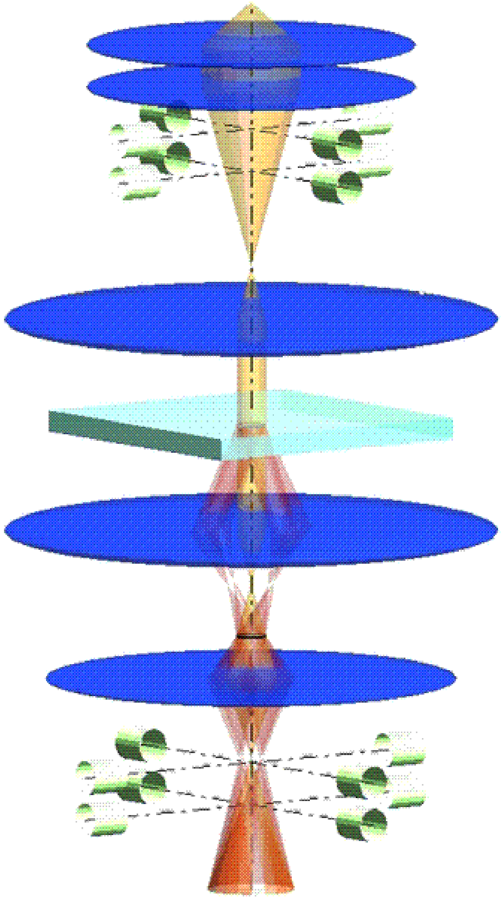
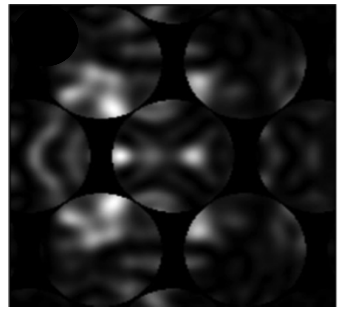
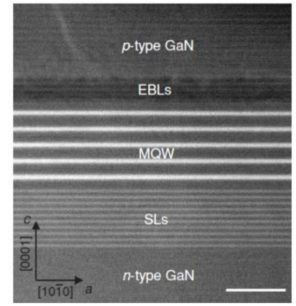
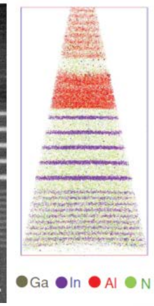
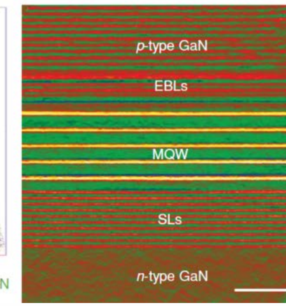
HUMBOLDT-UNIVERSITÄT ZU BERLIN

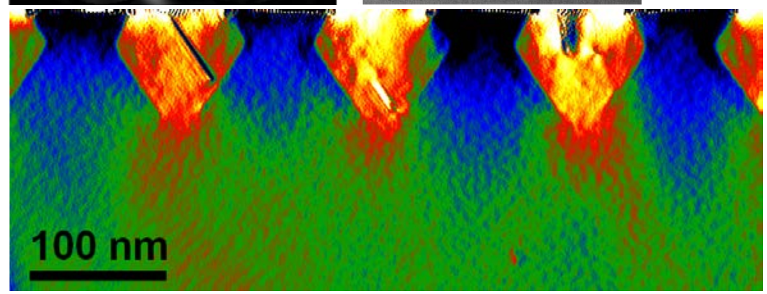


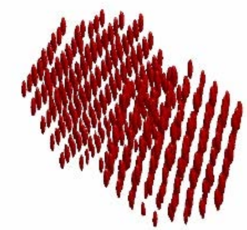


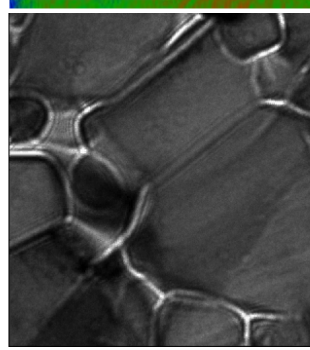


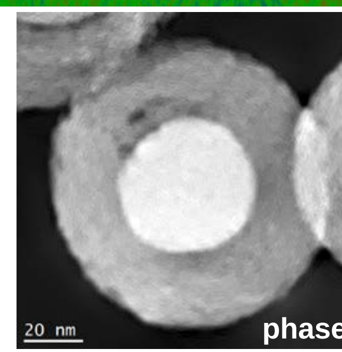


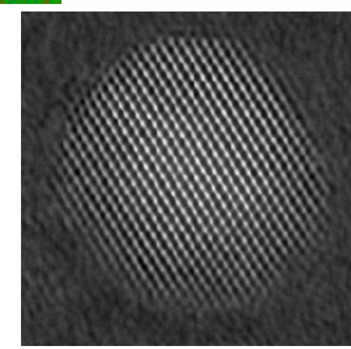












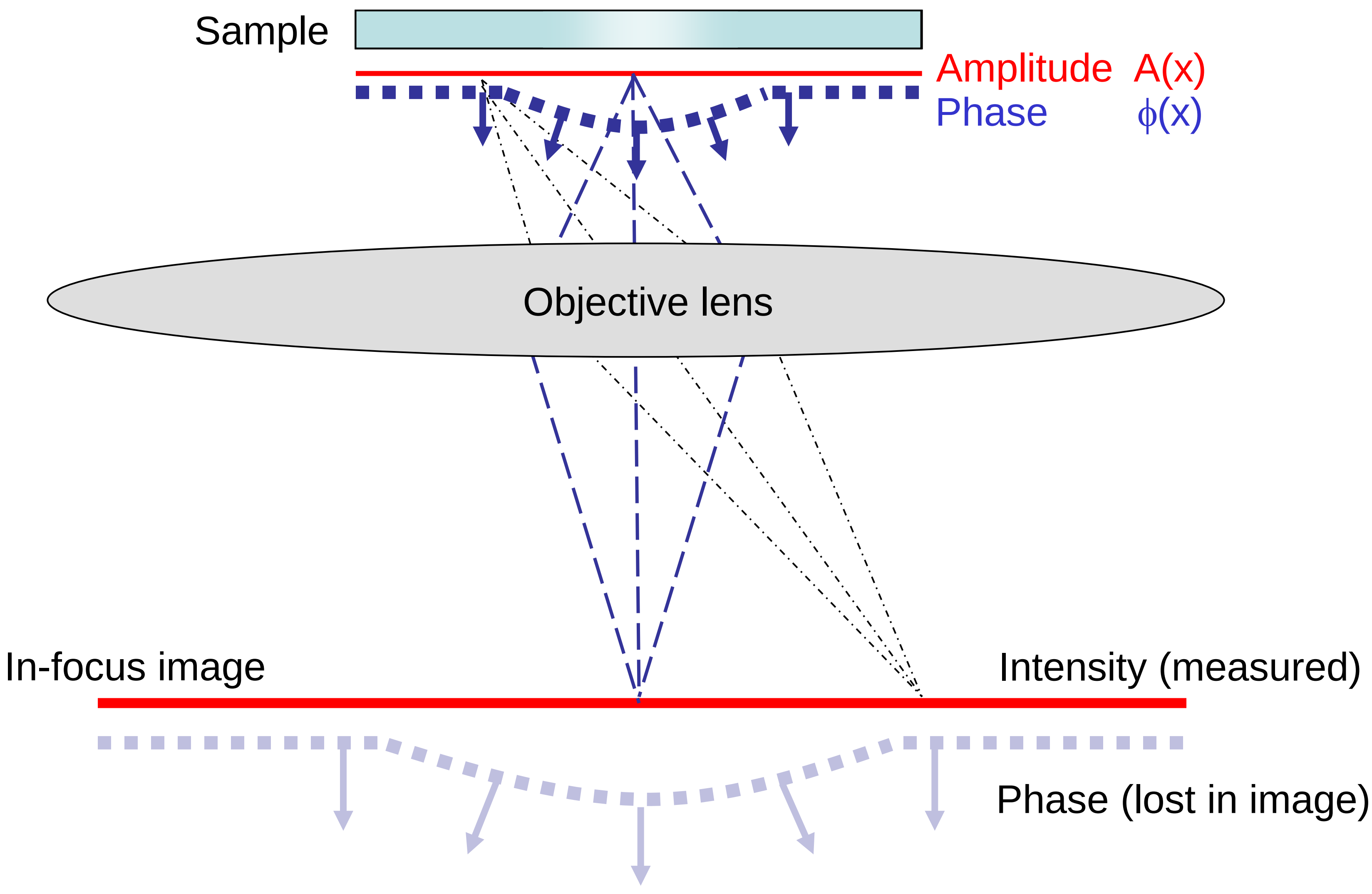
Inline and hybrid electron holography for mapping charges, potentials, and strain

Christoph T. Koch | Institut für Physik | HU Berlin

Outline

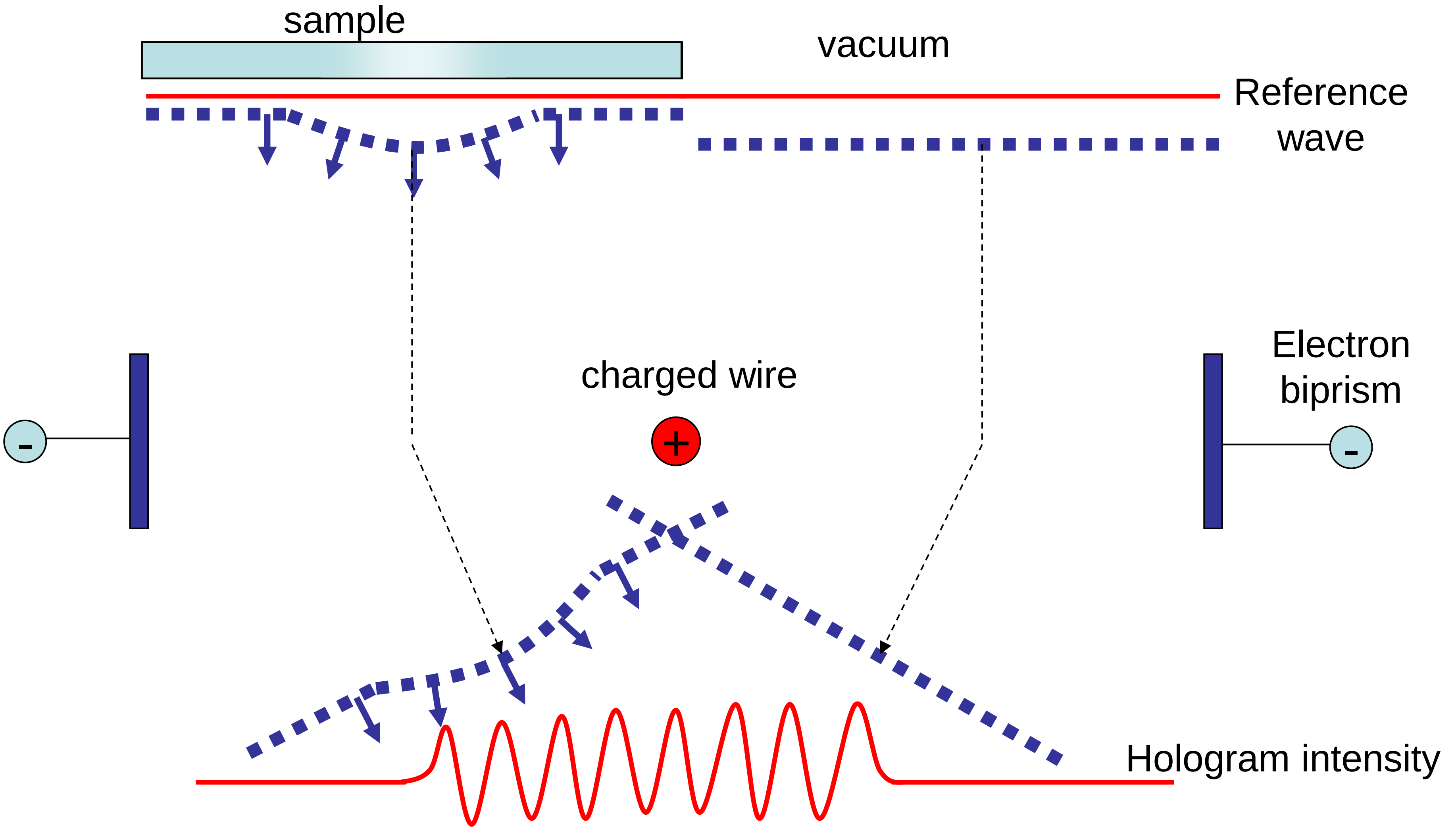
- Introduction: What is inline holography?
- Applications: HRTEM Aberration compensation & Strain Mapping
- Recovering low spatial frequencies by
  - Hybrid holography
  - Gradient-flipping inline holography
- Introducing the full-resolution wave reconstruction (FRWR) code
- Data Acquisition at the TEM

The Phase Problem in Imaging



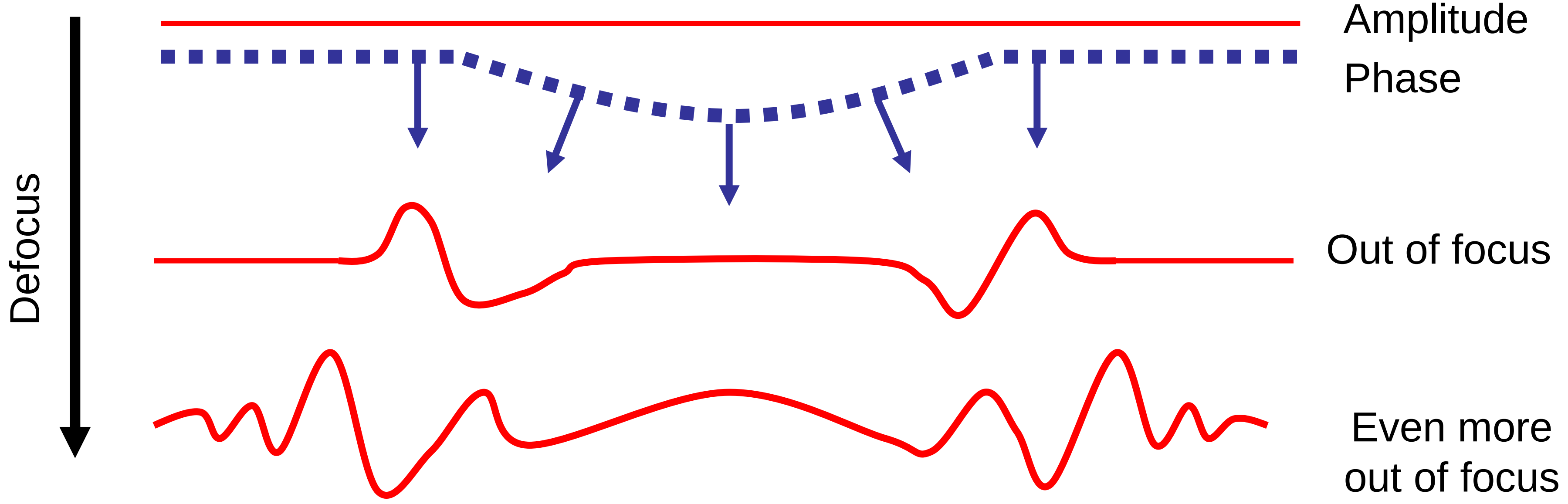
Holography in the TEM: a) Off-axis Electron Holography

Pioneered by Gottfried Möllenstedt in Tübingen



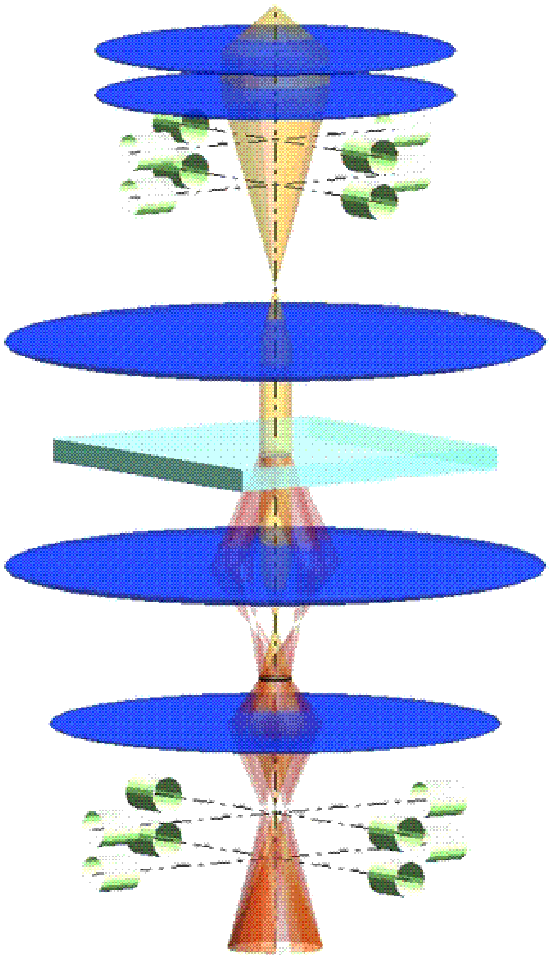
Interference pattern
(phase shift reconstructed by linear algebra methods)

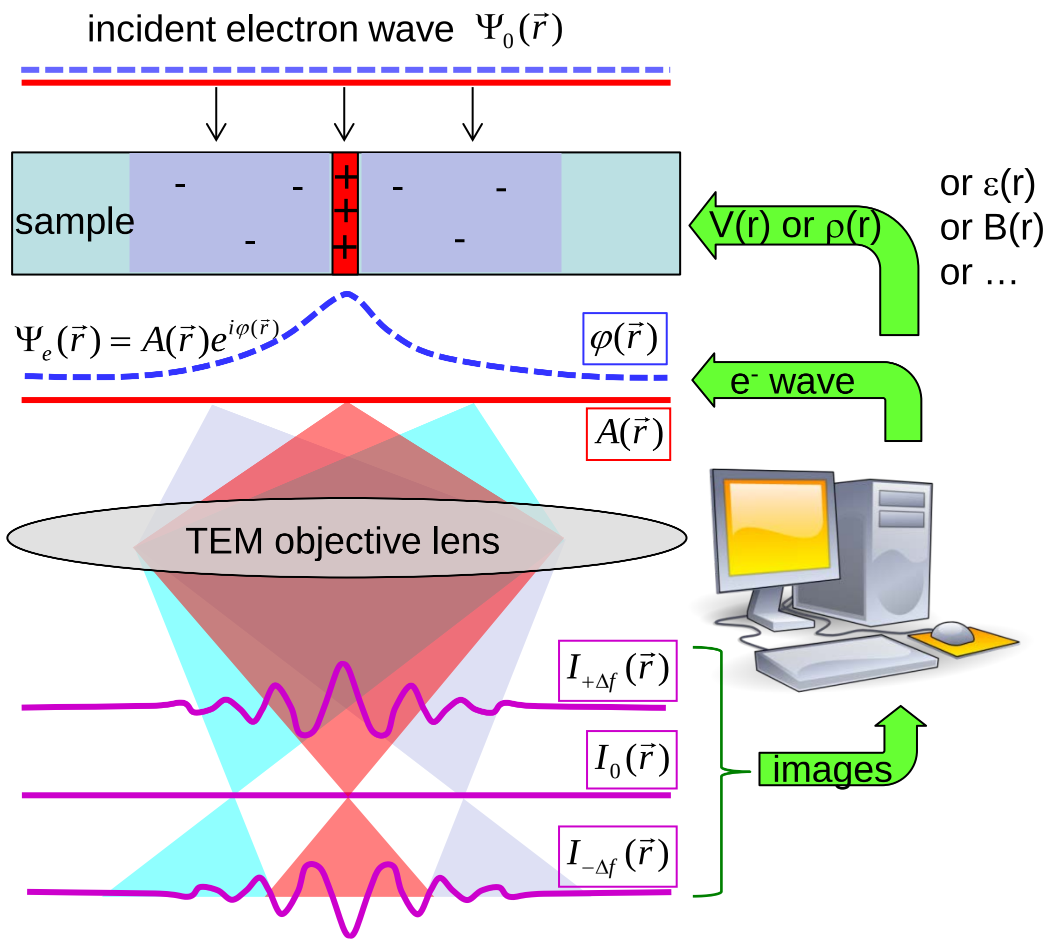
Holography in the TEM: b) Inline Electron Holography



Variations in projected mass thickness => Fresnel fringes

How Inline Holography Works in the TEM





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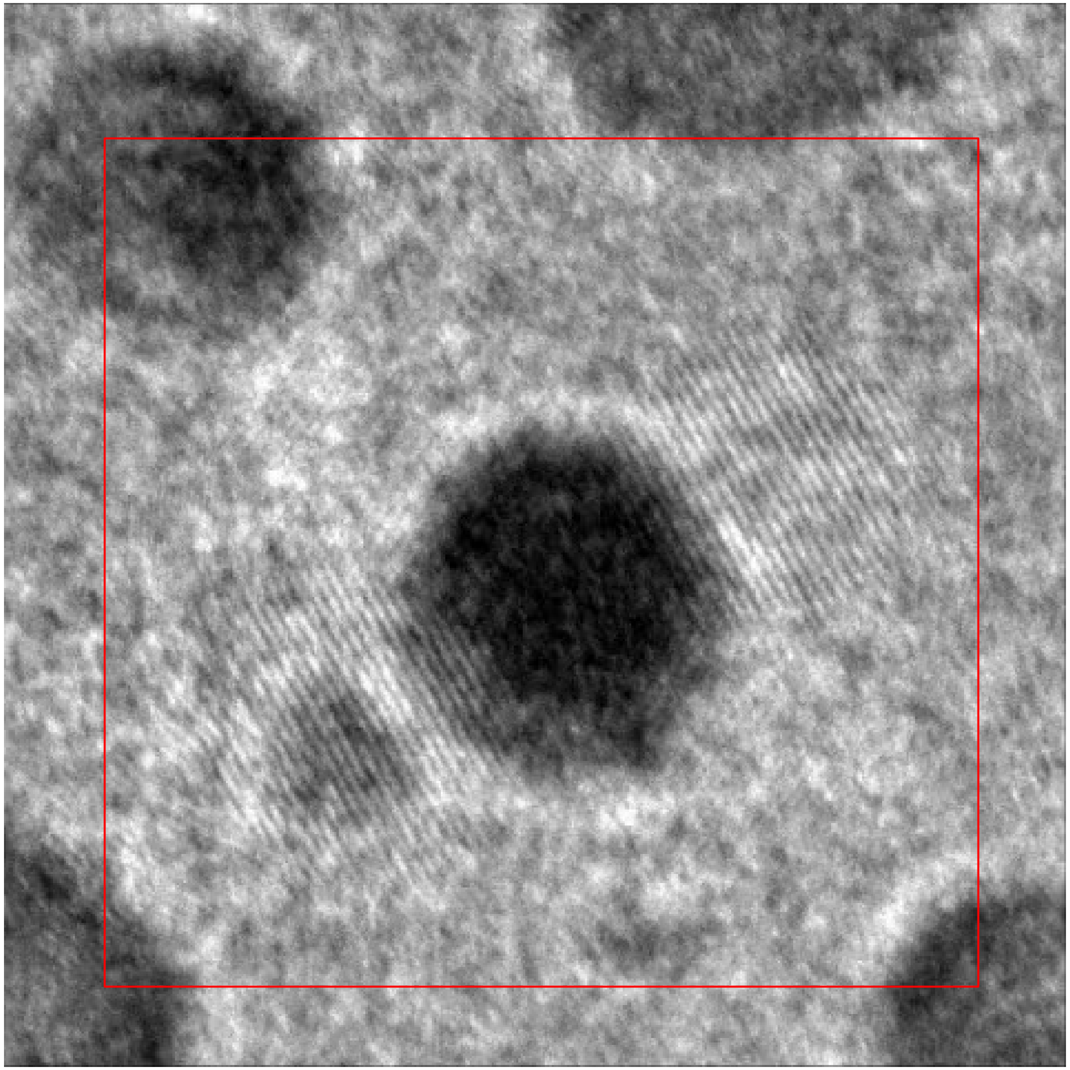
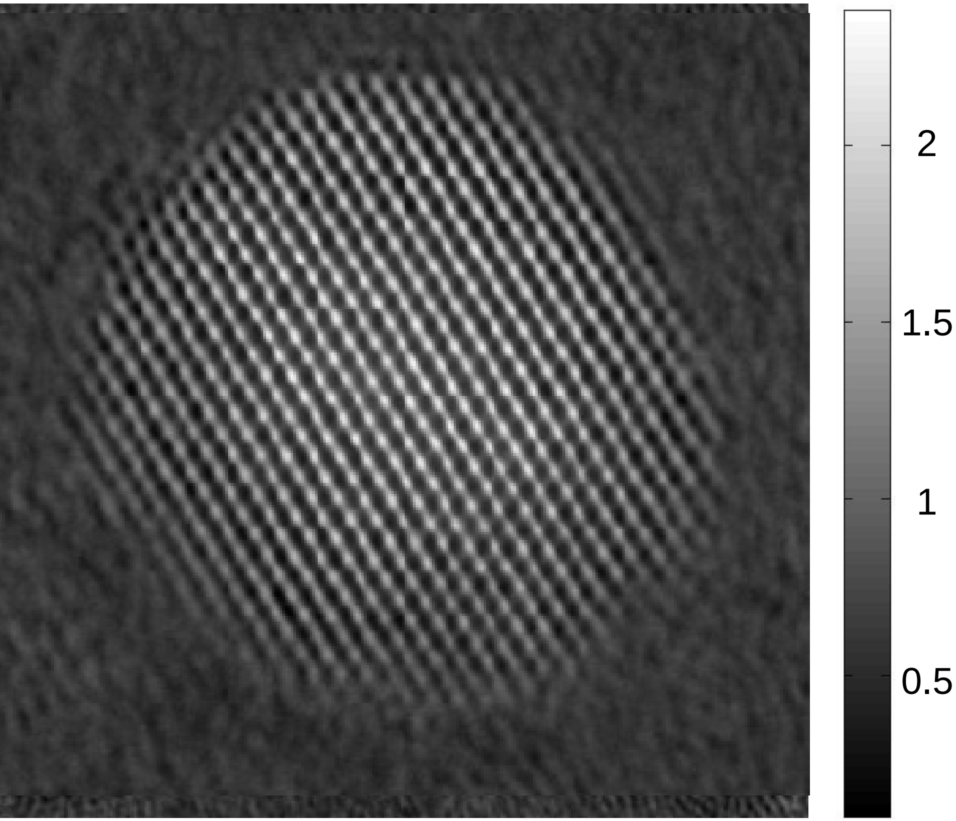
Iterative Focal Series Reconstruction in HRTEM

21 images
Δf=-605 .. -679nm

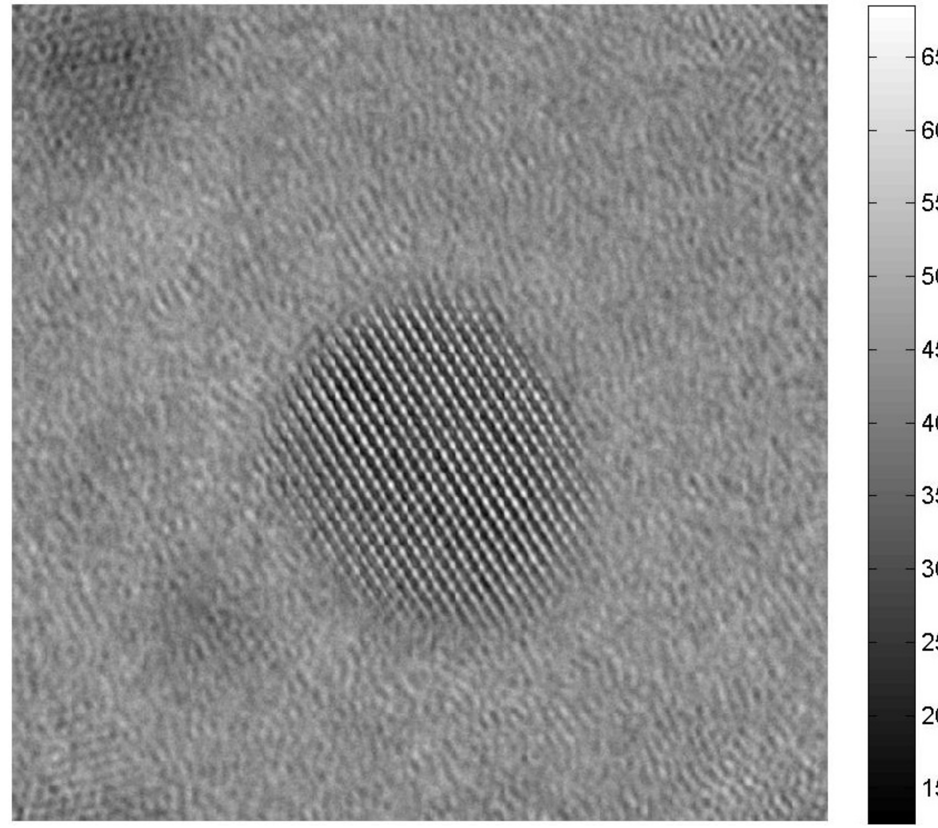


Data: M. Pelsozy, F. Ernst, T. Zawodzinski (Case Western Reserve University)
Gold particle on thin amorphous Ge film

Atomic-Resolution Inline Electron Holography



Phase

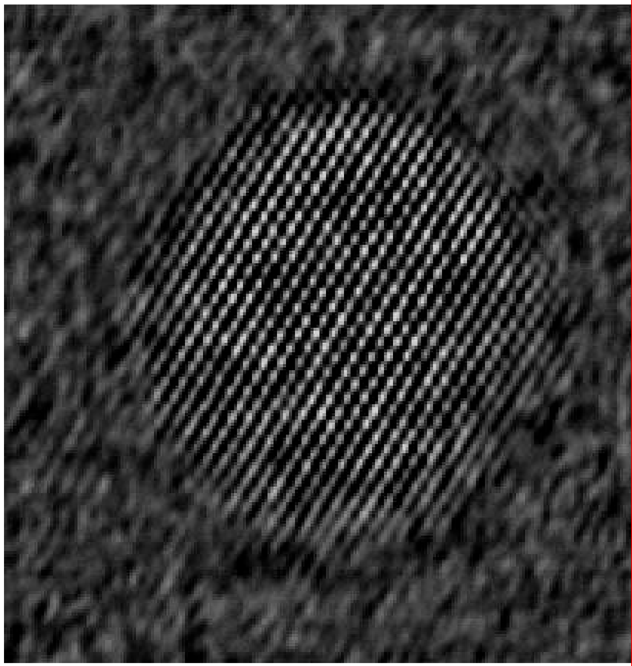


Amplitude

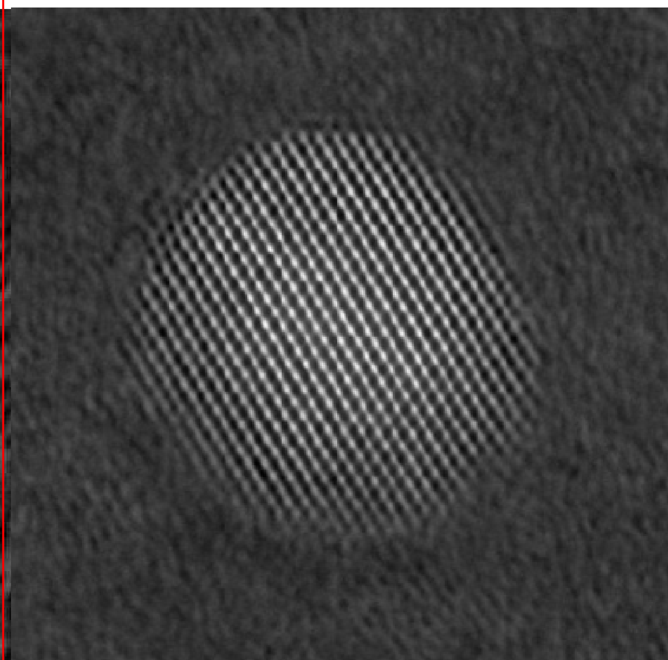
Phase and amplitude reconstructed using FRWR from focal series of a Gold particle on a thin Carbon film.

