Antiphase Domains and Coherent X-rays

L.-M. Stadler, B. Sepiol, R. Harder,
I.K. Robinson, F. Zontone, and G. Vogl

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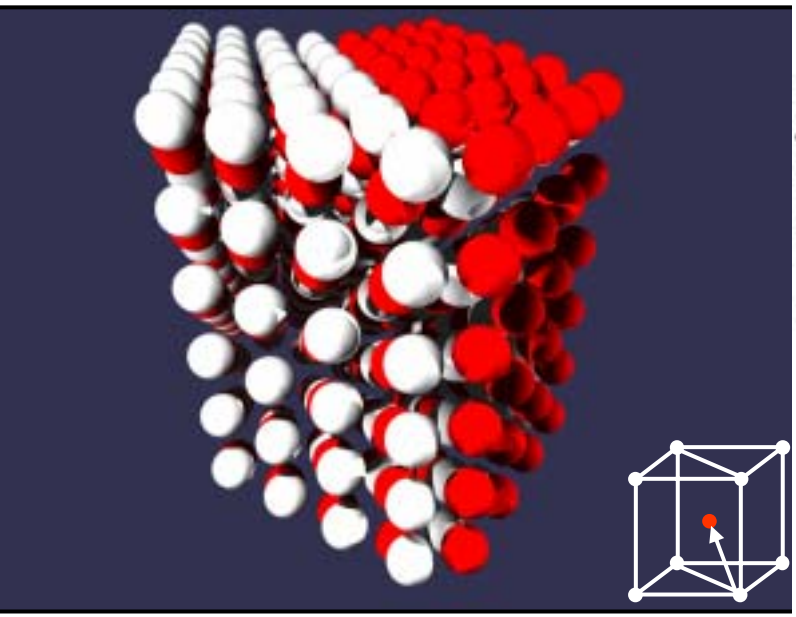
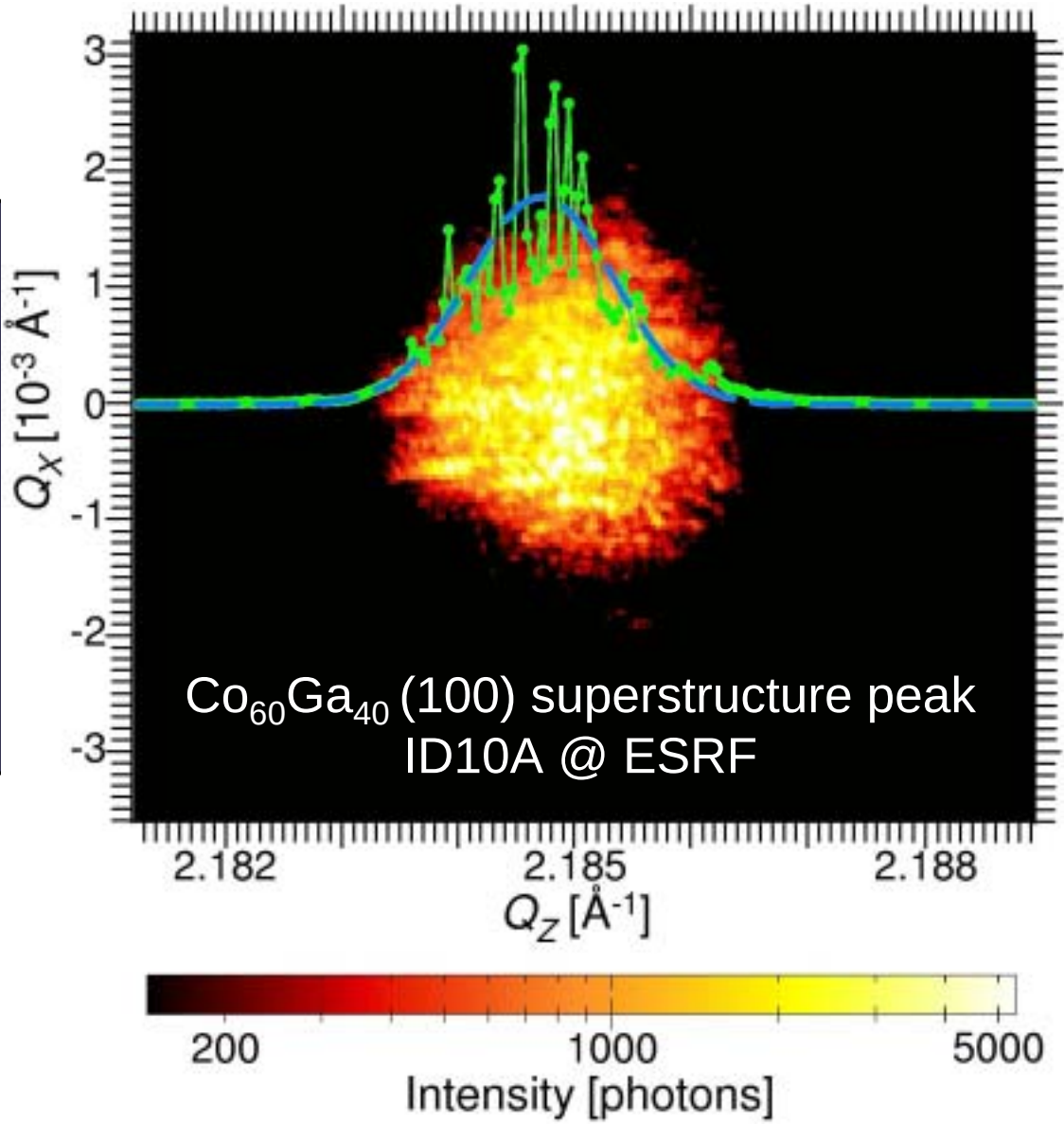
wien

Antiphase domains in B2 intermetallic phases





L.-M. Stadler *et al.*, PRB **69**, 224301 (2004);
ESRF Highlights 2004.

Detrended Fluctuation Analysis

• We construct the profile $Y(j) = \sum_{i=1}^{j} I_i$

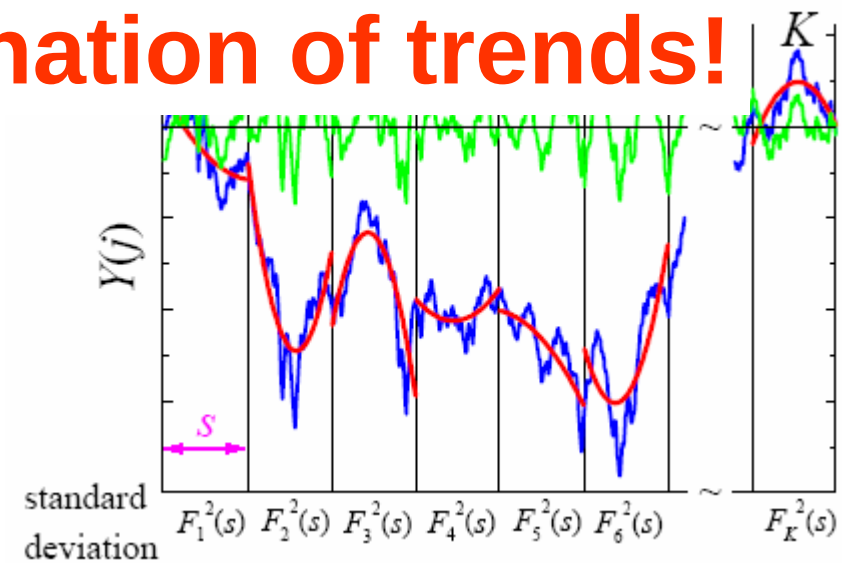
If we consider I_i as ***steps*** of a random walker, $Y(j)$ corresponds to its position after j time steps.

• We split $Y(j)$ into intervals of scale length **s** and perform a **polynomial fit** in each interval (DFA*1*: linear fit, DFA*2*: quadratic fit and so on).

• $F_n^2(s)$ is the **variance** in each segment. $F(s)$ is obtained by averaging over all segments and taking the square root, $F(s) = \sqrt{\left\langle F_n^2(s) \right\rangle_n}$.

In analogy to above $F(s)$ corresponds to the RMS displacement of the random walker.

