Discrete Tomography in Materials Science

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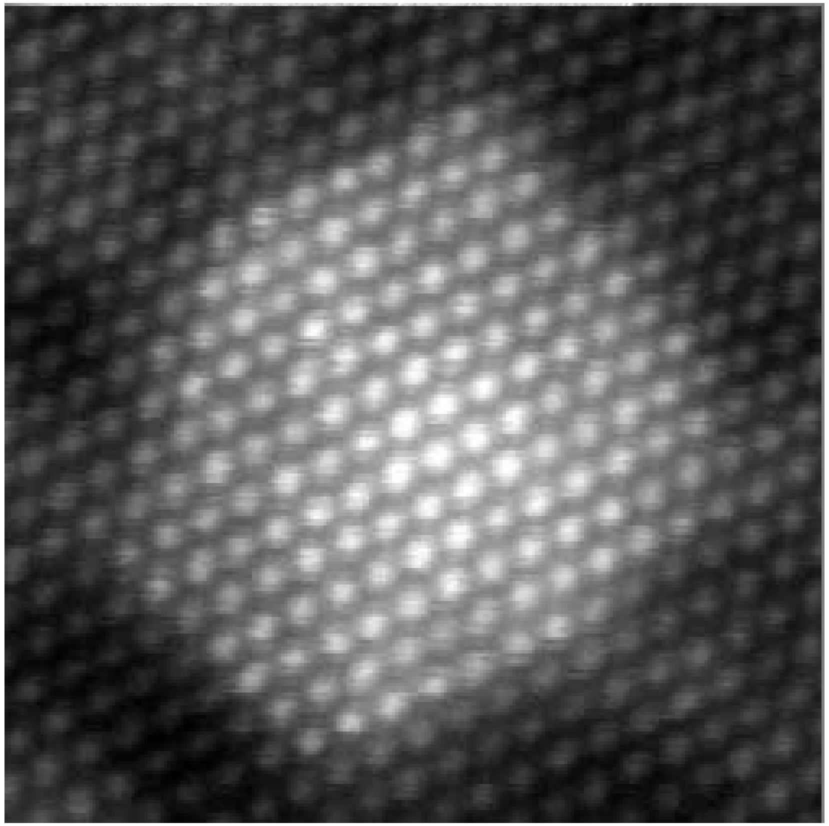
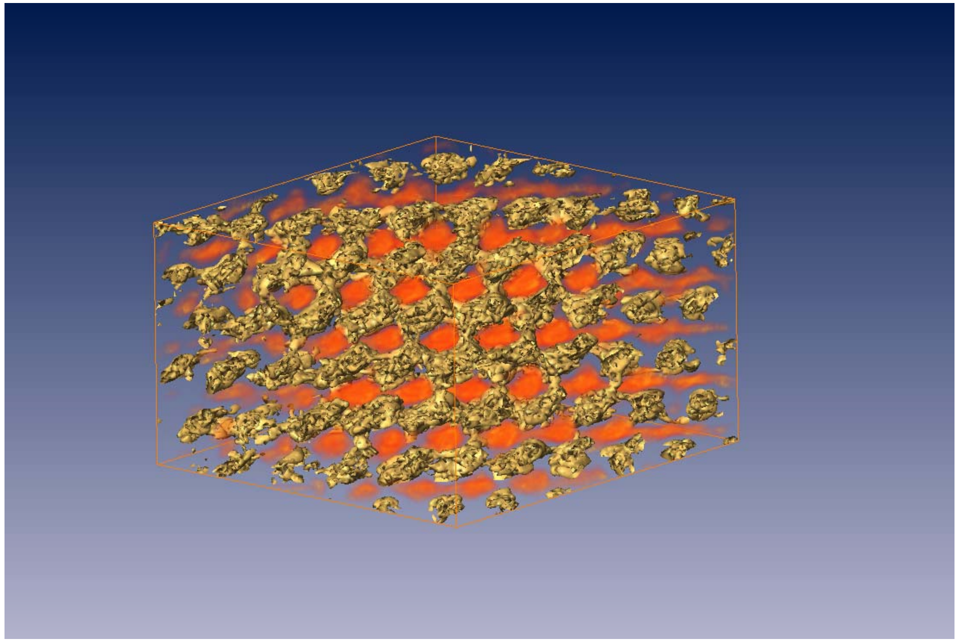
Overview

- Introduction to tomography
- Electron tomography
- Discrete electron tomography
- Outlook

