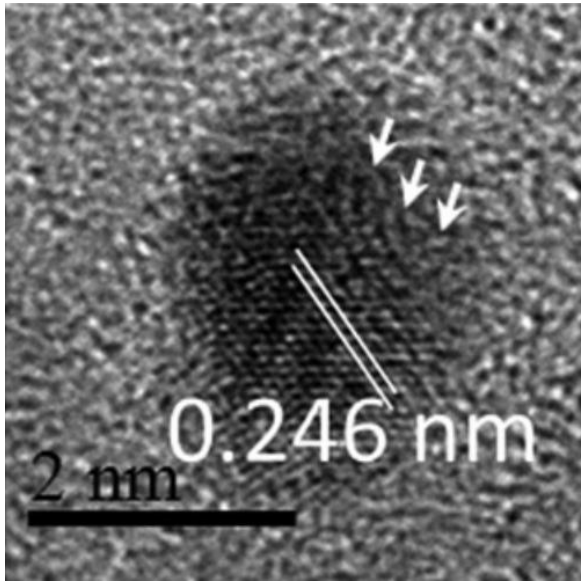


ICMN
Interfaces, Confinement, Matériaux et Nanostructures

Daniel Förster

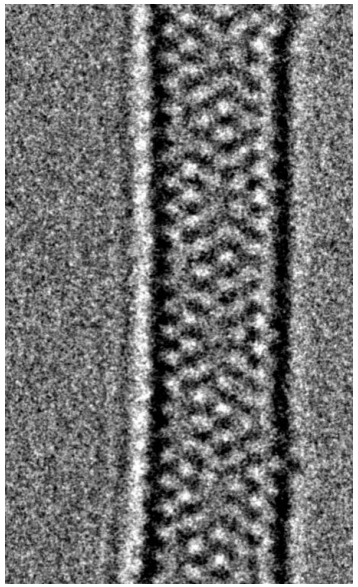
HRTEM for structure analysis

Co/Ag nanoalloys



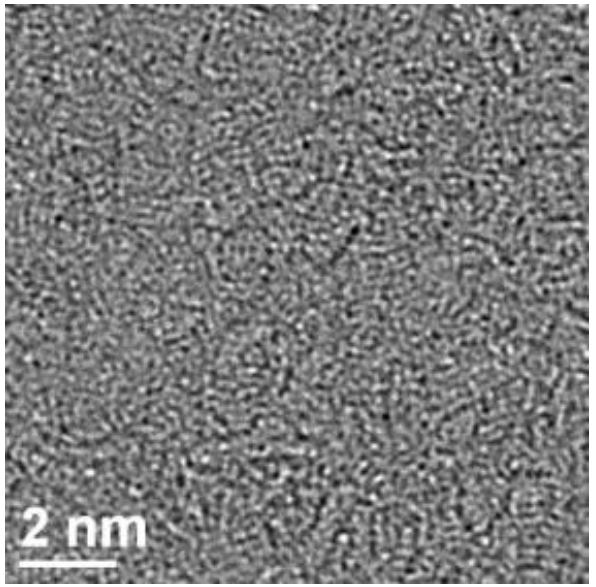
Int. J. Hydrogen Energy **42**, 21751 (2017)

Carbon nanotubes



Carbon **169**, 465 (2020)

Amorphous carbon



Microsc. Microanal. **23**, 2268 (2017)

Individual objects at atomic resolution

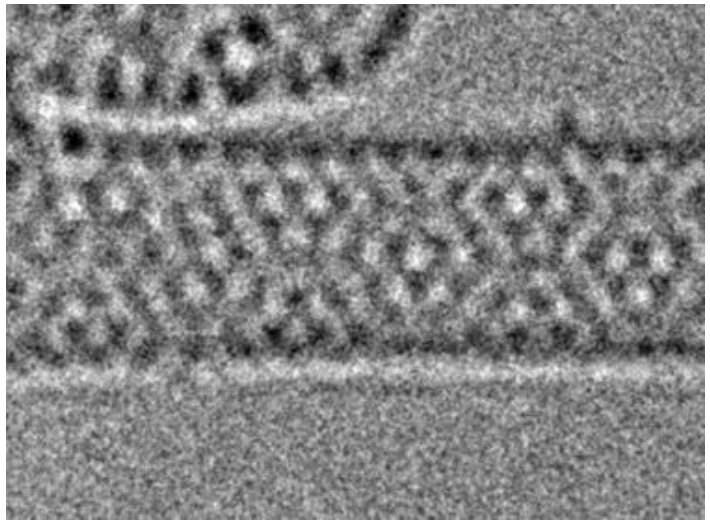
However **large number of images** necessary for sample characterization

Outline

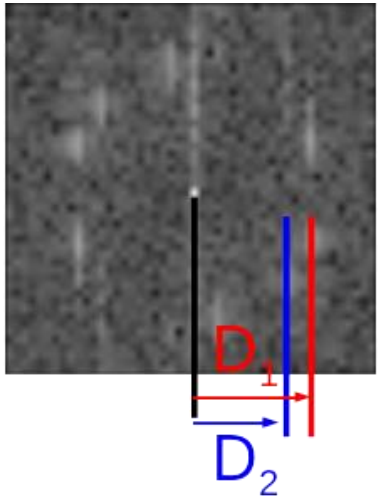
- Interpretation of HRTEM images and difficulties
- Data driven approach
  - Atomistic simulation
  - HRTEM image generation
  - Convolutional neural networks for analysis
- Application to images from experiments