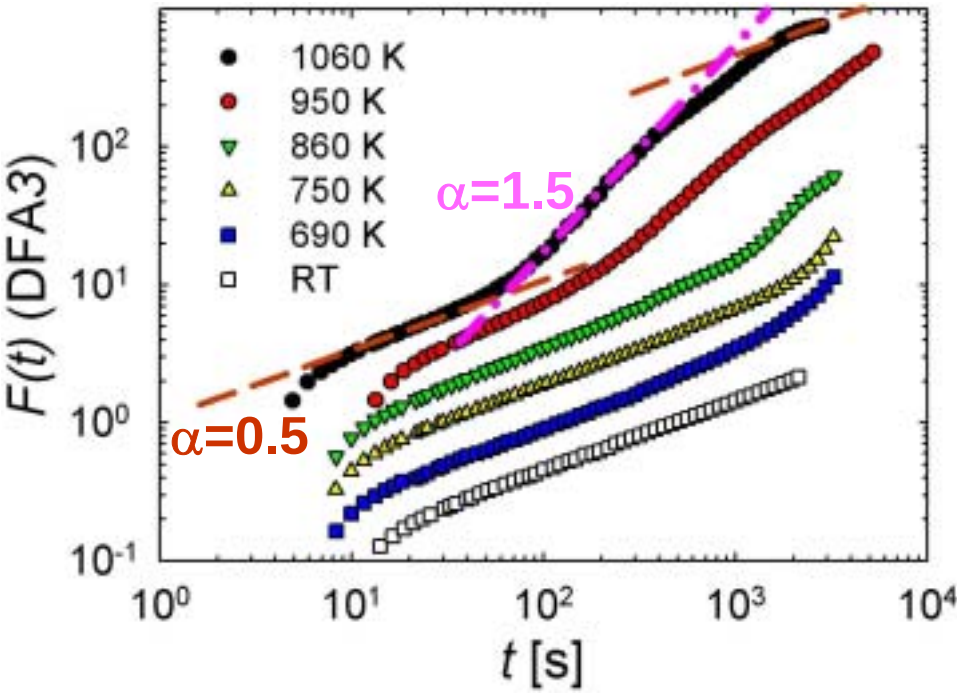
=> Systematic elimination of trends!



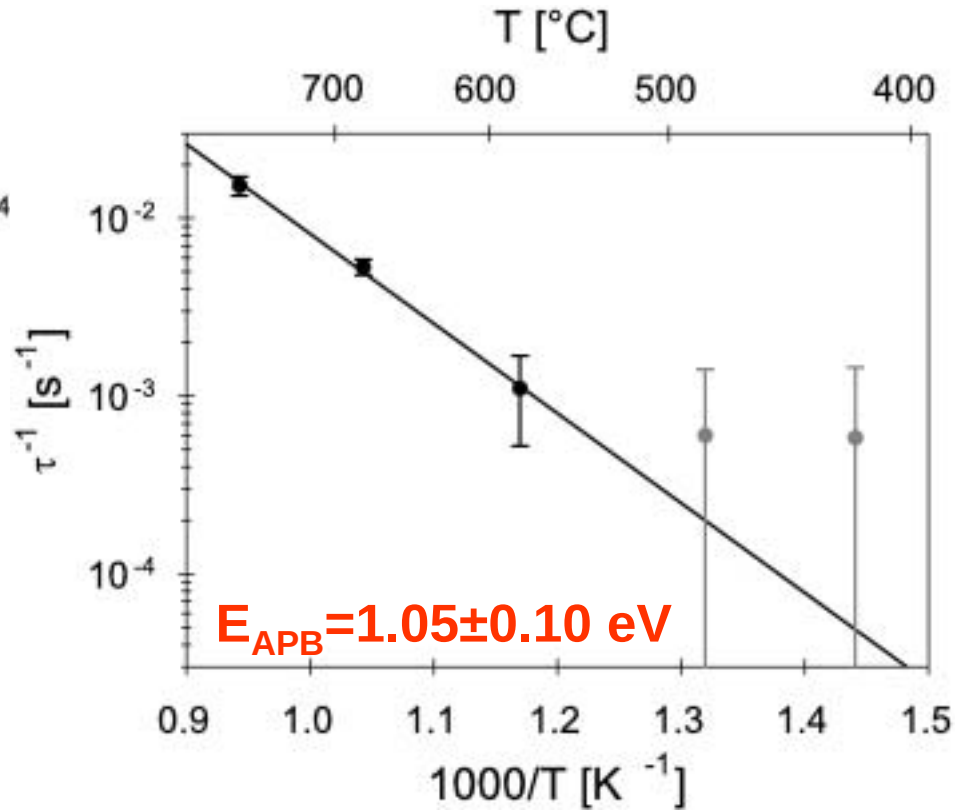
Uncorrelated fluctuations: $F(s) \propto s^{1/2}$

Random walk fluctuations: $F(s) \propto s^{3/2}$

Analysis of the correlations in the $Co_{60}Ga_{40}$ (100) superstructure peak:



For DFA and XPCS,
see also poster of **B. Pfau**



R. Weinkamer *et al.*, PRB **58**, 3082 (1998).

Is there a possibility to gain information on the exact structure of the antiphase domains?

=> Solve the phase problem!

APDs are indistinguishable by their electron density - they are **phase objects**

=> APD structure is mirrored in the reconstructed phases

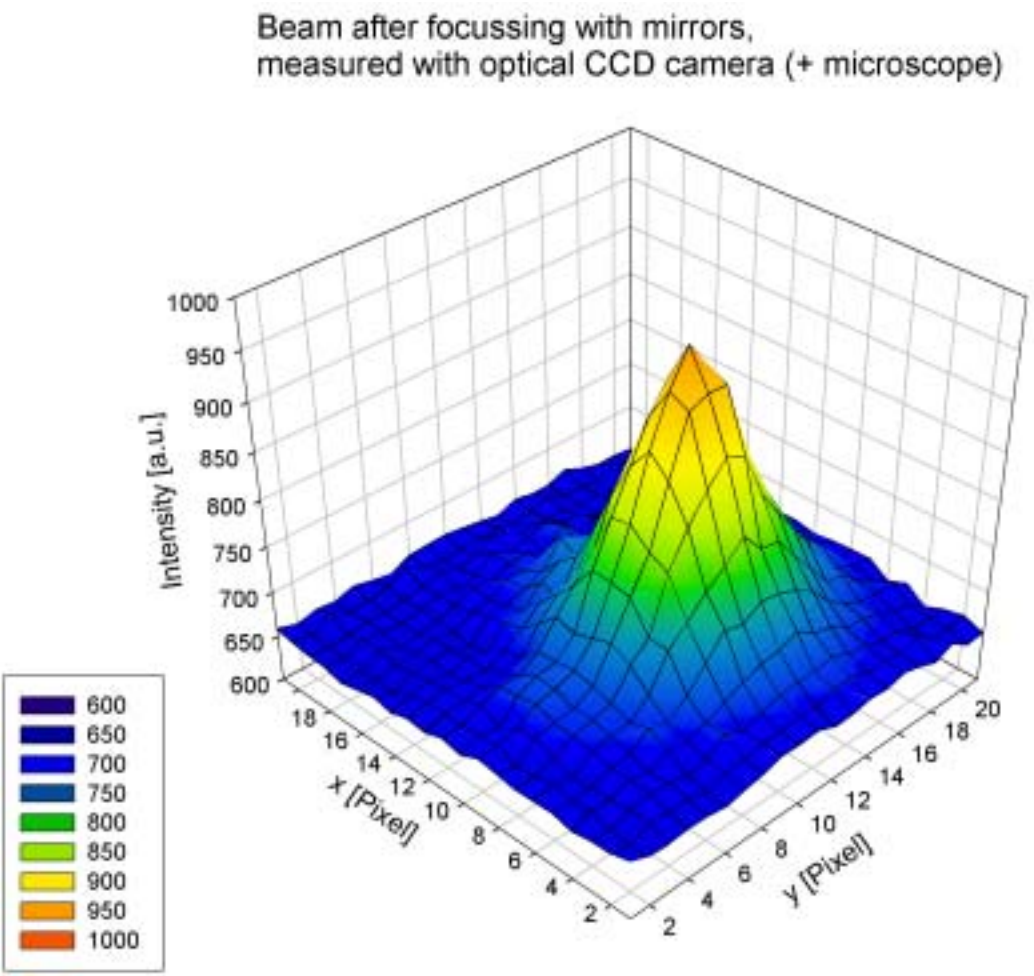
Challenge: Can we reconstruct the phases of a non-compact object?