Electron microscopy

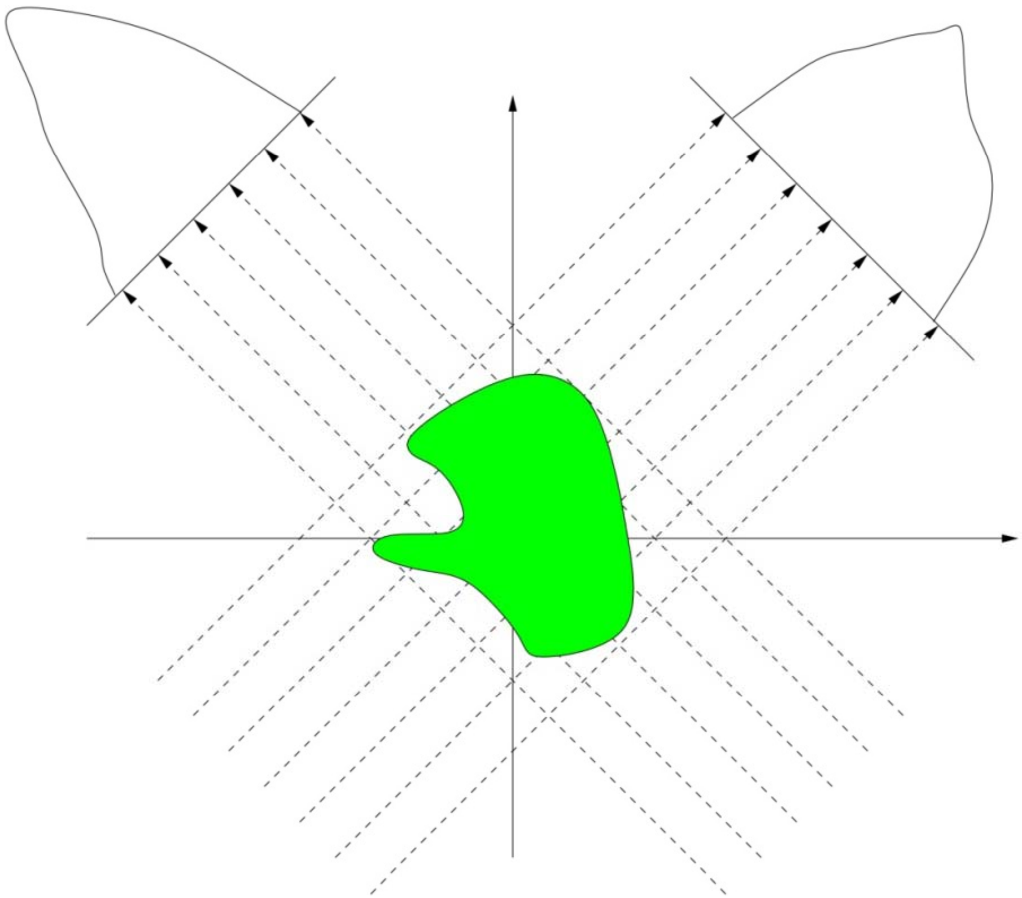


Electron tomography



Sara Bals, K. Joost Batenburg, Duoduo Liang, Oleg Lebedev, Gustaaf Van Tendeloo, Alexander Aerts, Johan A. Martens, and Christine E. A. Kirschhock, J. Am. Chem. Soc., 131(13), 4769, 2009

Tomography: principle



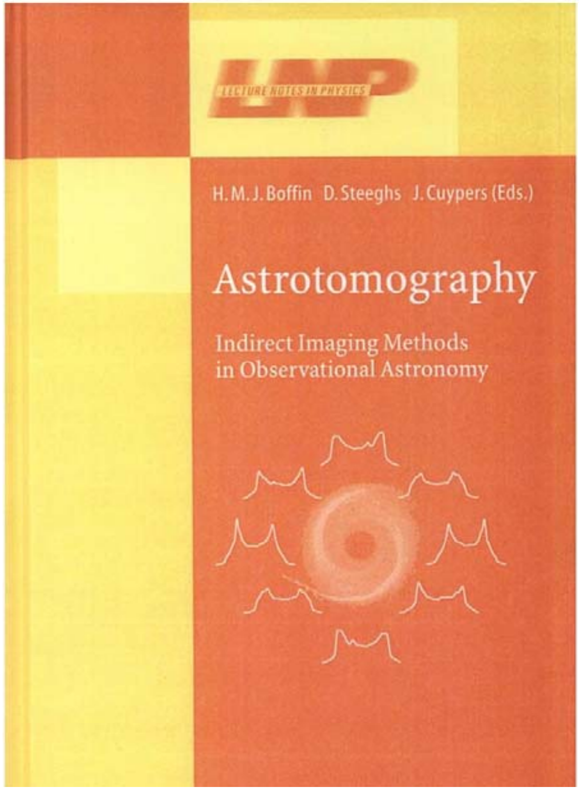
$$N_d = N_{in} e^{-\int_{\mathrm{ray}} f(x,y)\,\mathrm{d}s}$$

$$\int_{\mathrm{ray}} f(x,y)\,\mathrm{d}s = \log \frac{N_{in}}{N_d}$$

Tomography at all scales

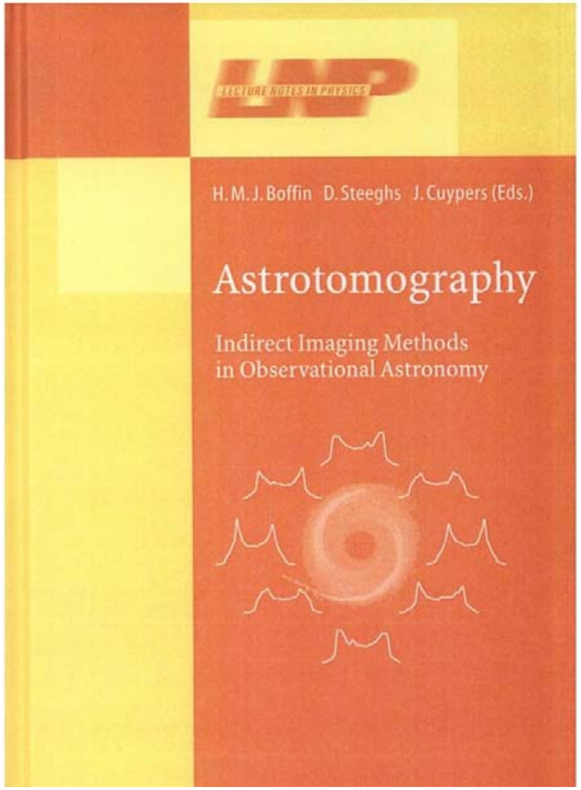
- Medical tomography (CT) is by far the most common subfield of tomography research
- Tomography is also being used outside of CT, at all imaginable scales, from light years down to sub-nm
- Electron tomography covers the smallest of these scales

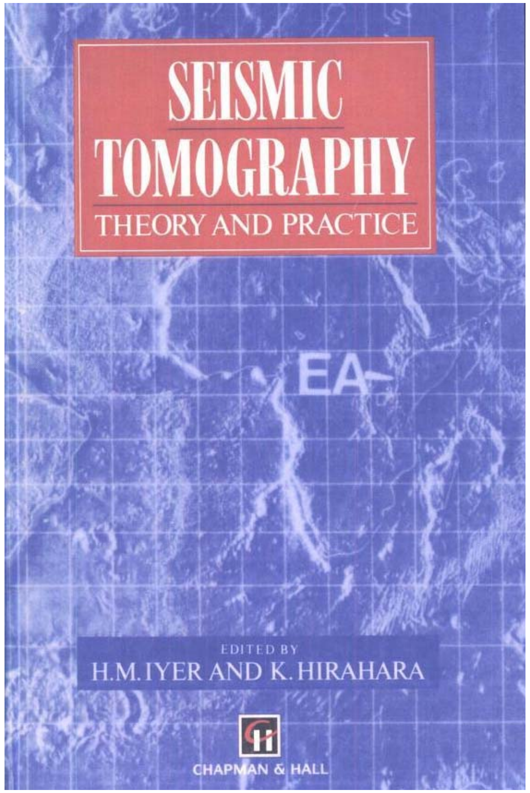
Tomography at all scales: astrotomography