"Classical" approach

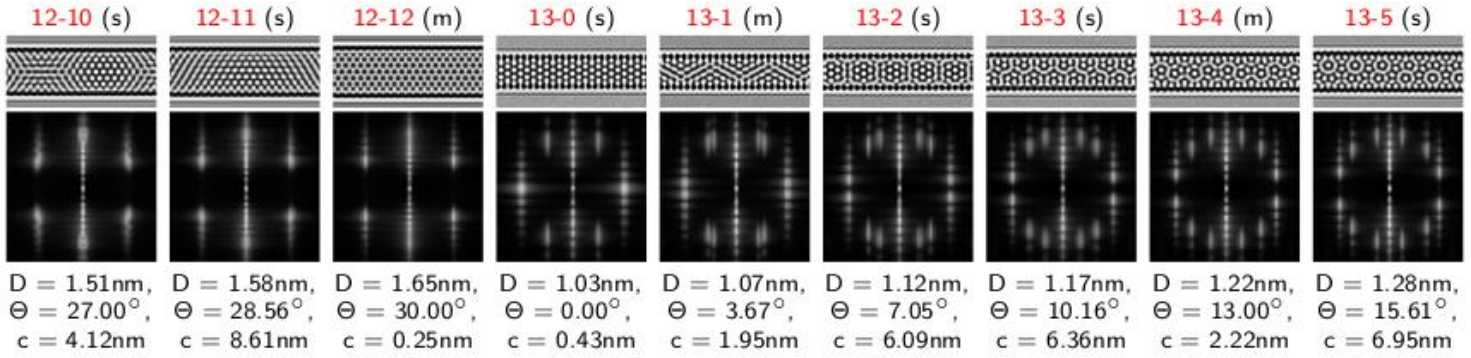
HRTEM image

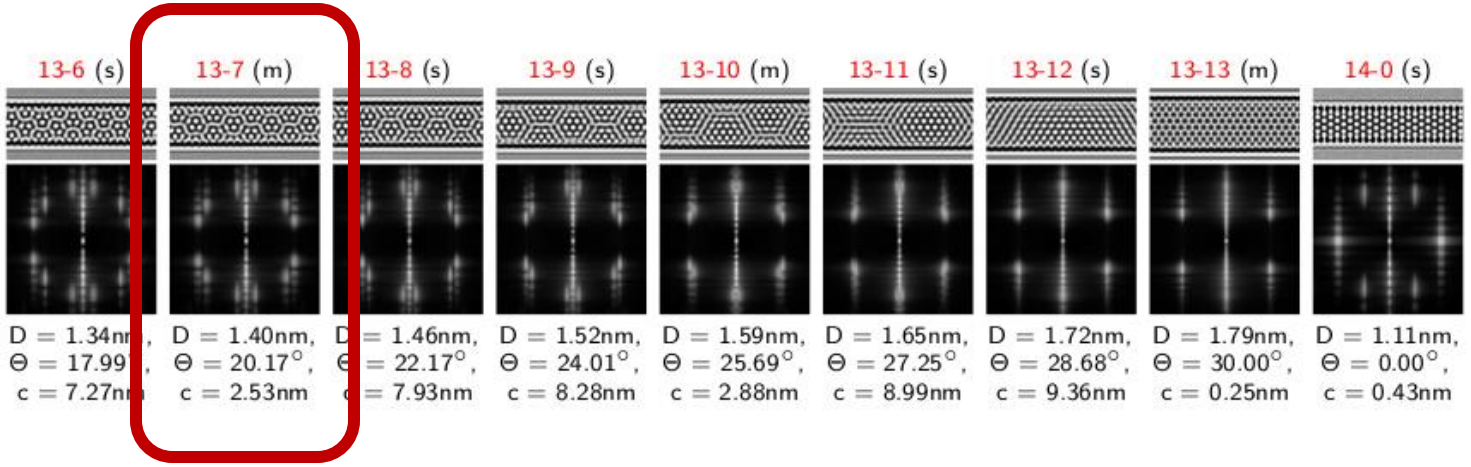


Fourier transform

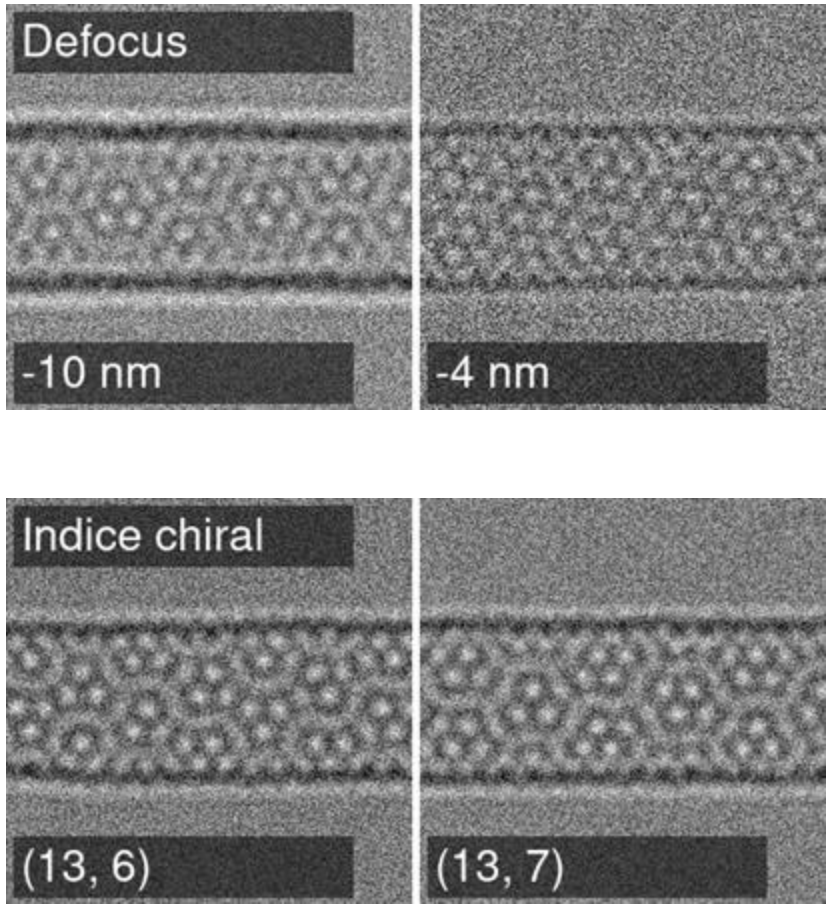


Comparison with simulated images





Challenges for the interpretation of HRTEM images



- Microscopy aberrations
- Pattern depend on object orientation
- Defects
- Image noise

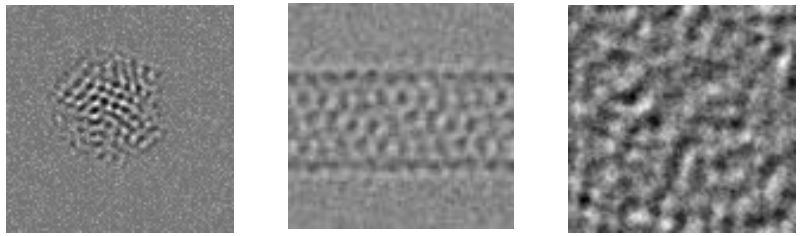
New method based on convolutional neural networks

1

Simulations

Atomistic simulations

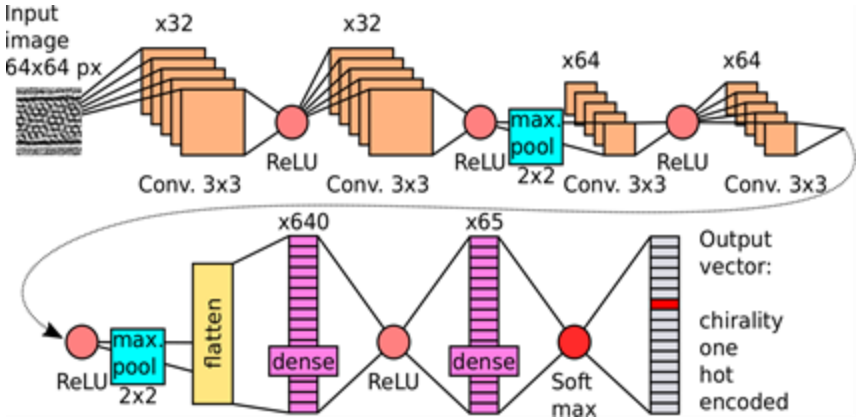
HRTEM images of simulated structures



2

Training

Deep learning: convolutional neural network for classification, regression, and denoising