Measurement of the (001) superstructure peak of $Fe_{65}Al_{35}$ (UNICAT 34 ID, APS)

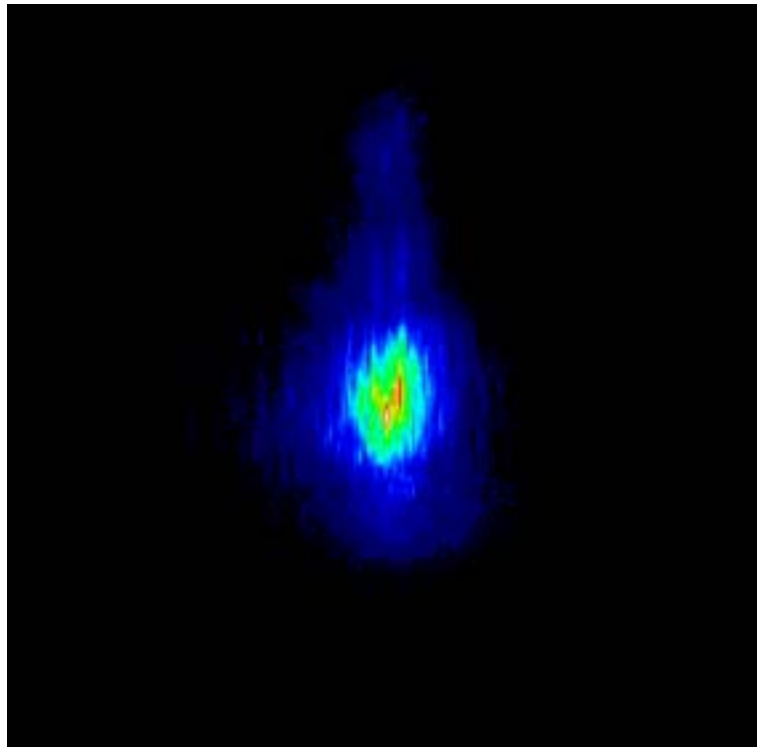
Pixel size 22.5 ◈ 22.5 μm²; 401 pixels in *y* direction