Light year

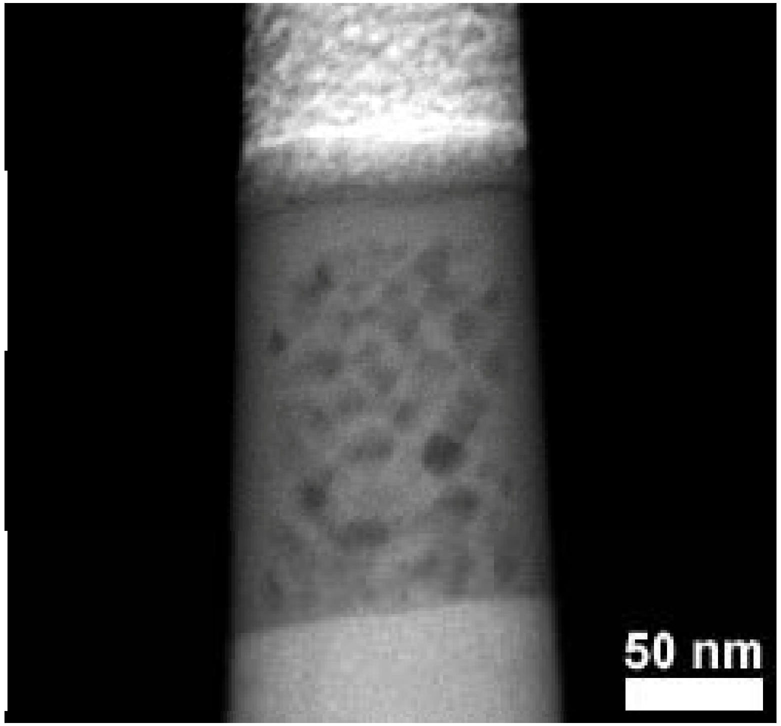
Tomography at all scales: seismic tomography





Light year • • • km

Tomography at all scales: Electron tomography



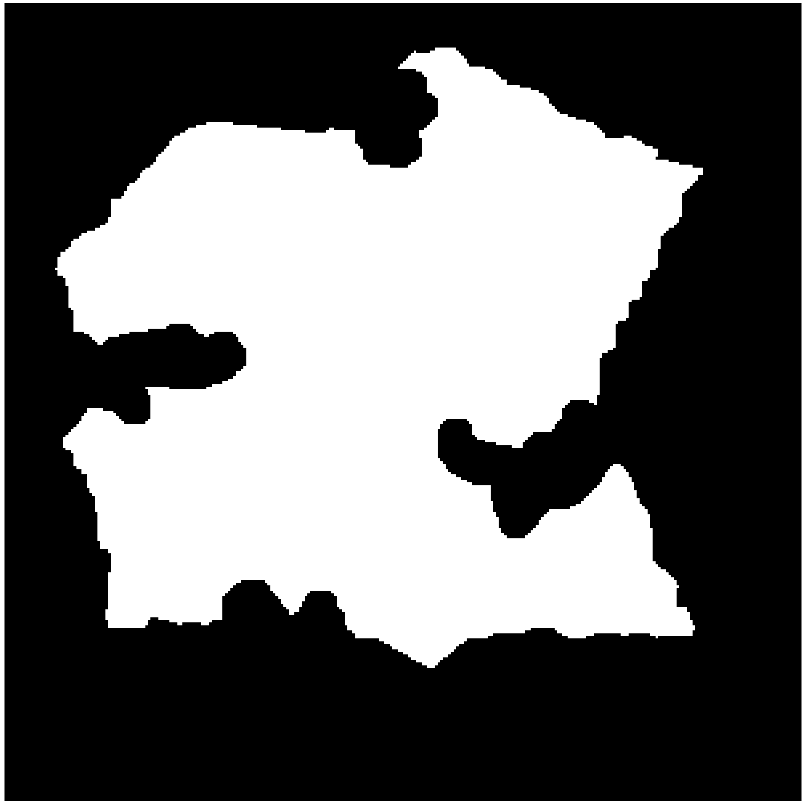
STEM image of LZO, Ellen Biermans

Light year • • • km • • • mm • • • µm • • • nm

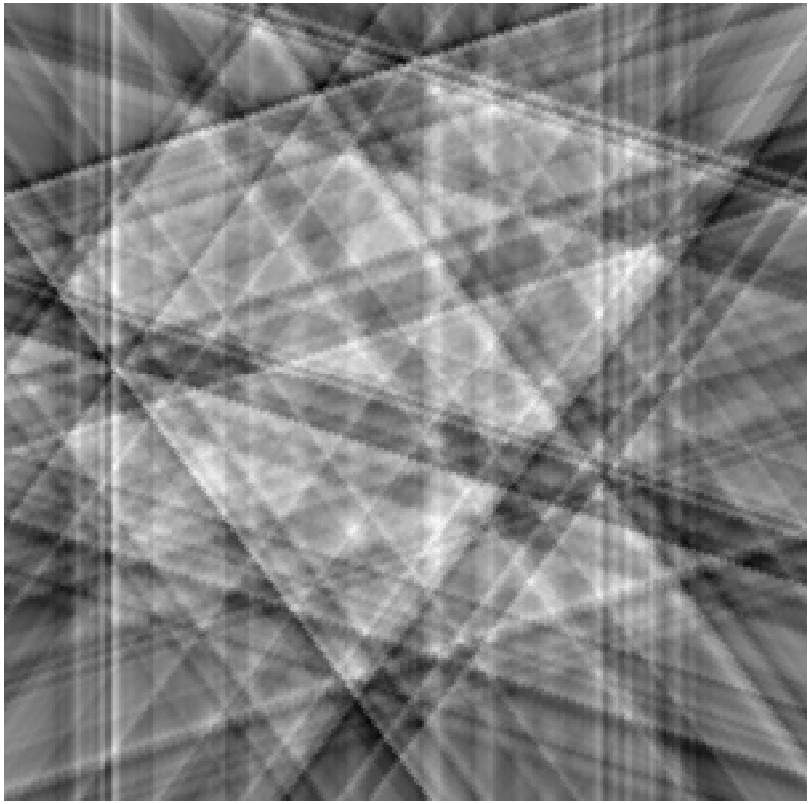
Electron tomography: Key limitations

- Tomography requires a large number of projection angles
  - Beam damage
  - Time consuming
- … sampled at regular intervals
  - Full angular range is needed