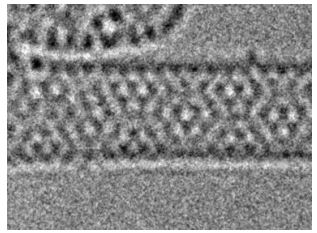


3

Application to images from experiments

microscope JEOL- ARM 200F

- automatized analysis
- interpretation of experimental data

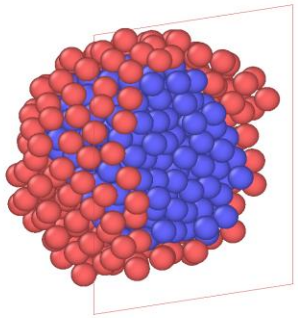


Molecular dynamics

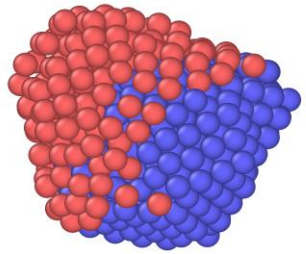
- TB-SMA for Ag/Co alloy system
- Tersoff interatomic model for carbon

- rapid quench
  - **Stabilization of different nanoalloy chemical orderings**
  - **defects**
  - **thermal fluctuations**

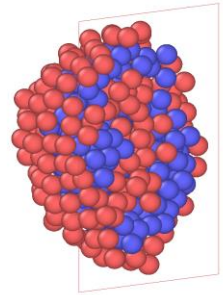
- Several 100,000 simulation runs



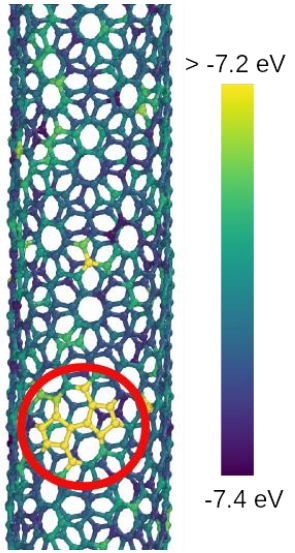
core-shell



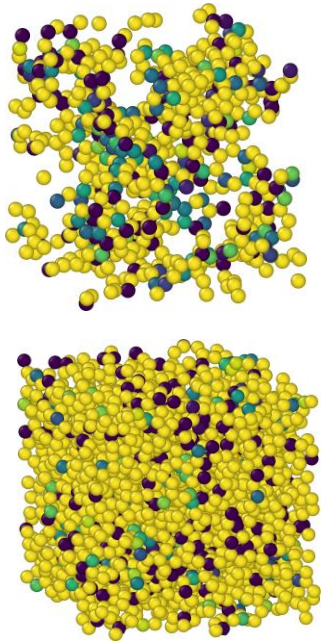
Janus



disordered alloy



carbon nanotubes



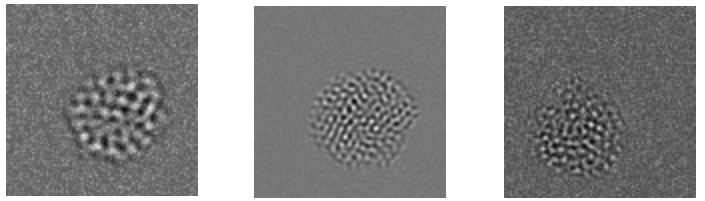
amorphous carbon

Multi-slice simulations

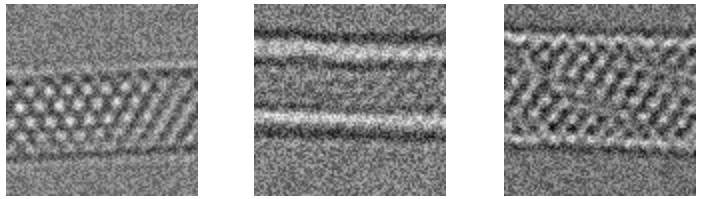
Multi-slice simulation and generation of images (different resolutions, with and without shot noise)

Variability:

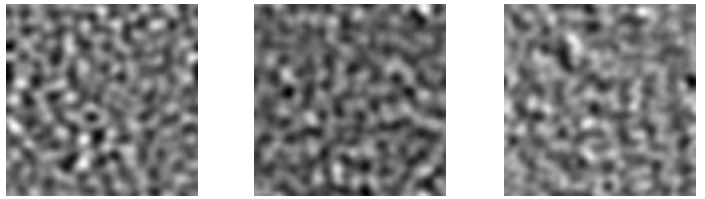
- position
- orientation (3 axes)
- zoom level
- **defocus**, aberration coefficients
- noise
- overall brightness