❶ ΔQ 2.9 ◈ 10^{-5} Å^{-1} ❷ 21.5 μm ❶ 54 nm resolution

Measurement results



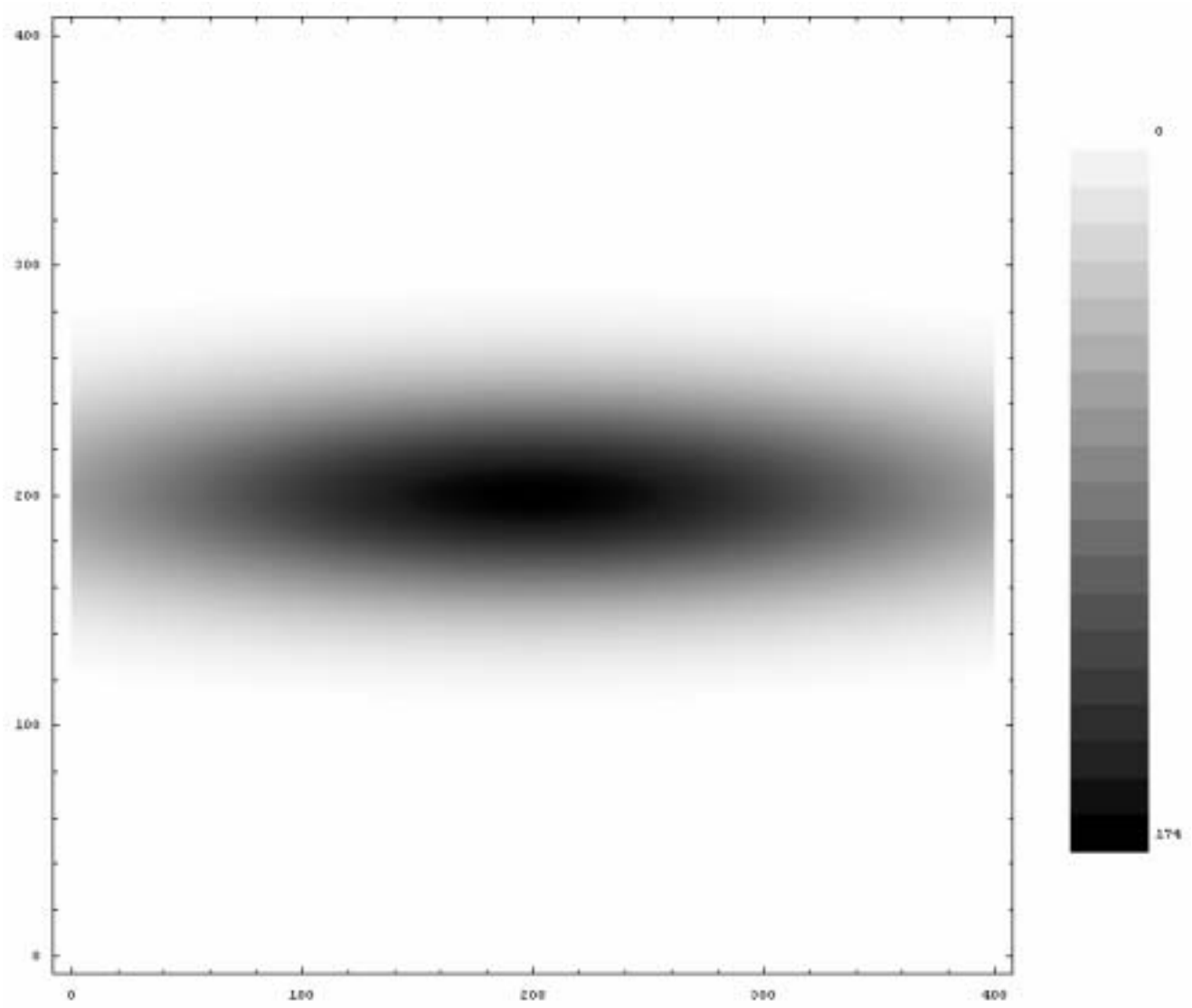
+



Mean APD size ≈ 800 nm

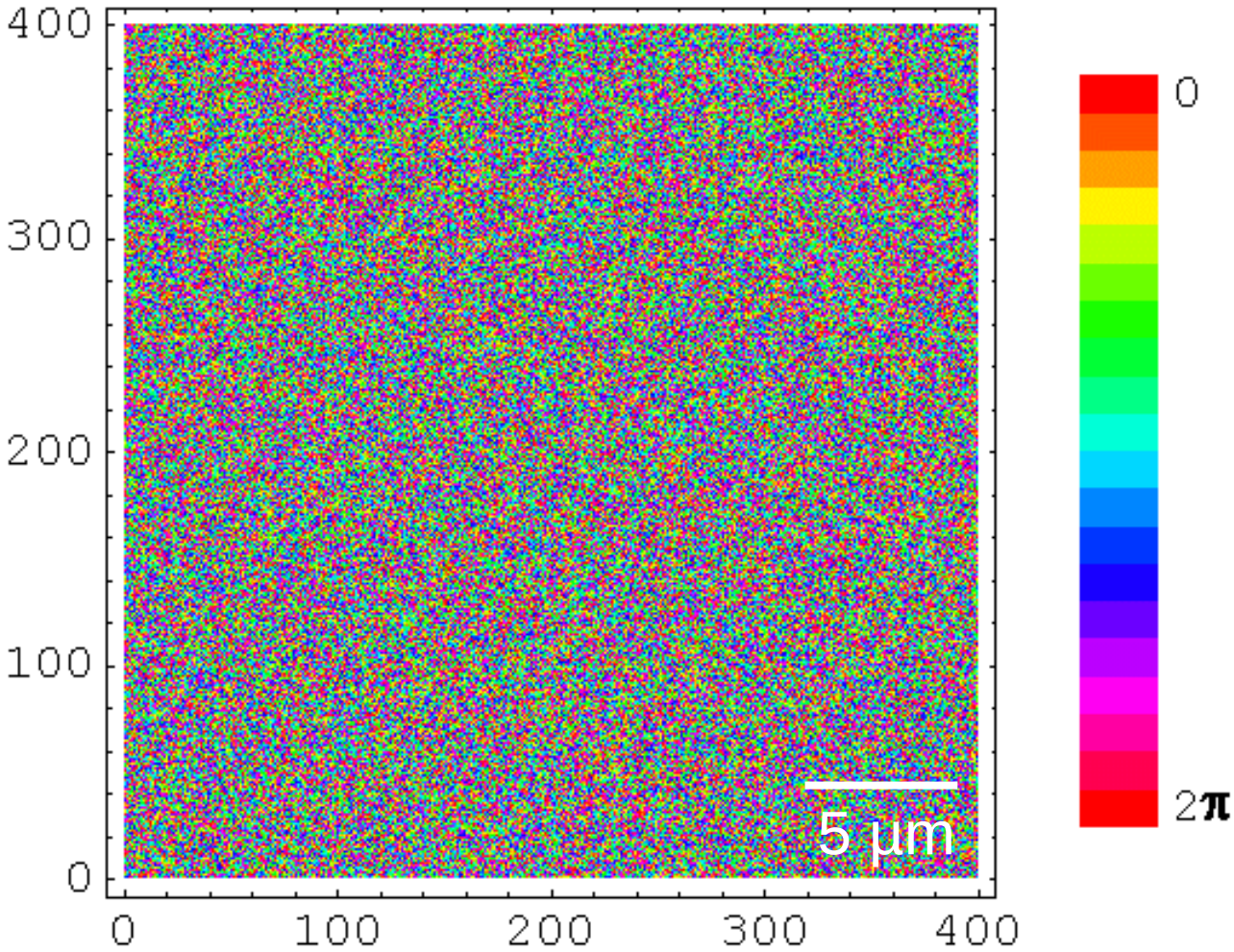
1 pixel=0.45 µm

The naive Gerchberg-Saxton (GS) approach



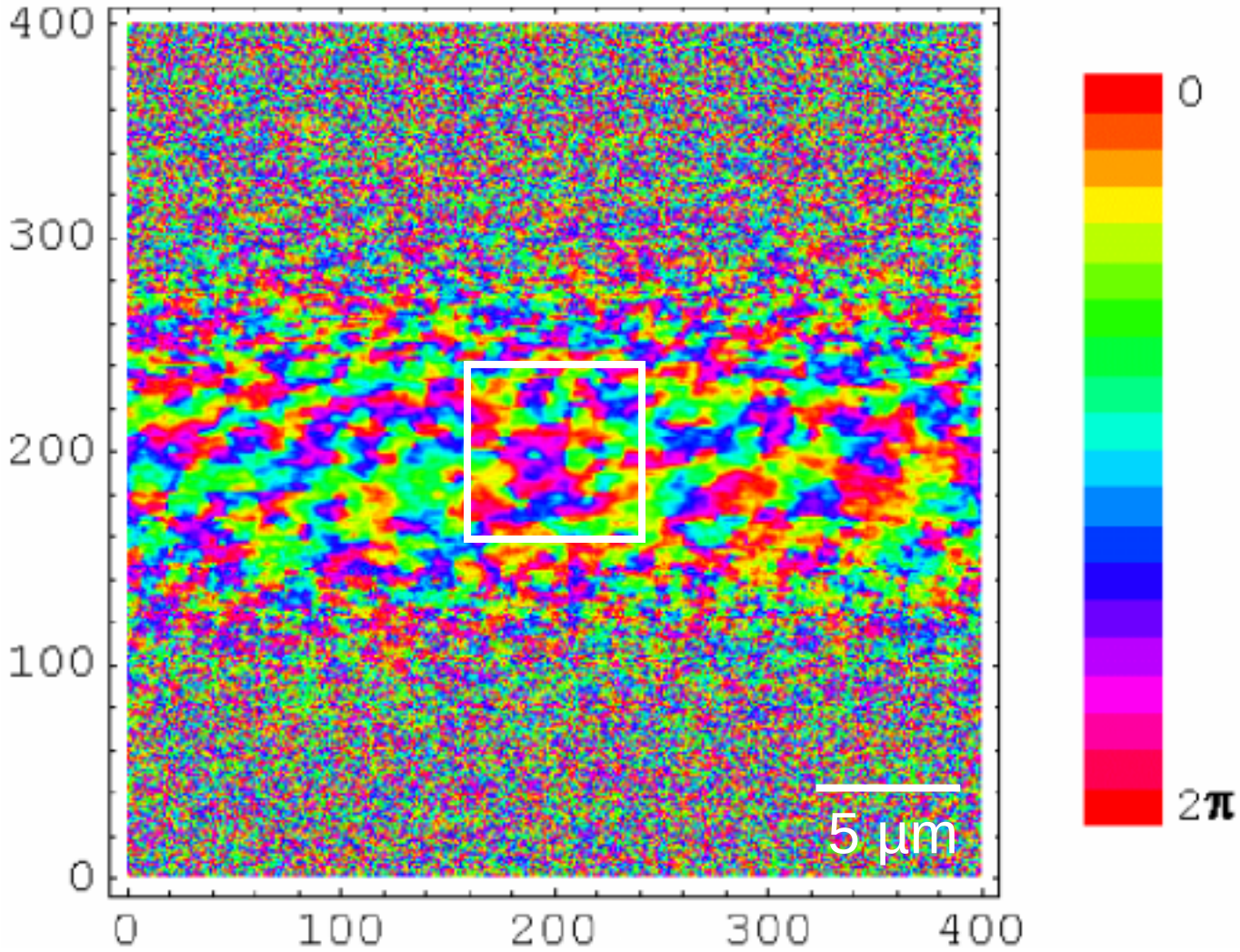
Illumination function = image in the object domain