Same Data – Different Algorithms

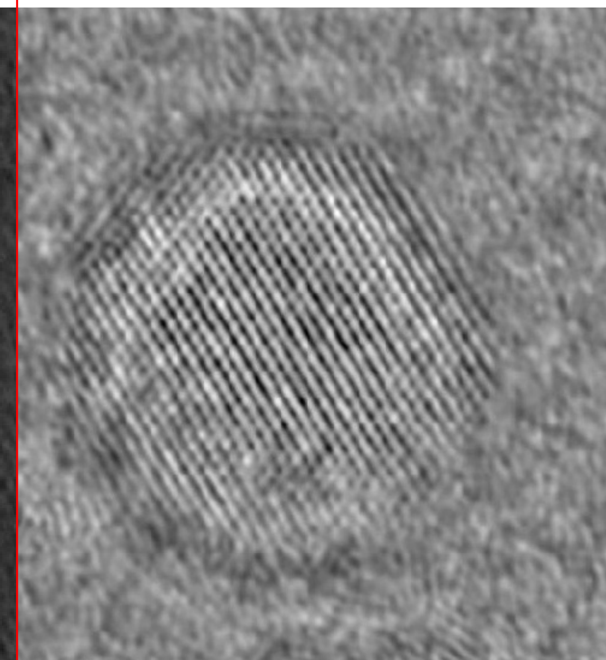
Algorithm 1



FRWR



Algorithm 3



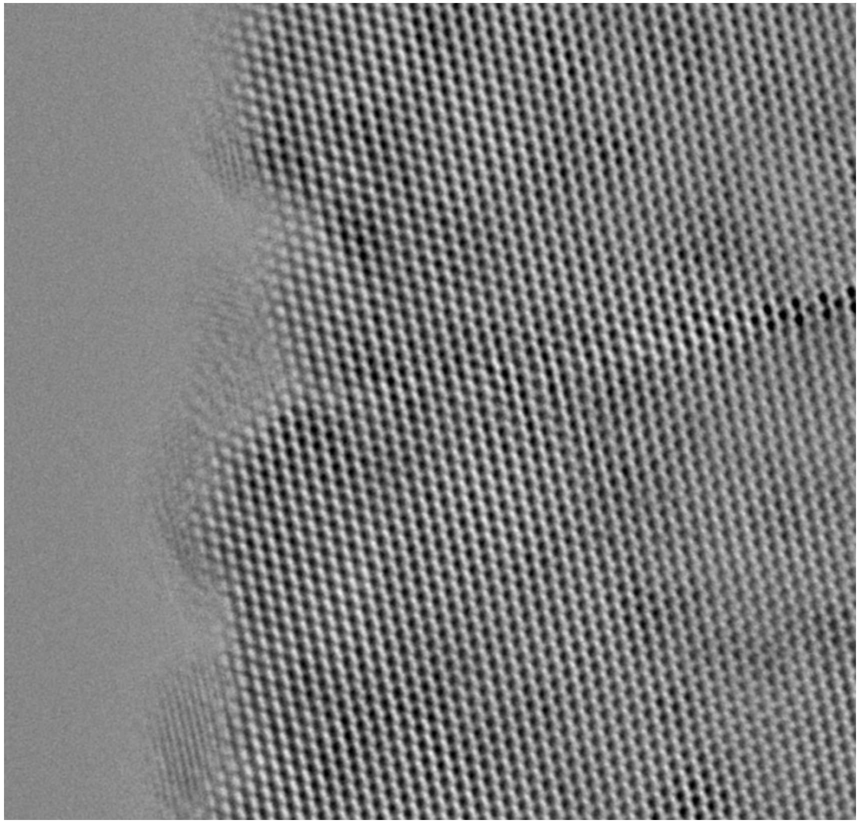
Phase of reconstructed exit-face wave function

Grain Boundary in $SrTiO_3$

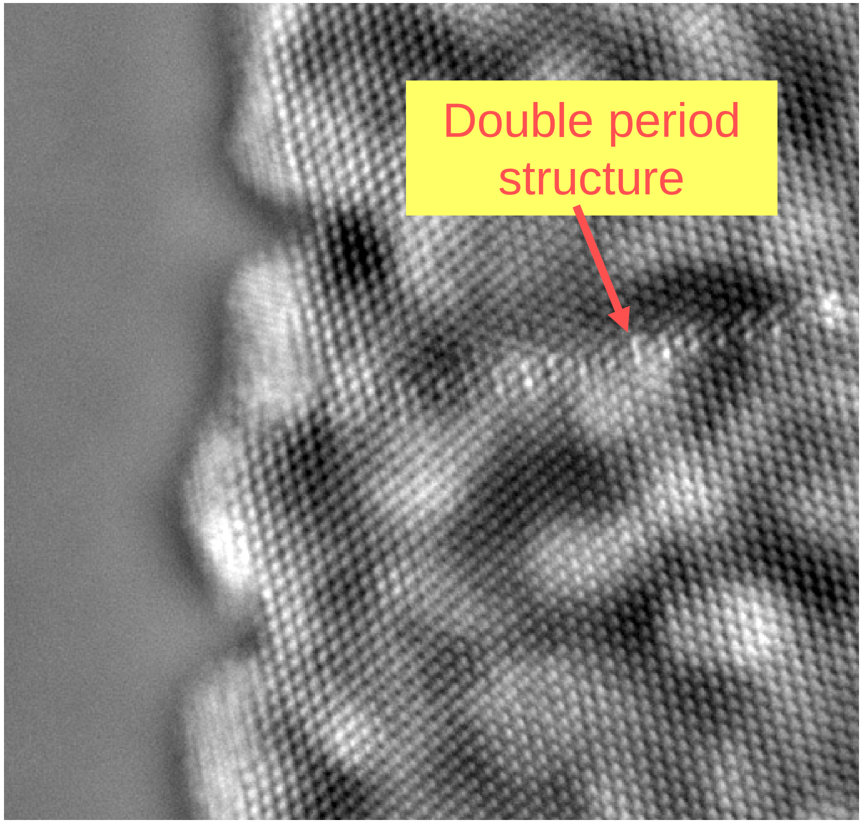
Complex electron wave function reconstructed from inline holograms using the FRWR Algorithm[1]

(experimental data provided by K. Dudeck, Oxford)

Amplitude

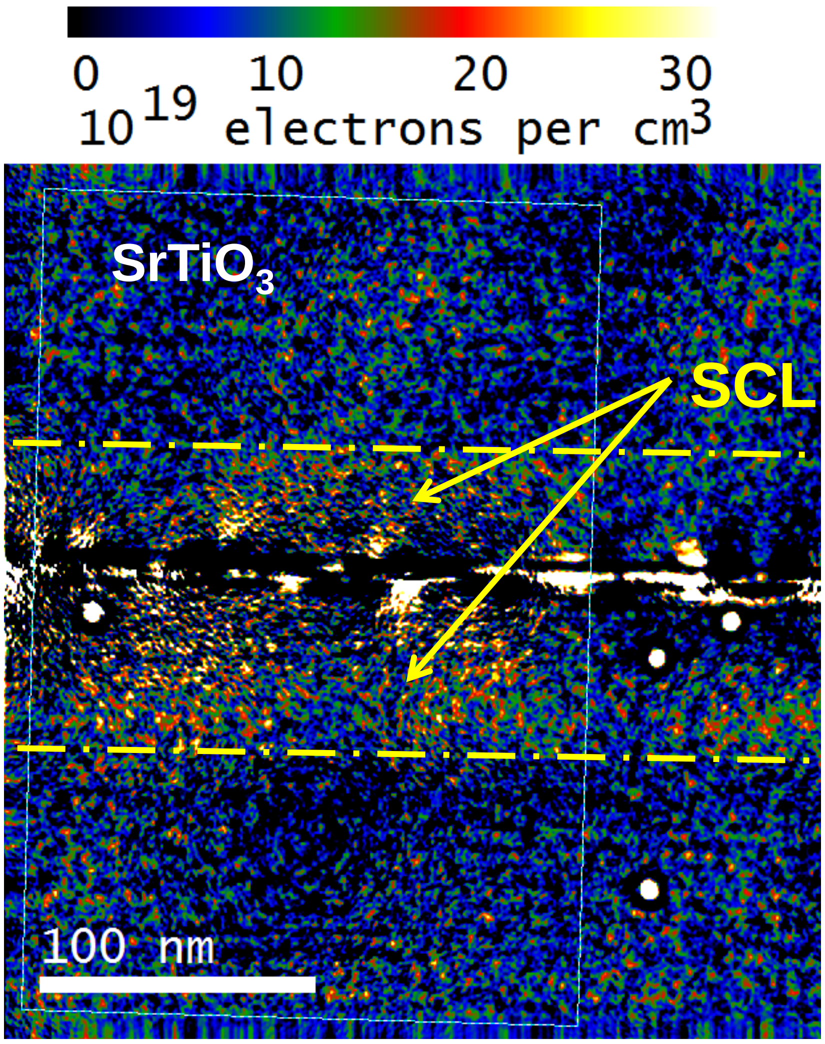


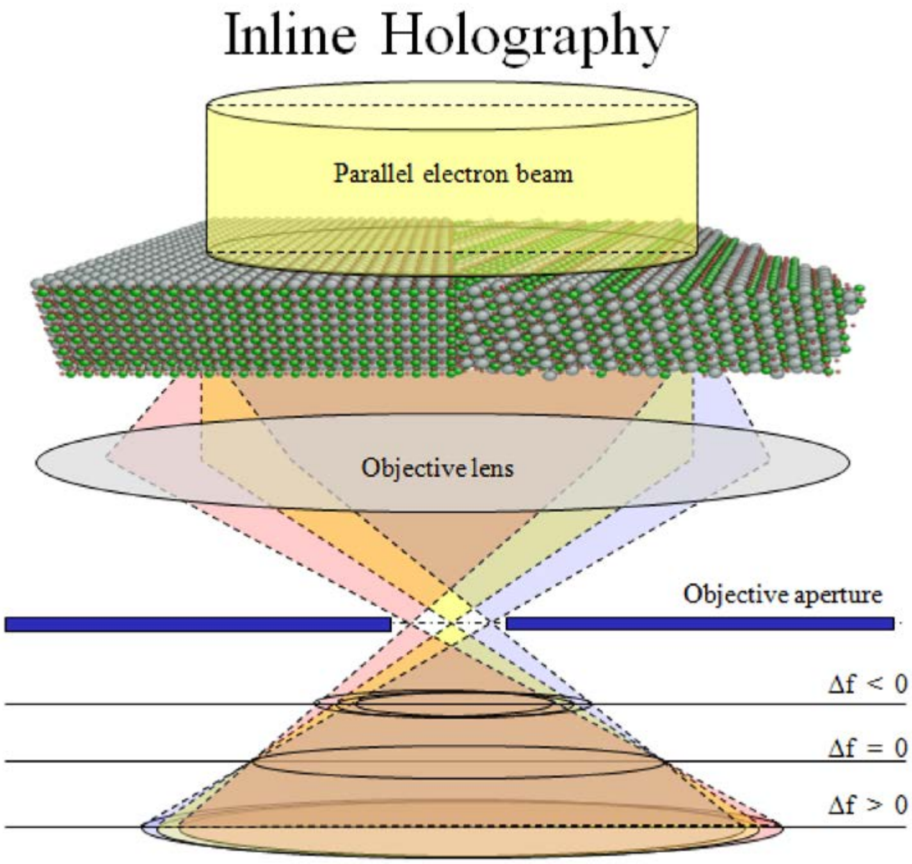
Phase



[1] C.T. Koch, Ultramicroscopy 108, 141-150 (2008)

Mapping Space Charge in Ceramics

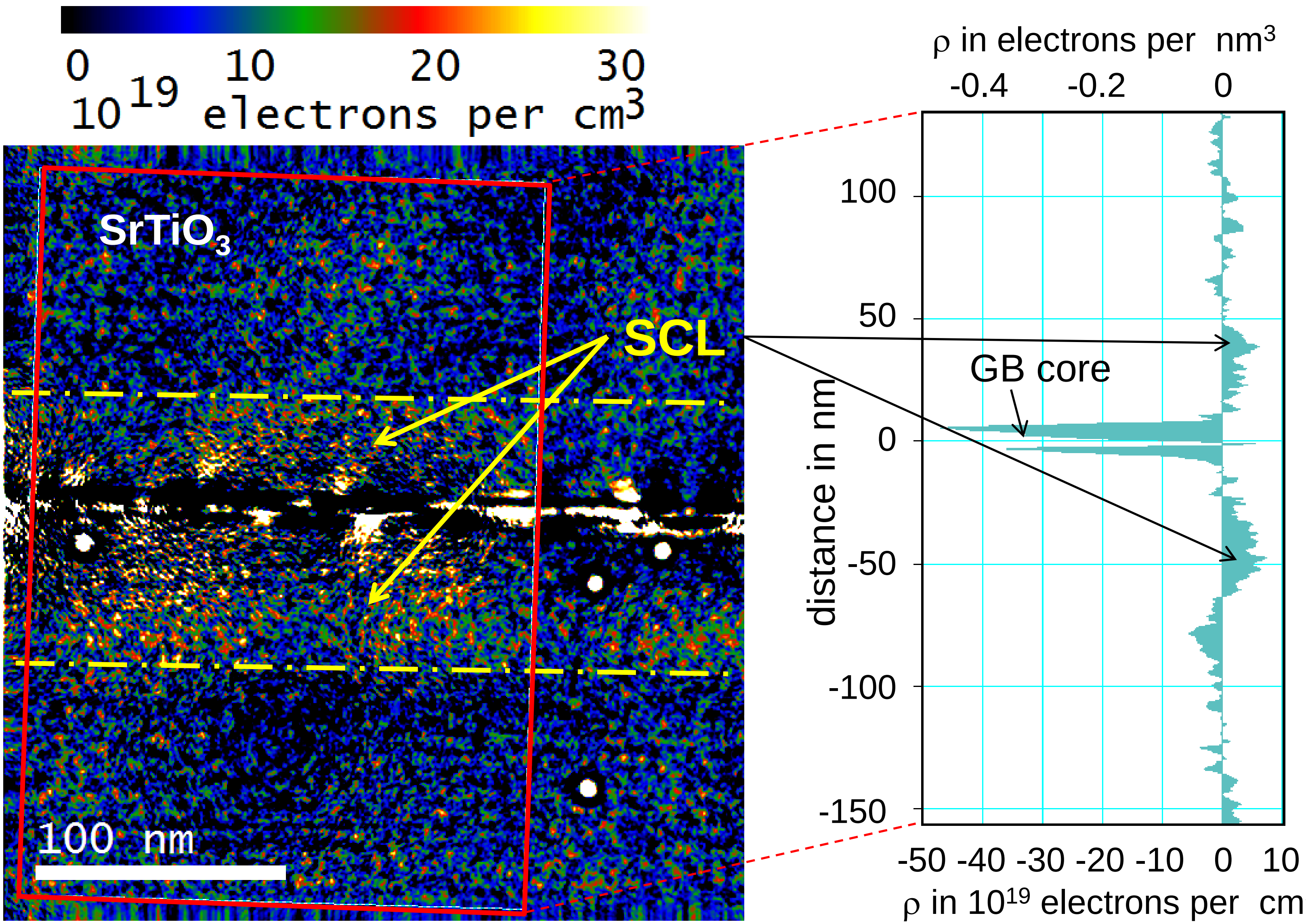




Spatial resolution: ≈ 1 nm

C.T. Koch, International Journal of Materials Research **2010/01** (2010) 43-49

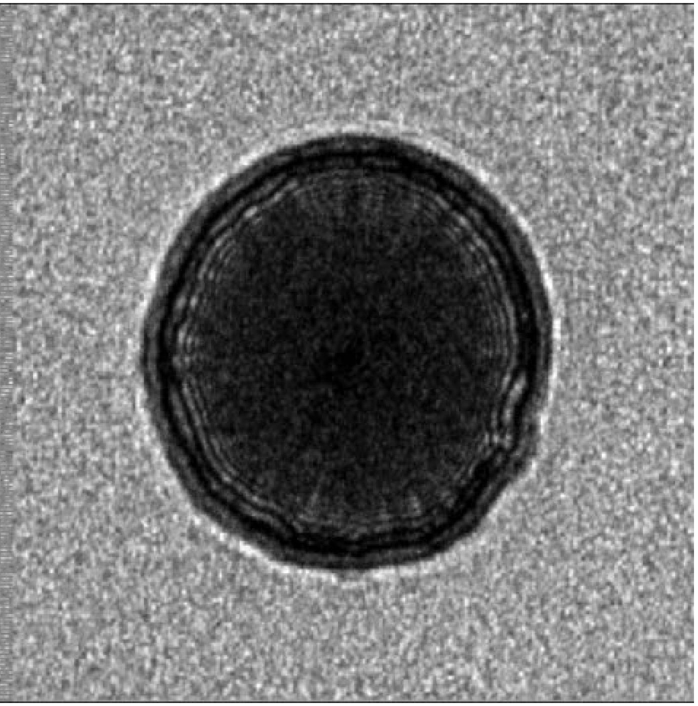
Space charge @ Σ3(112) GB in $SrTiO_3$

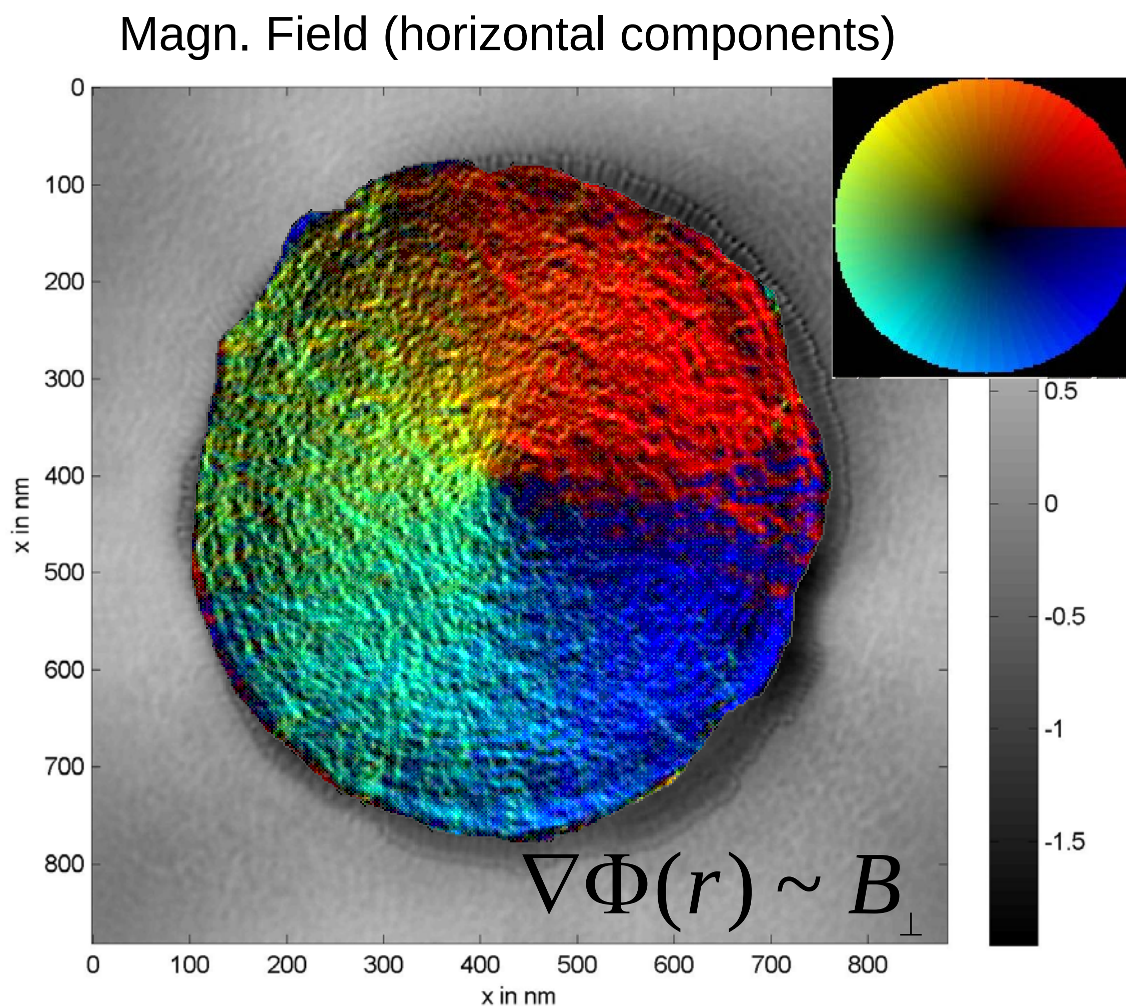


S. von Alfthan, et al., Annu. Rev. Mater. Res. **40** (2010), 557–99

E = 200 kV, t = 170 nm, ε_{STO} = 230 (probably closer to 100 because of high E-field)

Imaging Magnetic Fields by Inline Electron Holography





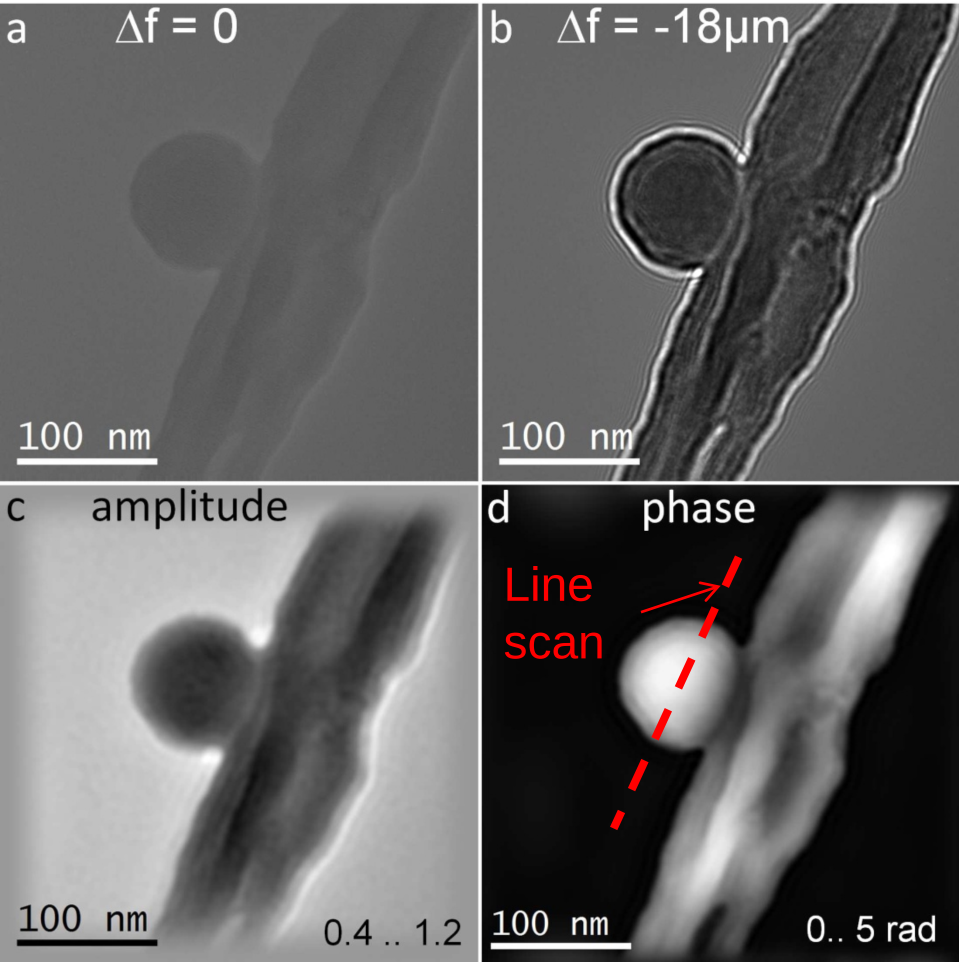
Lorentz focal series of a lithographically patterned magnetic structure

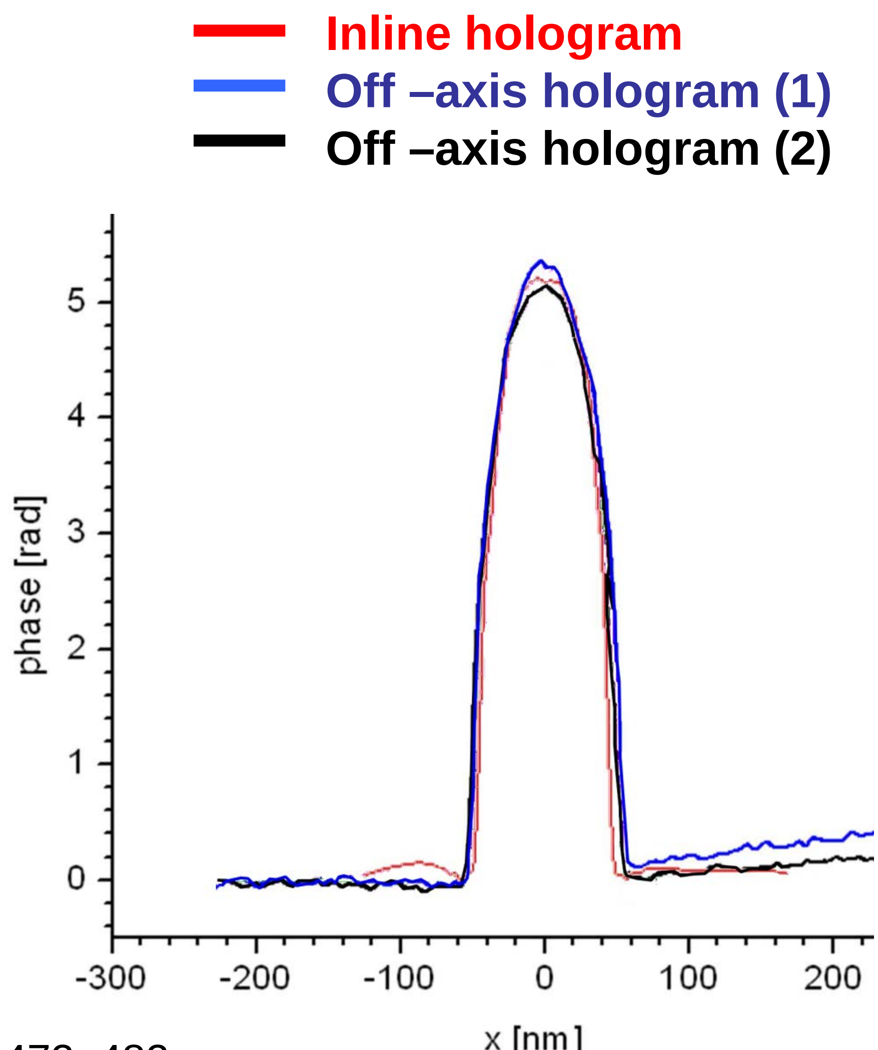
Image size: 1.2 x 1.2 µm^2
Data: S. McVitie (Glasgow)

Reconstruction using FRWR software

Reconstruction of Inline Holograms

Reconstruction from 1 in-focus and 1 out-of-focus image
by an iterative (non-linear) reconstruction algorithm





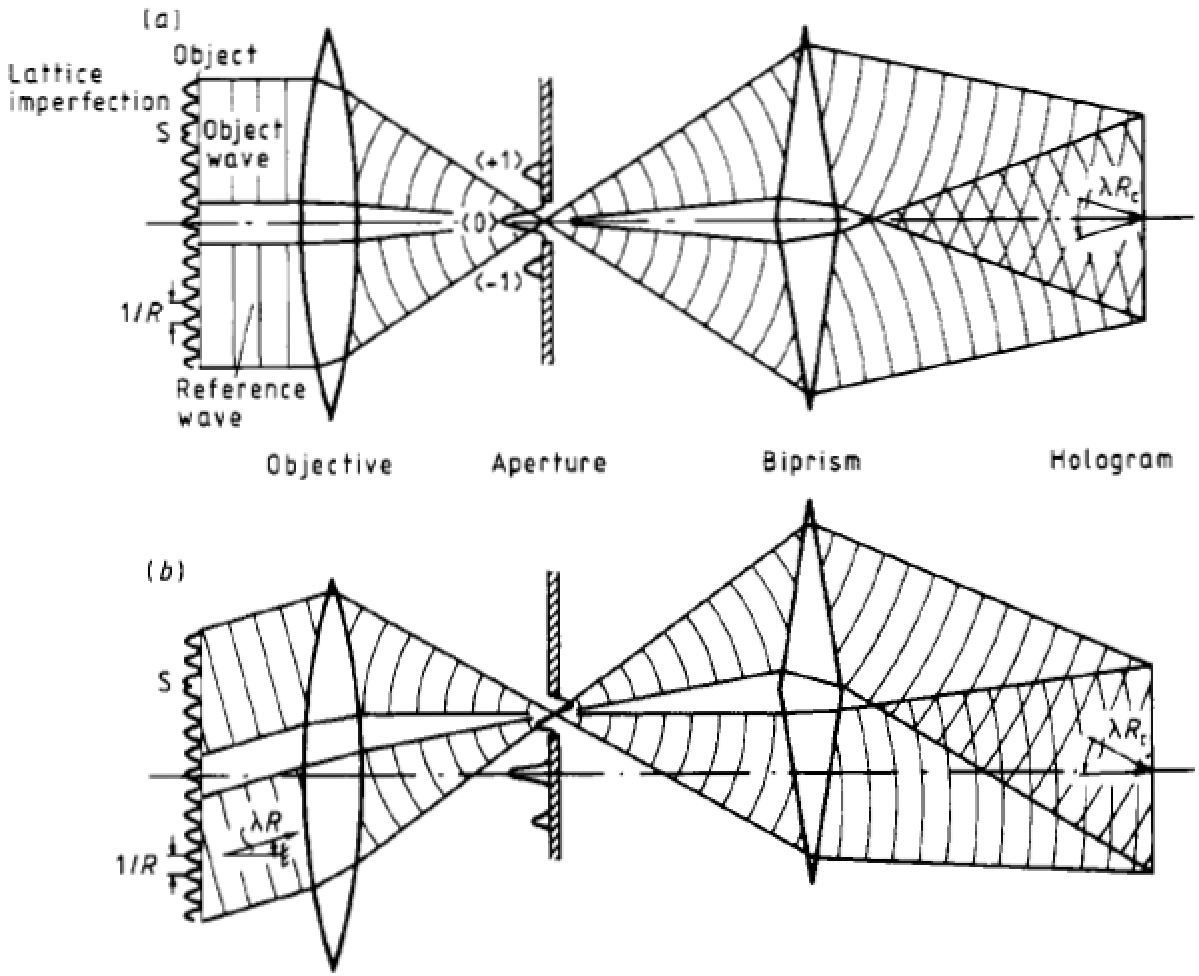
Experiment: P. Formanek (Dresden)