Ag/Co nanoalloys



Carbon nanotubes



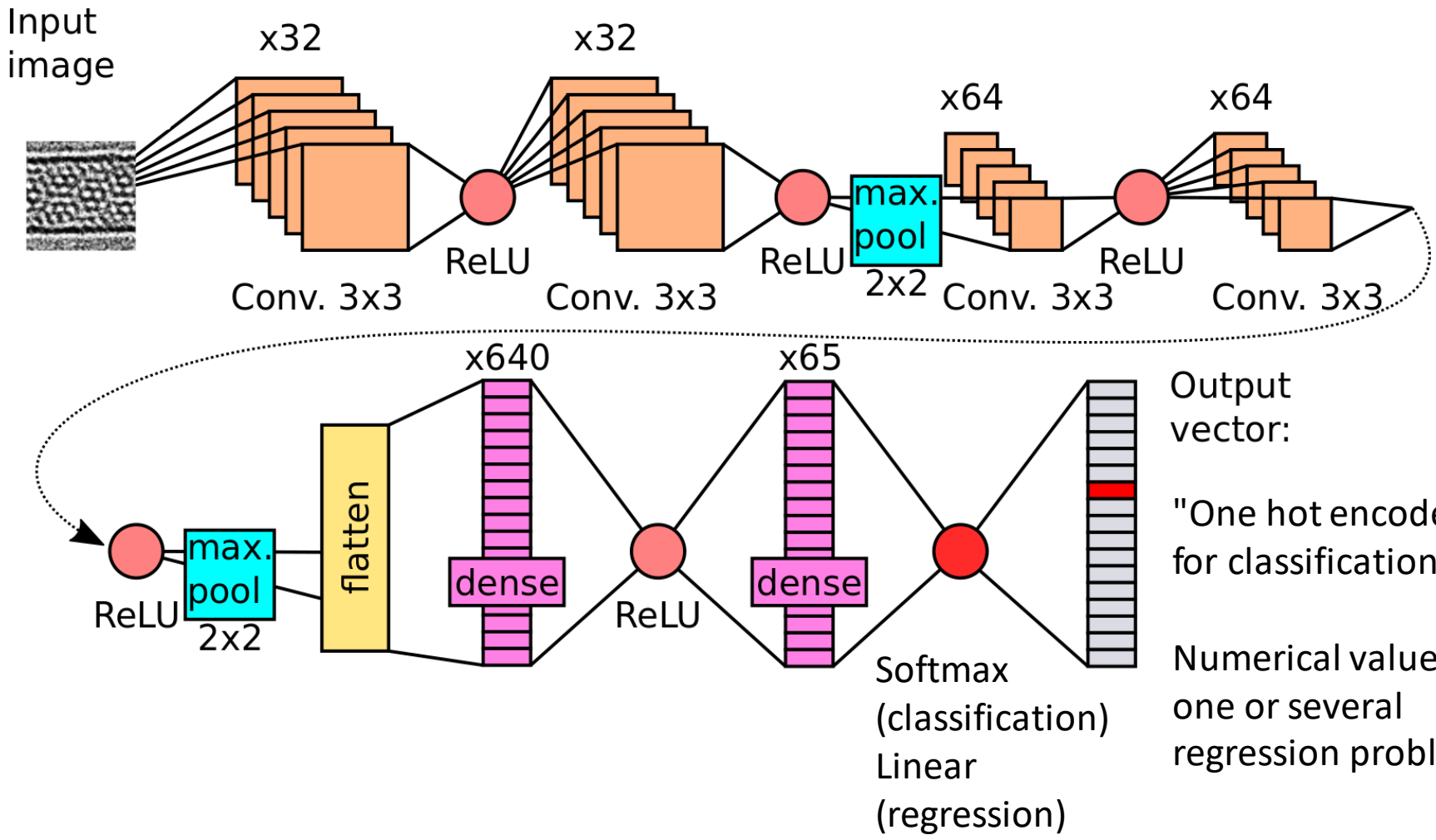
Amorphous carbon

Convolutional neural network

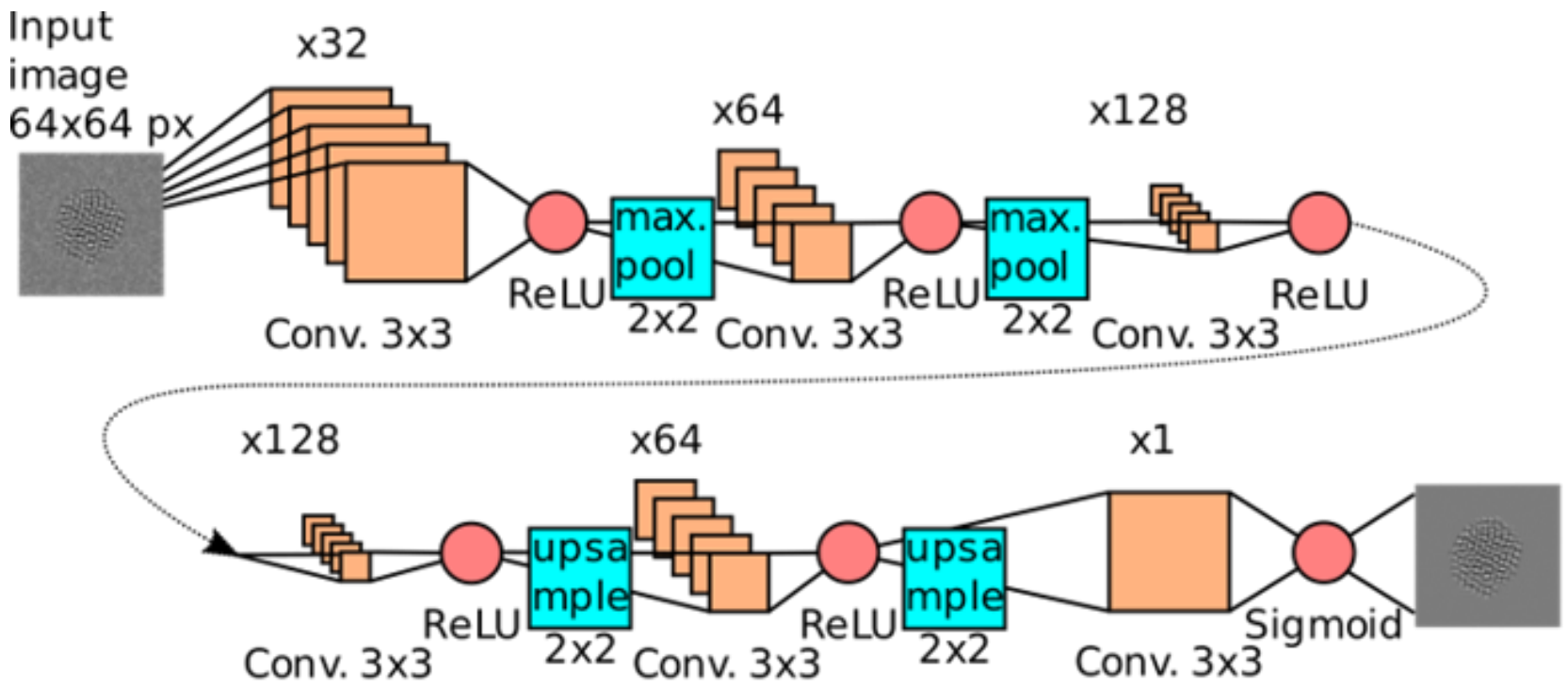
- Image classification
- Sort images into a finite number of predefined categories
- Requires large number of examples with known categories

Proc. of the IEEE **86**, 2278 (1998)