Phases: random start configuration



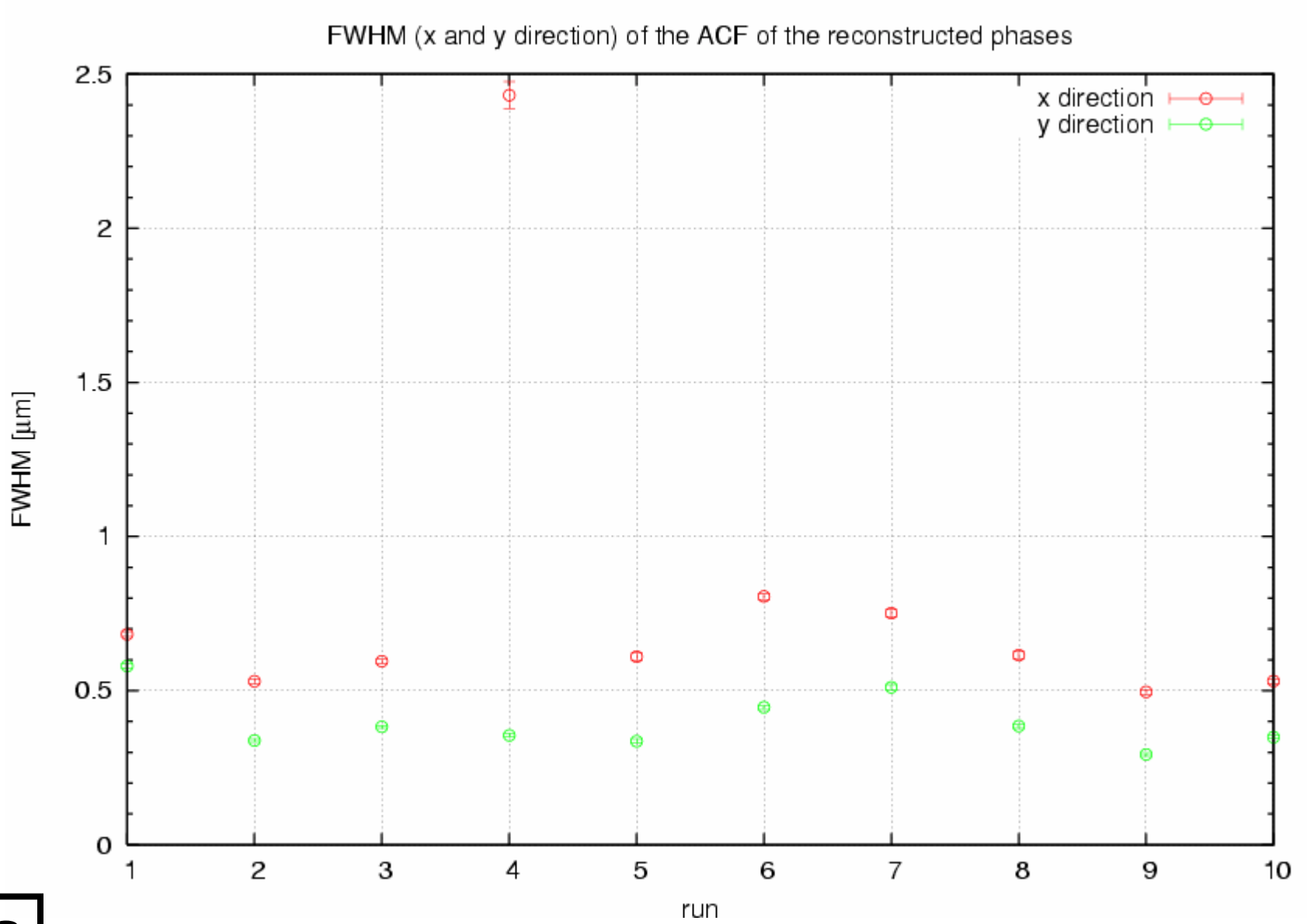
GS

Reconstructed phases (5000 iterations)