Few projections

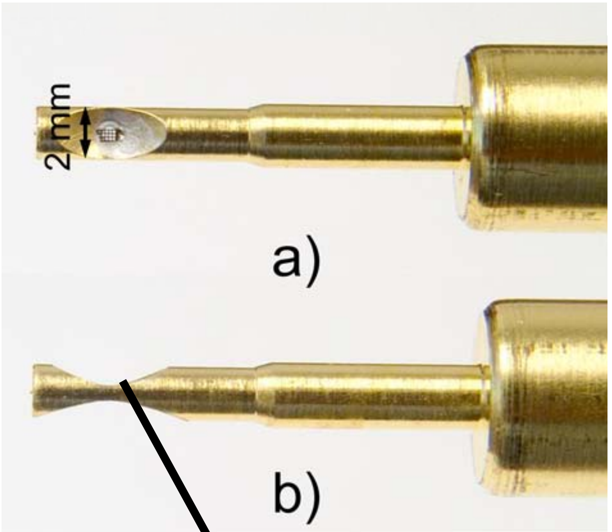


Original image



Filtered backprojection, 5 projections

Electron tomography: Tomography holder



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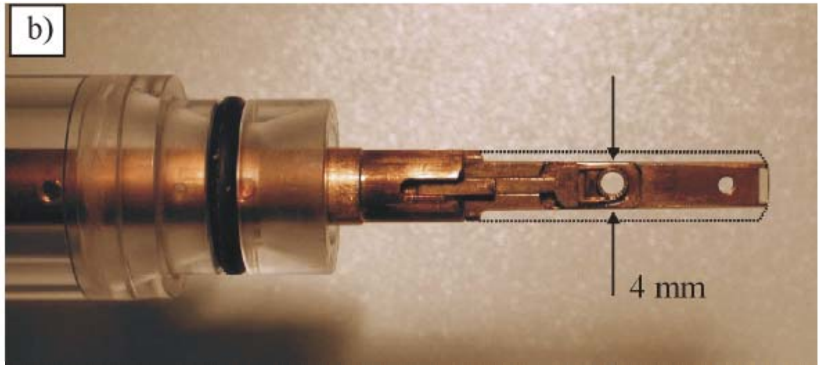
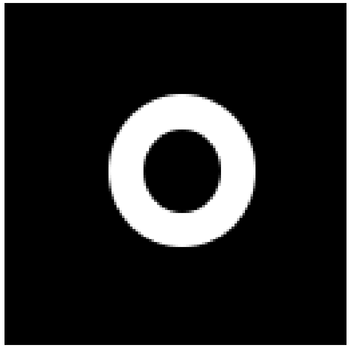
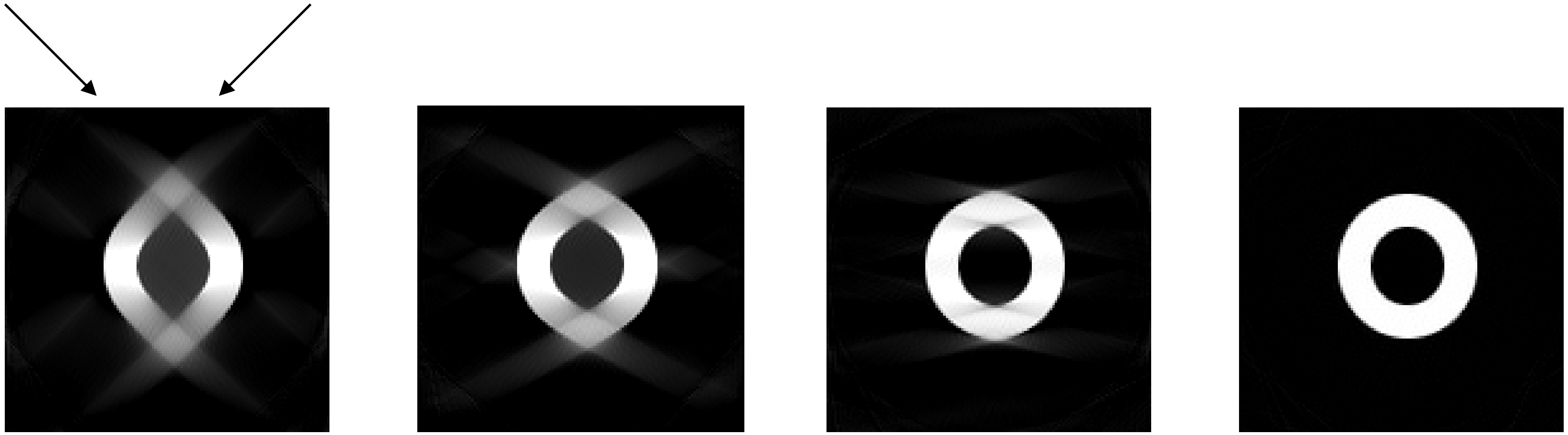