Convolutional neural network for classification/regression



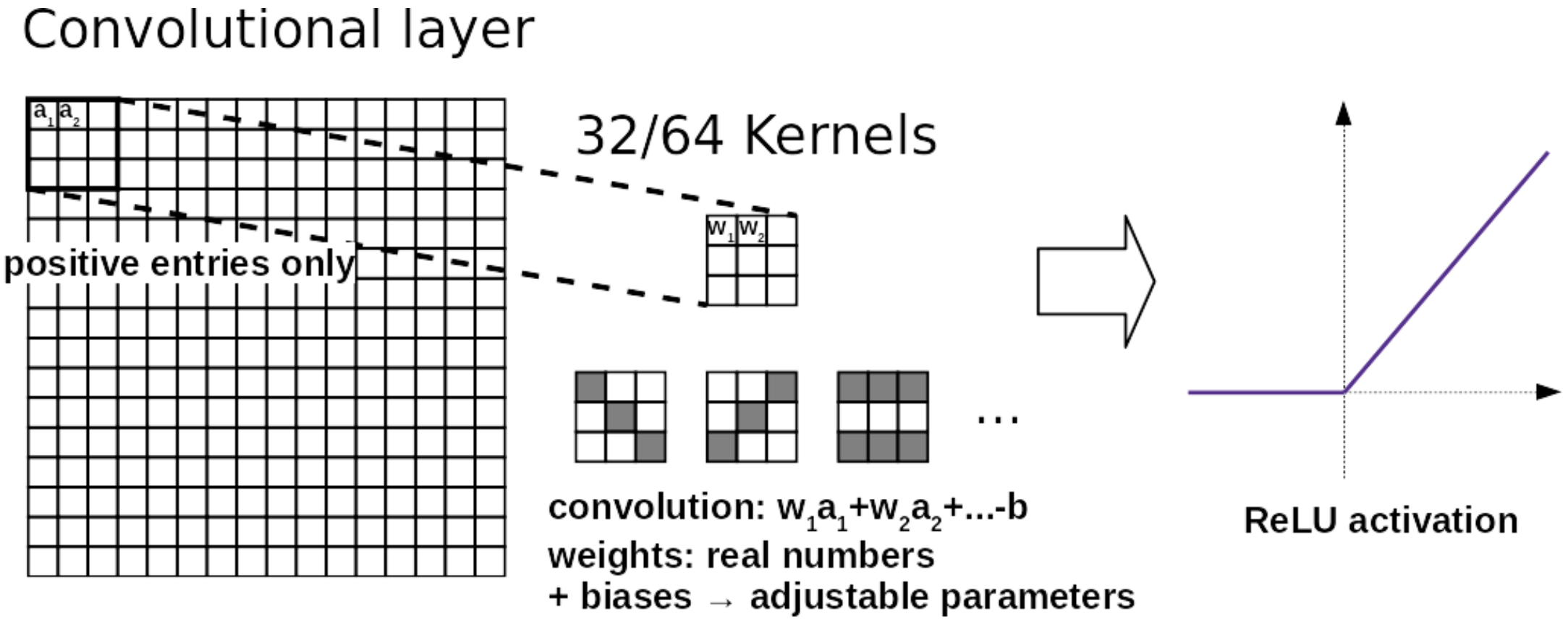
Convolutional neural network for denoising (autoencoder)



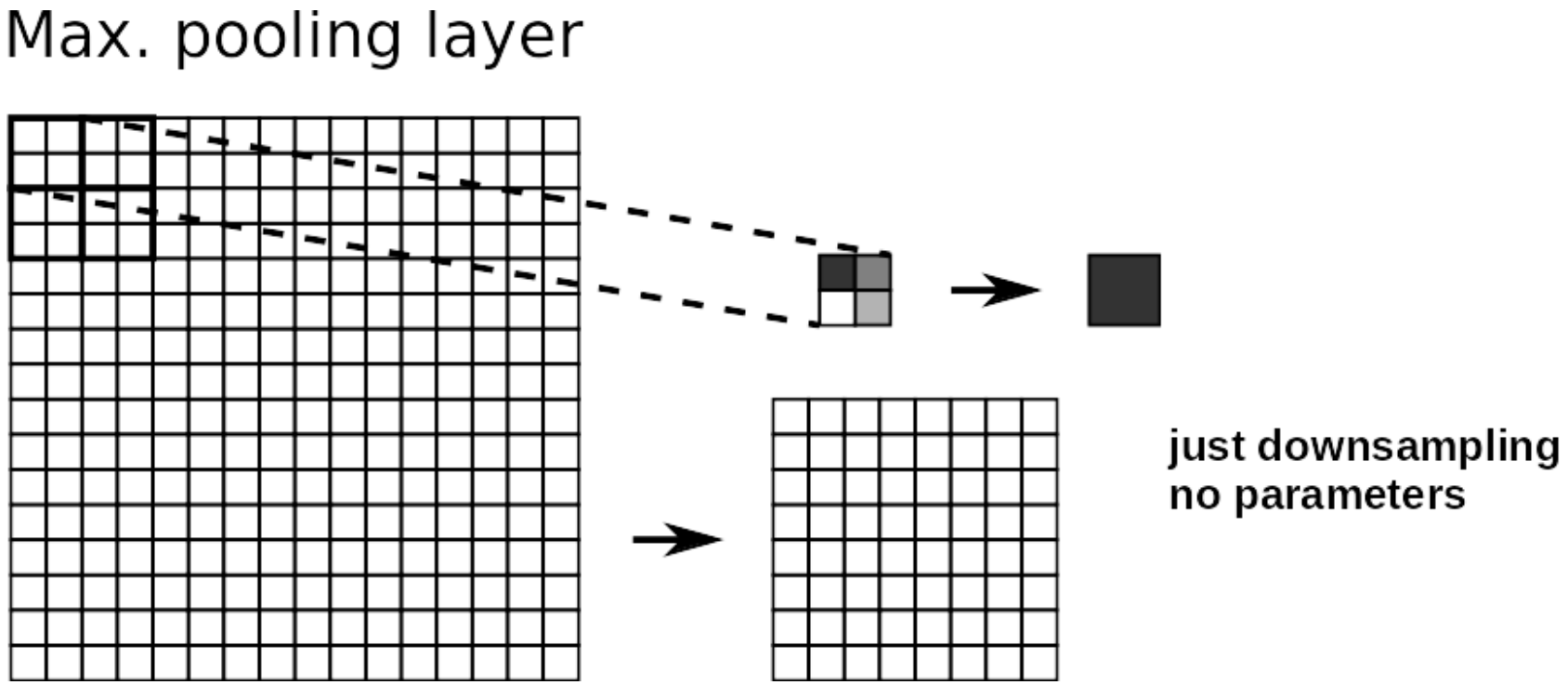
Output matrix as image:

without image noise
without microscopy aberrations
improved resolution

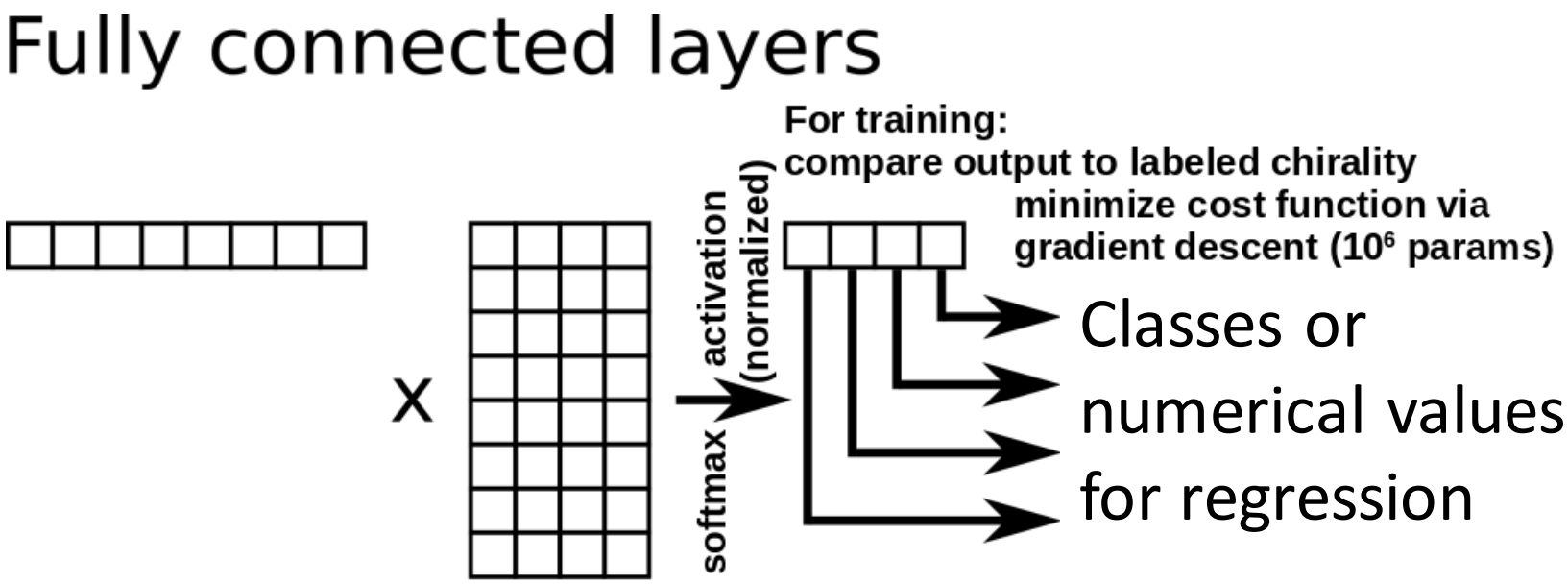
Convolutional neural networks



Convolutional neural networks

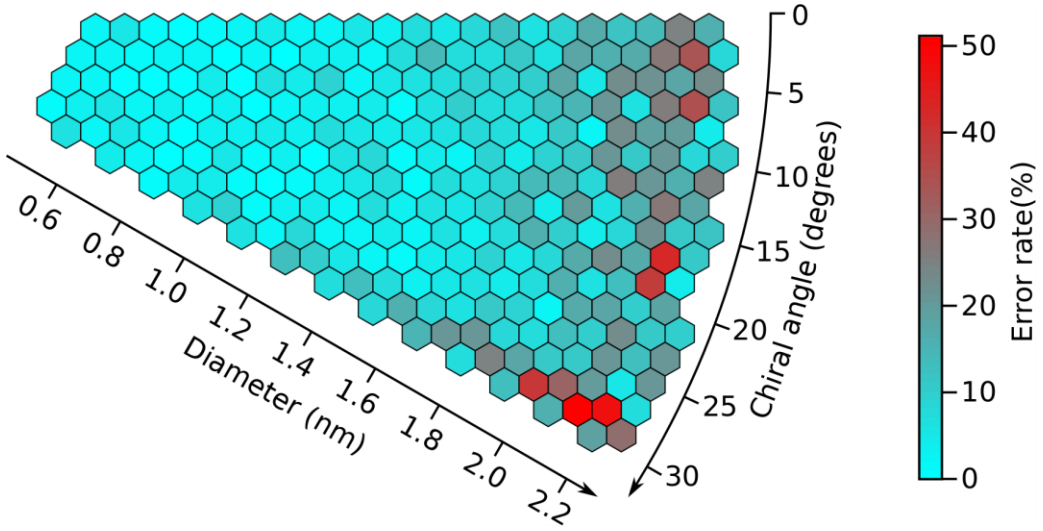


Convolutional neural networks



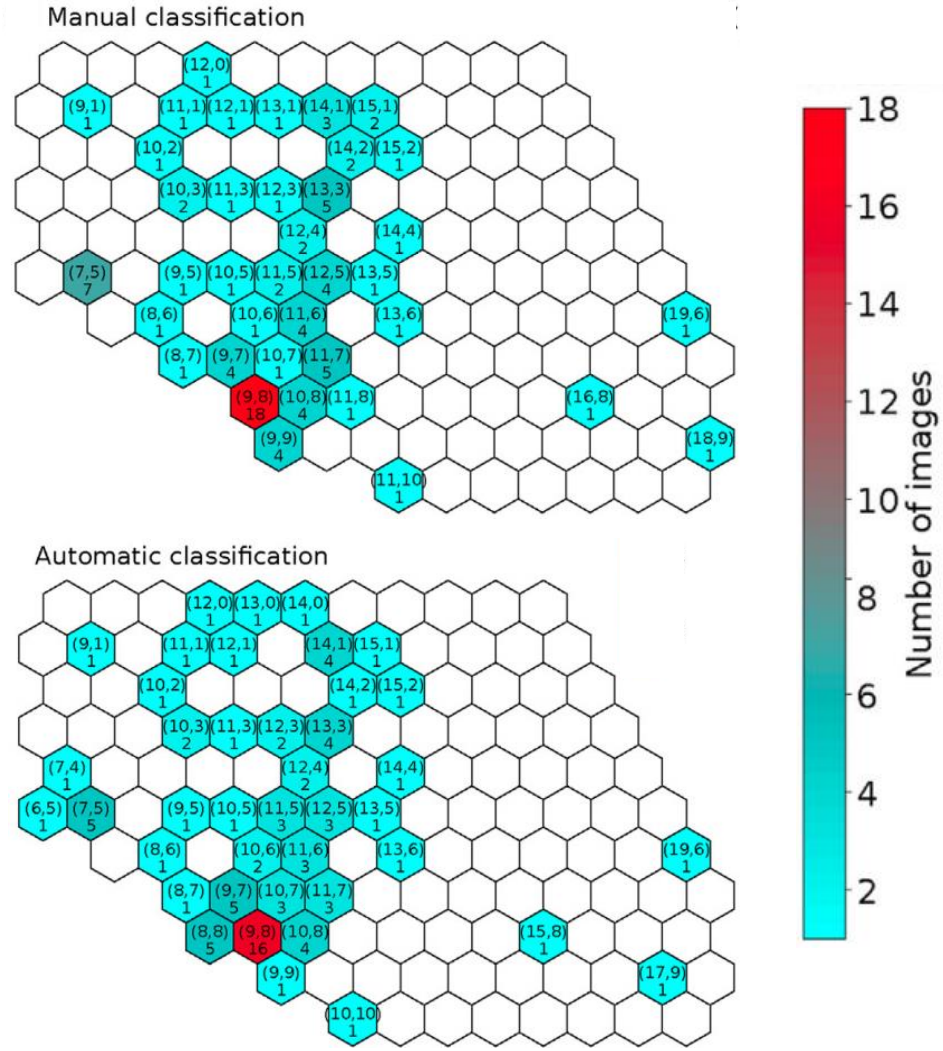
Classification: Carbon nanotube structure (chirality)