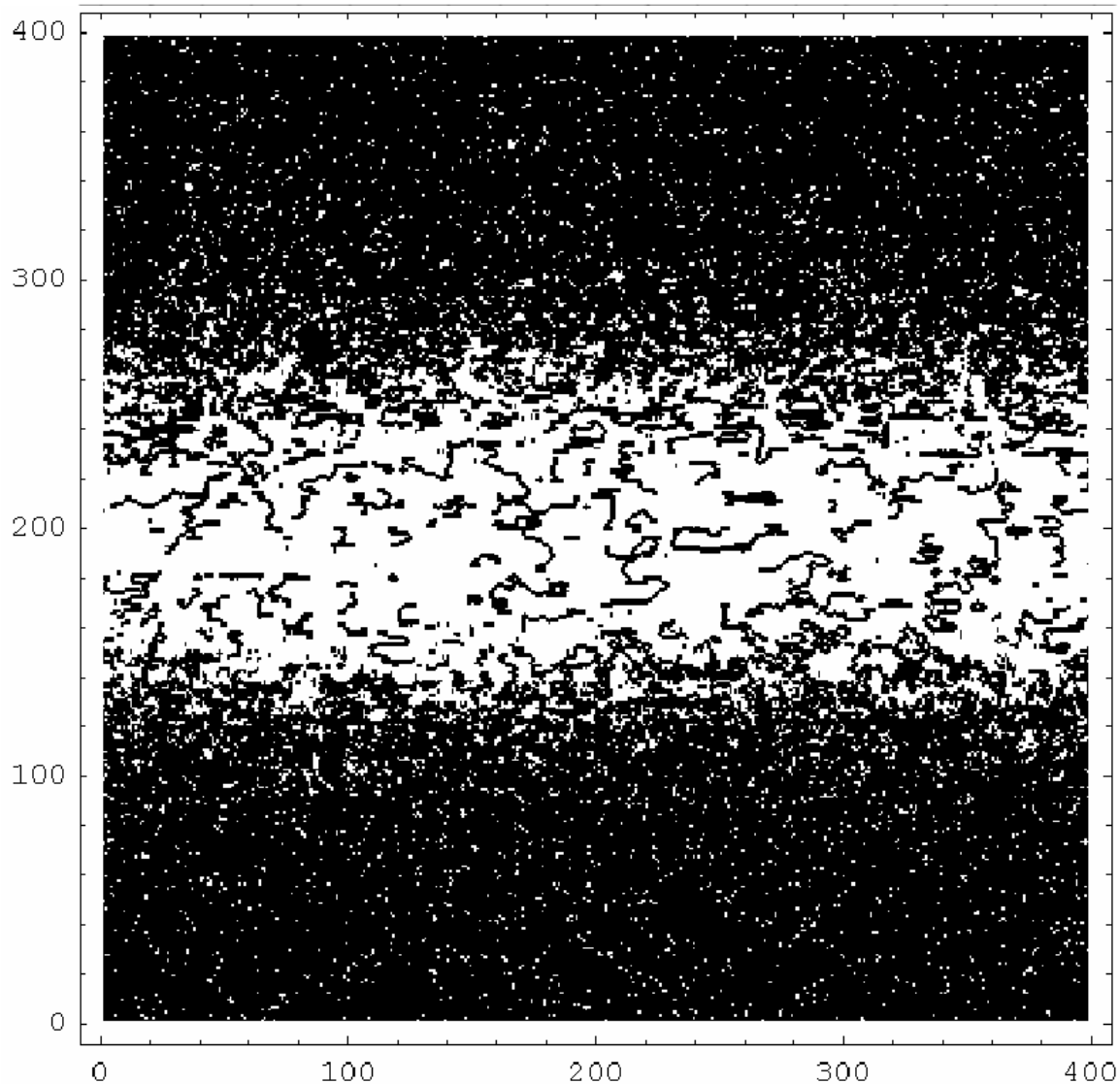
GS

Domain size: Autocorrelation function of the reconstructed phases



GS

Looking for phase jumps that indicate antiphase boundaries

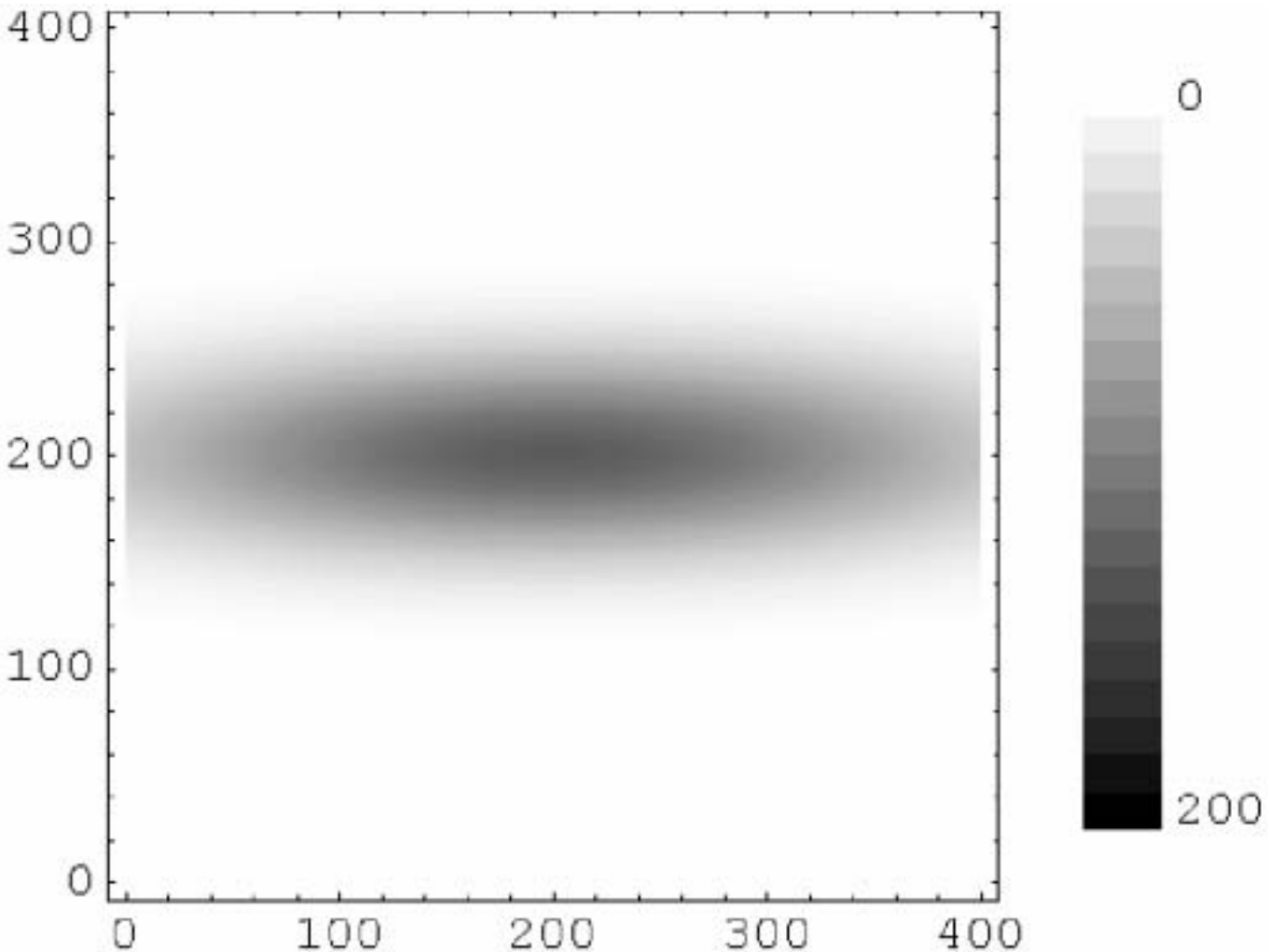


$\Delta\Phi < \pi/10$

$\Delta\Phi \geq \pi/10$

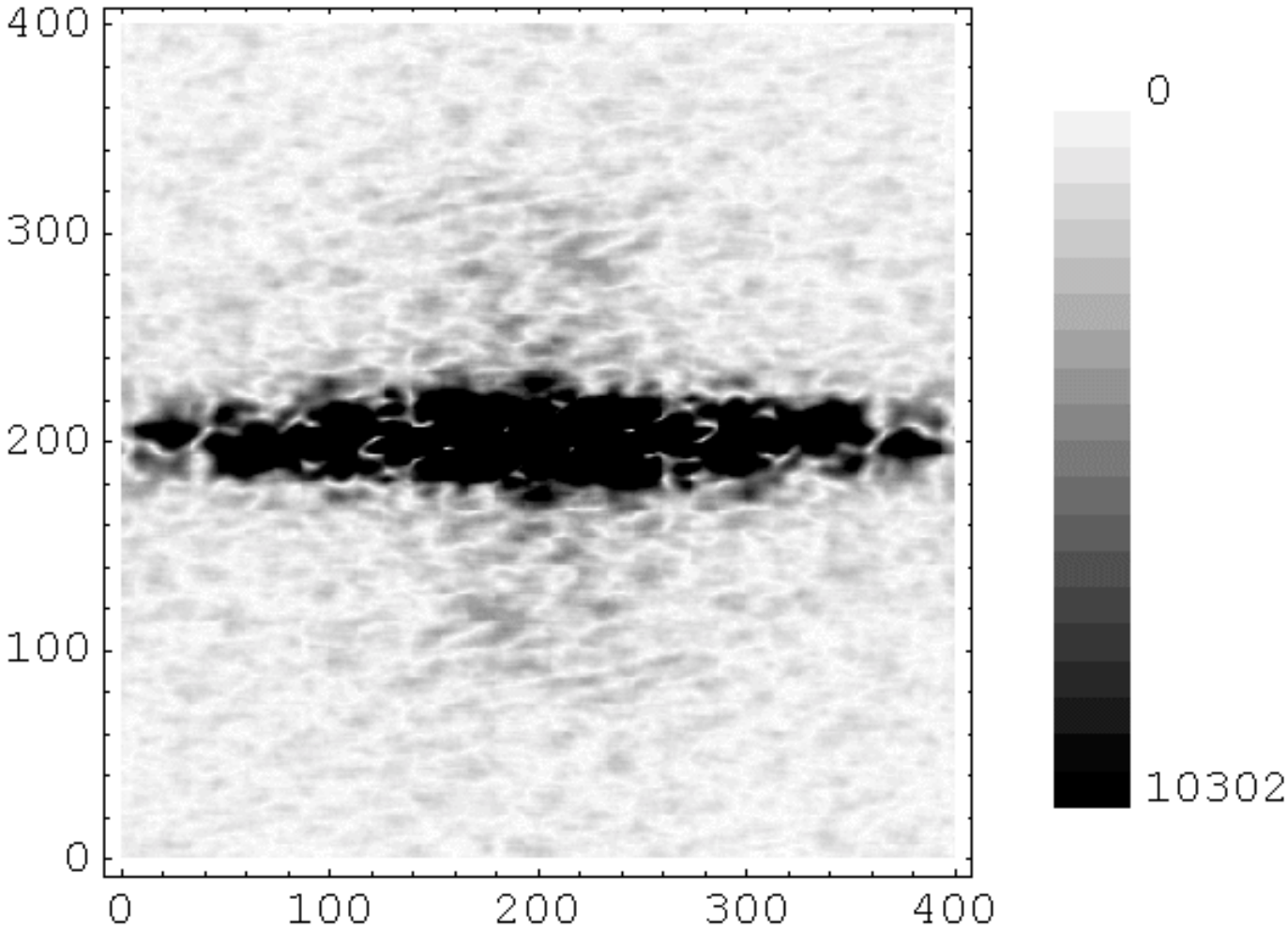
GS

Reconstructed amplitudes in real space (5000 iterations)



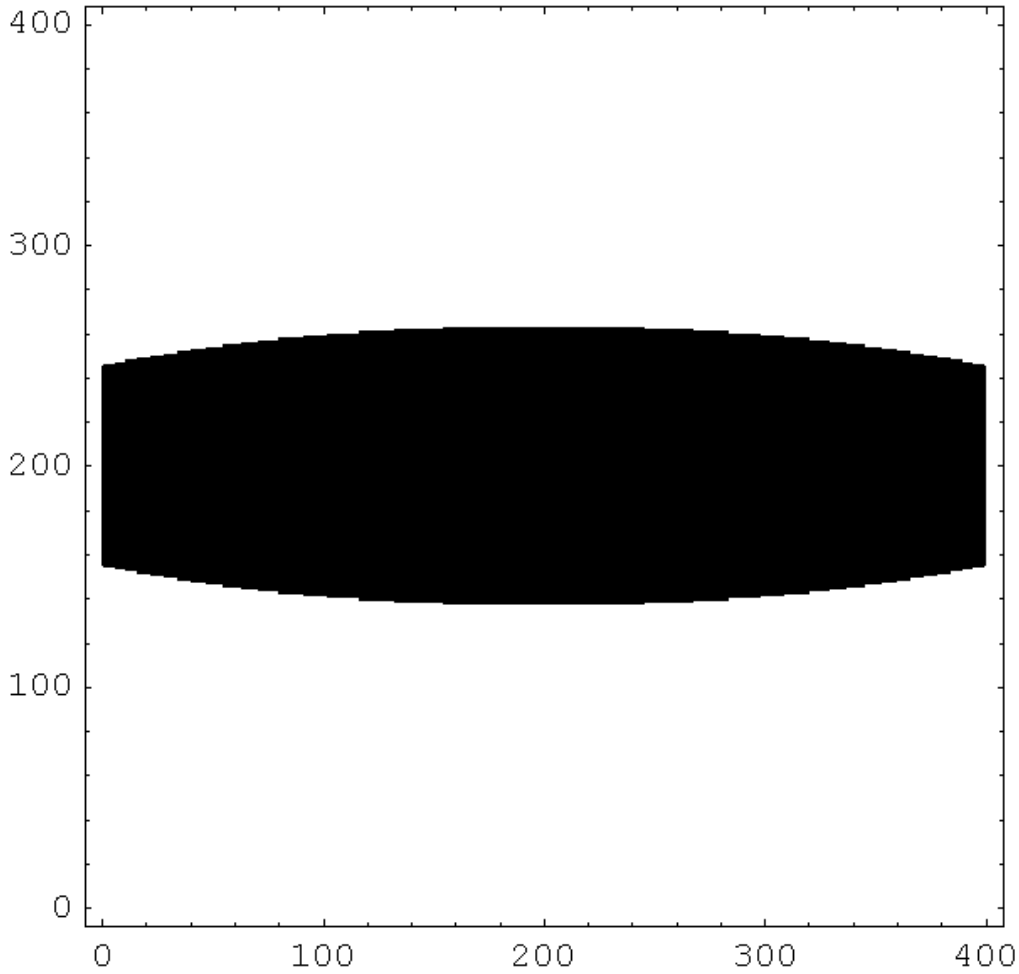
GS

Error-reduction algorithm (50 steps) + HIO (200 steps)