Fischione

Missing wedge

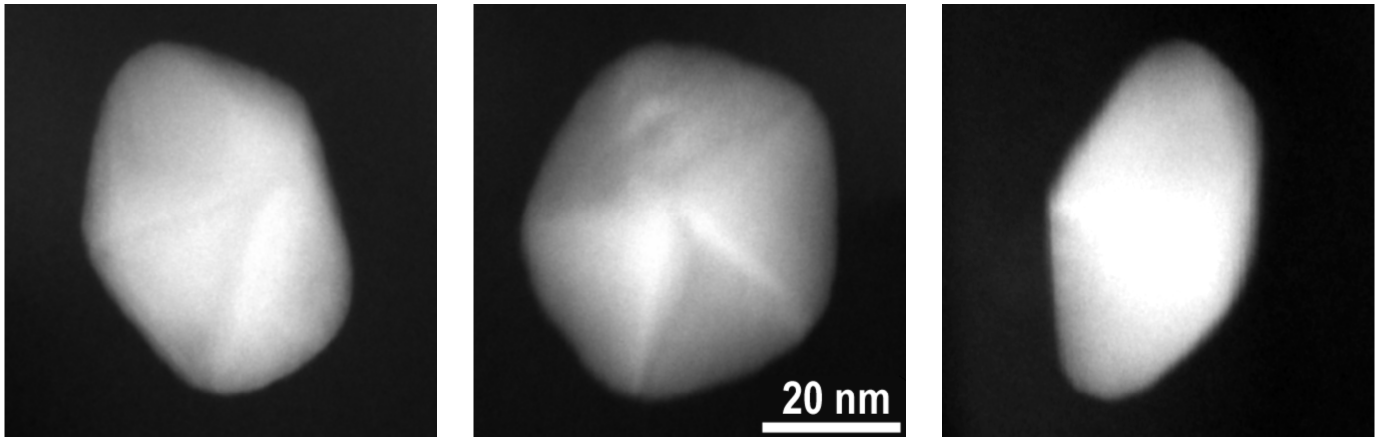


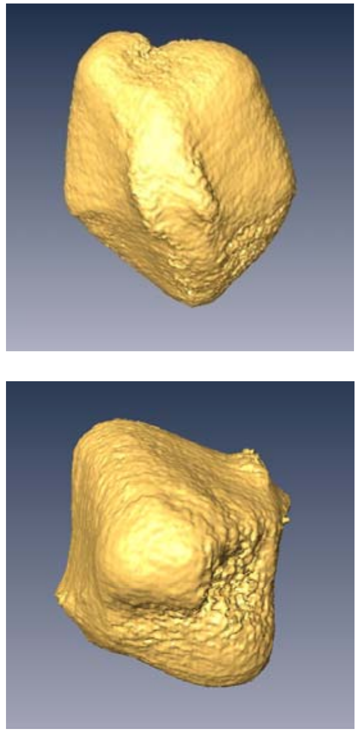


-45° - +45°   -60° - +60°   -75° - +75°   -90° - +90°

Missing wedge artefacts

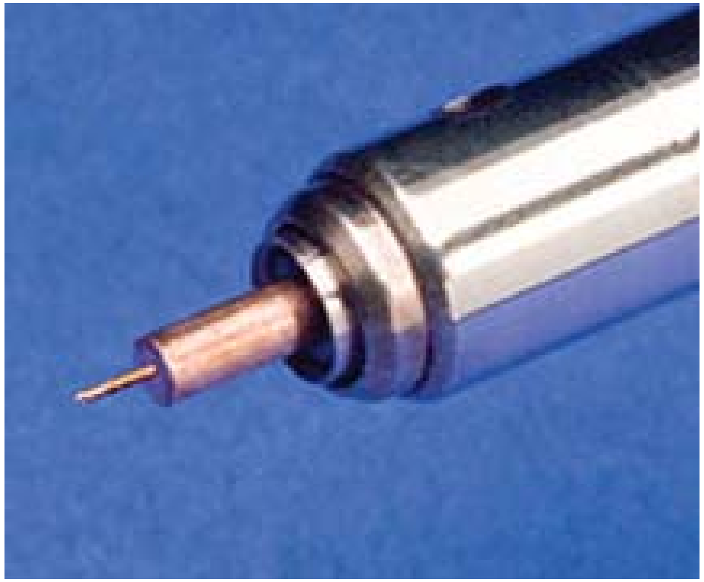
- Insufficient number of projections
- Limited angular range

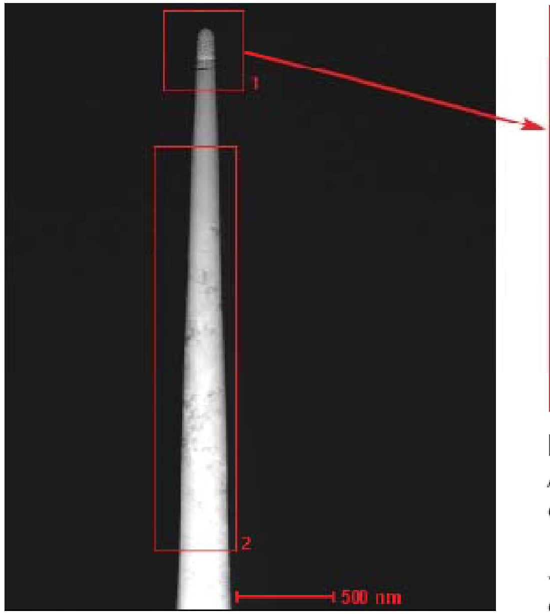




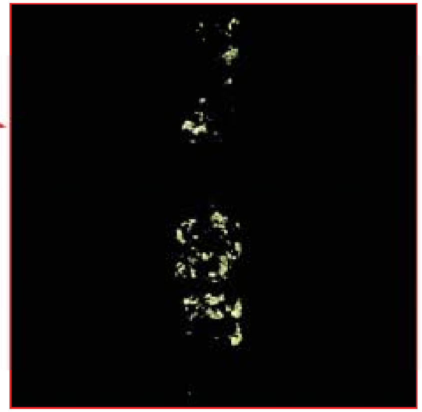
K.J. Batenburg, S. Bals et al.,
Ultramicroscopy, 109(6), 730-740, 2009

Electron Tomography: Tomography holder





HAADF STEM image of a Ni specimen containing alumina particles. The needle-shape was created using an FEI DB 235 DualBeam Instrument equipped with an Omniprobe nanomanipulator for specimen lift-out.

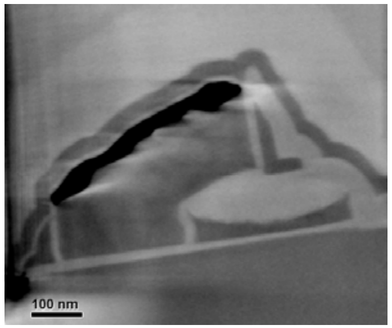


Reconstruction of alumina particles. An FEI Tecnai F30 TEM was used to collect 19 x-ray spectral images, 500 x 100 pixels by 1024 channels at a rate of 50msec/pixel. The specimen was rotated on-axis in 10° increments from −90° to +90°. Total data acquisition was approximately one million x-ray spectra taken in the course of 4 days. Analysis was conducted simultaneously with the Sandia multivariate statistical analysis software. In the image, Ni is shown as red and the alumina component is shown after image alignment in green.

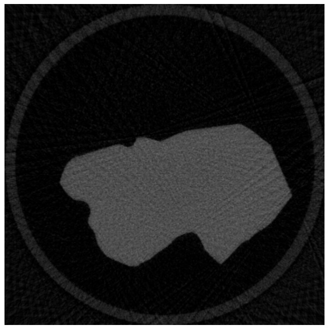
Images couresy of P. Kotula, Sandia National Laboratories, U.S.A., L.A. Giannuzzi, FEI Company, U.S.A., and F. de Haas, FEI Company, The Netherlands.

Discrete tomography

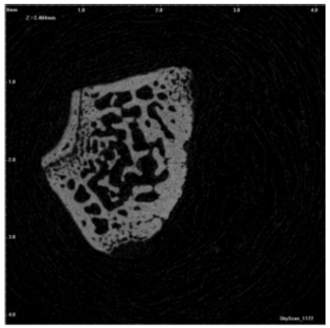
- Fixed set of possible intensities (grey values)
- Materials should be known in advance
- Use prior knowledge about the materials in the reconstruction



C. Kübel, FEI



DiamCAD NV



Skyscan NV

Algorithm: DART

- **DART: Discrete Algebraic Reconstruction Technique**
  - Iterative method
  - Input: projection images + set of intensities
  - Output: segmented image