T. Latychevskaia, et al. Ultramicroscopy 110 (2010) 472–482

BF and DF off-axis Electron Holography

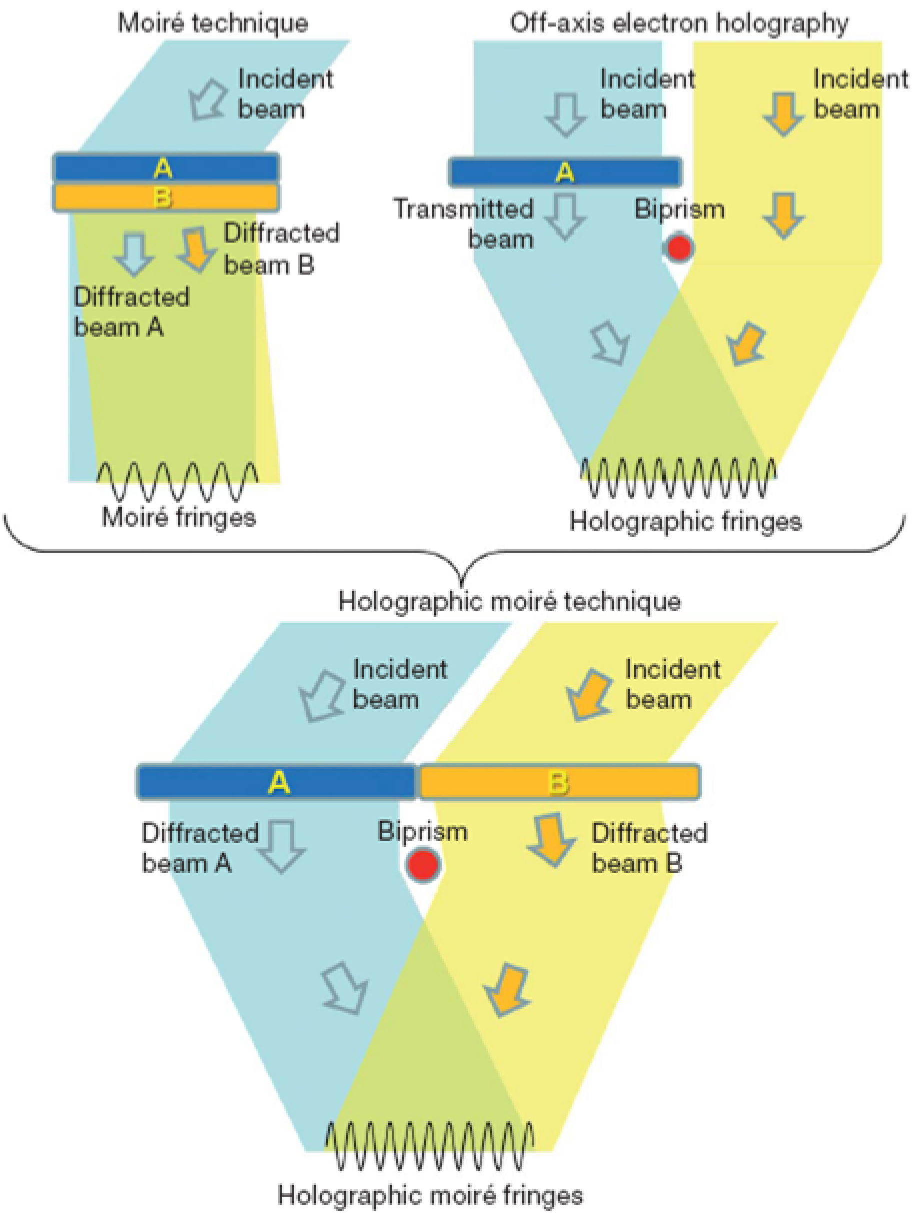
Bright-field

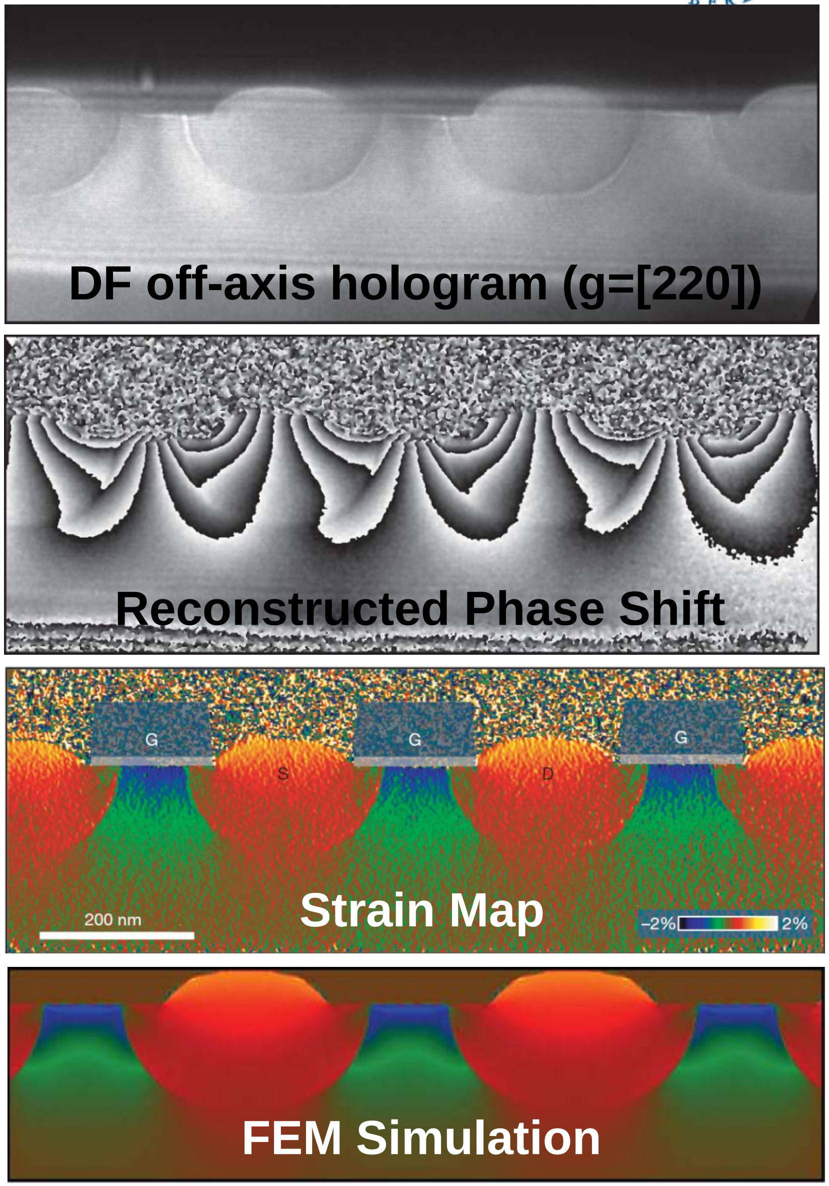
Dark-field



K.-J.Hanszen, J. Phys. D: Appl. Phys. **19** (1986) 373-395

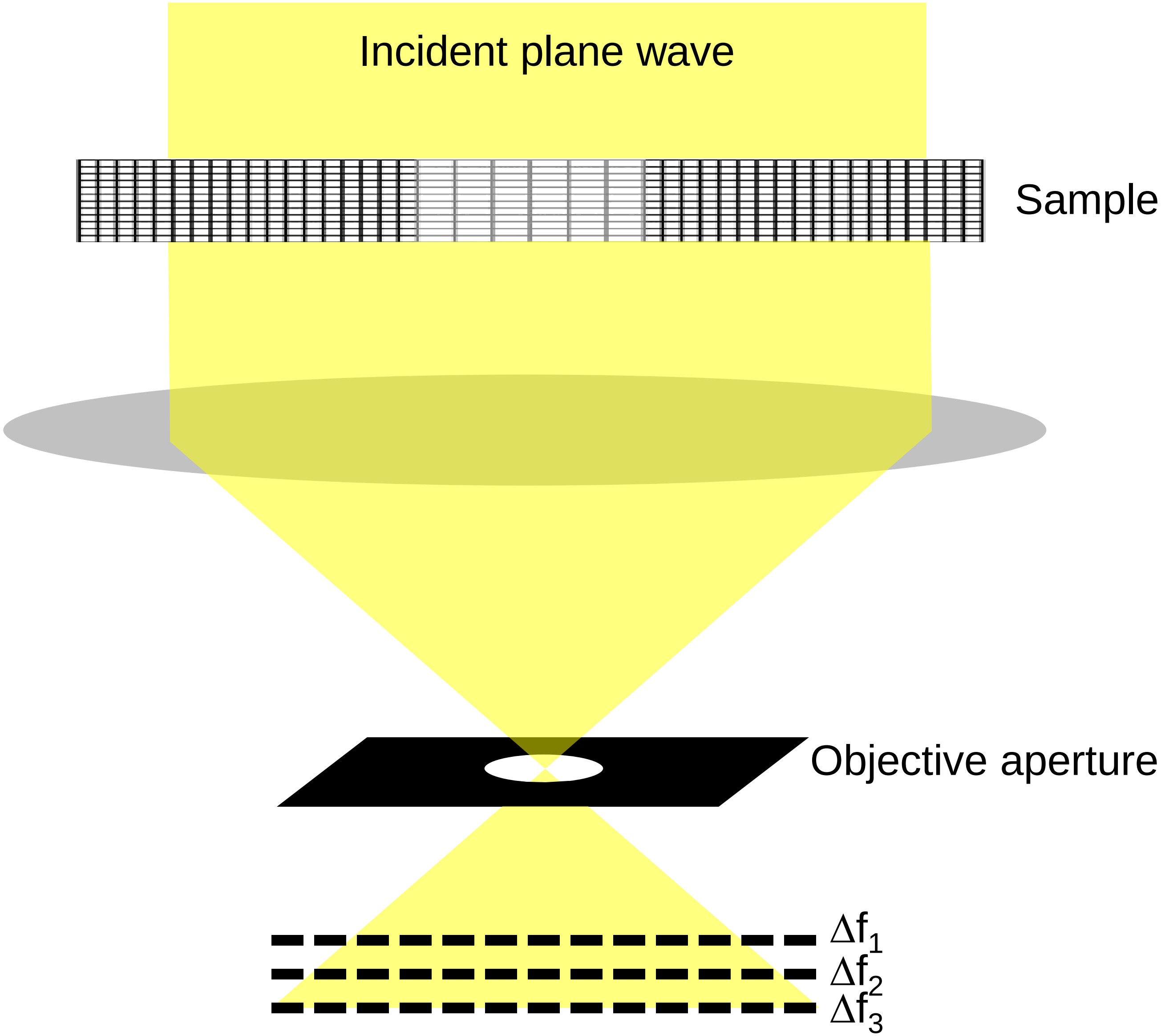
Strain Mapping by Dark-field Holography



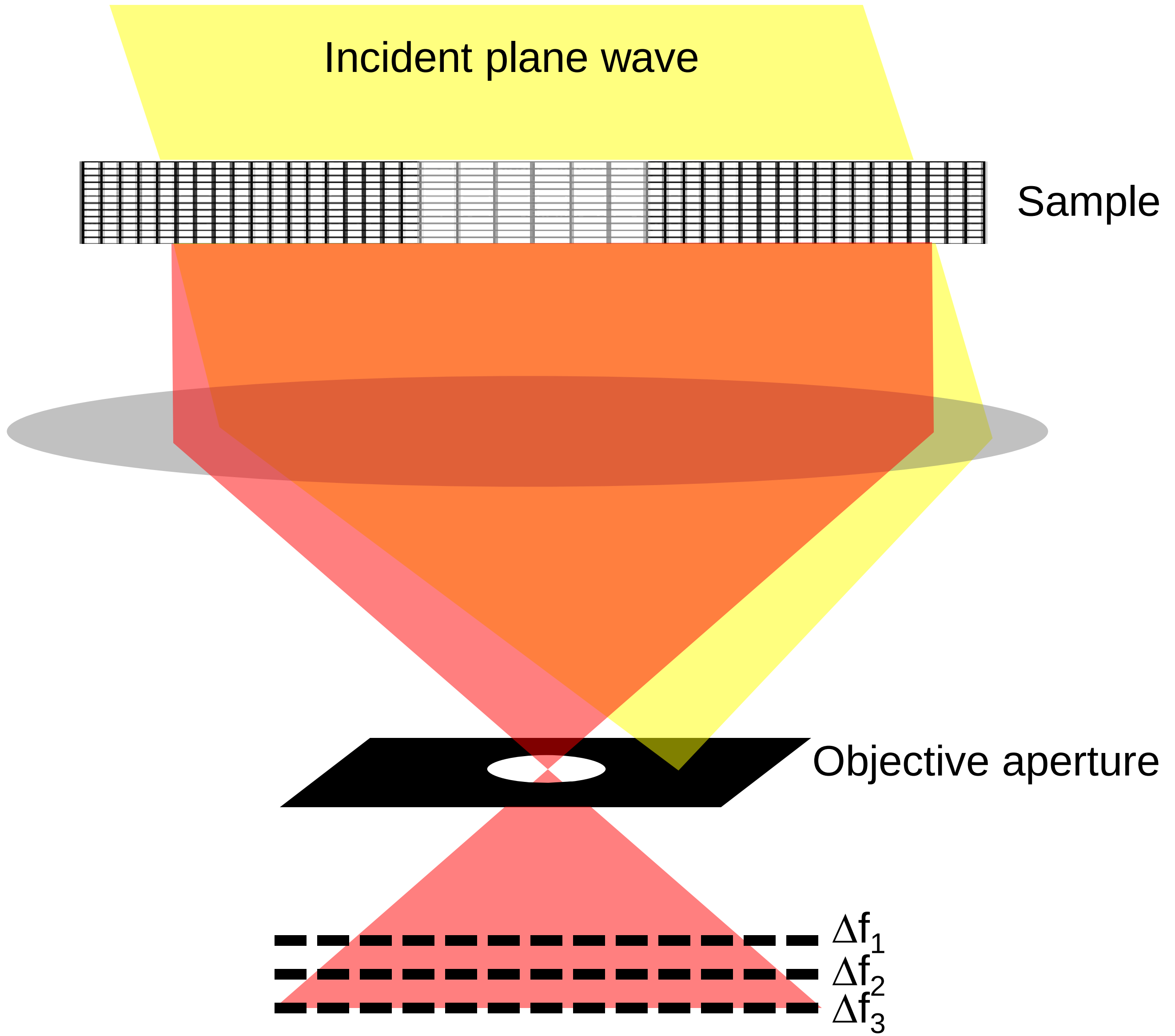


M. Hytch et al, Nature **453** (2008) 1086

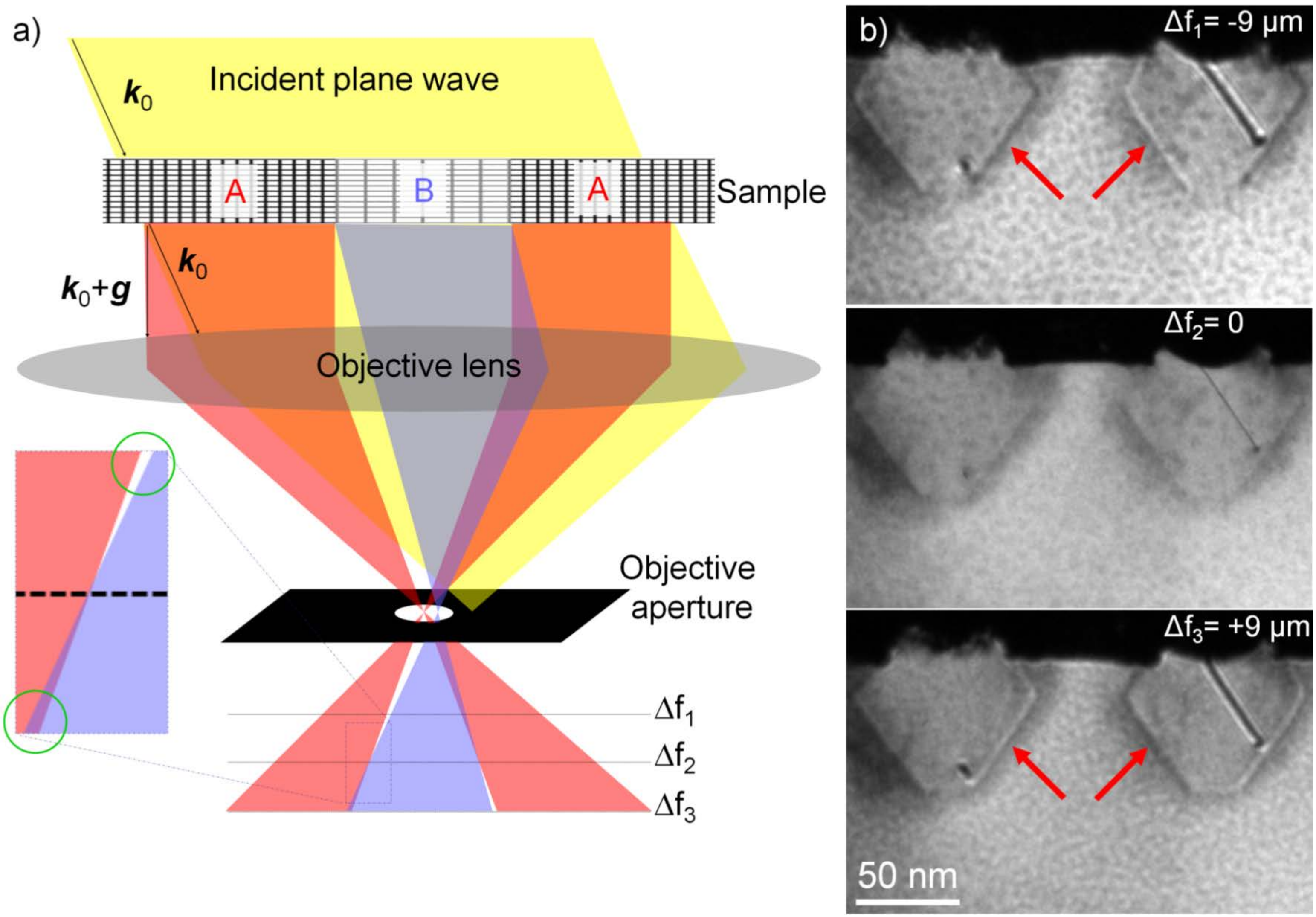
Bright-Field Inline Electron Holography



Dark-Field Inline Electron Holography (DIH)

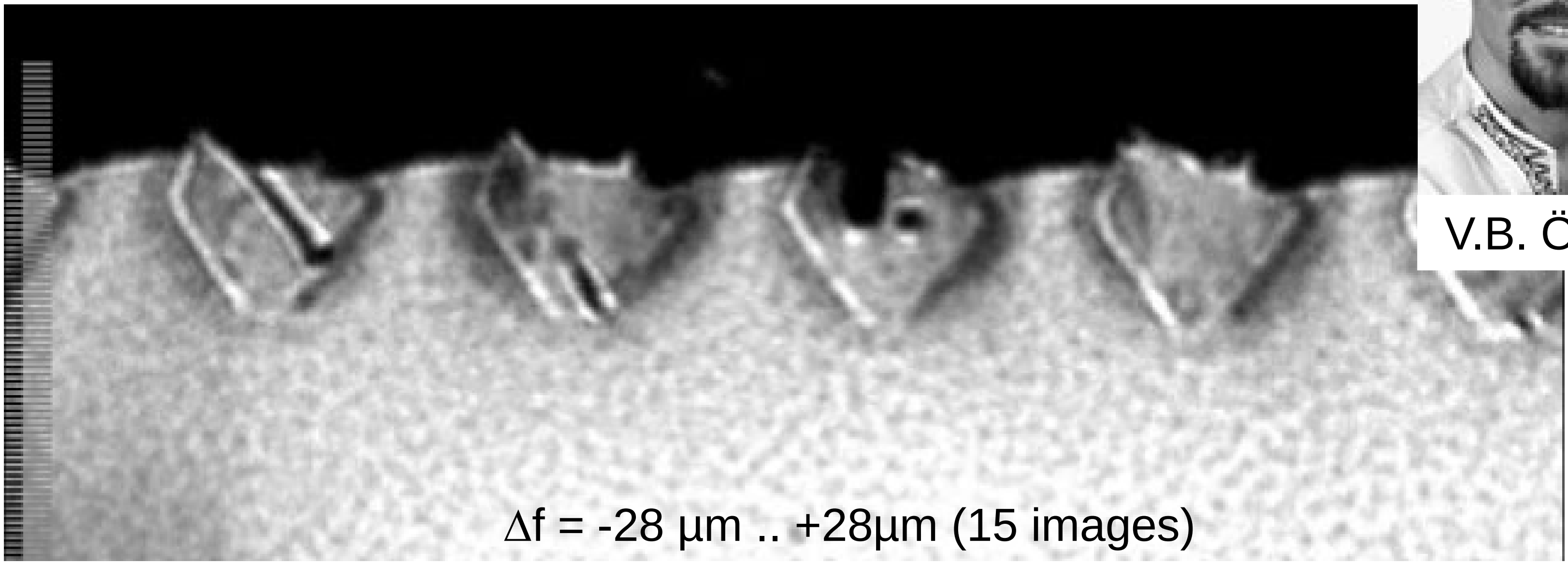


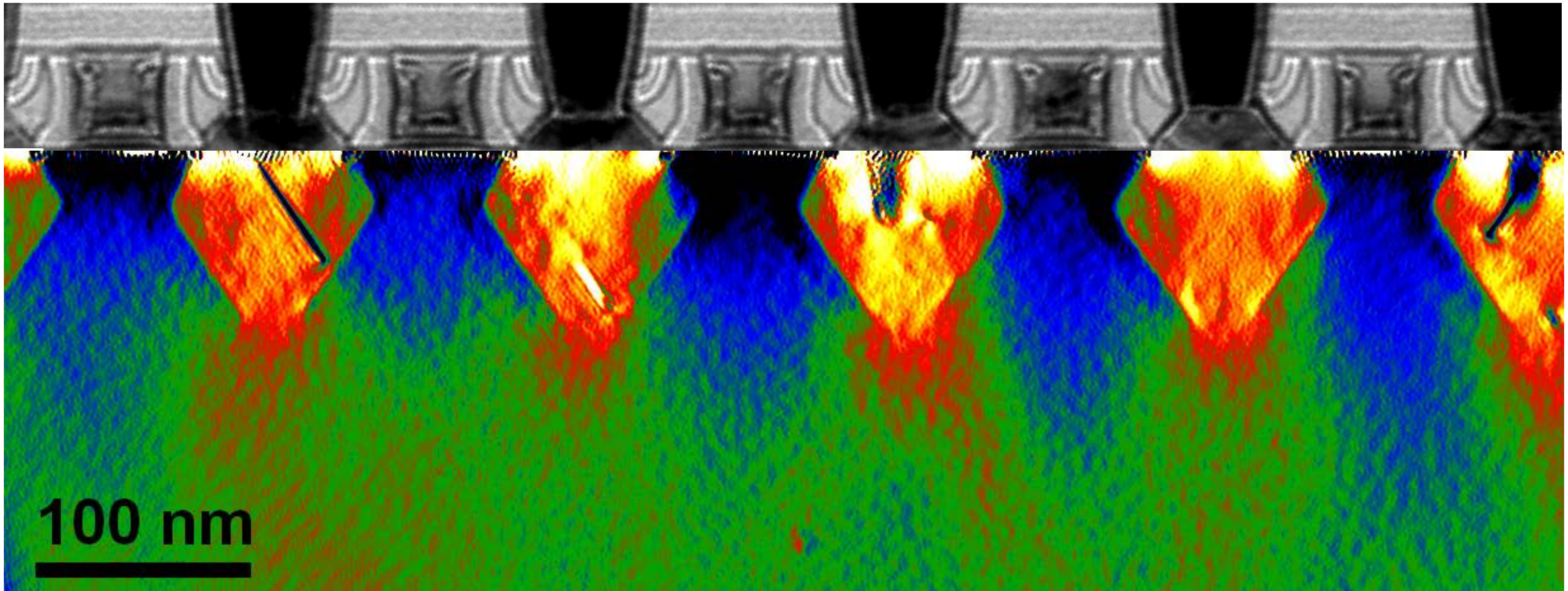
Dark-field Inline Holography (DIH)