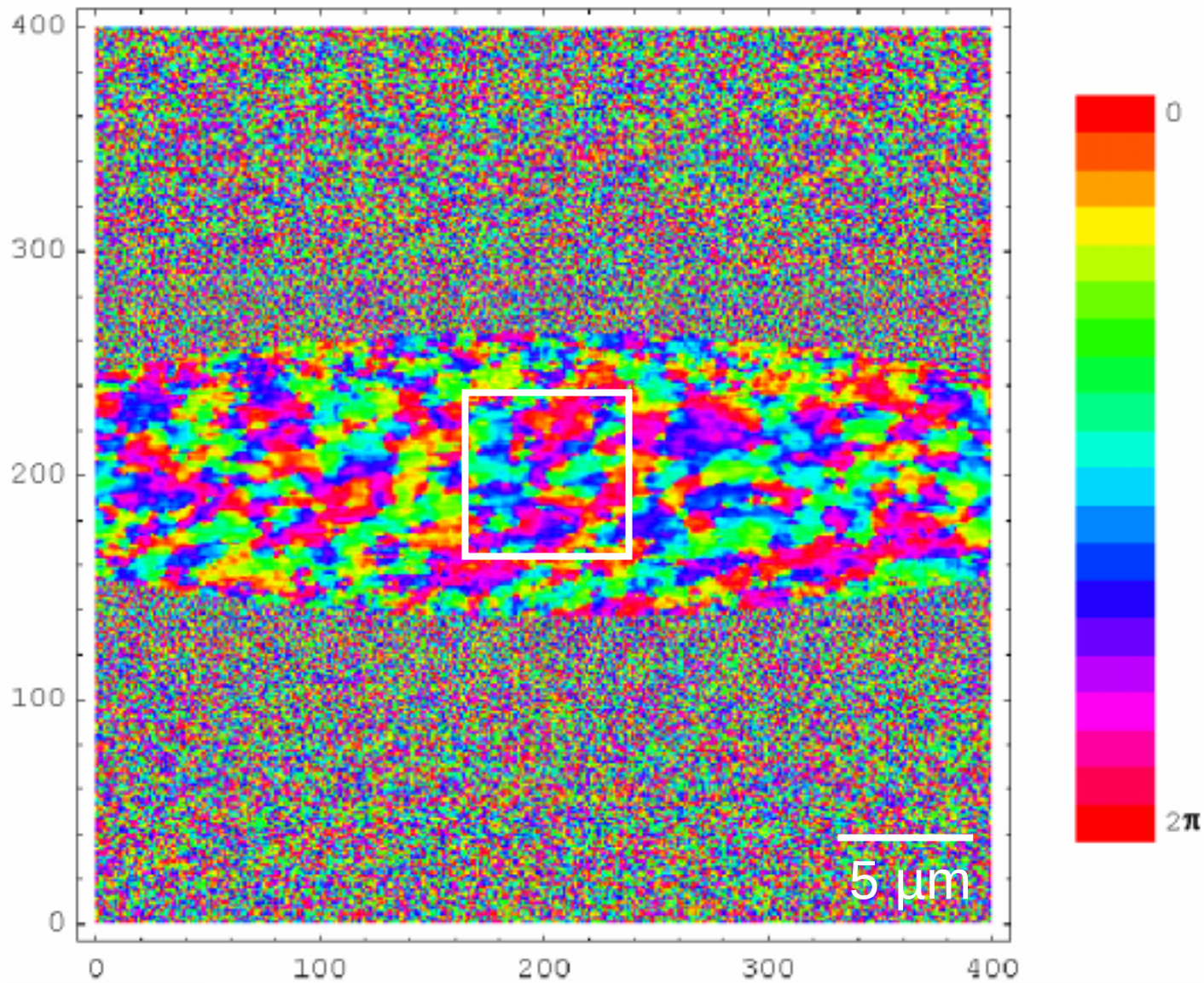
ER-HIO

Defining the support as 2-sigma region of the Gaussian illumination function



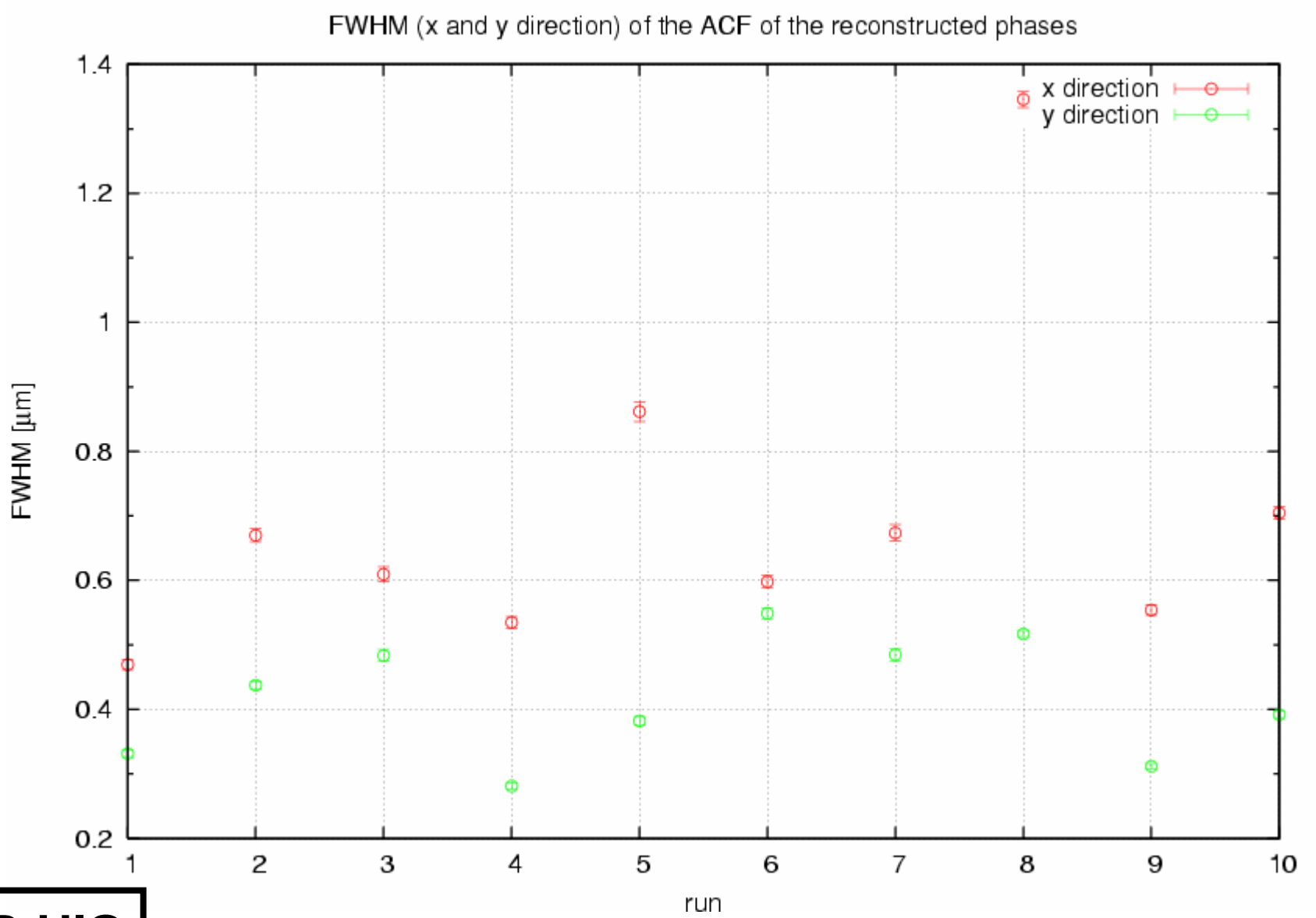
ER-HIO

Reconstructed phases (10050 iterations)