DART

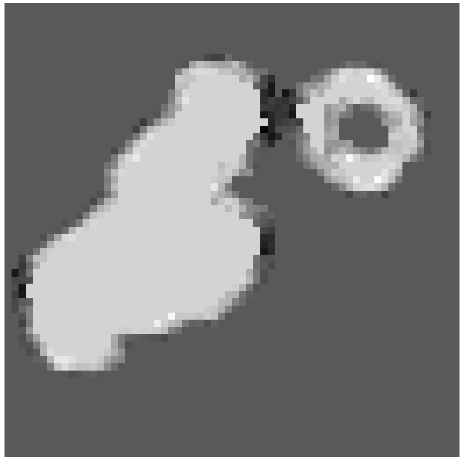
Simulation image

13 projections
-60/+60 degrees

SIRT reconstruction

SIRT reconstruction, thresholded

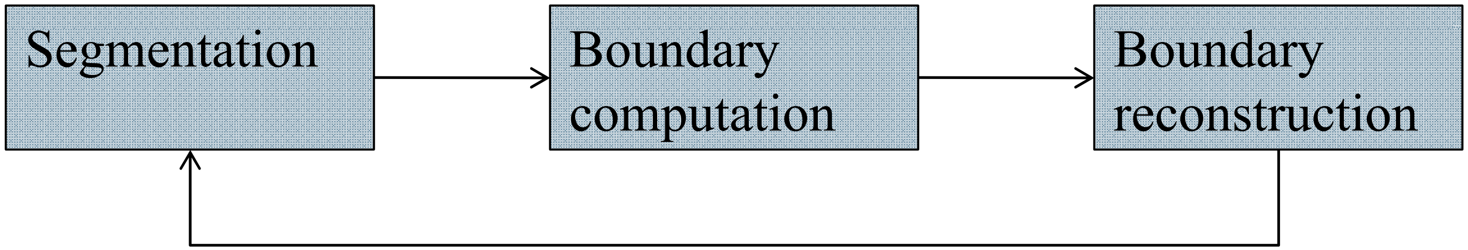
K.J. Batenburg, S. Bals et al.,
Ultramicroscopy, 109(6), 730-740, 2009



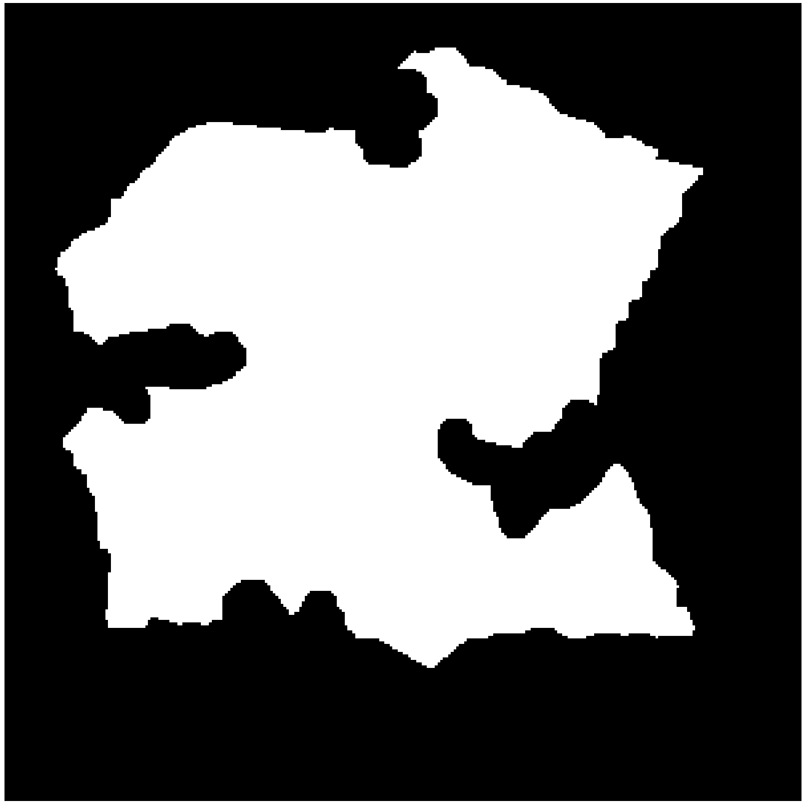
Intermediate reconstruction

Final reconstruction (3 iterations)