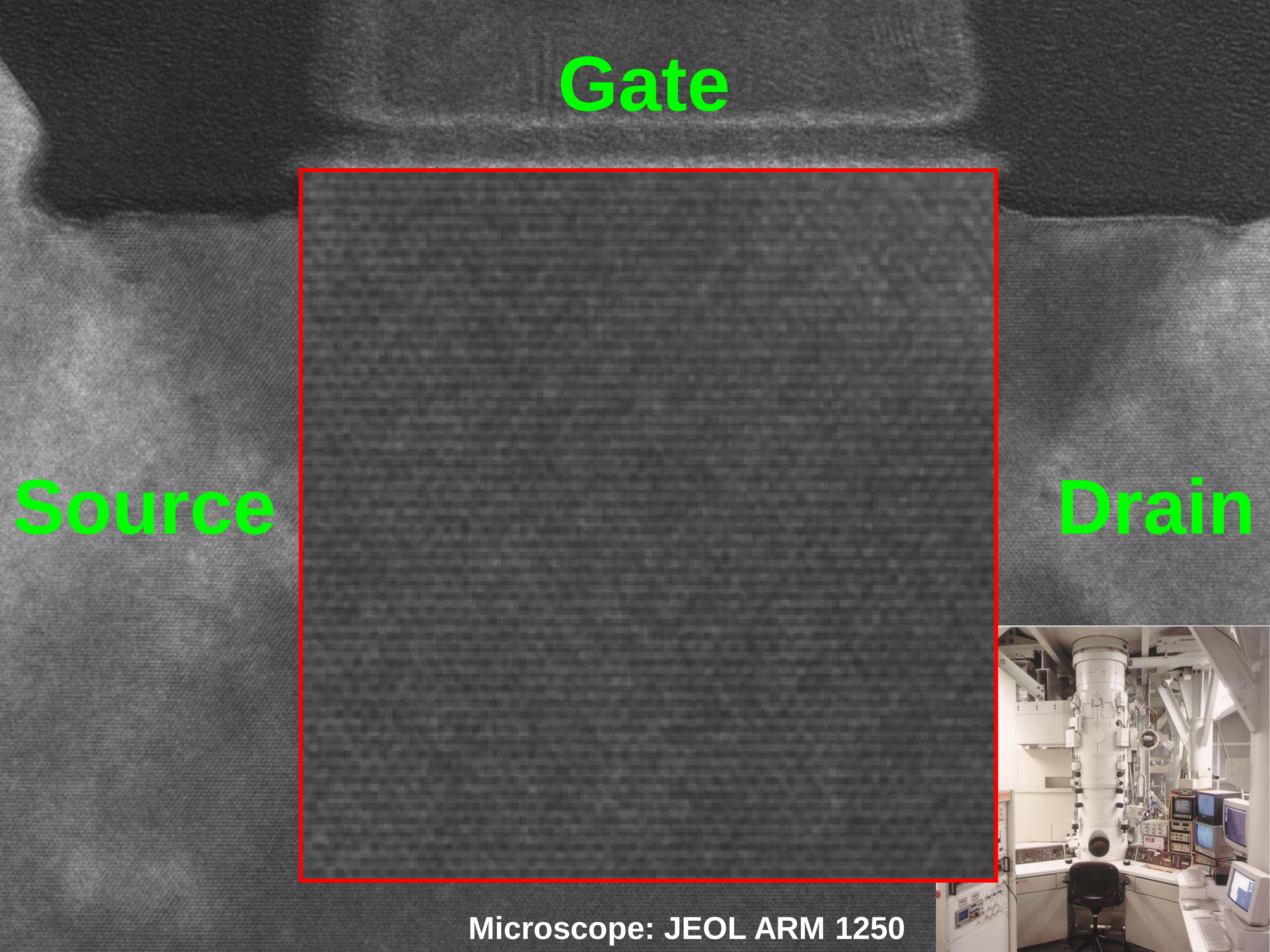


C.T. Koch, V.B. Özdöl, P.A. van Aken, APL **96,** (20010) 091901

DIH of 45nm CMOS transistor structure



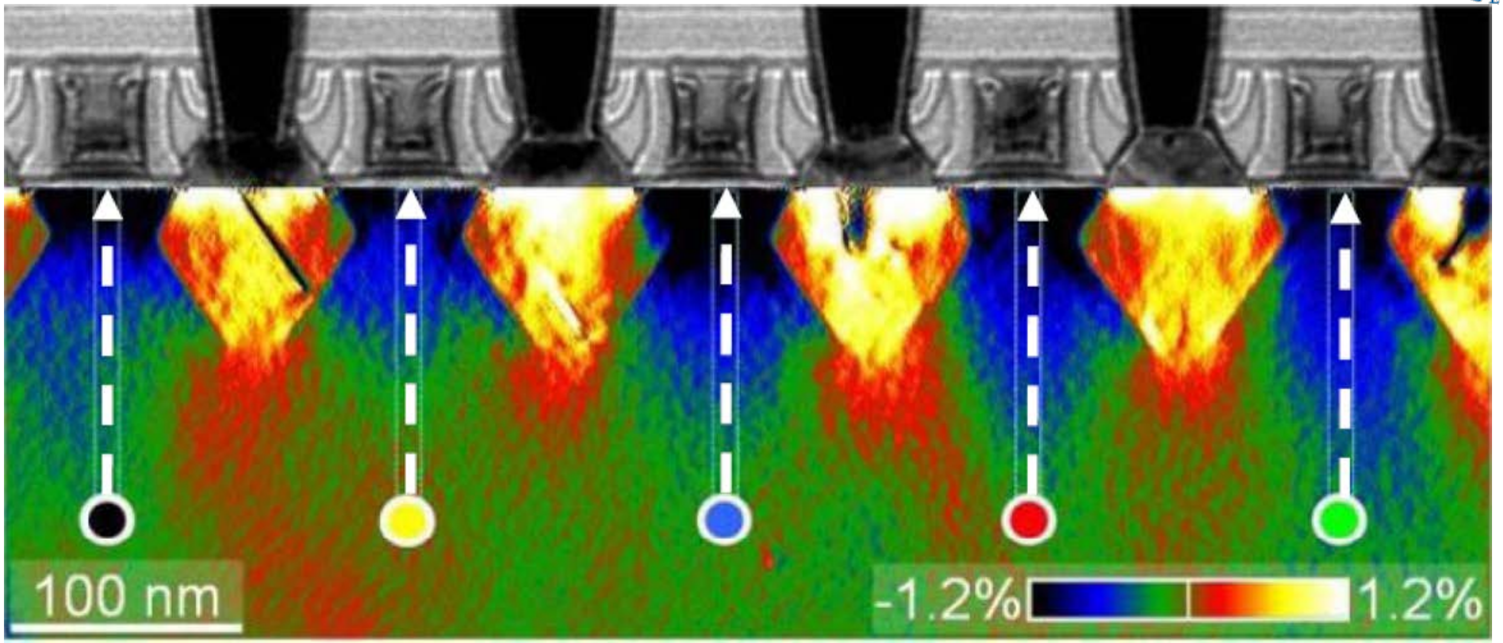


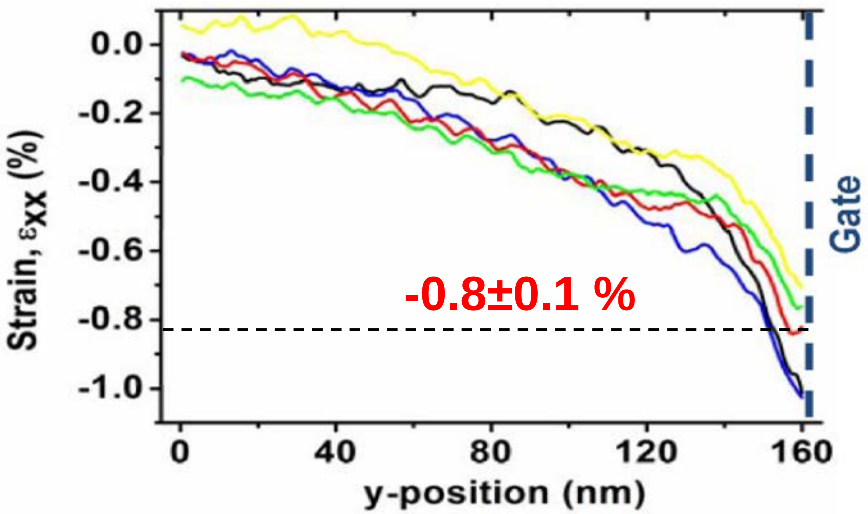


Microscope: JEOL ARM 1250

Quantitative DIH of 45nm CMOS transistor structure

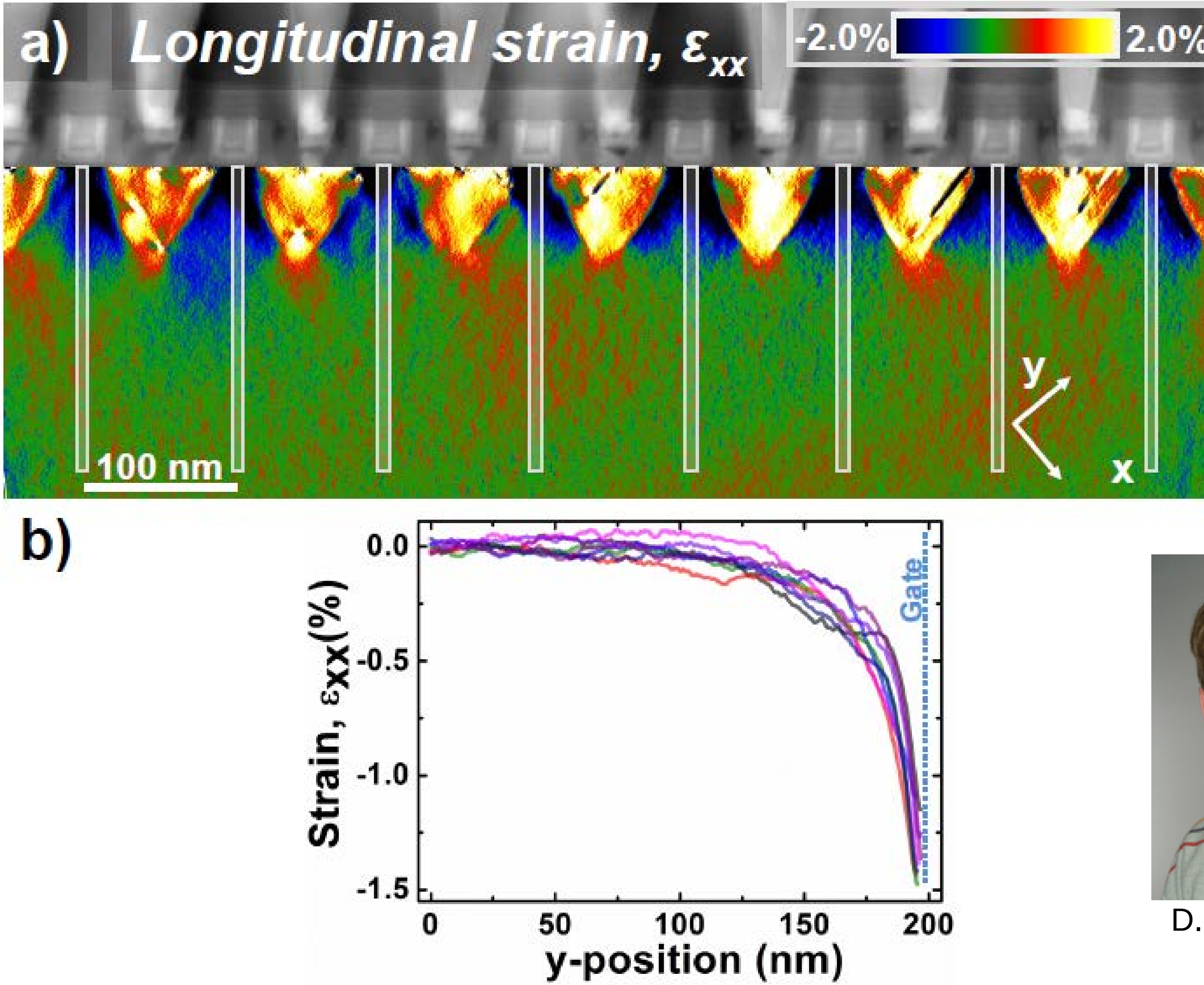
Horizontal strain





C. T. Koch et al, APL **96** (2010) 091901

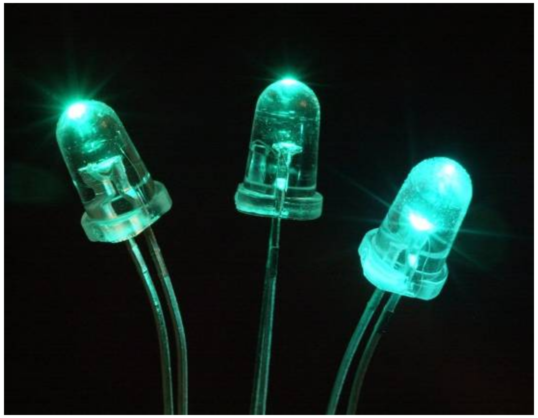
32nm PMOS Transistor Structure

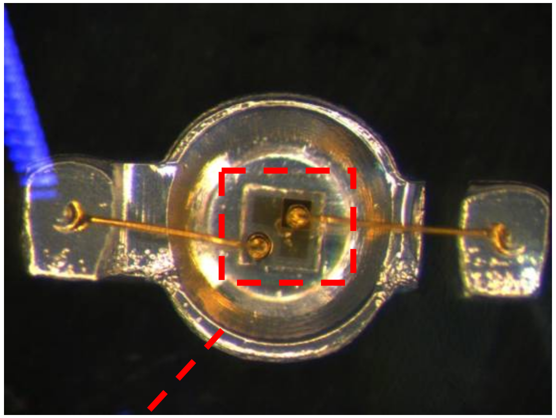


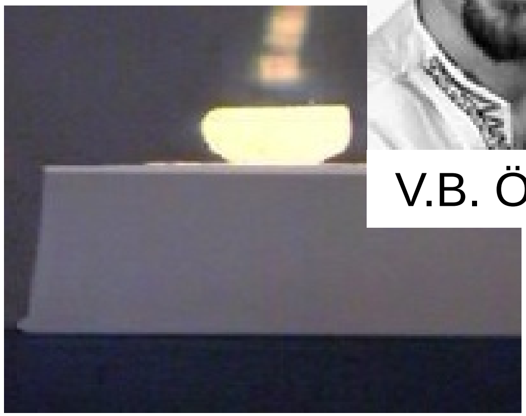
D. Tyutyunnikov

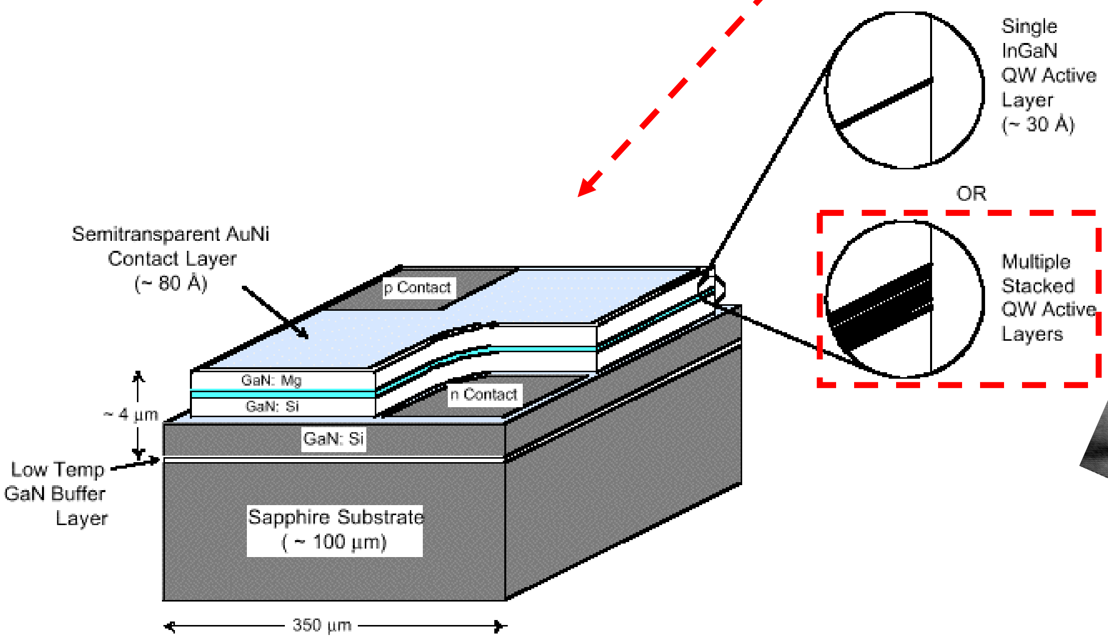
B. Özdöl, D. Tyutyunnikov, C.T. Koch, and P.A. van Aken,, Cryst. Res. Technol. **49** (2014) 38-42

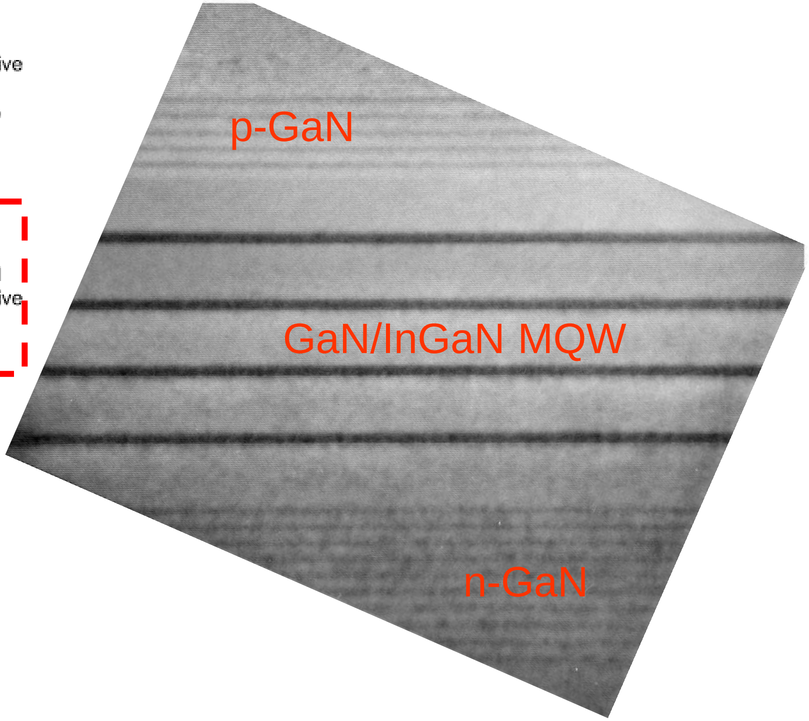
InGaN MQWs in efficient green LEDs



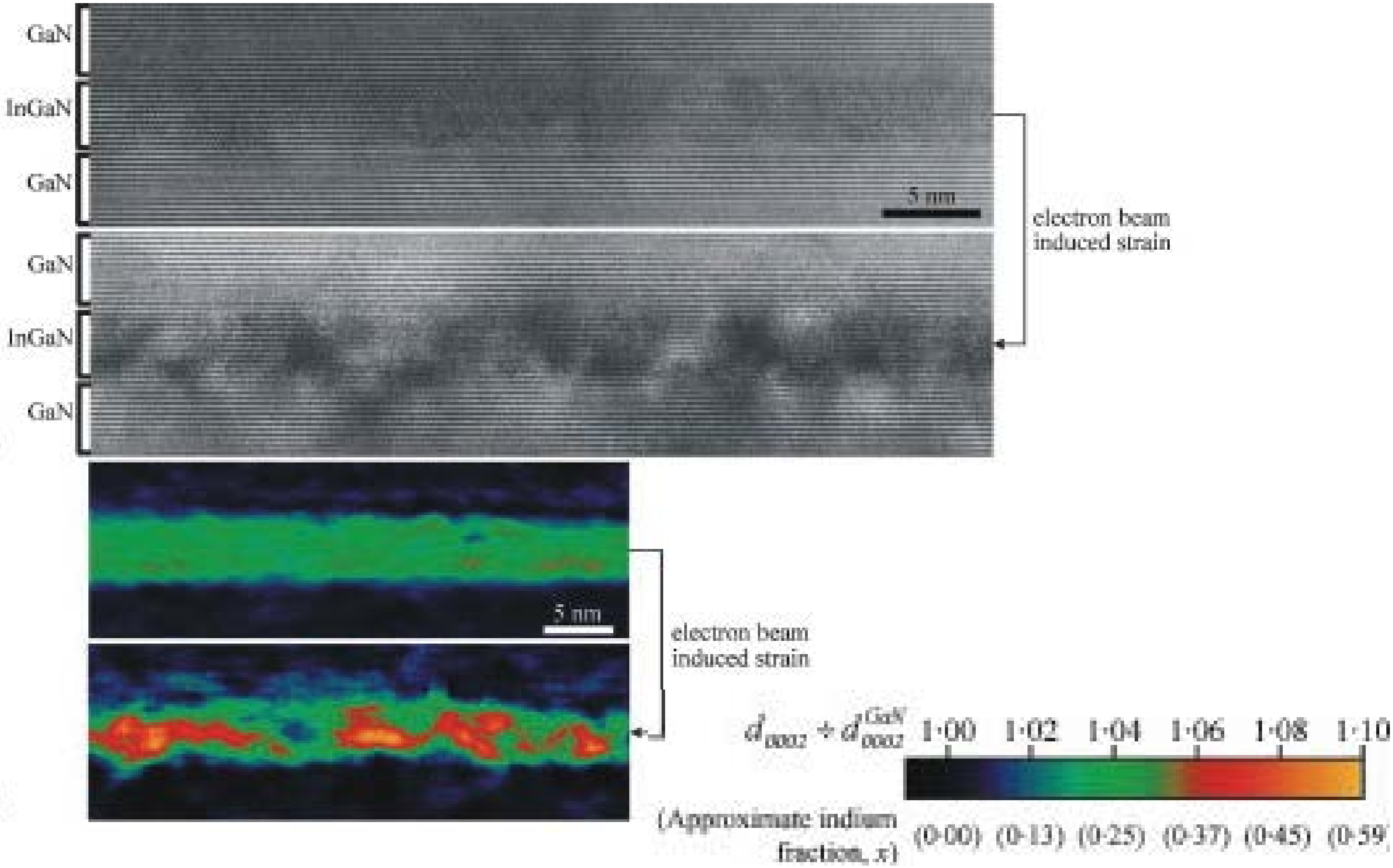








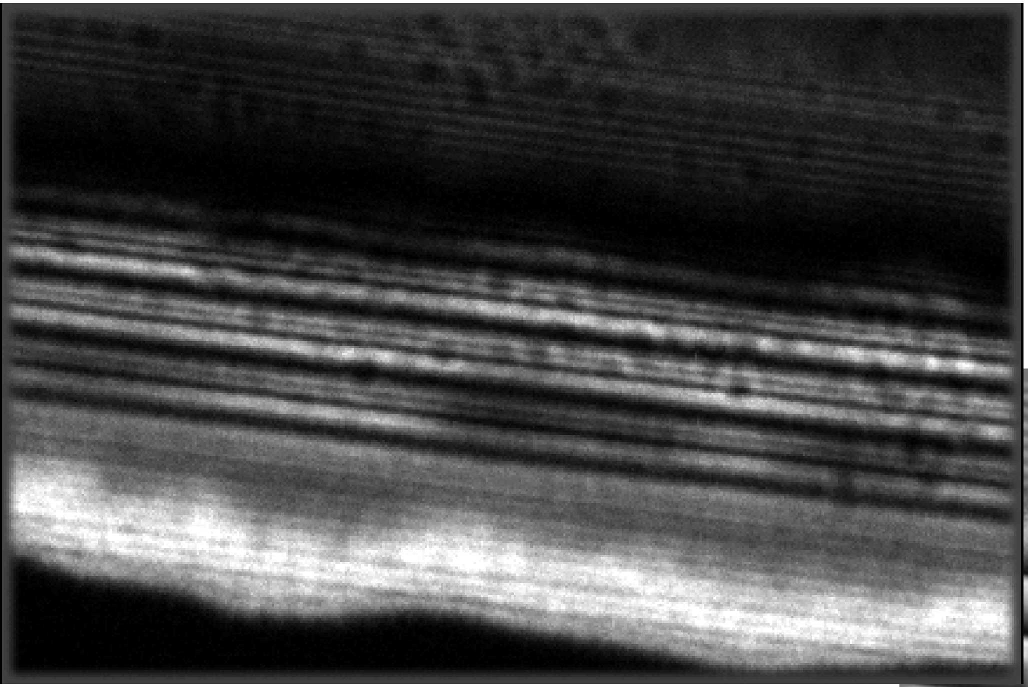
HRTEM Strain Mapping May Damage!



R. A. Oliver, M. J. Galtrey and C. J. Humphreys, Materials Science and Technology **24** (2008) 675

DF Inline Holography of GaN/InGaN

Focal series of (0002) DF images



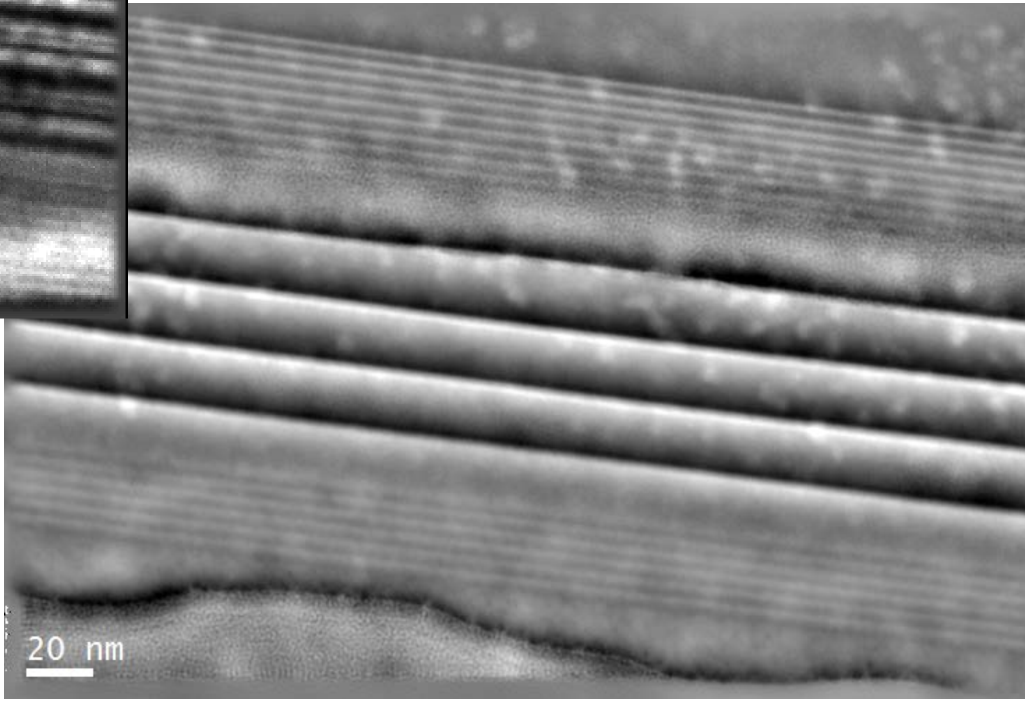
50 nm

Experiment only possible with energy filter, otherwise the Fresnel fringes will be drowned by diffuse inelastic scattering.

Sampling:	0.2 nm
Electrons / pixel:	32
Resolution:	1.04 nm

Reconstruction using FRWR[1] algorithm

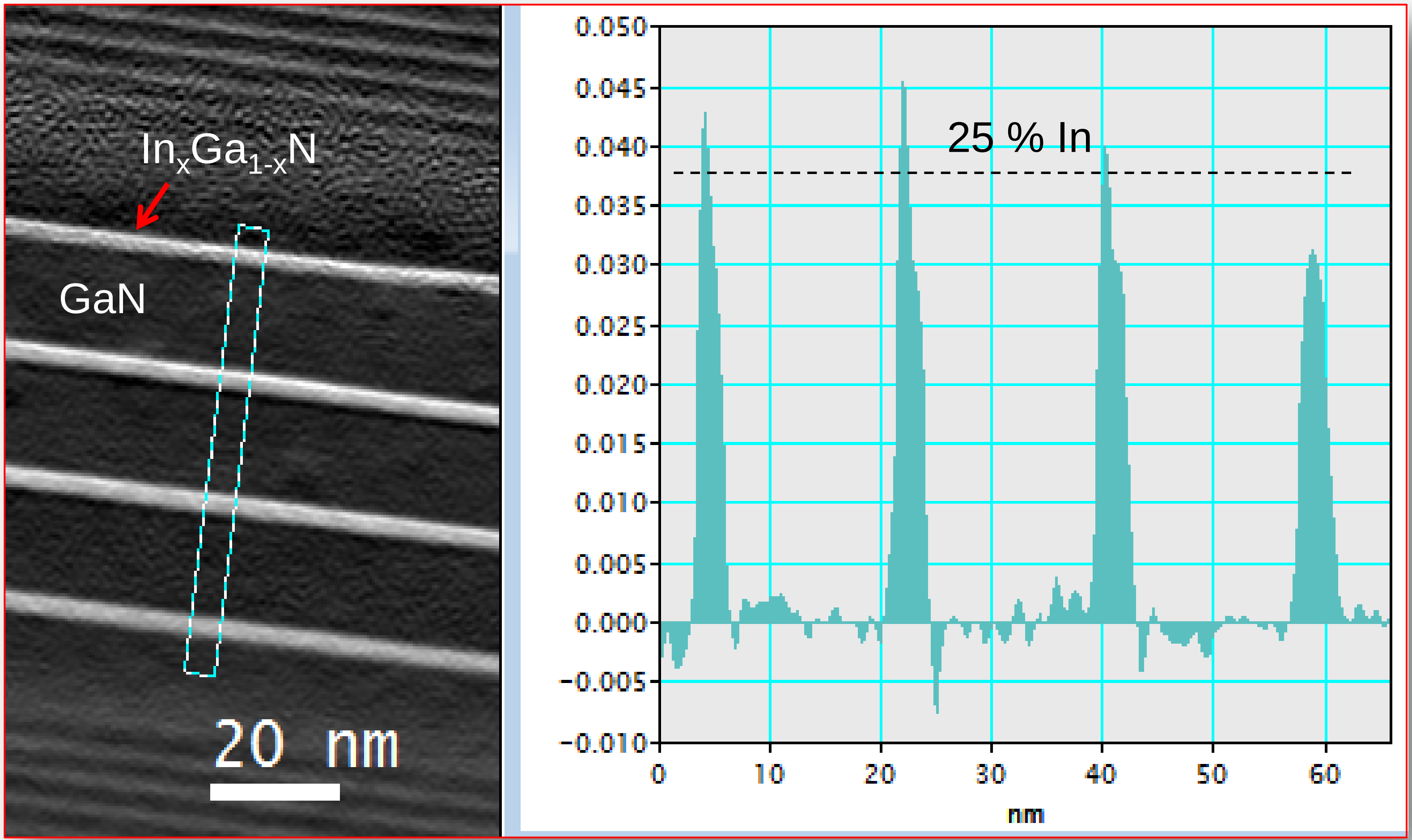
Reconstructed geometric phase



[1] C.T. Koch, Ultramicroscopy **108**, 141-150 (2008)

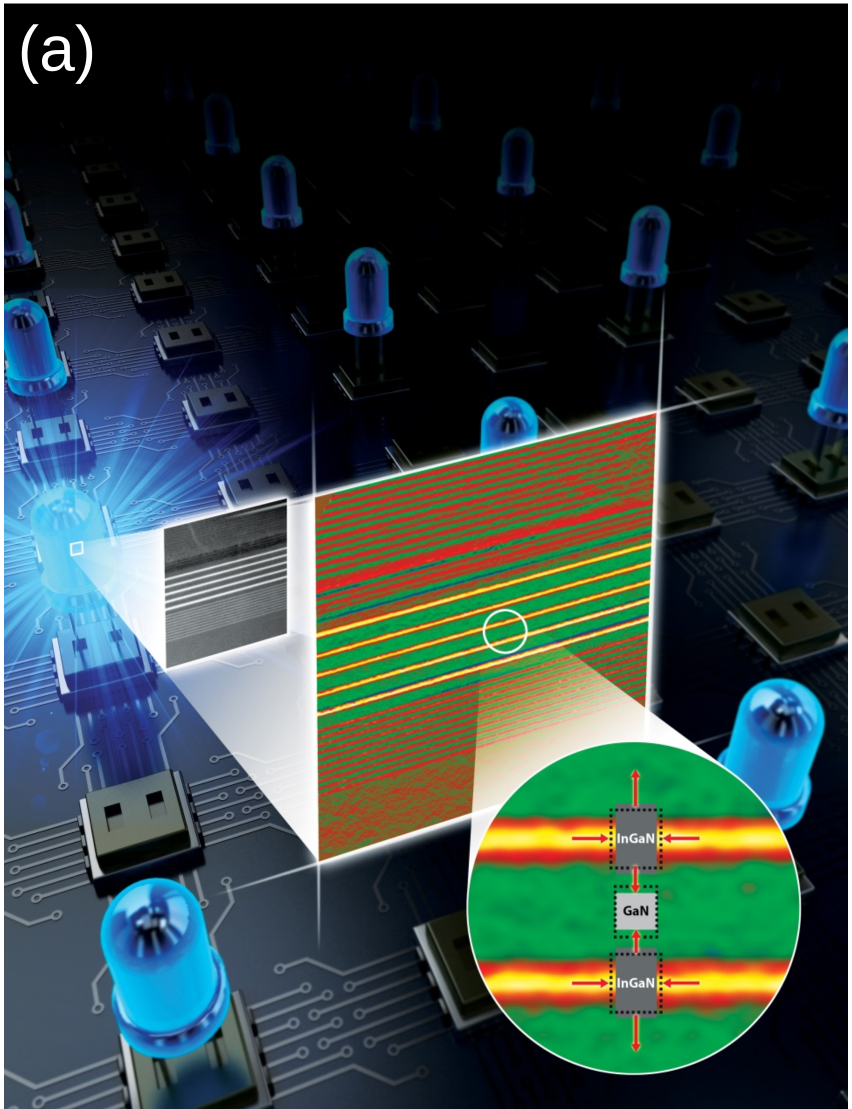
In mapping by Dark-field Inline Holography

GaN / InGaN multiple quantum wells: Zone axis: [$11\bar{2}0$]



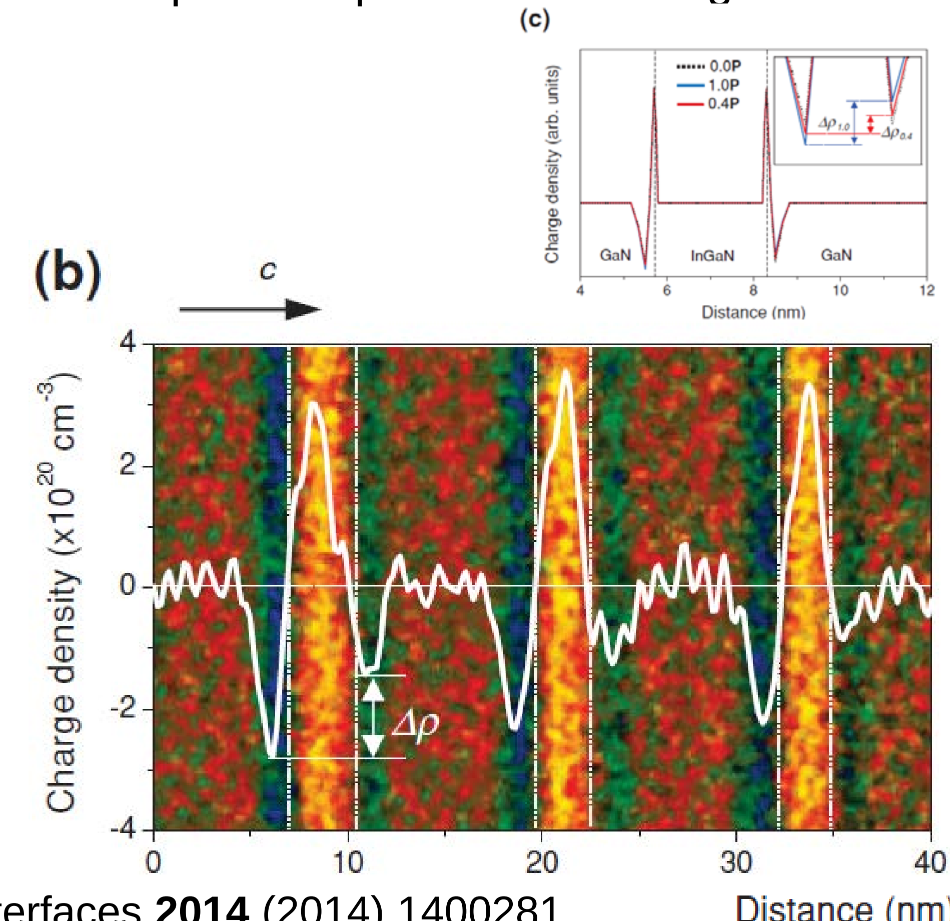
V.B. Özdöl, C.T. Koch, P.A. van Aken, J. Appl. Phys **108** (2010) 056103

Mapping piezoelectric fields



Combining Dark-field and Bright-field Inline Electron Holography

Mapping of sheet charges which compensate polarization charge



K. Song, C.T. Koch et al. Advanced Materials Interfaces **2014** (2014) 1400281

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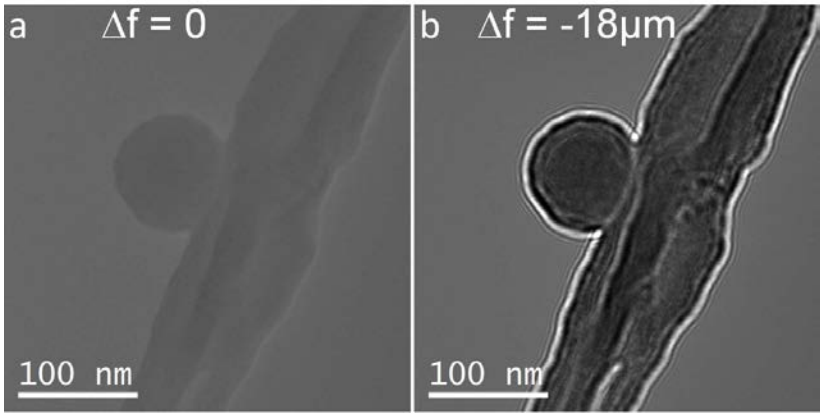
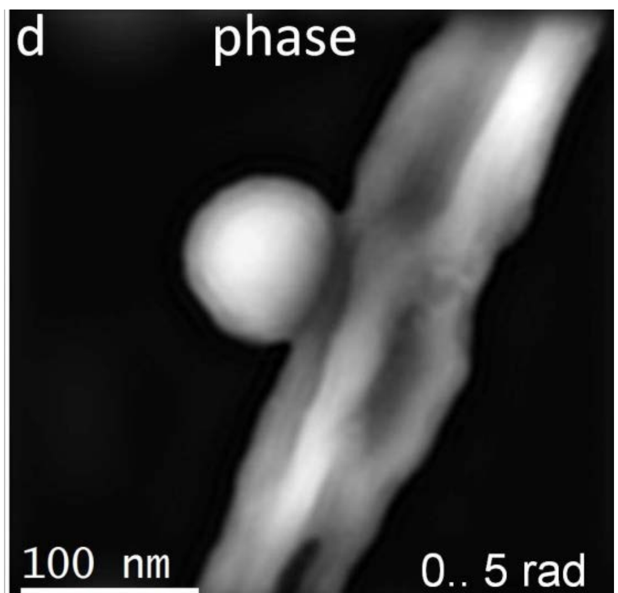
Still Problems at Very Low Spatial Frequencies