Synthetic images



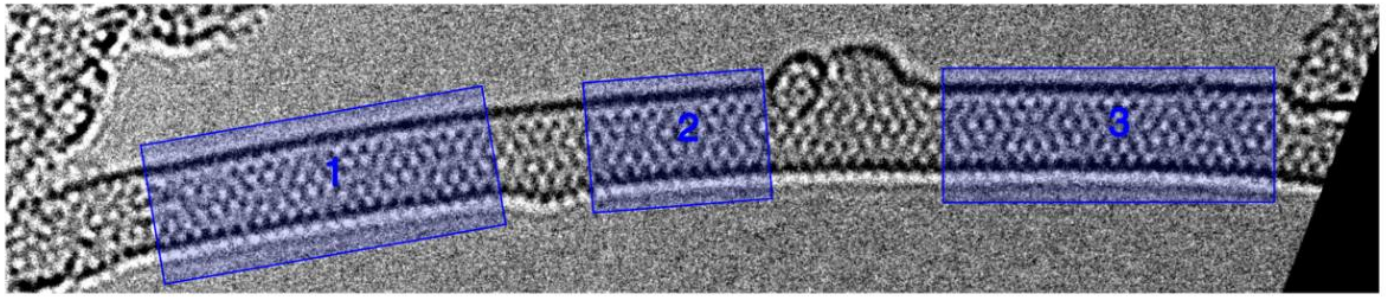
Overall accuracy >90%

Experimental images

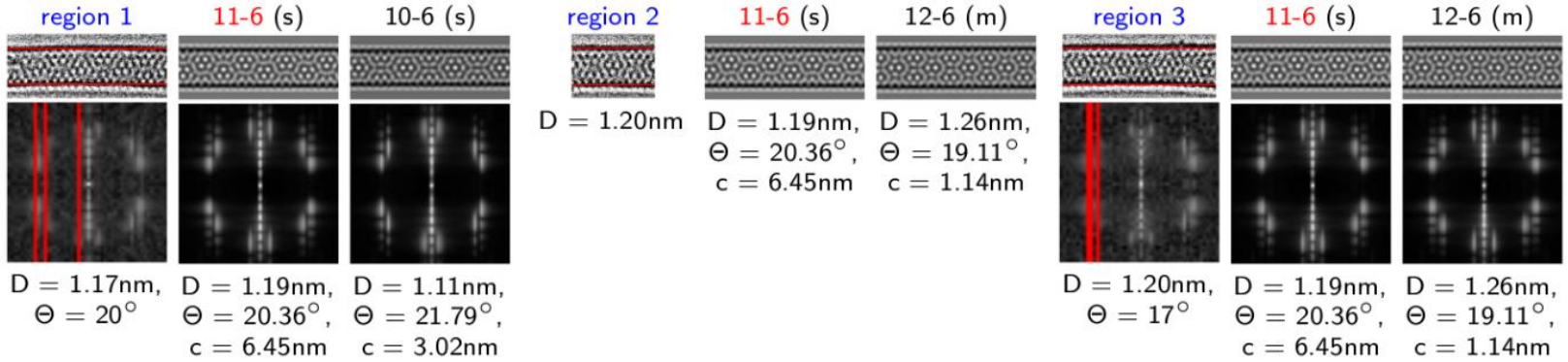


same result: 71% of 91 cases

Application to real, experimental images



region	chirality 1	prob. 1	chir. 2	prob. 2	chir. 3	prob. 3
1	11-6	**85.5 %**	10-6	11.3 %	11-5	3.0 %
2	11-6	**91.8 %**	12-6	5.2 %	11-7	2.9 %
3	11-6	**95.5 %**	12-6	2.8 %	11-7	1.3 %

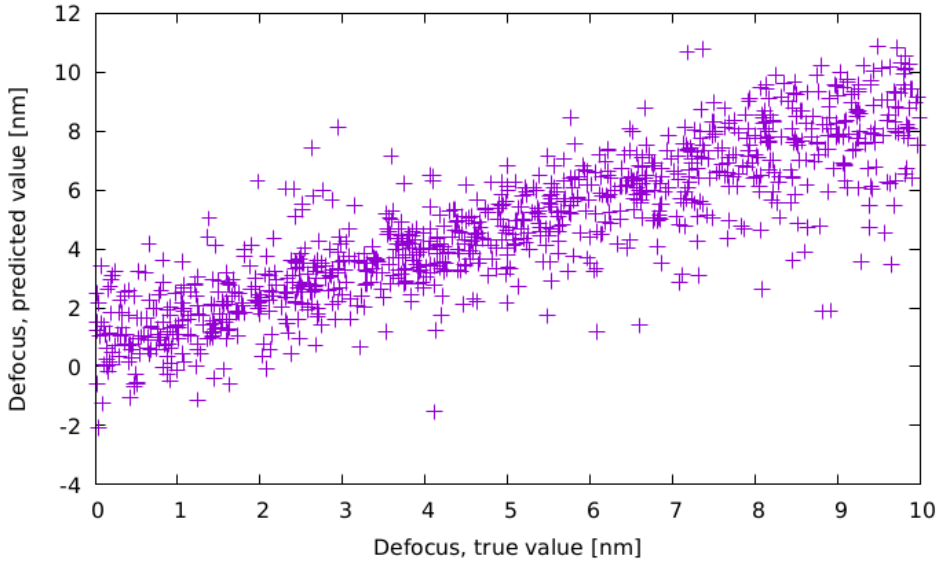


Publication: Carbon **169**, 465 (2020)
hrtem-analysis.fr

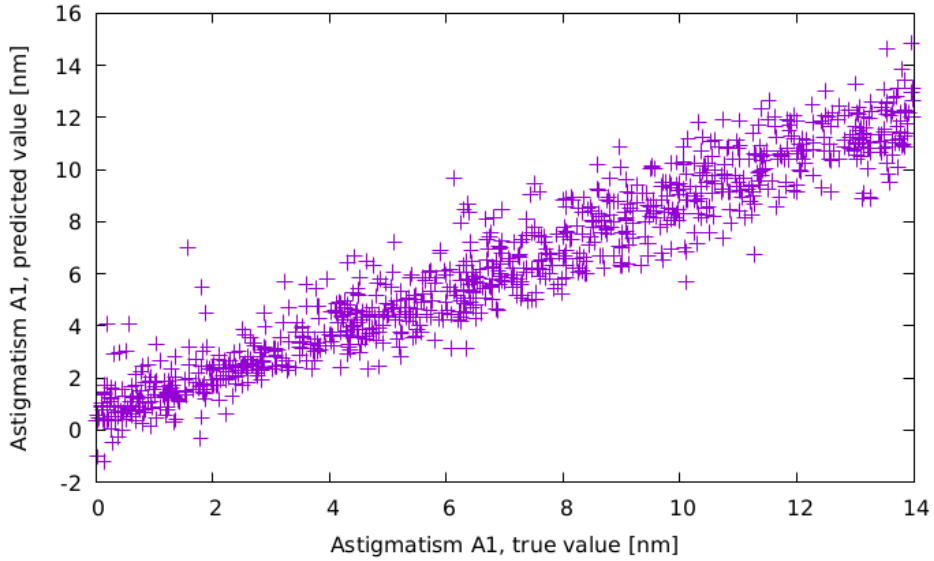
Regression: microscope defocus and astigmatism