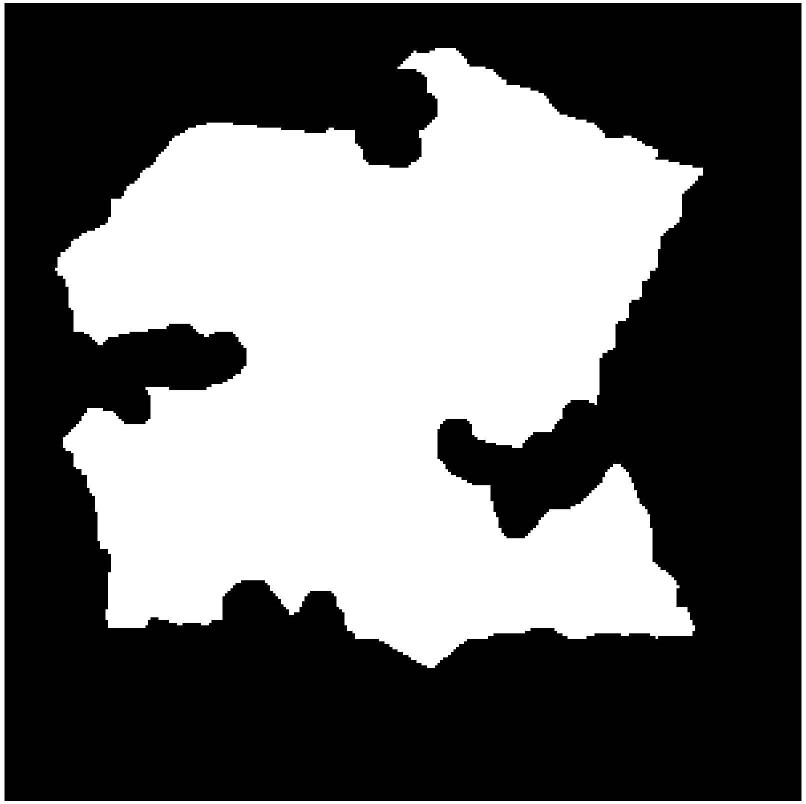
Original image



DART from few projections



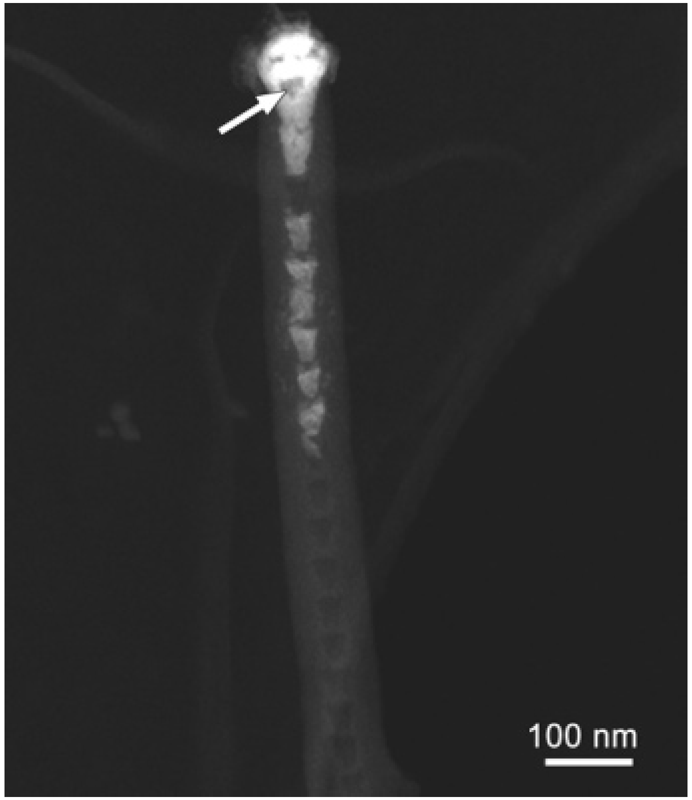
Original image



Discrete tomography, 5 projections

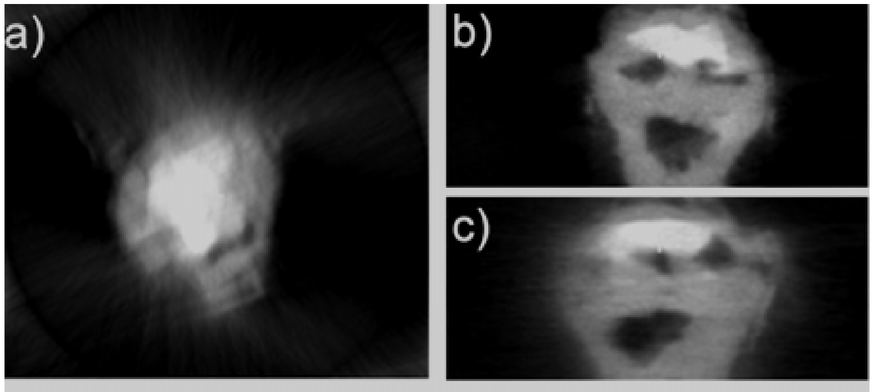
Example:
electron tomography of a nanoparticle

HAADF STEM imaging, FEI Titan microscope

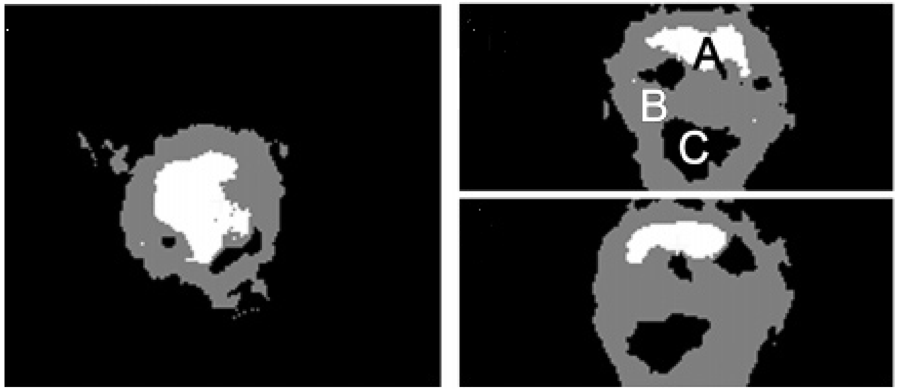


Example:
electron tomography of a nanoparticle

HAADF STEM tomography, FEI Titan



Classical reconstruction,
using the SIRT algorithm

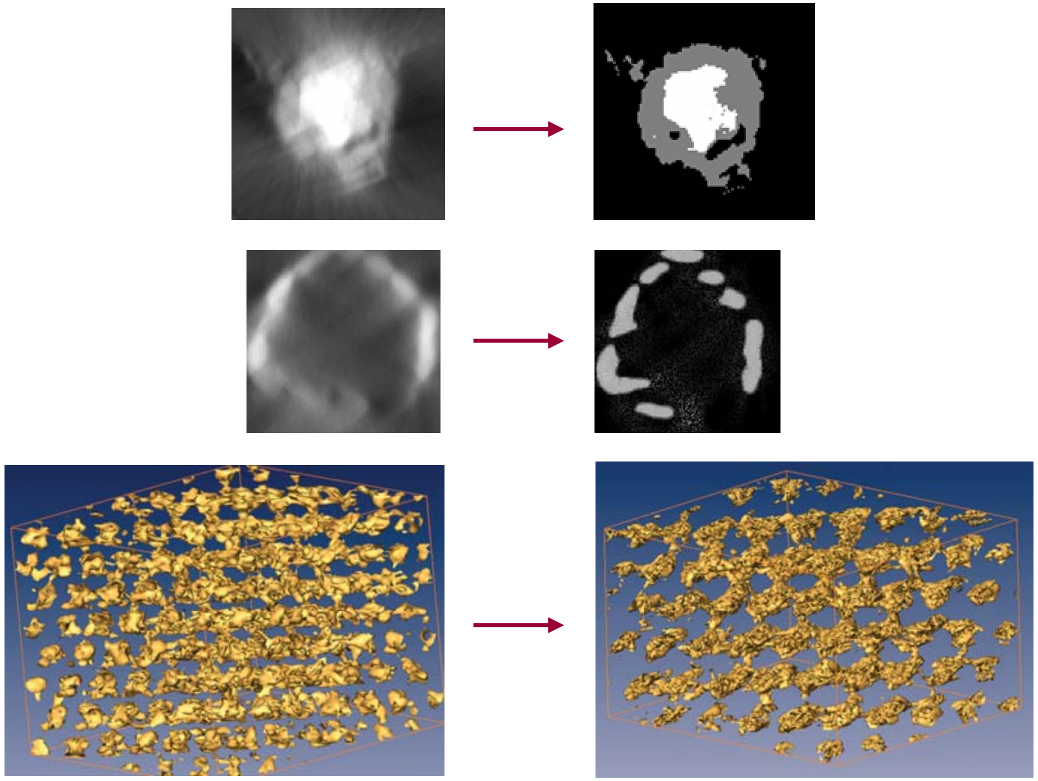


DART reconstruction

S. Bals, K.J. Batenburg et al., Nano Letters 7(12), 3669-3674 (2007)

K.J. Batenburg, S. Bals et al., Ultramicroscopy 109(6), 730-740 (2009)