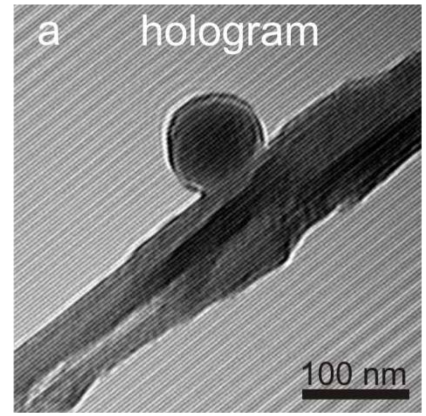
(partly due to inelastic/incoherent scattering)

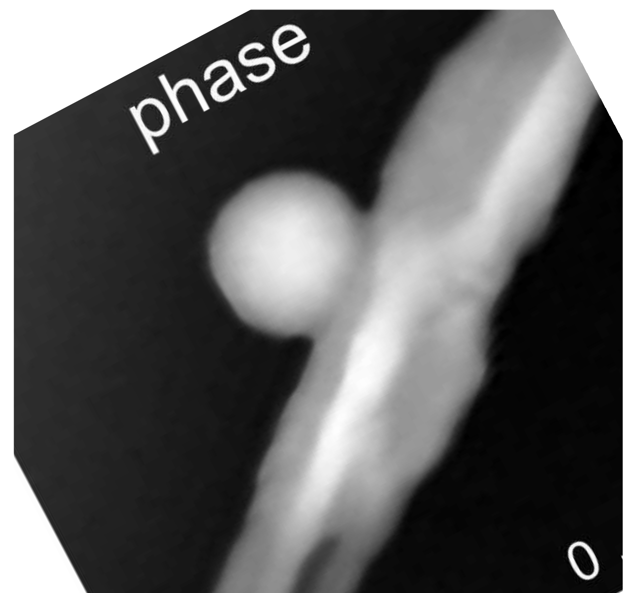
Inline holography





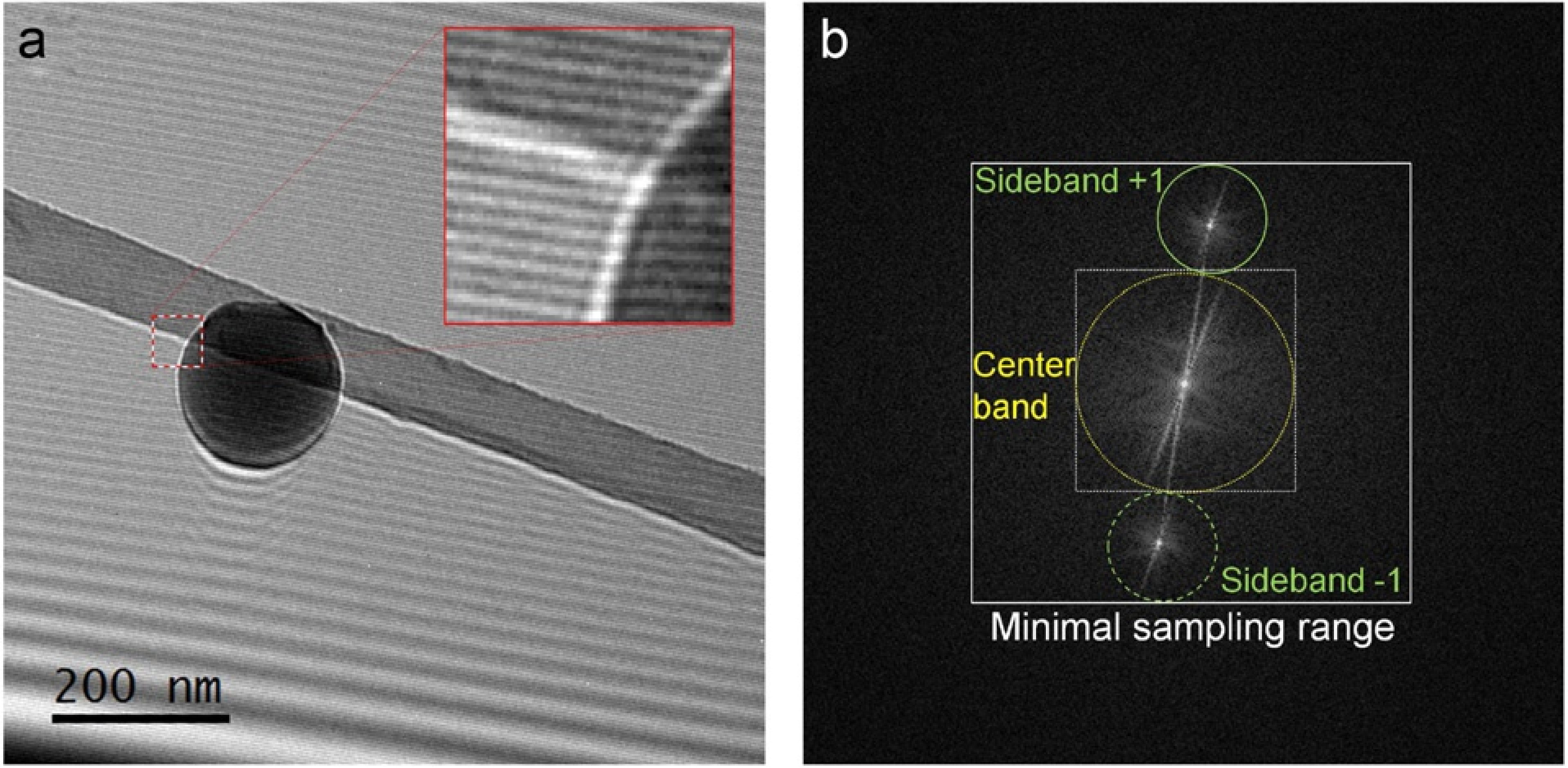
Off-axis holography





T. Latychevskaia, et al. Ultramicroscopy 110 (2010) 472–482

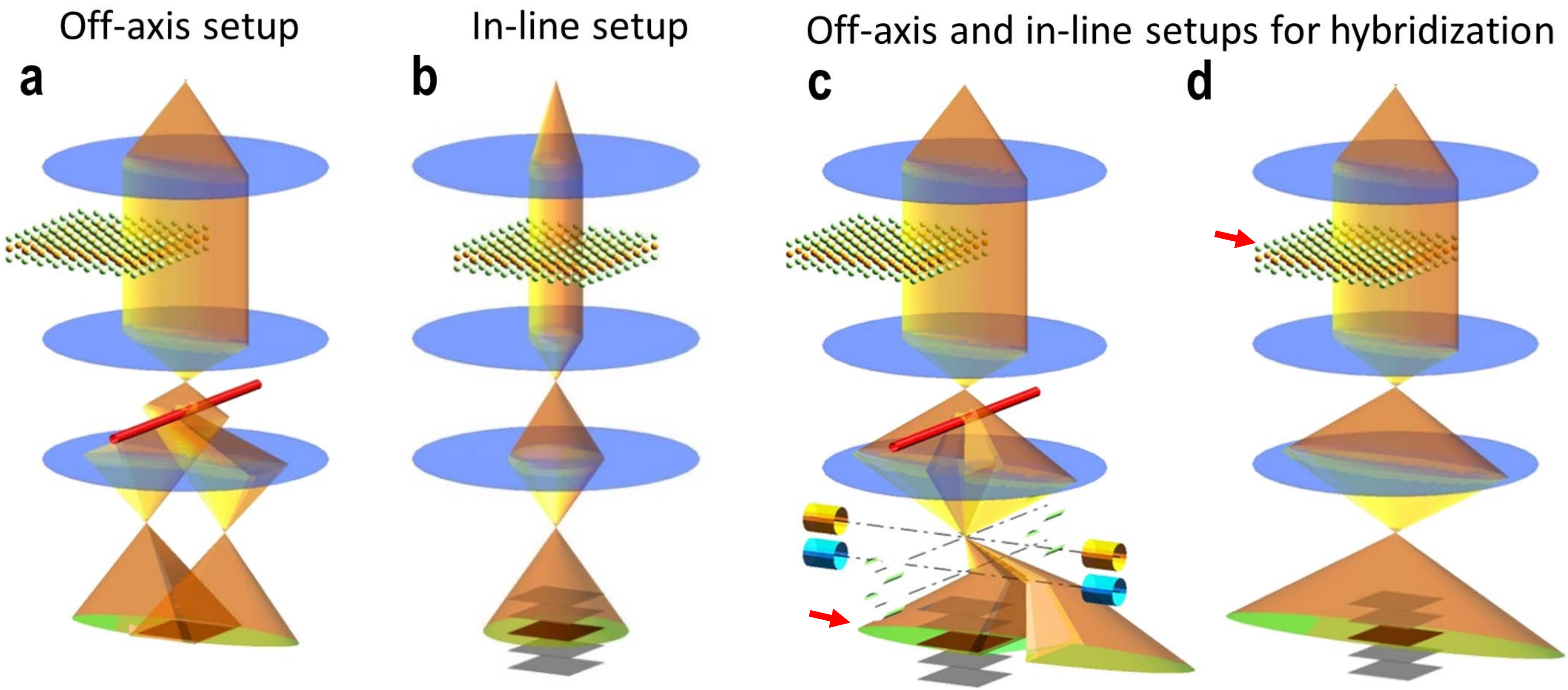
Oversampling in Off-axis Holography



The necessary oversampling reduces the counts per pixel and thus increases the noise and requires thus **long exposure times**.

C. Koch and A. Lubk Ultramicroscopy **110** (2010) 460–471

Synergy: Combining Off-axis and Inline Holography

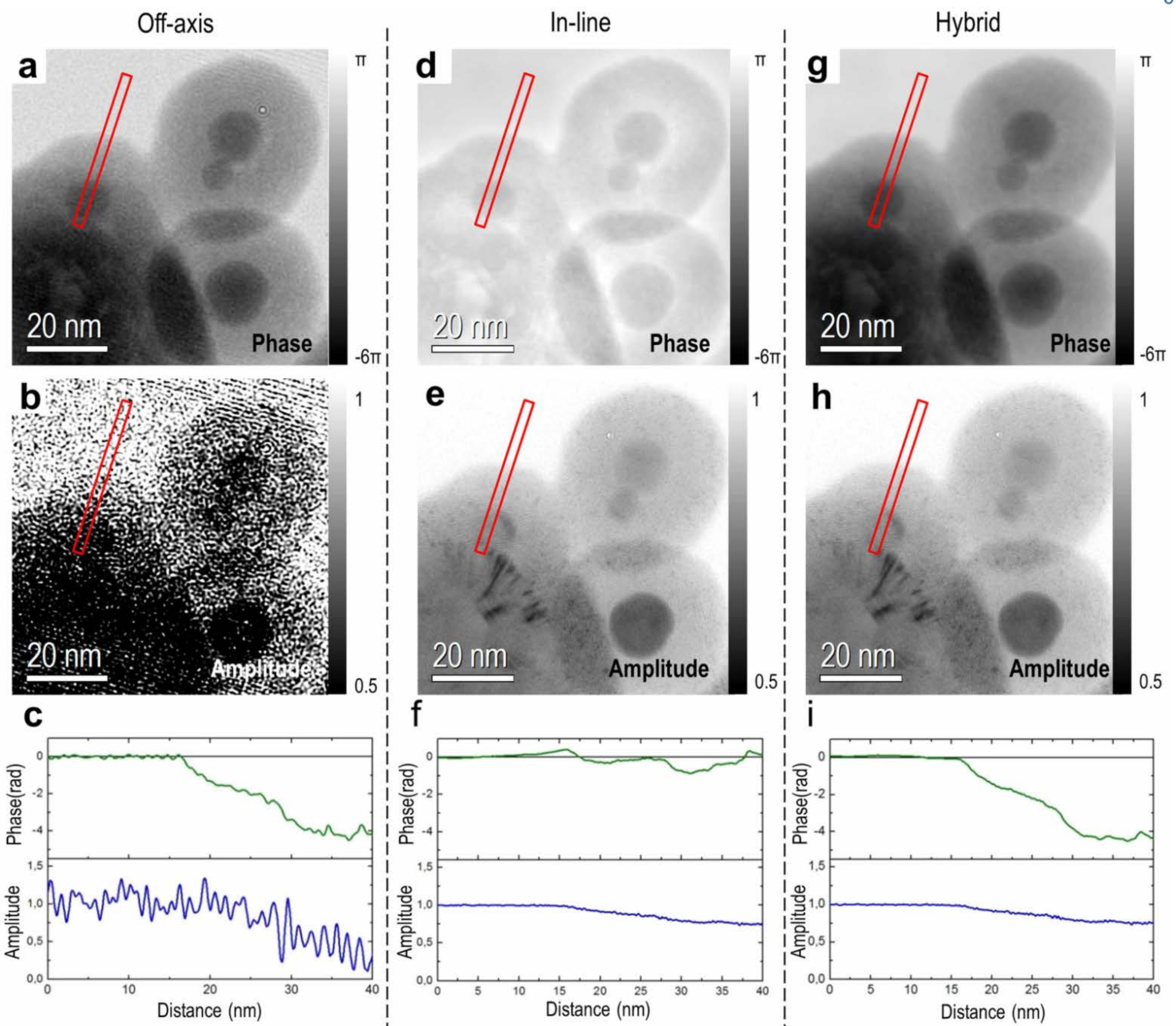


Advantages:

- Low spatial frequencies through off-axis holography (even if data is very noisy)
- High spatial frequencies from inline holography (at least two times better resolution)

C. Ozsoy Keskinbora et al. Scientific Reports **4** (2014) 7020

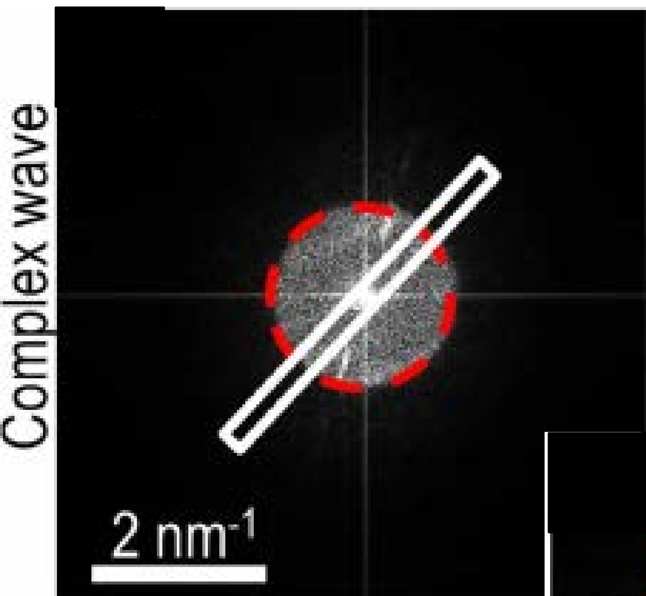
Experimental results



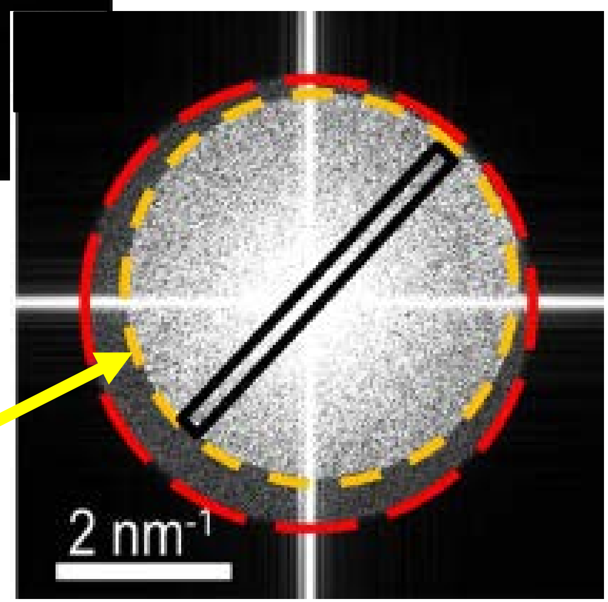
C. Ozsoy Keskinbora et al. Scientific Reports **4** (2014) 7020

Comparison of Spatial Resolution

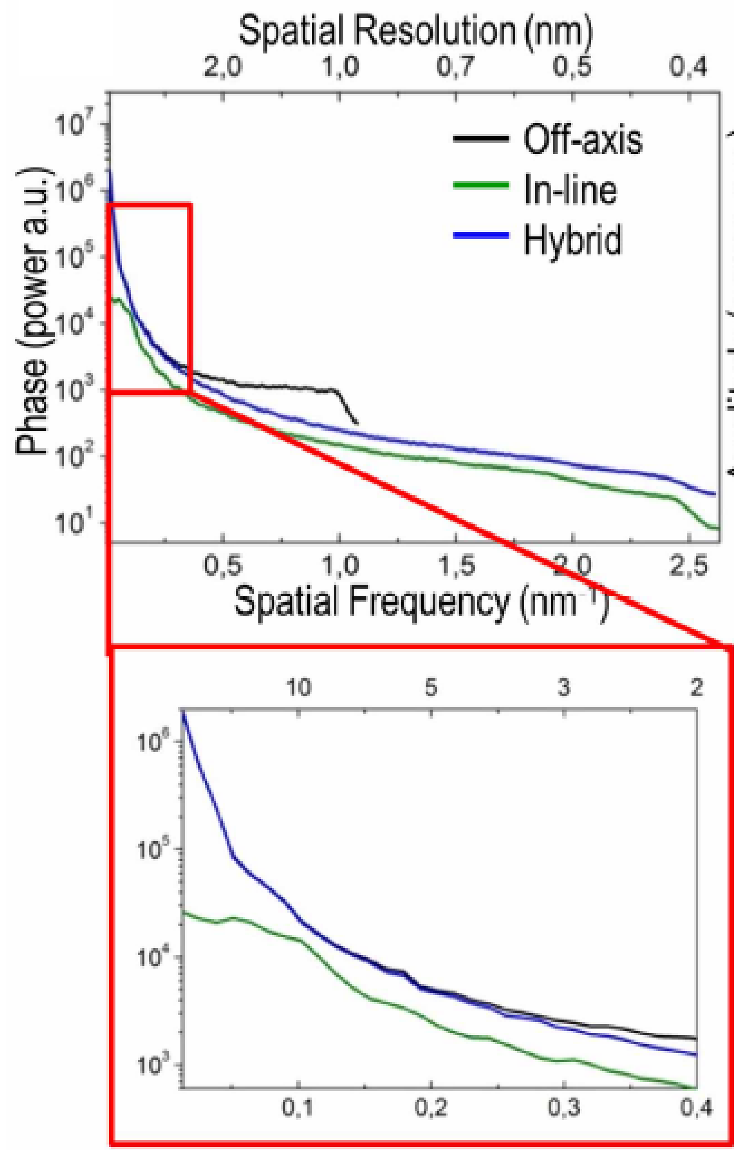
Off-axis



Hybrid



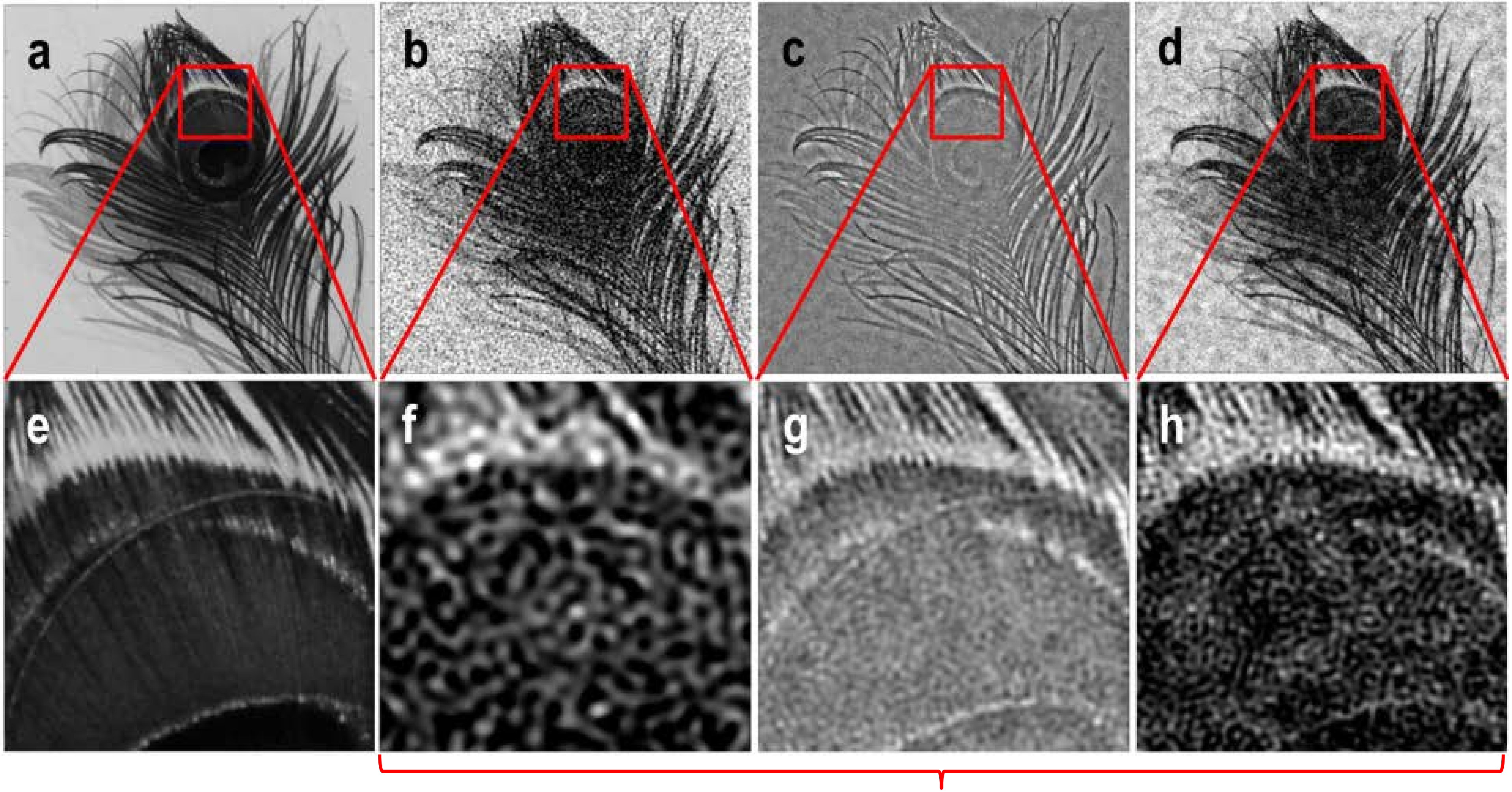
Objective aperture used during experiment



C. Ozsoy Keskinbora et al. Scientific Reports **4** (2014) 7020

Verification by Simulation

Original phase | Off-axis phase | Inline phase | Hybrid phase



Equal electron dose in all 3 cases!

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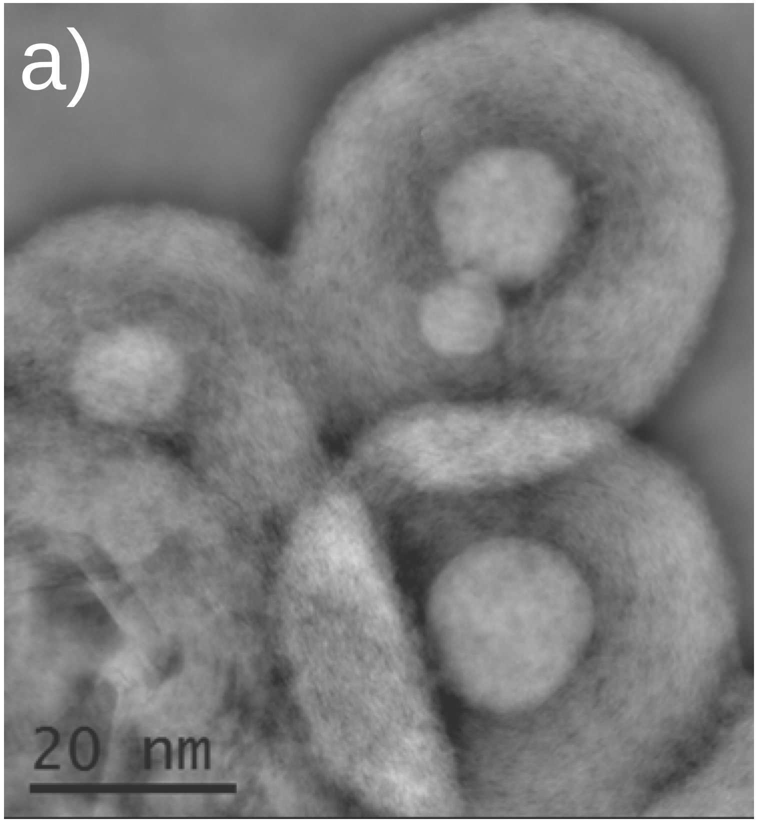
Outline

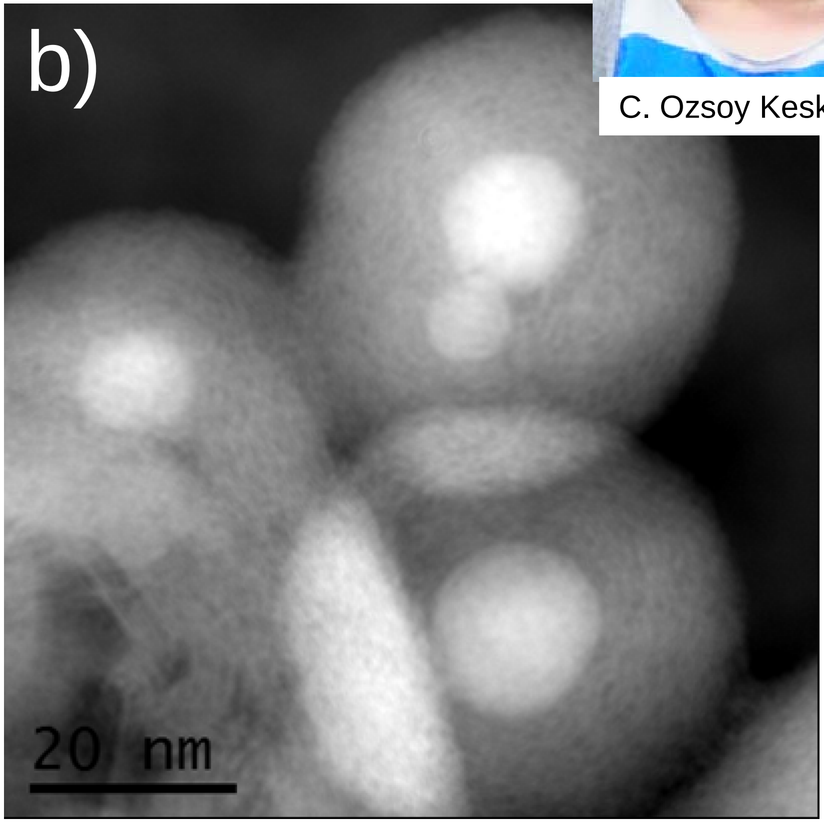
- Introduction: What is inline holography?
- Applications: HRTEM Aberration compensation & Strain Mapping
- Recovering low spatial frequencies by
  - Hybrid holography
  - Gradient-flipping inline holography
- Introducing the full-resolution wave reconstruction (FRWR) code
- Data Acquisition at the TEM

Dealing with low spatial frequencies

C. Ozsoy Keskinbora



Conventional reconstruction algorithm

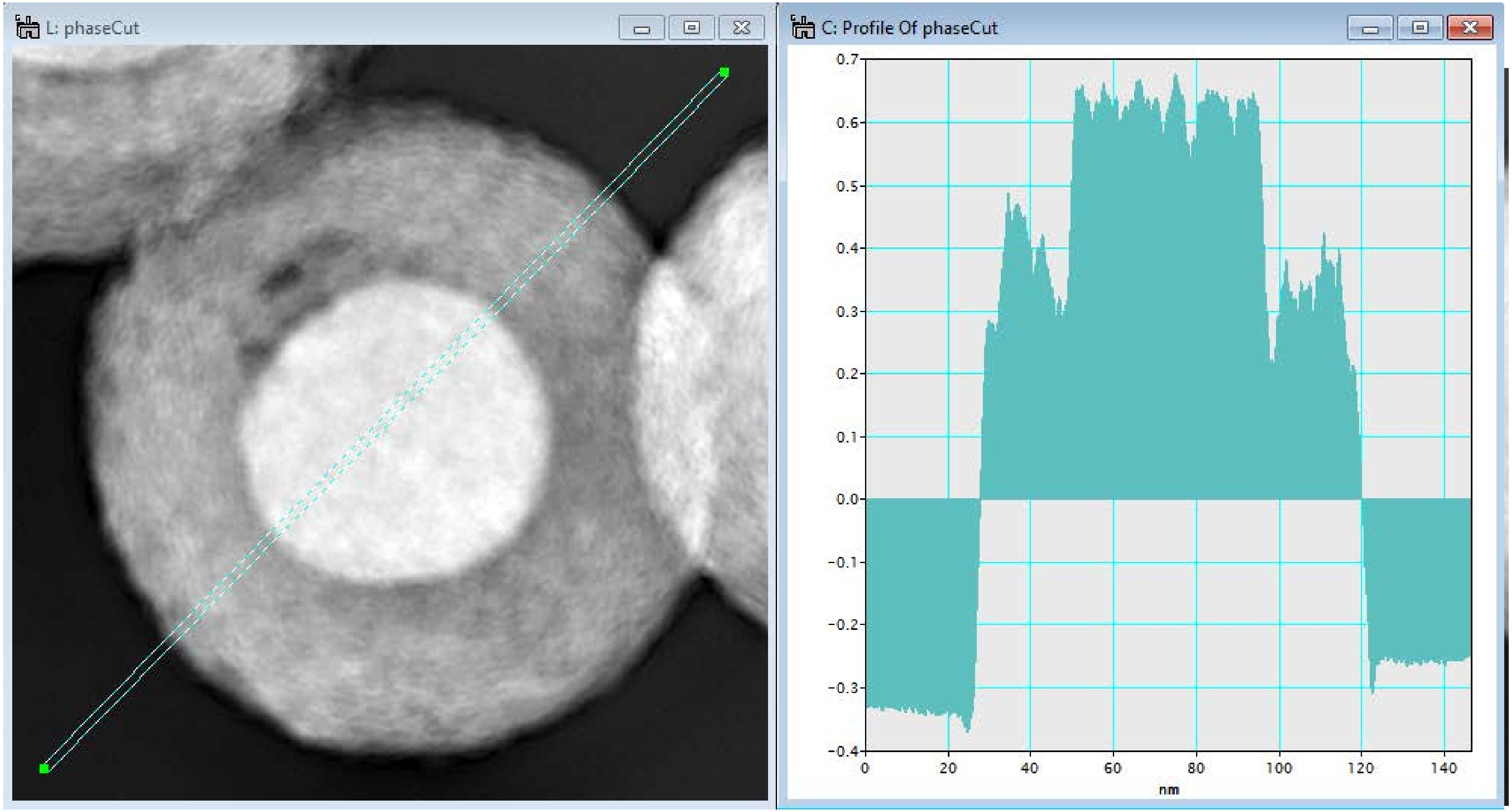


Regularized reconstruction

Both reconstructions are equally consistent with the focal series data

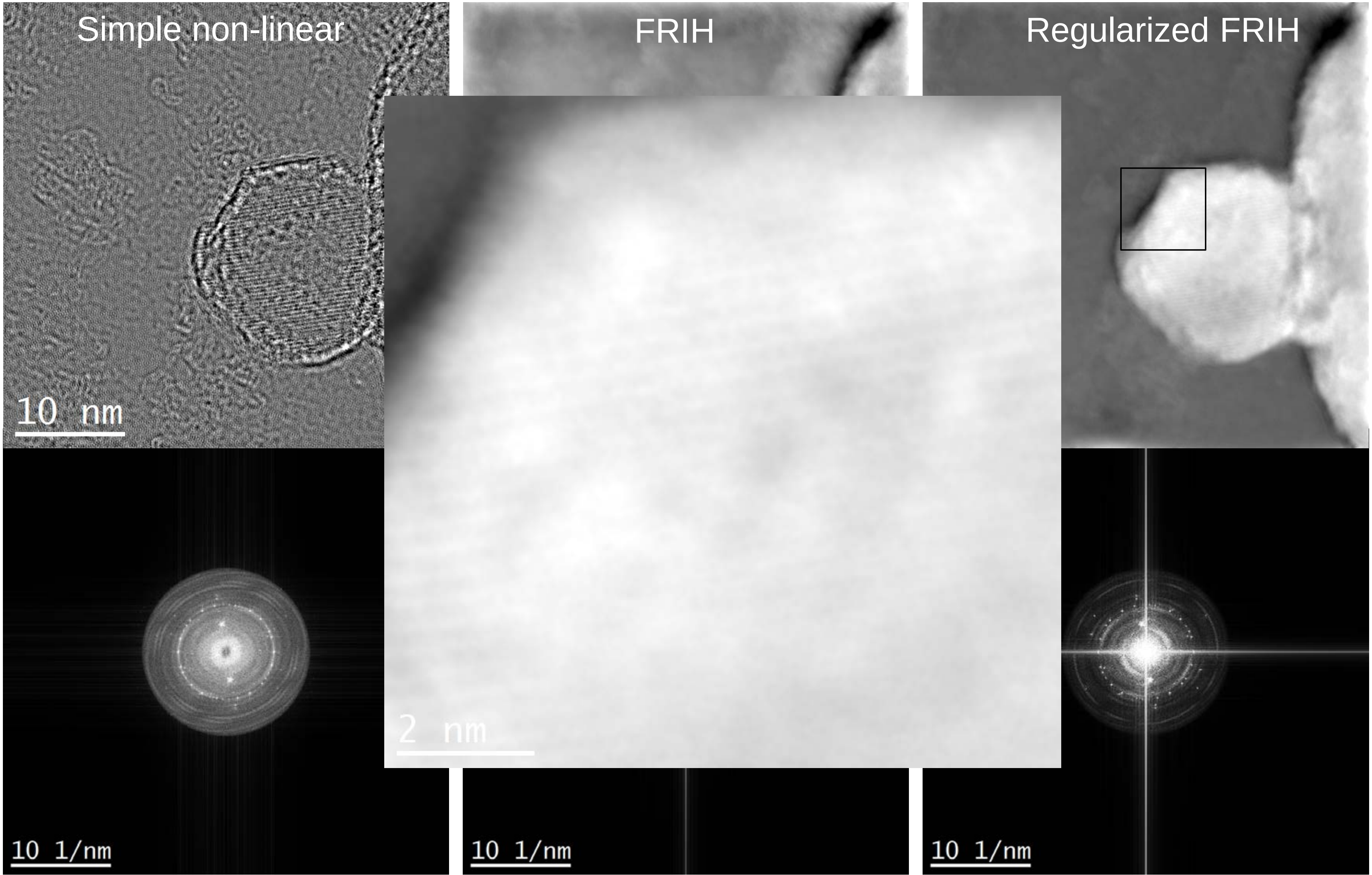
data: C. Ozsoy Keskinbora (MPI-Stuttgart) at FZ Jülich (R. Dunin-Borkowski & C. Boothroyd)