Based on synthetic Ag/Co nanoalloy images

Defocus



Astigmatism



Valuable information for microscopists

Perspective: Regression on **structural and energetic observables**

Denoising: convolutional autoencoder

Carbon nanotube

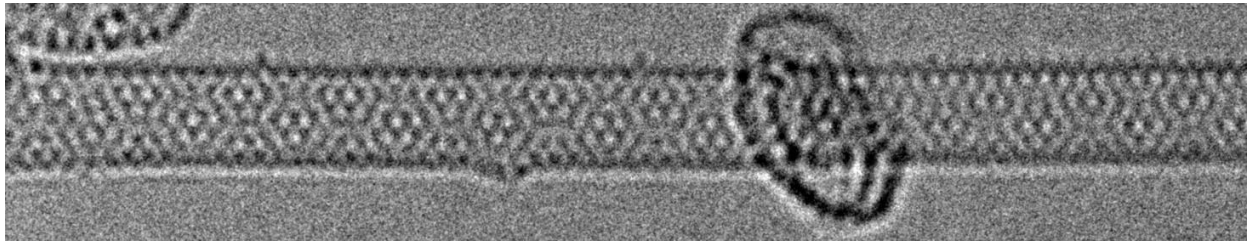
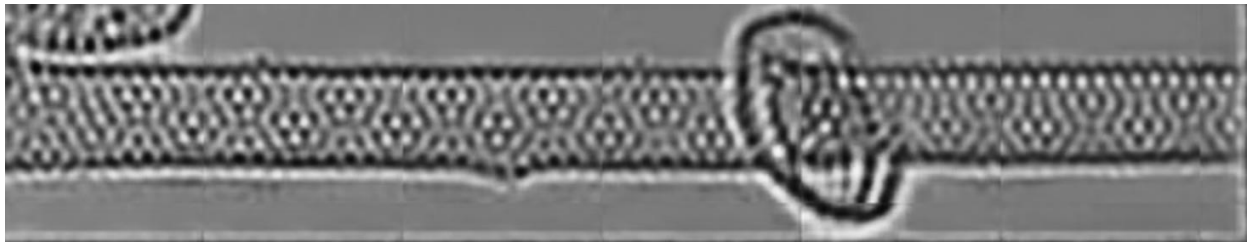


Image from experiment



Denoised image

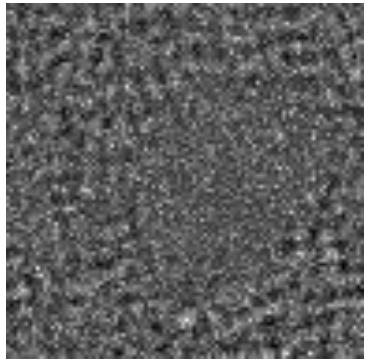
Reduction of irradiation damage

Faster image acquisition

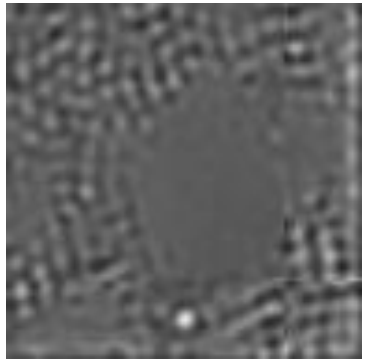
Improved resolution

Perspective: Reduction of microscope aberrations

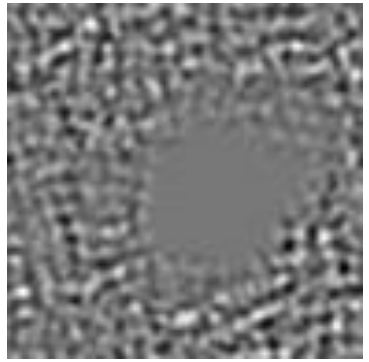
Amorphous carbon (synthetic images)



Noisy image (shot noise)

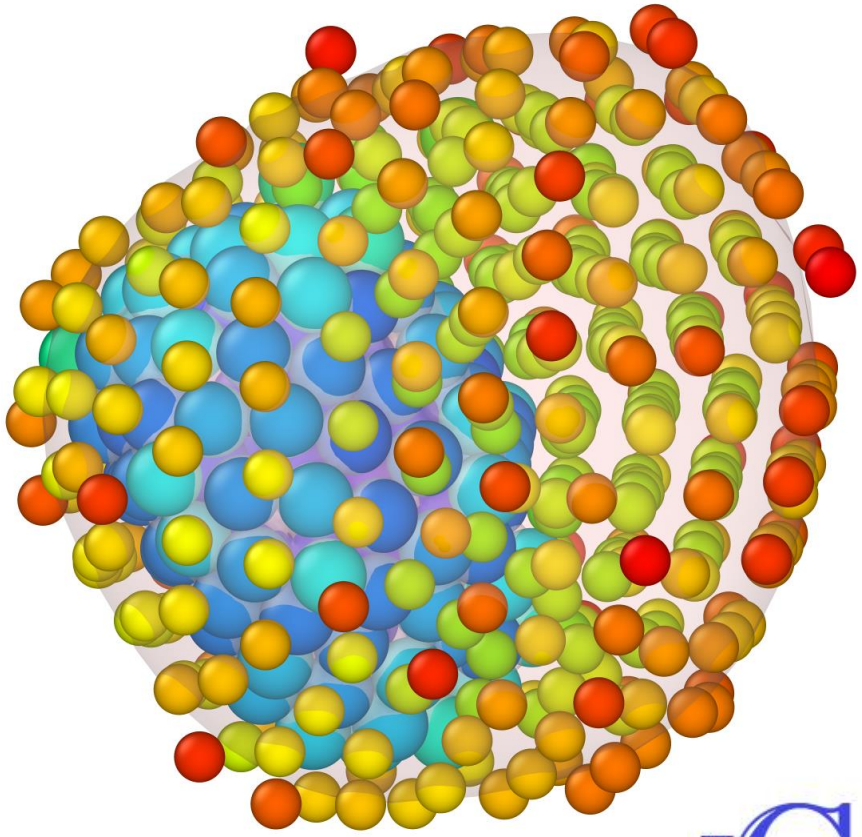


Denoised image



Ground truth

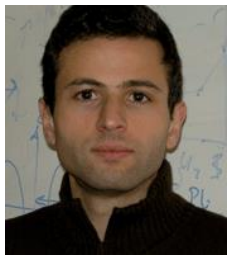
Value of deep learning for HRTEM image analysis



Many thanks to

Alice Castan Frédéric Fossard Damien Alloyeau Jaysen Nelayah






Hakim Amara Annick Loiseau Matthieu Larger Hiba Idrissi Caroline et Pascal Andreazza

Thank you for your kind attention!

Daniel Förster