Discrete Electron Tomography



Conventional reconstruction

Discrete Tomography

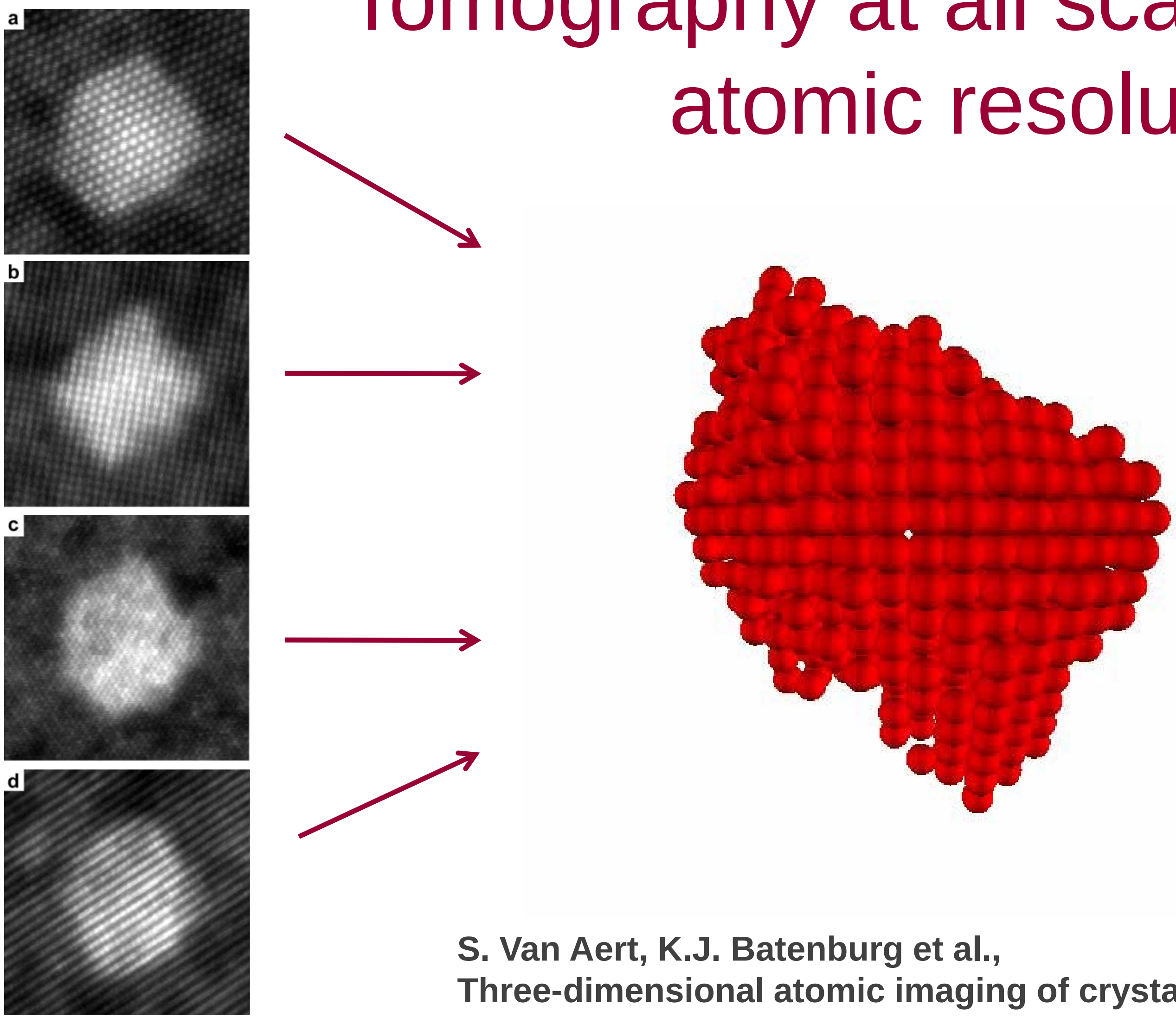
S. Bals, K.J. Batenburg et al.,
Nano Letters,
7(12), 3669-3674, 2007

S. Turner, S.M.F. Tavernier et al.,
J. Nanoparticle Research,
12(2), 615-622, 2009

S. Bals, K.J. Batenburg et al.,
J. Am. Chem. Soc.,
131(13), 4769-4773, 2009

- **By exploiting prior knowledge, more accurate reconstructions can be computed from *the same* measured data.**

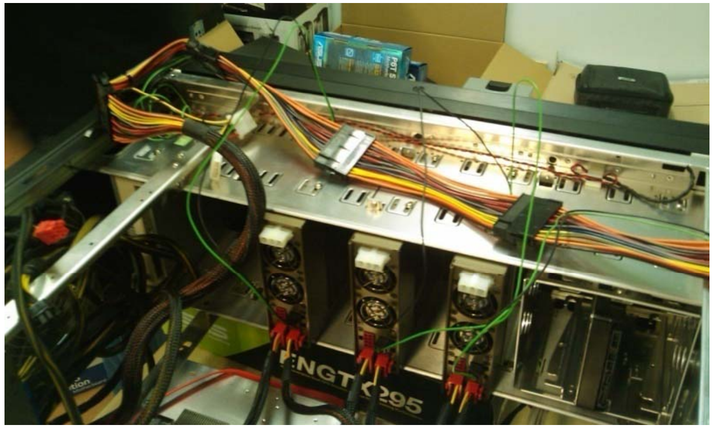
Tomography at all scales: atomic resolution



S. Van Aert, K.J. Batenburg et al., Three-dimensional atomic imaging of crystalline nanoparticles, Nature 470, 374-377 (2011).

Light year • • • km • • • mm • • • µm • • • nm • • • sub-Å

Supercomputing for tomography



- **FASTRA II: 12 TFLOPS supercomputer on your desk**
- **13 NVIDIA GPUs**
- **http://fastra2.ua.ac.be**

Outlook and Conclusions

- For effective nanometrology, the 3rd dimension is crucial
- Electron tomography is a versatile tool for 3D nanometrology
- New instruments and computational models can overcome traditional limitations
- Discrete tomography allows accurate imaging at the nanoscale, up to the atomic level

TY for your attention

Acknowledgements

- CWI, Amsterdam
- EMAT, Antwerp
- Vision Lab, Antwerp
- Fraunhofer, KIT, DiamCAD, Skyscan, NVIDIA, …