Very Low Frequencies in the Phase Unreliable by Inline Holography



data: C. Ozsoy Keskinbora (MPI-Stuttgart) at FZ Jülich (R. Dunin-Borkowski & C. Boothroyd)

Different reconstruction versions



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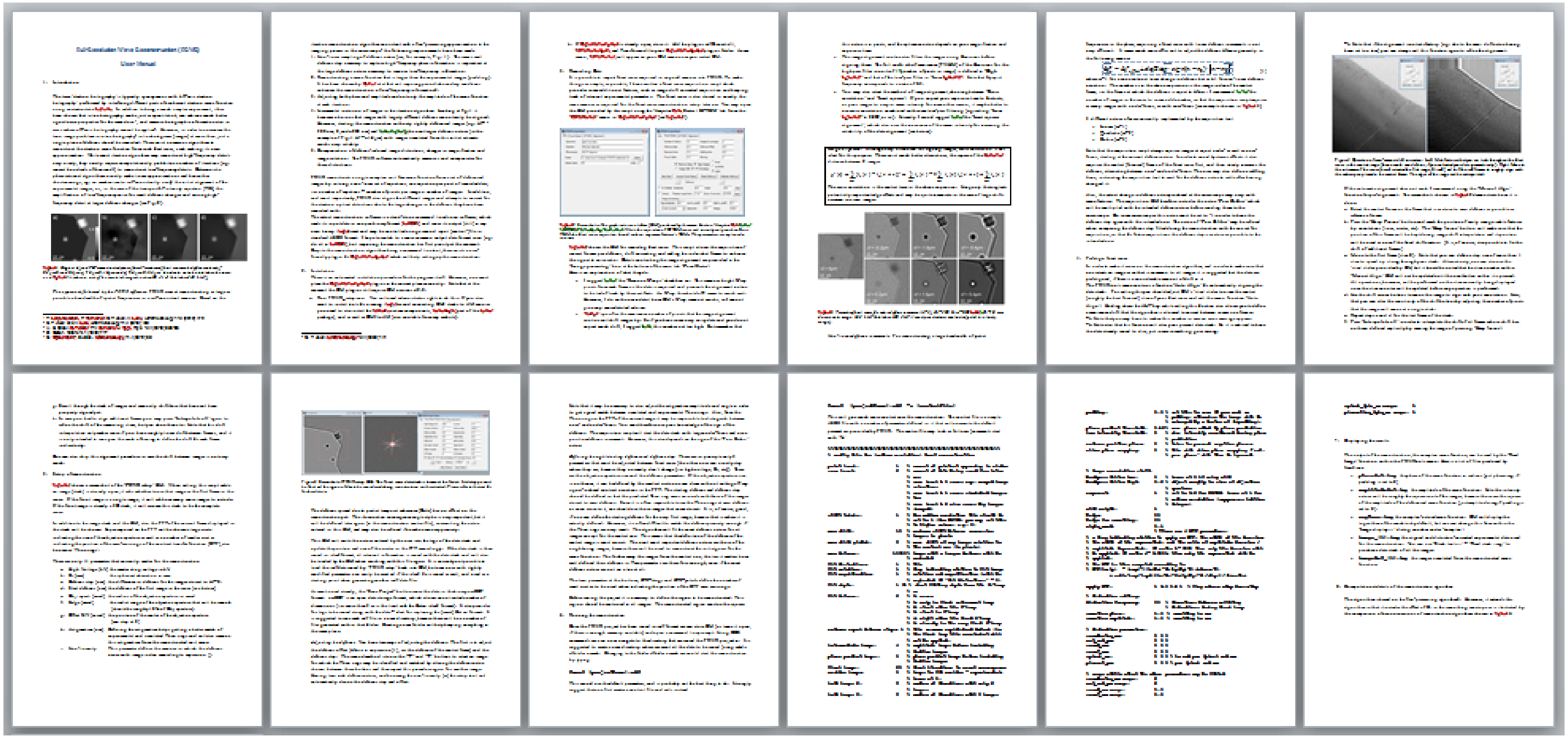
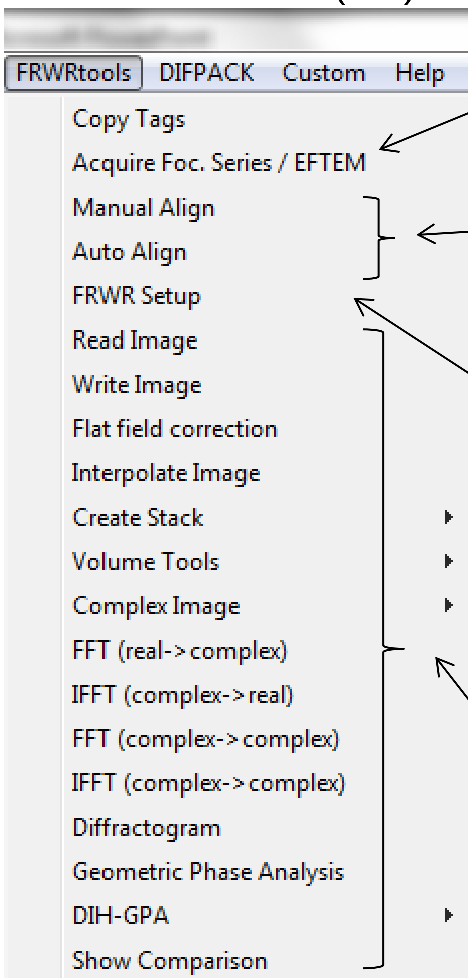
User Manual



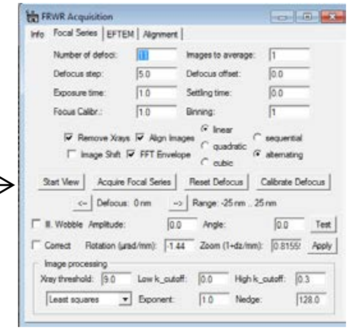
Not fully up to date ☹, but still highly recommended

FRWR Workflow

FRWRtools menu (DM)

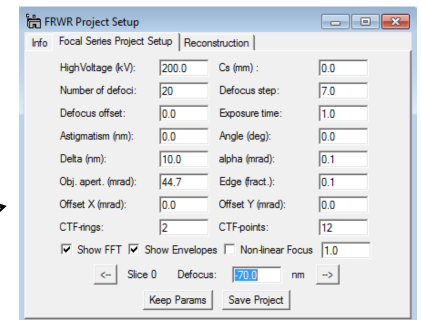


1. Data acquisition



2. Data pre-alignment (further details in manual)

3. Setup of reconstruction



4. Running the reconstruction (results saved in .img format)

5. Read results into DM and process the data (e.g. for strain mapping)

Towards Full-Resolution Inline Holography (FRIH)

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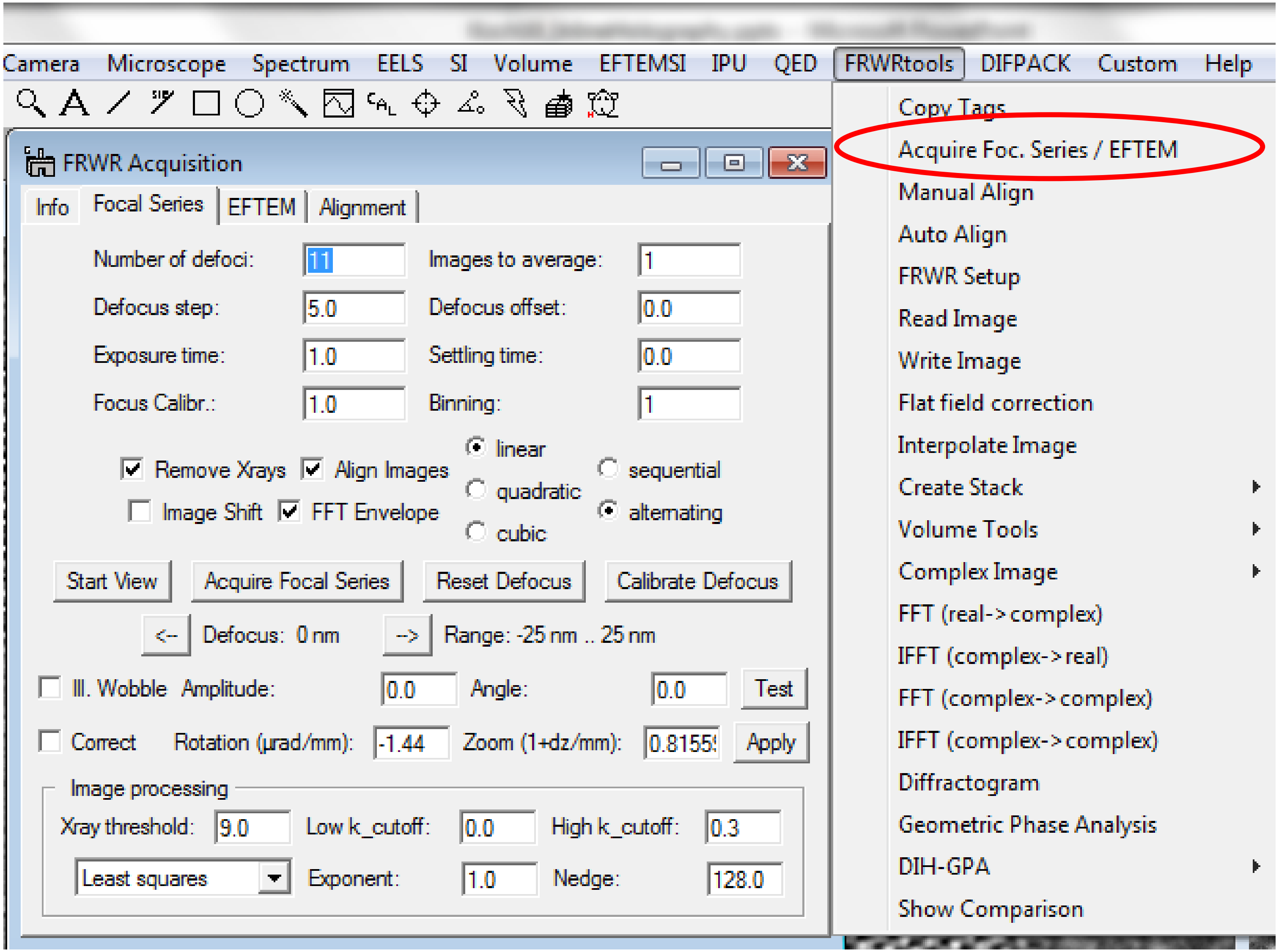
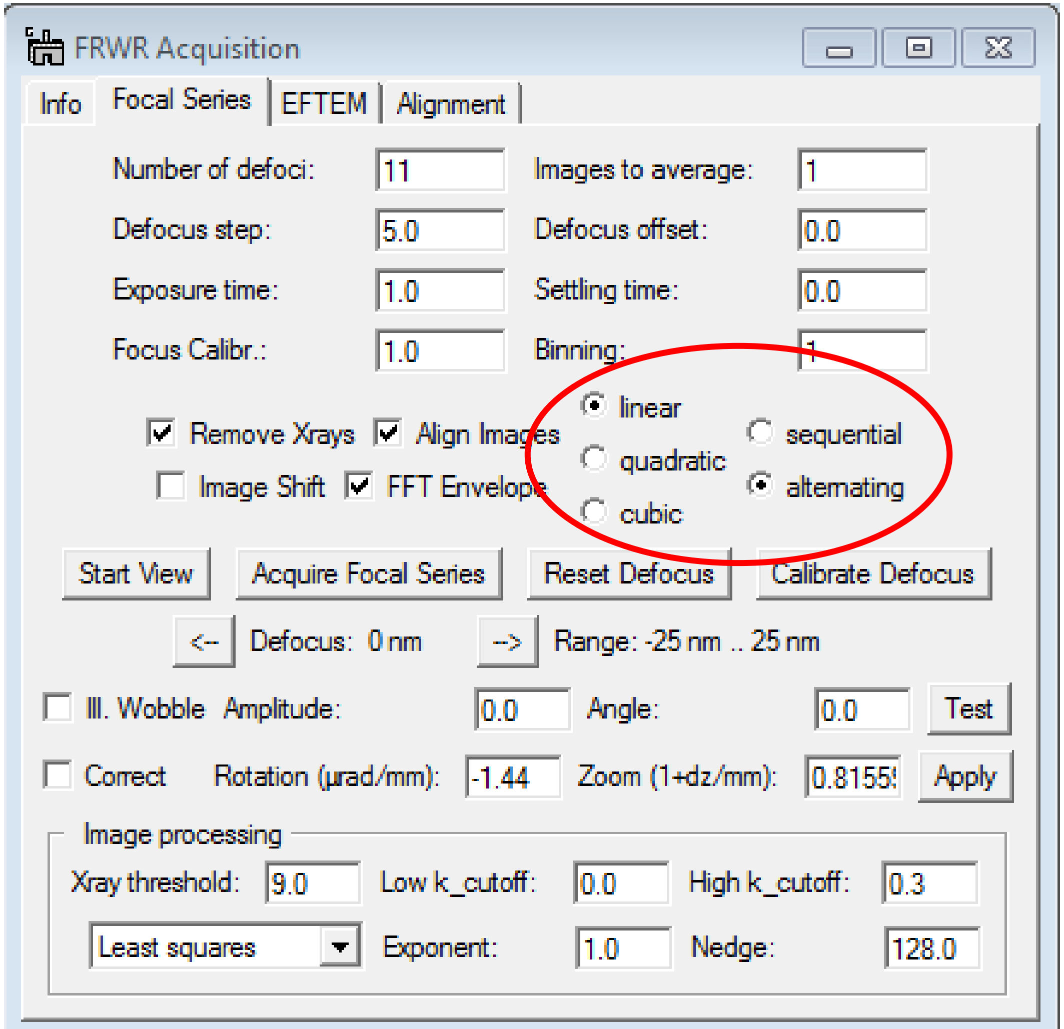
The FRWRTools Plugin



Free download: https://www.physik.hu-berlin.de/en/sem/software/software_frwrtools

The Acquisition Tool



Non-linear defocus increments:
(n=1 [linear], 2 [quadratic], or 3 [cubic])

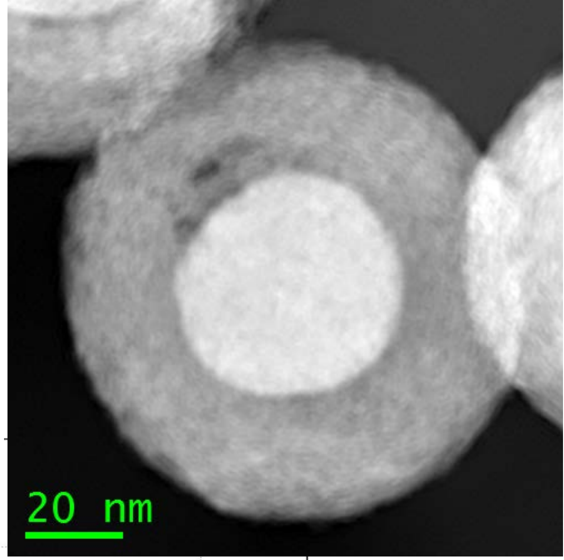
$$\Delta f_n = \Delta f_{offset} + defStep \cdot sign(n - n_0) \cdot |n - n_0|^m$$

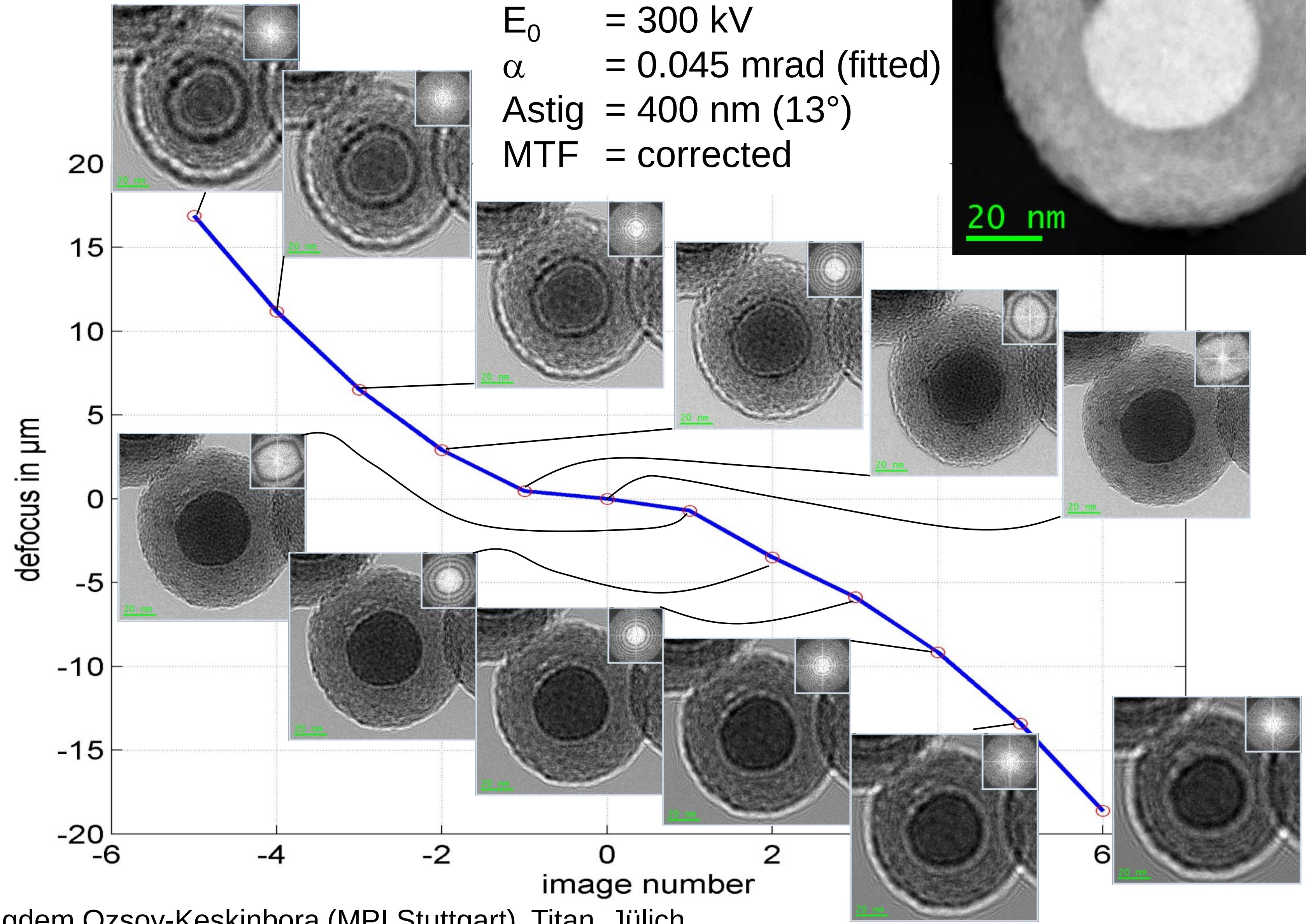
Sequential acquisition:

- Aim is to have accurate defocus at small defocus values
- Sequential acquisition first jumps to lowest underfocus (if defstep > 0) => hysteresis!
- Alternating acquisition uses the following sequence: df = 0, -1, +1, -2, +2, -3, +3, …

Nonlinear defocus sampling

E_0 = 300 kV
α = 0.045 mrad (fitted)
Astig = 400 nm (13°)
MTF = corrected





data: Cigdem Ozsoy-Keskinbora (MPI Stuttgart), Titan, Jülich

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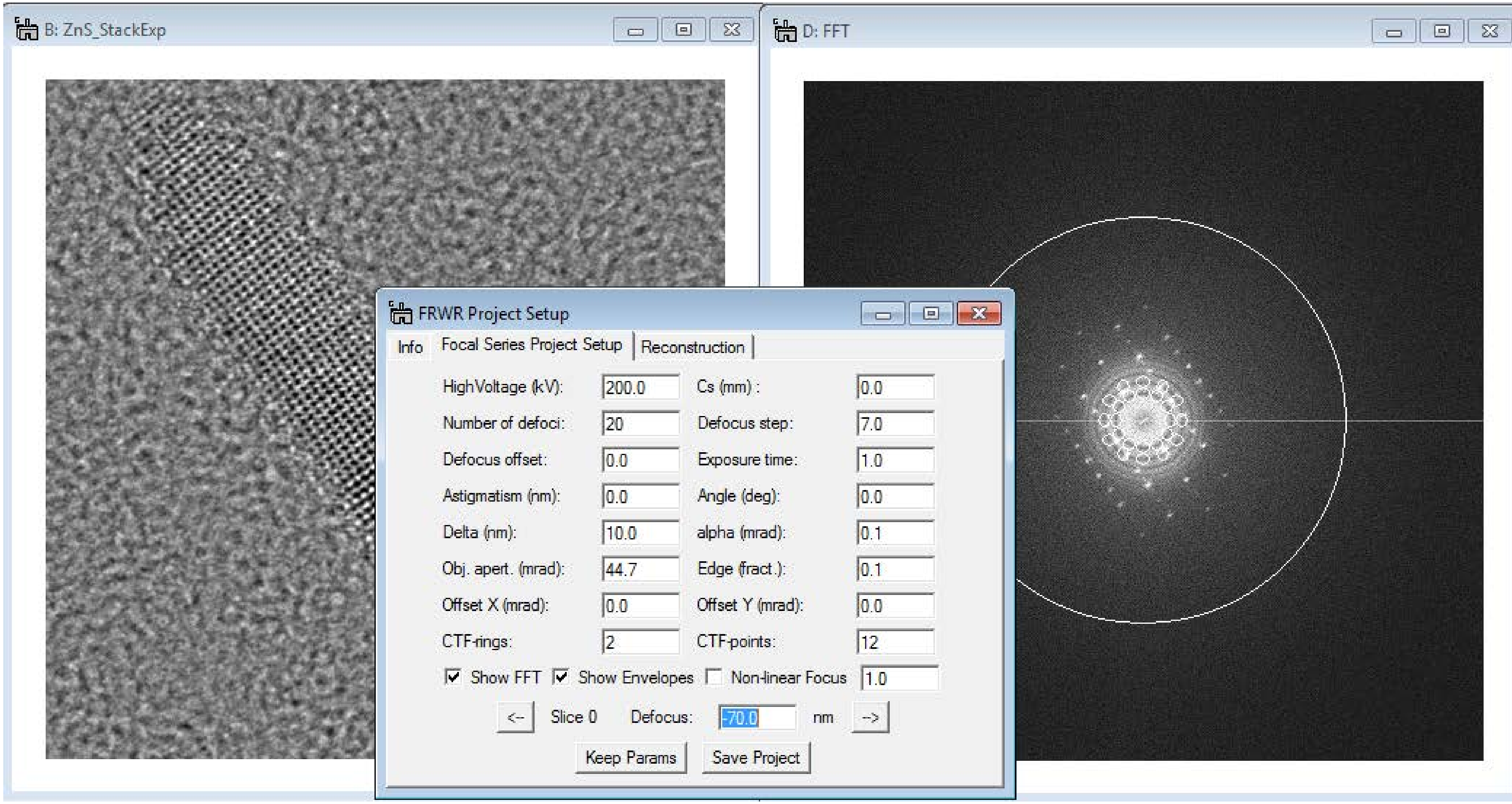
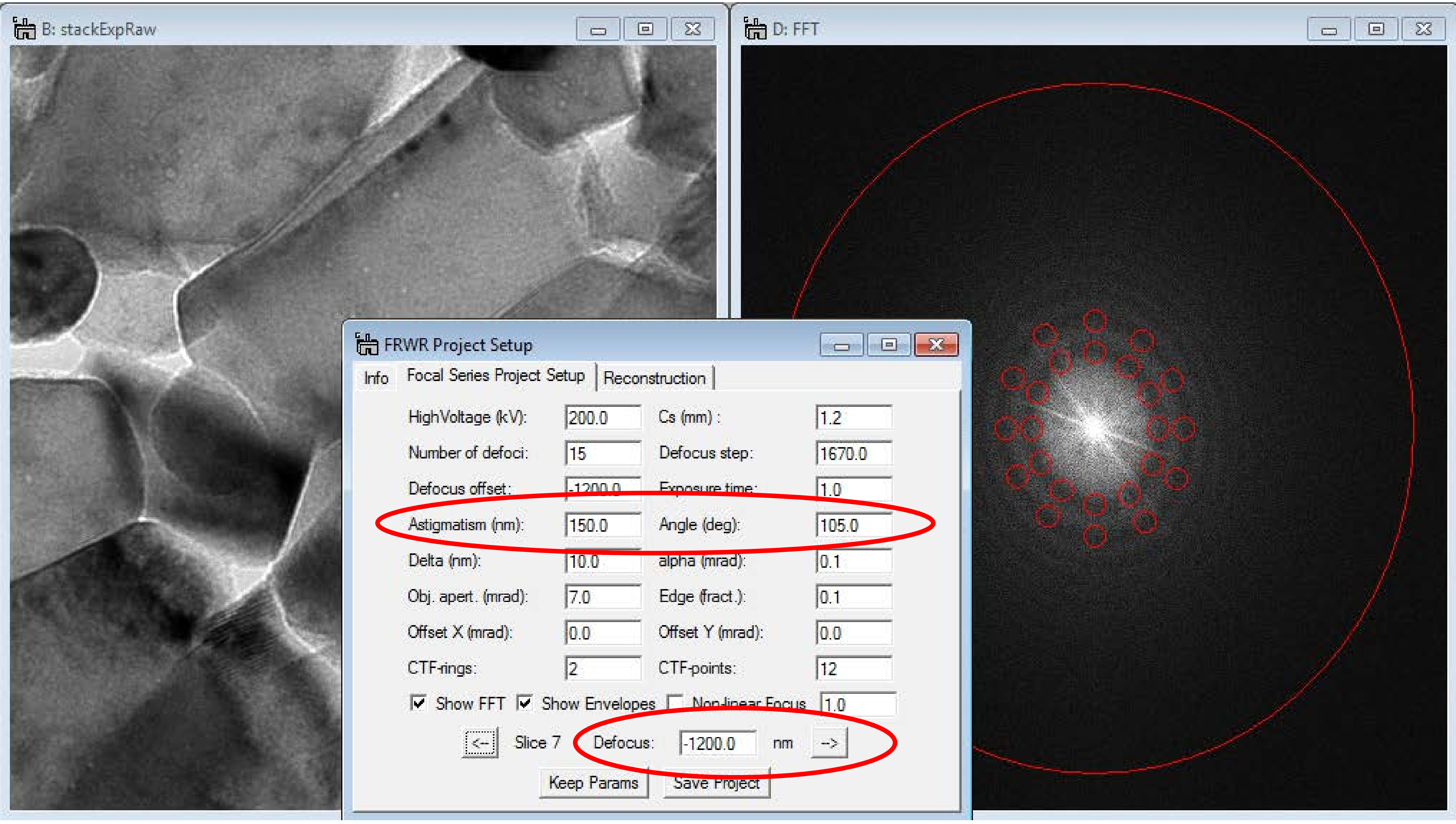
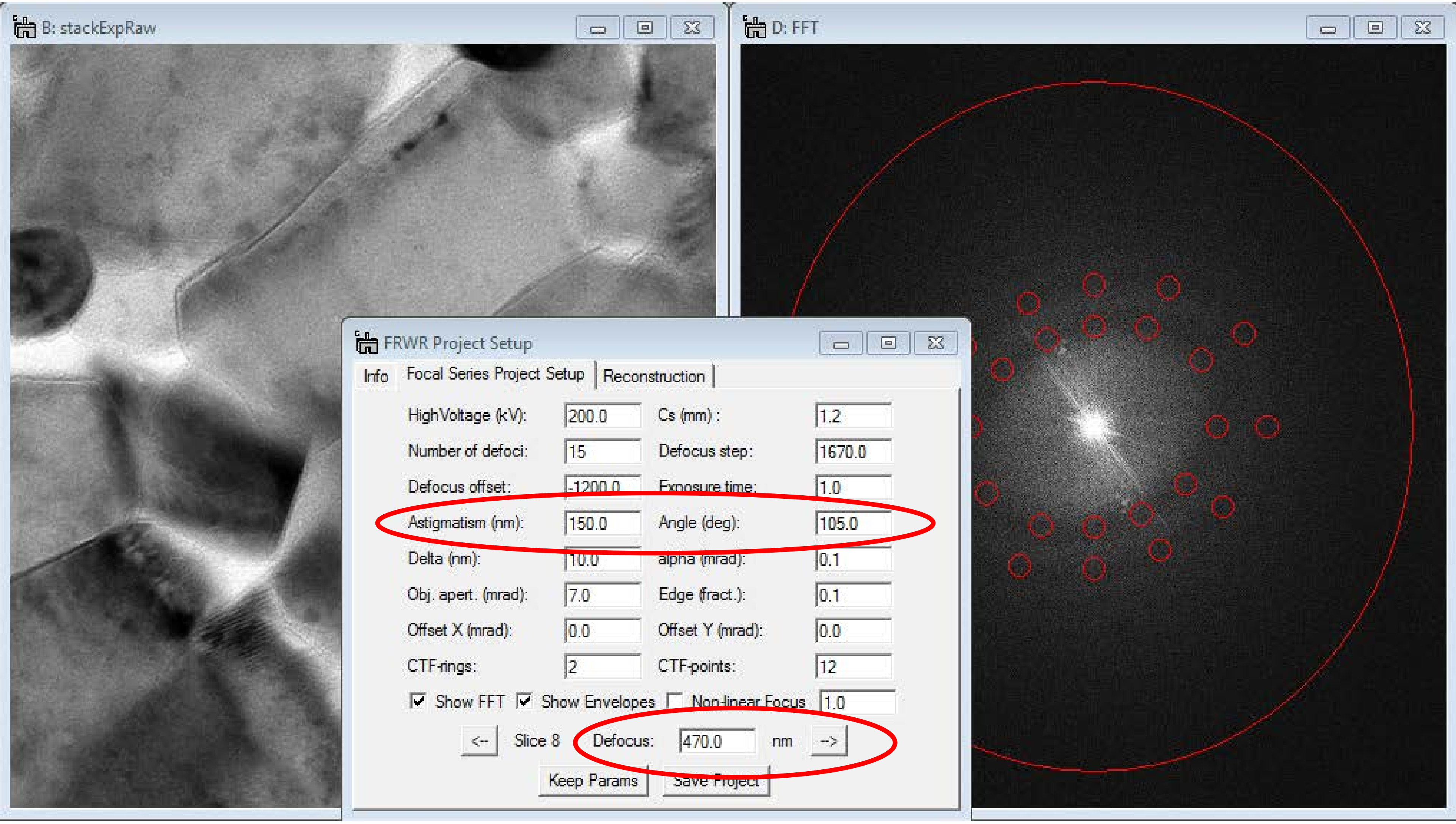
Setup Tool


B: ZnS_StackExp
D: FFT
FRWR Project Setup
Info
Focal Series Project Setup
Reconstruction
HighVoltage (kV): 200.0
Cs (mm) : 0.0
Number of defoci: 20
Defocus step: 7.0
Defocus offset: 0.0
Exposure time: 1.0
Astigmatism (nm): 0.0
Angle (deg): 0.0
Delta (nm): 10.0
alpha (mrad): 0.1
Obj. apert. (mrad): 44.7
Edge (fract.): 0.1
Offset X (mrad): 0.0
Offset Y (mrad): 0.0
CTF-rings: 2
CTF-points: 12
Show FFT
Show Envelopes
Non-linear Focus 1.0
<--
Slice 0
Defocus: -70.0 nm
-->
Keep Params
Save Project

Adjust defocus & Astigmatism at Underfocus



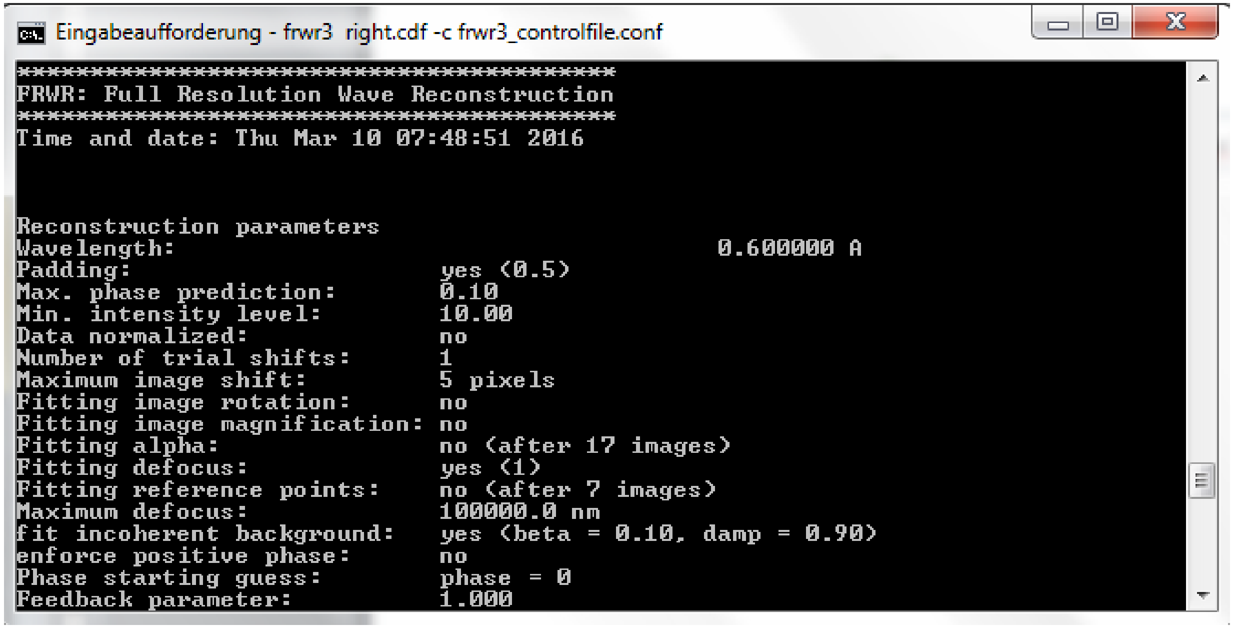
Adjust defocus & Astigmatism at Overfocus



Running the reconstruction

Open a command window, navigate to the folder where you want to store the results, and start the reconstruction using the command

```
frwr3  [projectName].cdf  –c [controlFile]
```



Because of extensive hard disc access this reconstruction may run for quite some time, especially if distortion correction is turned on.

Reconstructions can always be interrupted (Ctrl + C) and resumed with the command

```
frwr3  [projectName].cdf  –c [controlFile] -r
```

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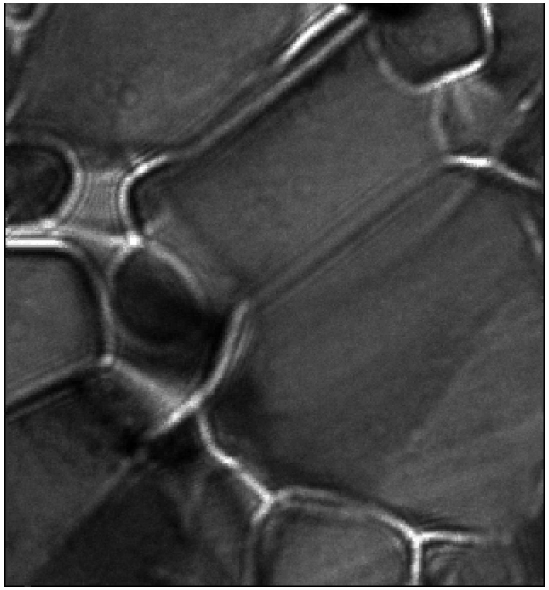
Low Spatial Frequencies: Compensate Distortions !

Raw experimental data



Distortions (amplified x5)

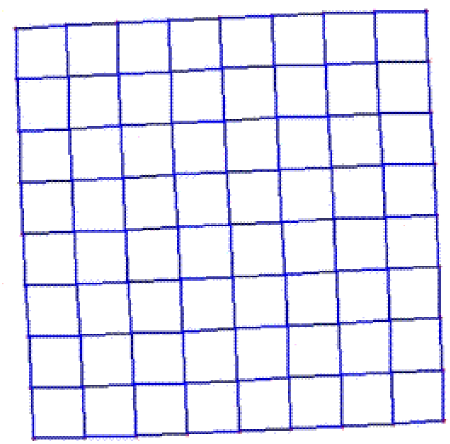
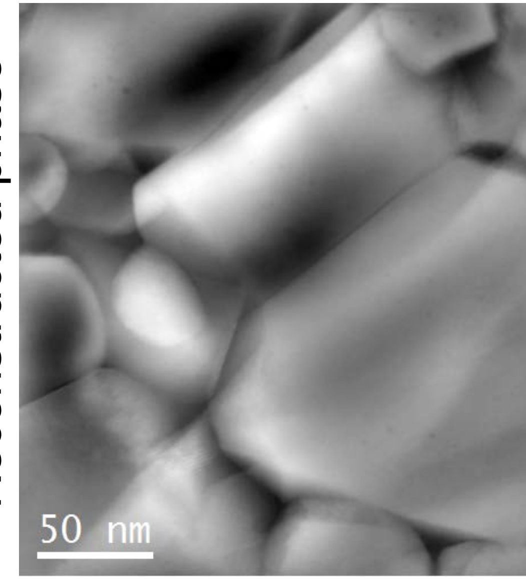
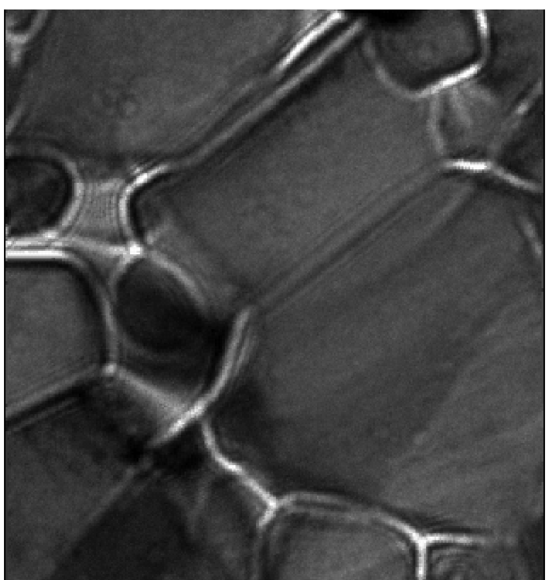


Image 3, Defocus = -12184 nm

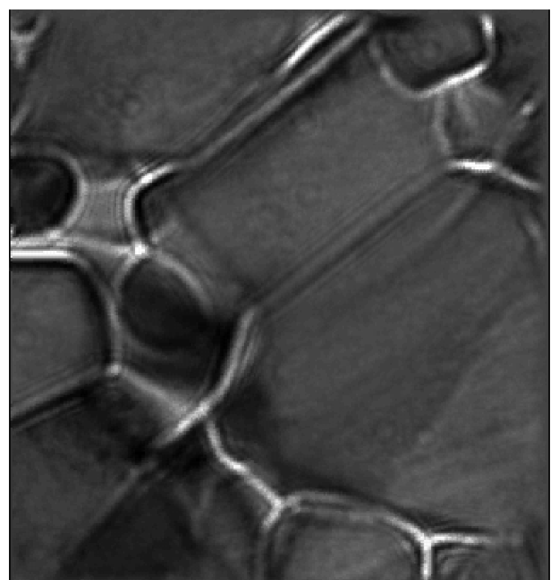
Reconstructed phase



Distortions corrected



Simulated from wave



Use simulated focal series for verifying the result

How to control distortion fitting

A few lines from the control file:

```
fit distortions:            1
fit rotation:               1
fit magnification:          1
```

Turns distortion fitting on/off

Controls fitting rotation and magnification separately (only if ‚fit distortions' =1)

```
zoomFactor_mm: 0 0 0
rot_rad_mm:    0 0 0
zoomX_mm:      0 0 0
zoomY_mm:      0 0 0
spiral_mm:     0 0 0 % in rad per kpixel
pincush_mm:    0 0 0 % per kpixel and
```

Starting parameters for distortions
- microscope dependent
- can be obtain from previous reconstructions

```
zoomFactor_mm range:  3
rot_rad_mm range:     2
zoomX_mm range: 0.1
zoomY_mm range: 0.1
spiral_kpix_mm range:      0.4
pincushion_kpix_mm range: 0.4
```

Range over which you allow parameters to vary
- microscope dependent
- always per mm of defocus
  => small defocus => small distortions

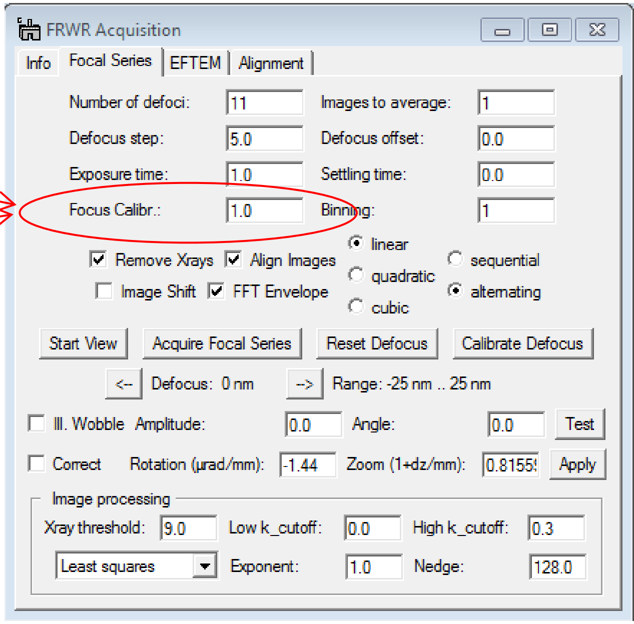
Reporting of Distortion Parameters: imgParams.log

```
defocus: -11468.386 -10206.851 -8843.599 -7370.959 -5878.288 -4378.202 -2817.284 -1244.810 500.000 2039.198 3660.883 5279.983 6853.055 8481.858 10028.473
rotation: 0.000321 0.000320 0.000302 0.000268 0.000222 0.000169 0.000111 0.000054 -0.000000 -0.000035 -0.000052 -0.000044 -0.000008 0.000066 0.000175
zoom: 0.000836 0.000787 0.000721 0.000637 0.000537 0.000426 0.000299 0.000162 -0.000000 -0.000149 -0.000310 -0.000473 -0.000633 -0.000797 -0.000950
zoomX: -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
zoomY: -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
spiral: 0.001318 0.000840 0.000455 0.000171 -0.000001 -0.000080 -0.000091 -0.000057 0.000000 0.000035 0.000027 -0.000060 -0.000250 -0.000587 -0.001068
pincushion: 0.001293 0.001117 0.000941 0.000765 0.000601 0.000446 0.000296 0.000153 -0.000000 -0.000131 -0.000268 -0.000407 -0.000546 -0.000696 -0.000847
alpha: 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930 0.033930
position: (48, 35) (48, 35) (47, 36) (48, 35) (48, 35) (48, 36) (48, 36) (48, 36) (48, 35) (48, 35) (49, 35) (49, 35) (48, 35) (48, 35) (49, 35)
```

Calibration=fitted def./requested def.

The fitted defocus step
(can also be used for microscope calibration):

```
defocus fit:   1628.79 1.99006 -1.76152 nm
```



The following section from imgParams.log can be copied into the control file for future reconstructions:

```
zoomFactor_mm: -0.0949699 -1.20323 74.5796
rot_rad_mm:    -0.0270412 2.646 222.616
zoomX_mm:      0 0 0
zoomY_mm:      0 0 0
spiral_mm:     0.0307718 -3.13081 -1244.92 % in rad per kpixel and mm
pincush_mm:    -0.0859823 0.64515 -99.9325 % per kpixel and mm
```

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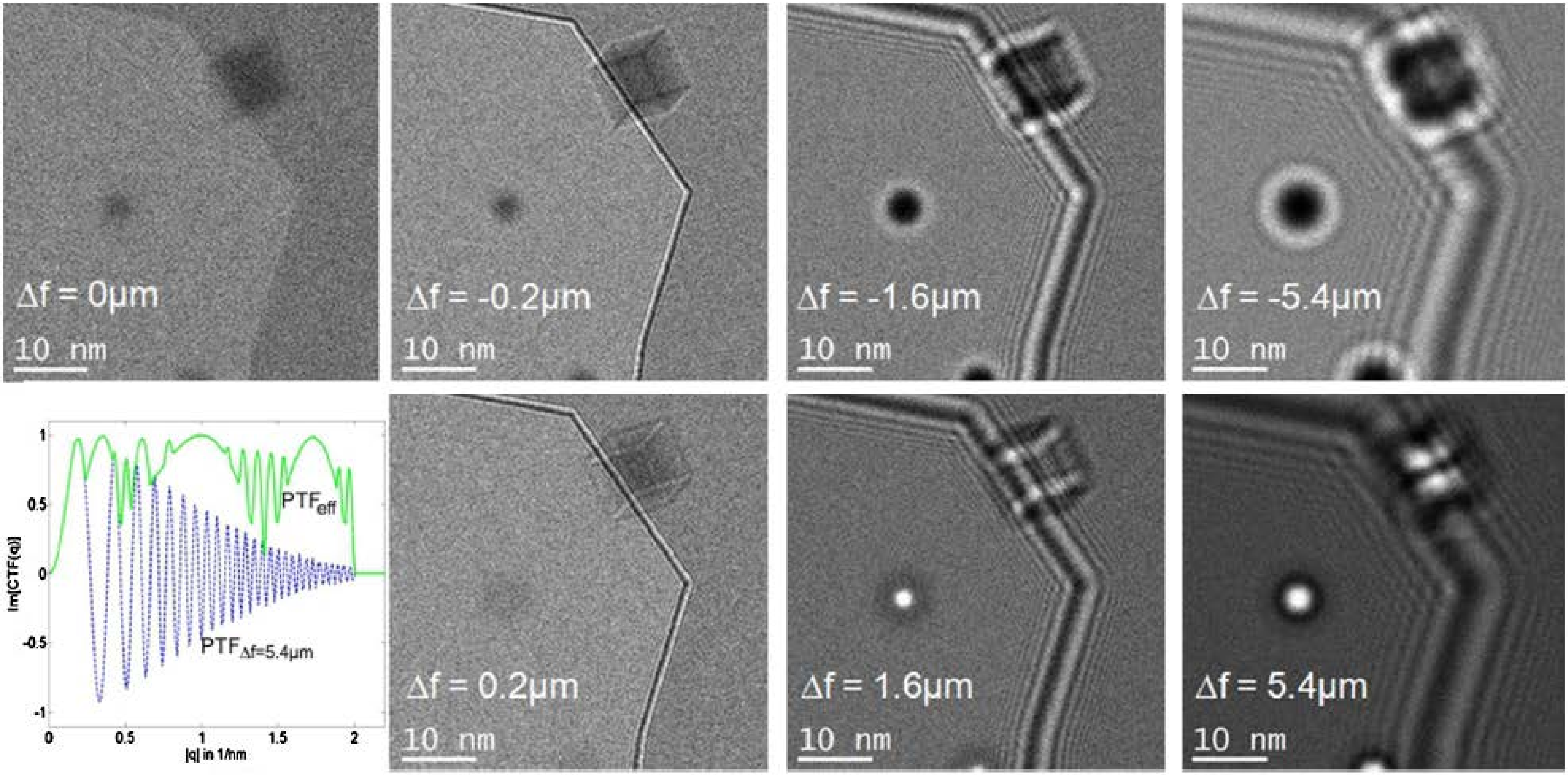
Recovering Low Frequencies Despite Low Spatial Coherence



Simulated focal series

Electron beam energy: 200 kV (λ = 2.51 pm)
Illumination convergence semi-angle: α = 0.05 mrad
Dose: 34.2 electrons / Å^2

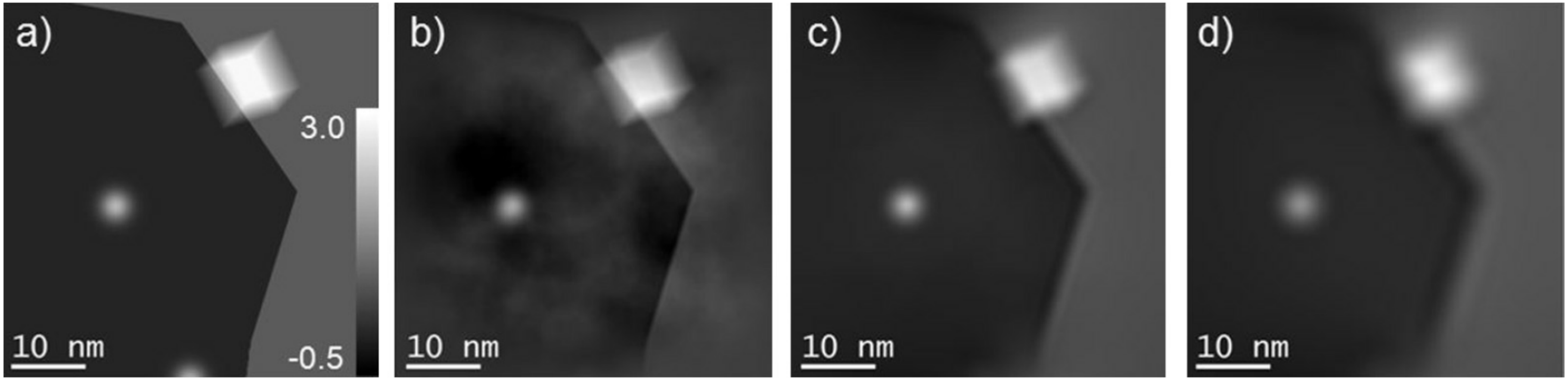
C.T. Koch, Micron **63** (2014) 69–75

Applying the Transport of Intensity Equation

$$\frac{2\pi}{\lambda}\frac{\partial I(\vec{r},\Delta f)}{\partial \Delta f} = \nabla_{x,y}\cdot[I(\vec{r},\Delta f)\nabla_{x,y}\phi(\vec{r},\Delta f)]$$

Solving the TIE extrapolates to low spatial frequencies irrespective of spatial coherence

Original phase | $\Delta f = \pm\ 0.2\ \mu m$ | $\Delta f = \pm\ 1.6\ \mu m$ | $\Delta f = \pm\ 5.4\ \mu m$

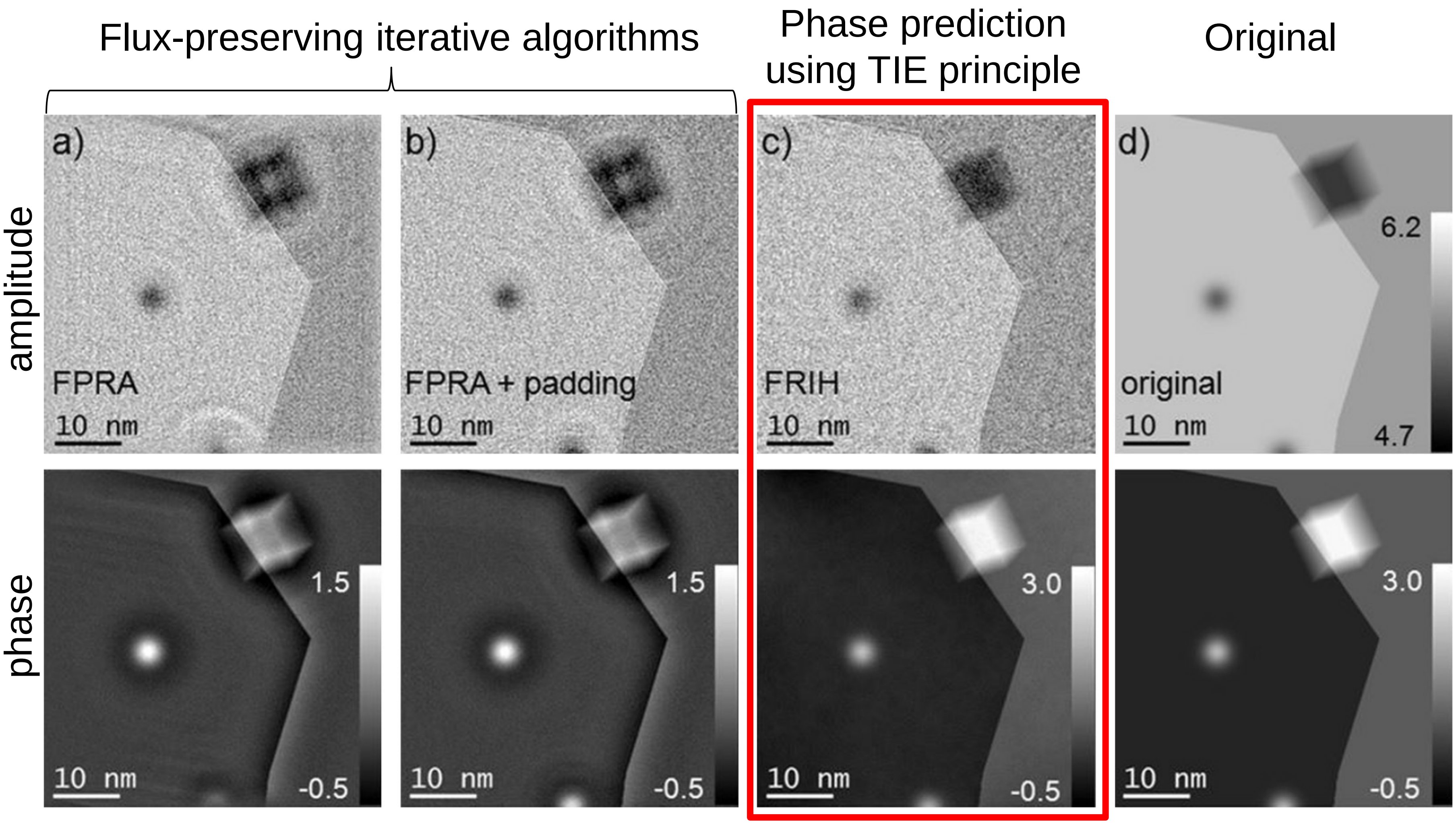


$\Rightarrow$ Compromise between low spatial frequency artefacts and resolution

DANGER The TIE is not self-consistent, requires boundary conditions DANGER

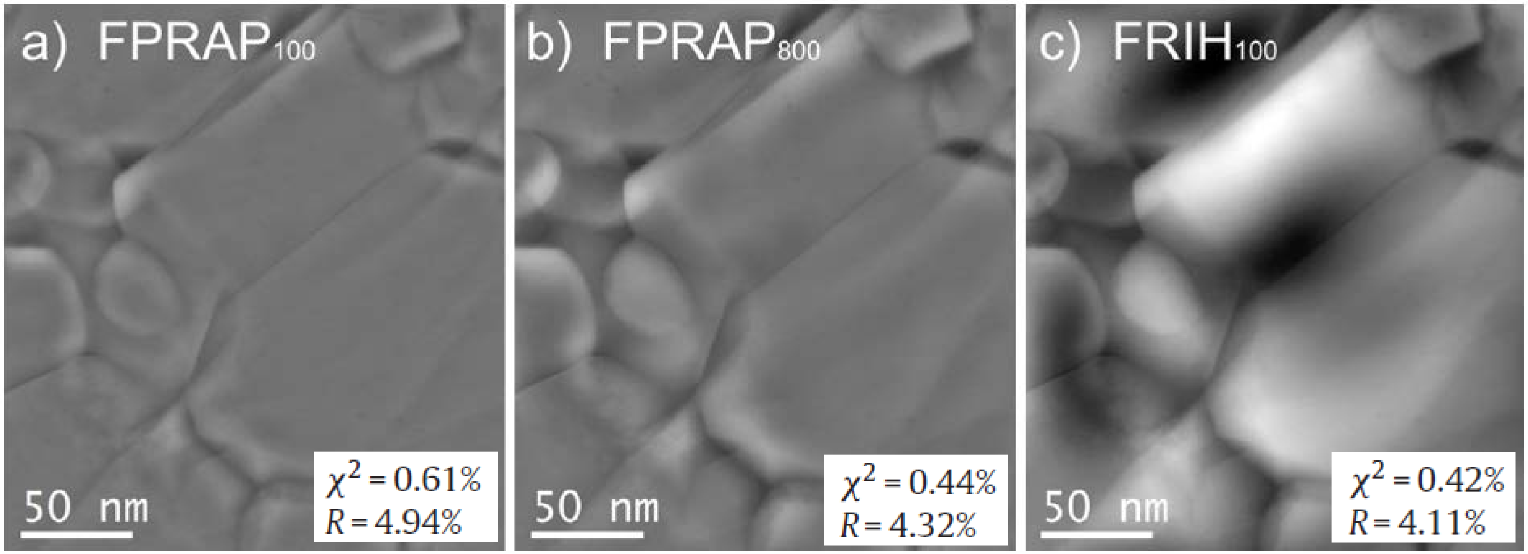
C.T. Koch, Micron **63** (2014) 69–75

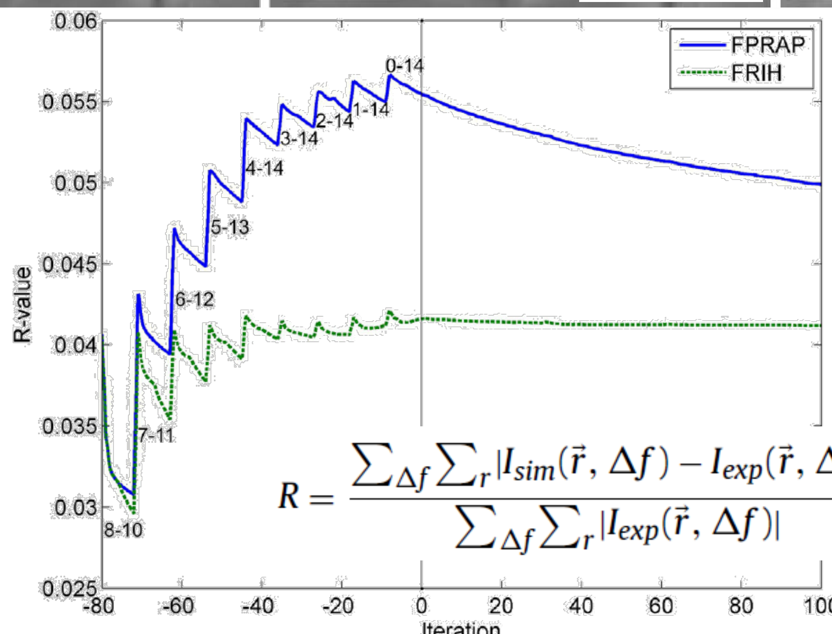
Full-Resolution Inline Holography (FRIH)



C.T. Koch, Micron **63** (2014) 69–75 (*open access*) DOI: 10.1016/j.micron.2013.10.009

Applying FRIH to Experimental Data



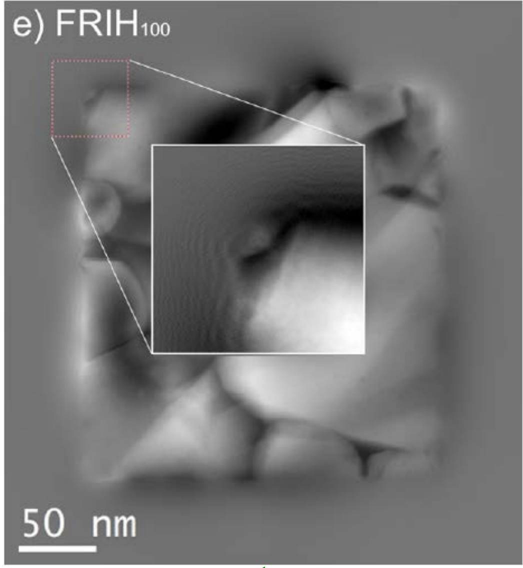


$$R = \frac{\sum_{\Delta f} \sum_{r} |I_{sim}(\vec{r}, \Delta f) - I_{exp}(\vec{r}, \Delta f)|}{\sum_{\Delta f} \sum_{r} |I_{exp}(\vec{r}, \Delta f)|}$$

$FPRAP_{iter}$: flux-preserving reconstruction algorithm with padding

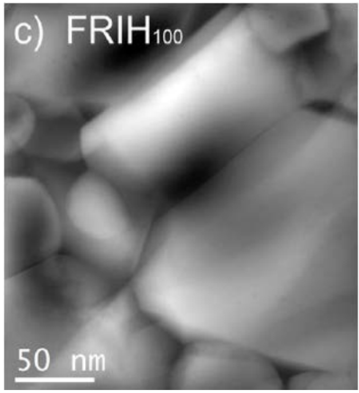
C.T. Koch, Micron **63** (2014) 69–75

Phase Prediction in Control File




```
enforce equal defocus steps:    0
intermediate loops:          5
final loops:                 50
residue loops:               0

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Settings for Phase Prediction:
phase predict loops:         4  % applies TIE to residual
phase predict threshold:     0.025 % keep only small phase update
low intensity threshold:     5 % avoids dividing by zero in TIE
padding:                     0.25
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```




```
Average chi2: 0.00171284
Image 0: defocus: 0.0 nm, wave shift: (0, 0)
Image 1: defocus: -0.1 nm, wave shift: (0, 0)
Image 2: defocus: -0.2 nm, wave shift: (0, 0)
Image 3: defocus: -0.3 nm, wave shift: (0, 0)
Image 4: defocus: -0.4 nm, wave shift: (0, 0)
Mean defocus step = -0.1nm
Will read image 5
6-Loop 0: align=1, R-value=0.0174959
6-Loop 1: align=0, R-value=0.017343
6-Loop 2: align=0, R-value=0.0172945
6-Loop 3: align=1, R-value=0.017267
6-Loop 4: align=0, R-value=0.0172463
6-Loop 5: align=0, R-value=0.0172295 (P)
6-Loop 6: align=0, R-value=0.0172472 (P)
6-Loop 7: align=0, R-value=0.0172754 (P)
6-Loop 8: align=0, R-value=0.0172974 (P)
```

5 iterations with flux-preserving GS-like projections

4 iterations with phase predictions

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Successive Increase of Defocus Range

frame	0	1	2	3	4	5	6
defocus	-90	-40	-10	0	10	40	90

Control file

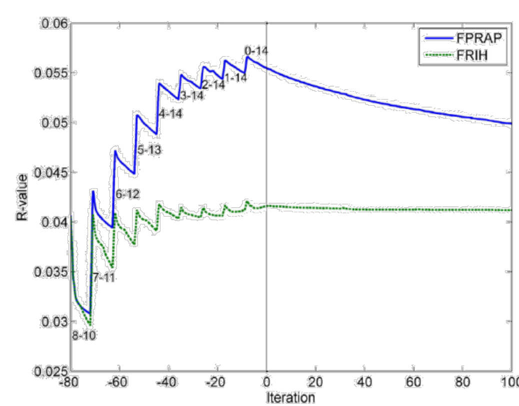
```
init loops 2:          5
init loops 3:          6
```

1. Find ut whether frame 4 or 2 correlates better with frame 3
2. Reconstruct from only those two frames (e.g. 5 iterations)
3. Try including a 3rd frame below or above (e.g. 6 iterations)

4. Initial reconstruction using 3 images only (3-loop)
5. Alignment of images simulated for Δf=+40 with exp. data

6. Reconstruction using 5 images only (5-loop)
7. Alignment of images simulated for Δf=±90 with exp. data

This procedure allows images with very different contrast to be aligned in a fully **automated** fashion quite **reliably**



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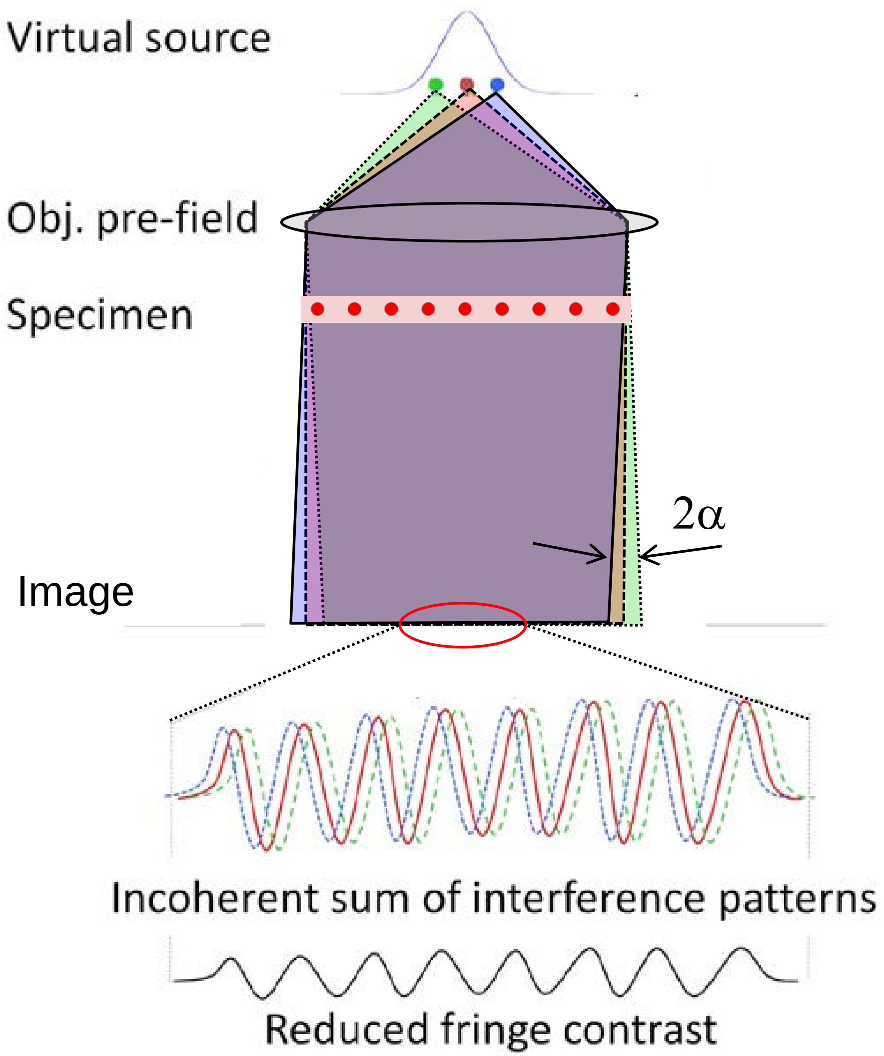
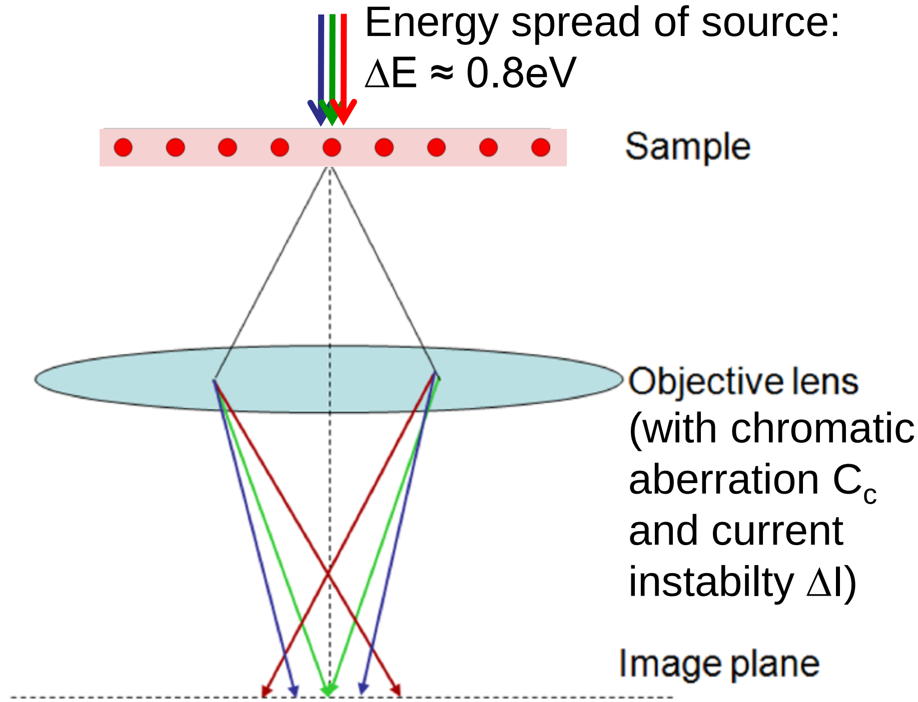
Partial Coherence

Partial **spatial** coherence



Partial **temporal** coherence



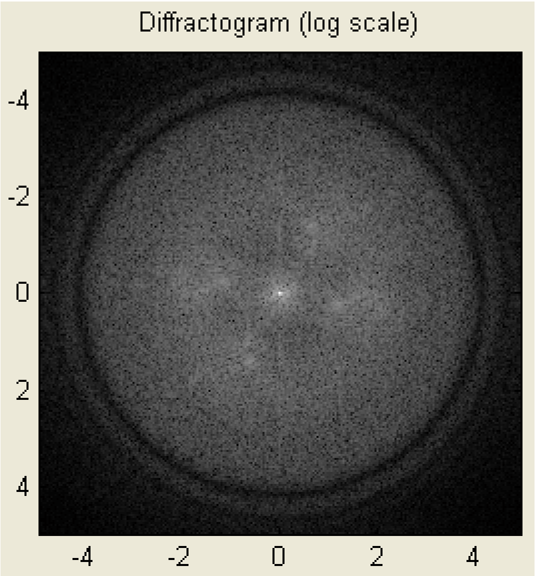
Parameters describing partial coherence

Spatial: illumination semi-convergence α

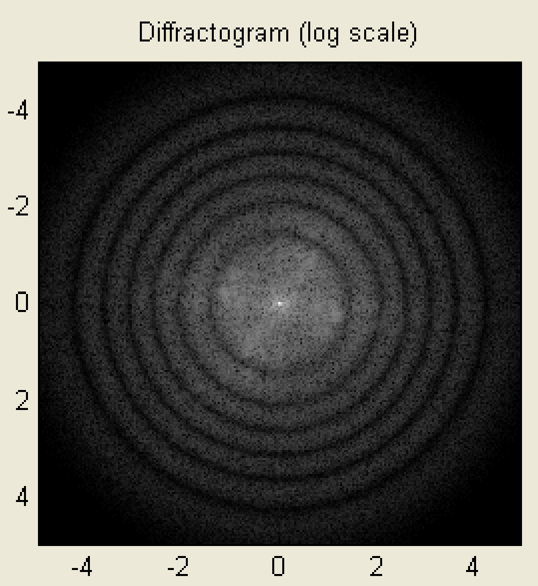
Temporal: focal spread $\Delta = C_c \sqrt{\frac{\Delta E^2}{E^2} + 2\frac{\Delta I^2}{I^2}}$

Effect of Partial Coherence in TEM

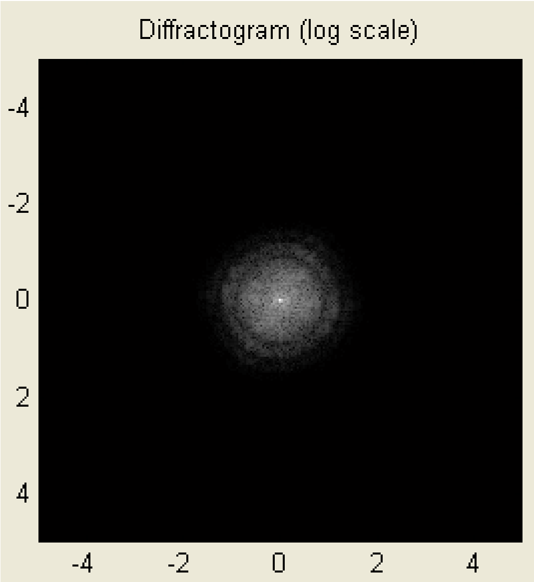
While coherent aberrations mingle amplitude and phase information in the images, partial coherence destroys information within the image all together.



C_s = 1.2mm, Δf = -65.7nm, Δ=20nm, α=1mrad



C_s = 1.2mm, Δf = -200nm, Δ=20nm, α=1mrad



C_s = 1.2mm, **Δf = -500nm**, Δ=20nm, α=1mrad

Finite values of Δ and α are a result of limited (partial) **temporal (longitudinal)** and **spatial (transversal)** coherence as well as chromatic aberrations.

The Transfer Cross Coefficient (TCC)

$$I(\vec{r}) = \mathrm{FT}^{-1}\left[\int \Psi_0(\vec{q}+\vec{q}')T(\vec{q}+\vec{q}',\vec{q}')\Psi_0^*(\vec{q}')d^2\vec{q}'\right]$$

Transmission cross coefficient (TCC)

$$TCC(q+q',q') = T_\Delta(q+q',q')T_s(q+q',q') \times exp\left(-i[\chi(q+q') - \chi(q')]\right)$$

Temp. Coherence: $T_\Delta(q+q',q') = \exp\left(-2(\pi\Delta_f)^2\left[\frac{\delta\chi(q+q')}{\delta\Delta f} - \frac{\delta\chi(q')}{\delta\Delta f}\right]^2\right)$

Spatial Coherence: $T_s(q+q',q') = \exp\left(-\left(\frac{\alpha}{2\lambda}\right)^2\left[\frac{\delta\chi(q+q')}{\delta(q+q')} - \frac{\delta\chi(q')}{\delta q'}\right]^2\right)$

Coherent Transfer: $\chi(q) = \pi\lambda\Delta f q^2 + 0.5\pi\lambda^3 C_s q^4$ + …

The quasi-coherent approximation

Spatial Coherence Envelope Function: $E_s(q) = \exp\left(-\left(\frac{\alpha}{2\lambda}\frac{\delta\chi(q)}{\delta q}\right)^2\right)$

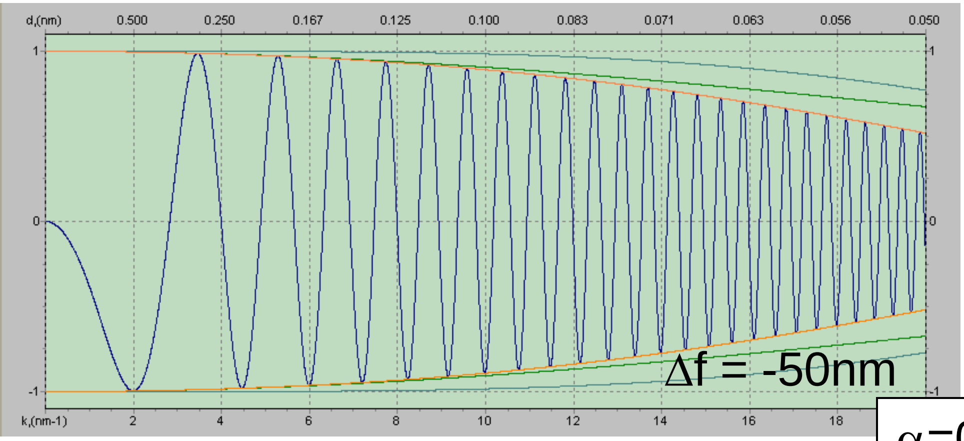
Temporal Coherence Envelope Function: $E_\Delta(q) = \exp\left(-2(\pi\Delta_f)^2\left[\frac{\delta\chi(q')}{\delta\Delta f}\right]^2\right)$

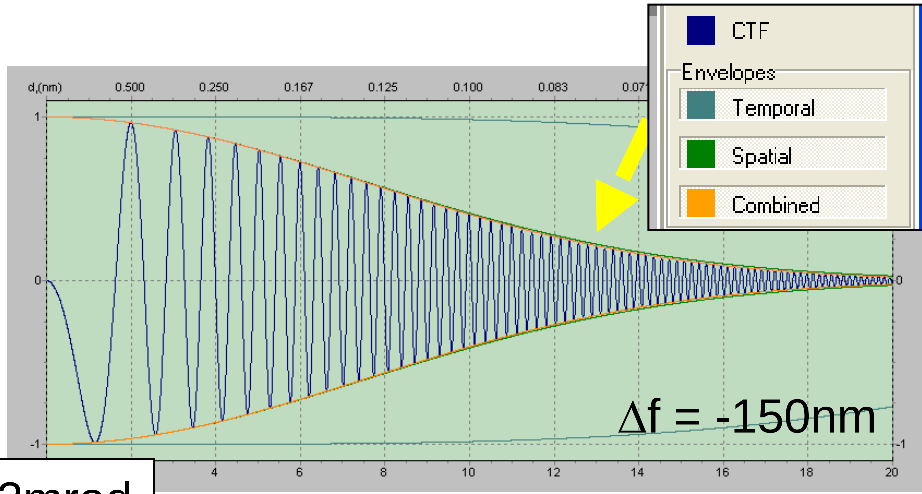
$$I(\vec{r}) = \left|\mathrm{FT}^{-1}\left[\Psi_0(\vec{q})exp(-i\chi(q))E_\Delta(q)E_s(q)\right]\right|^2$$

Problem: Multiplying the complex wave function with an envelope cuts away electrons!
(which is unphysical)

Will assume:

1. (dispersion free) monochromator: energy width 90meV => neglect $T_\Delta(q+q',q')$
2. C_s-corrector => $\chi(q) = \pi\cdot\lambda\cdot\Delta f\cdot q^2$

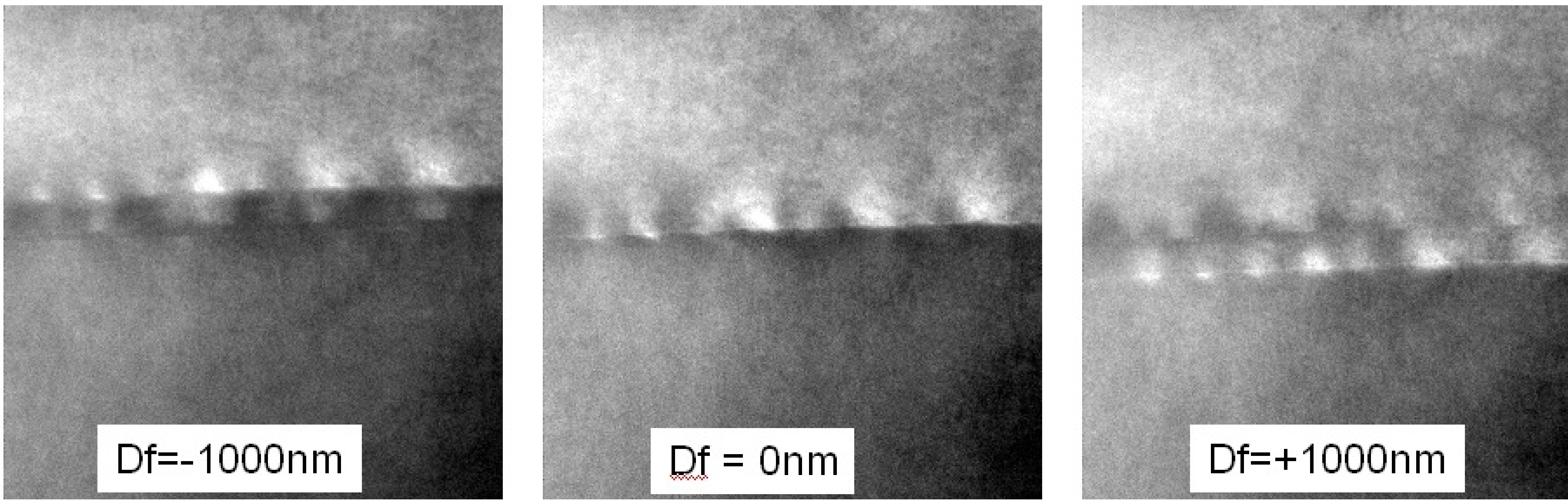




α=0.2mrad

Flux preservation important at large Δf

The **TCC** correctly predicts the presence of
DF images in defocused BF images
(in the quasi-coherent approximation these electrons would be missing)



Experimental BF images of a Σ5 grain boundary in SrTiO3.
Large Objective aperture, relatively large convergence angle.

⇒ see C.T. Koch, *A flux-preserving non-linear inline holography reconstruction algorithm for partially coherent electrons*, Ultramicroscopy 108 (2008) 141–150 for details

Partial Spatial Coherence & Defoci

Lines in control file:

```
alpha_mrad:      0.08
fit alpha:       1 7 % start fitting alpha @ 7-loop (1=on, 0=off)
```

In this example α will be assumed to be 0.08 mrad for the first iterations, until 7 images are included in the reconstruction.

Starting with the 7-loop alpha will be refined together with the defoci.

frwr3 will also **optimize the defocus** of each image, except for the reference image (the one with the smallest absolute value of the Δf):

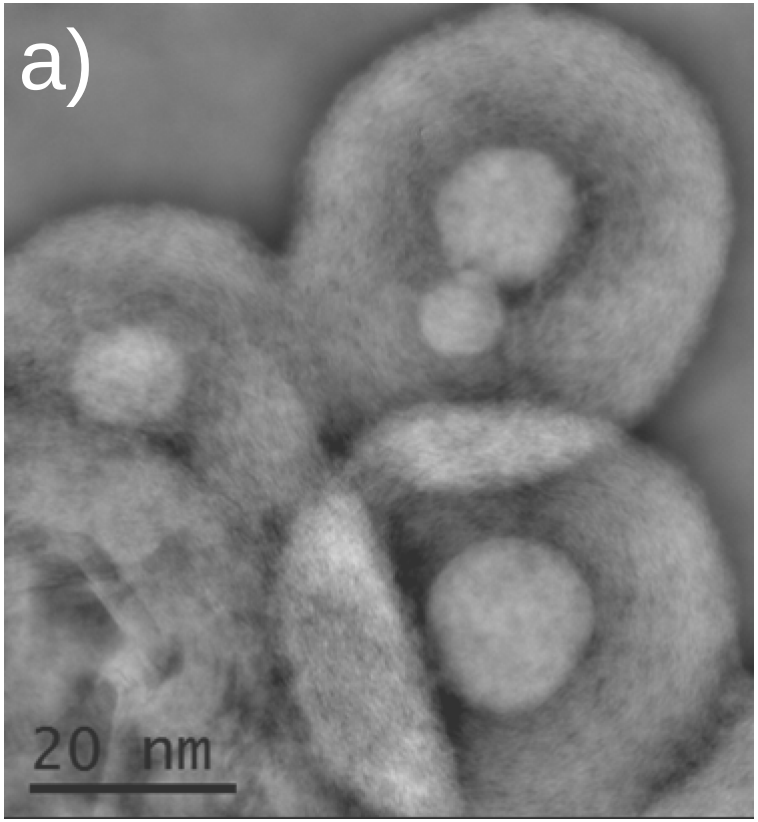
```
fit defocus:                2    % 0: never
                            % 1: only in final refinement loop
                            % 2: start after the 3-loop
                            % 3: start in 3-loop
                            % 4: right after the first 2-loop
                            % 5: already in the very first 2-loop
```

Towards Full-Resolution Inline Holography (FRIH)

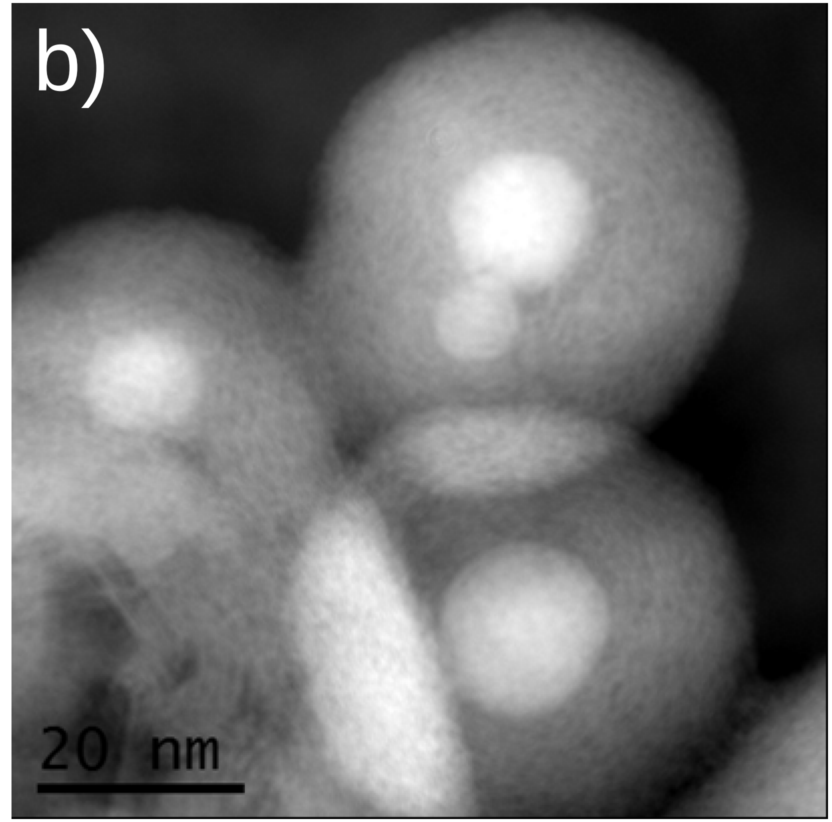
Features of the FRWR (full-resolution wave reconstruction) software:

- Non-linear defocus increments
- Fully automated acquisition in DM
- Setup of reconstruction in DM
- Compensation of distortions induced by changes in objective lens current
- Phase prediction - applies a variant of the TIE with $(I^{exp}-I^{sim})/df$ as input
- Flux-preserving model for partial spatial coherence
- Fitting of incoherent background (mimics incoherent scattering)
- **Different regularization functions for ‚improving‘ low spatial frequencies**

Regularization by, e.g. Gradient Flipping



Conventional reconstruction algorithm



Regularized reconstruction

Further details in the following 3 papers:

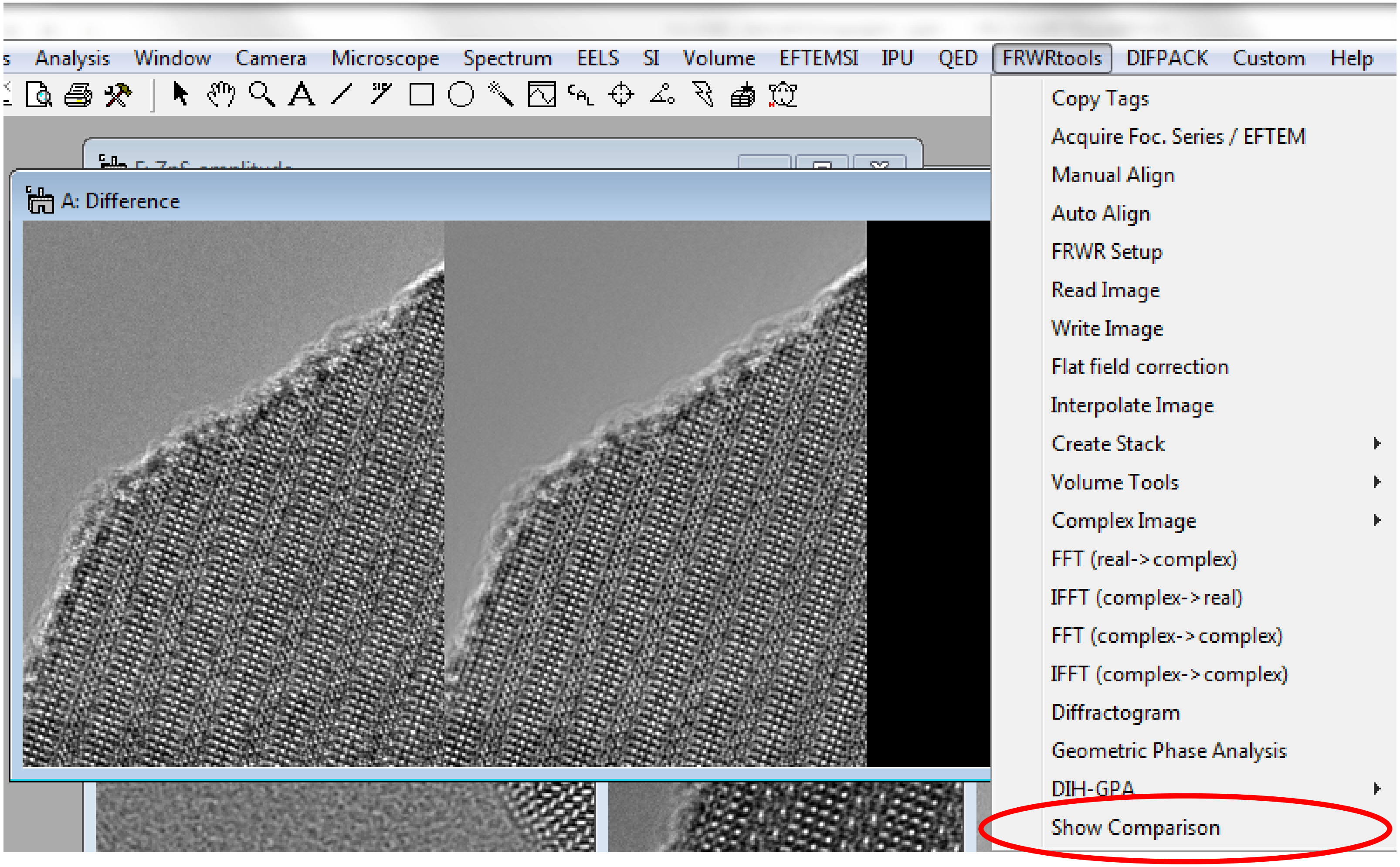
- A. Parvizi, W. Van den Broek, CTK, „Recovering low spatial frequencies in wavefront sensing based on intensity measurements “Advanced Structural and Chemical Imaging (2016) accepted
- A. Parvizi, W. Van den Broek, CTK, „The gradient flipping algorithm: introducing non-convex constraints in wavefront reconstructions with the transport of intensity equation“, Optics Express (2016) accepted
- C. Ozsoy Keskinbora et al. „Full-resolution high-contrast imaging of phase objects by gradient-flipping assisted full-resolution wave reconstruction“ (to be submitted)

How to apply Gradient Flipping (GF)

Section of the control file:

`%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%`	
`% Gradient flipping (GF):`	
`apply GF: 1`	Turn GF on/off
`GF flipping frequency: 3`	Apply GF every 3rd iteration
`GF beta: 0.85`	Mixing fraction of flipped & unflipped phase
`GF signal fraction: 0.92`	Initial value for fraction of pixels to be flipped
`GF adjust fraction:  1`	
`GF min signal fraction: 0.8`	Minimium fraction of pixels to be flipped
`GF threshold: 0.01 % will be adjusted`	Initial value for the flipping threshold
`GF length scale (nm): 1`	Flipping only affects spatial frequencies below this
`GF order: 1  % order=3 means flipping dx^2+dy^2  and dxdy`	
`GF 3rd order fraction: 0`	(experimental)
`%% end of gradient flipping`	
`%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%`	

Always verify the reconstruction



Some Additional Parameters

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% config file for frwr3 reconstruction

print level:                    2
save level:                     2

shift trials:                1 % try for N best alignments at start
max shift:                   12 % pixels between sucessive images
max shift global:            20 % pixels between any image and ref.
% first frame:               6  % define this image as reference

max defocus: 70000 % image with a larger defocus will be excluded

fit incoherent background: 1 0.1 0.9
```

Decide how much to print

Decide how much to save

Feedback parameter (< 0.5)

Parameters for alignment:

```
bandpass filter low:  0.04
bandpass filter high: 0.4
exponent:             0.4  % 1=cross, 0.5=mutual, 0=phase corr.
Nedge:                50
Nedge for smoothing:  30
```

Avoids low-frequency artefacts (e.g. moving bend contours)

Avoids high frequency noise