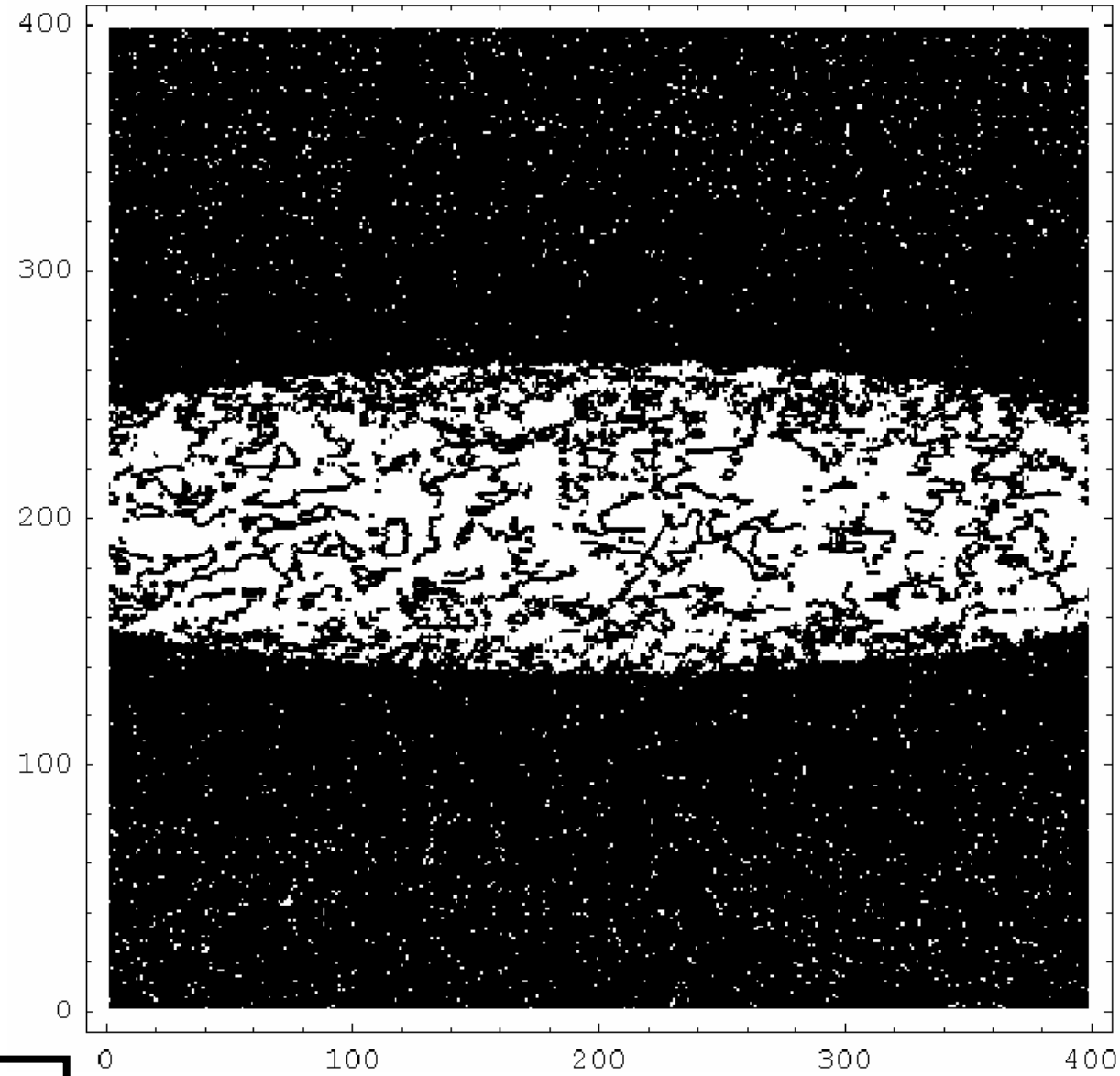
ER-HIO

Domain size: Autocorrelation function of the reconstructed phases



ER-HIO

Looking for phase jumps that indicate antiphase boundaries

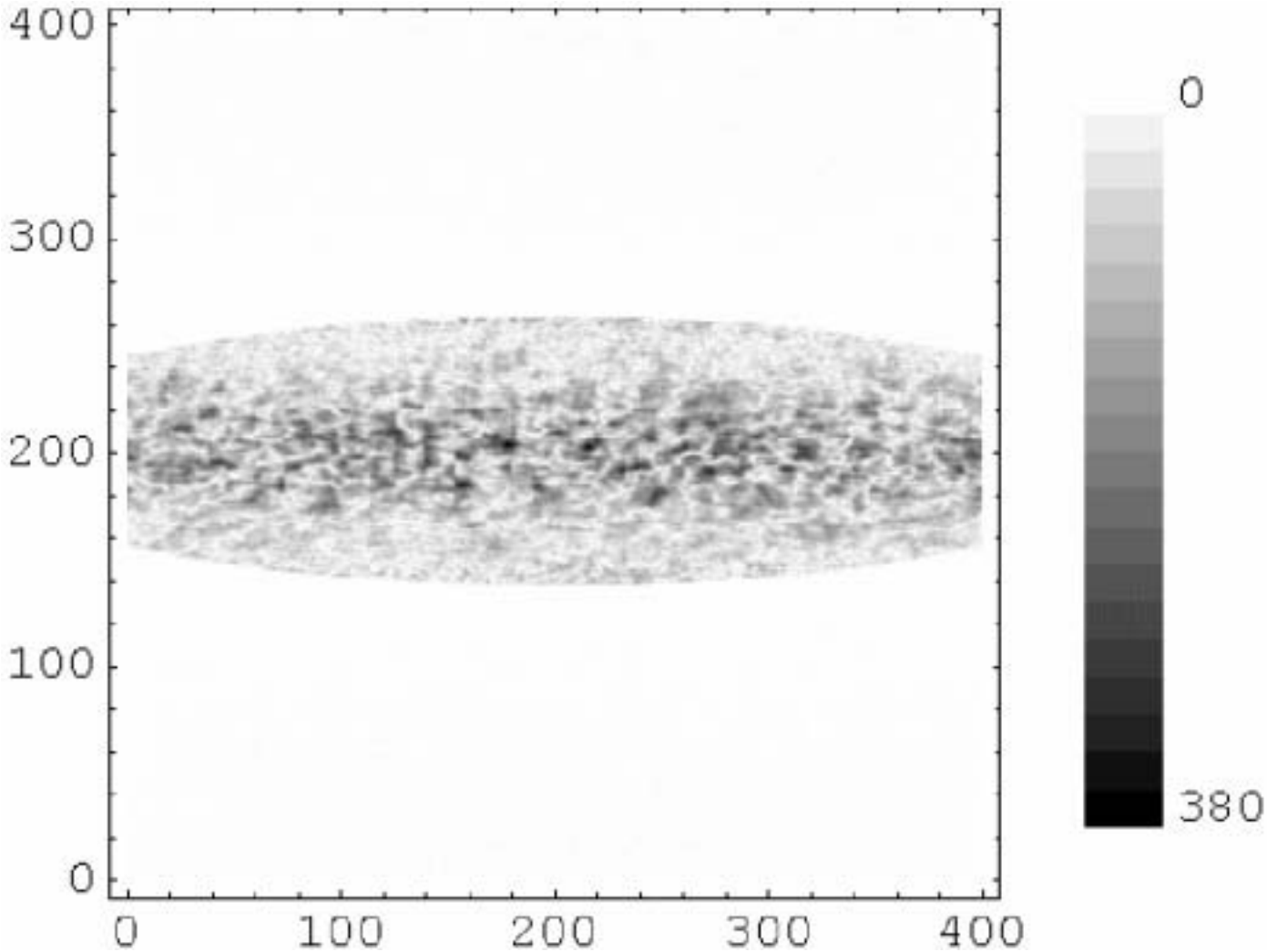


$\Delta\Phi < \pi/10$

$\Delta\Phi \geq \pi/10$

ER-HIO

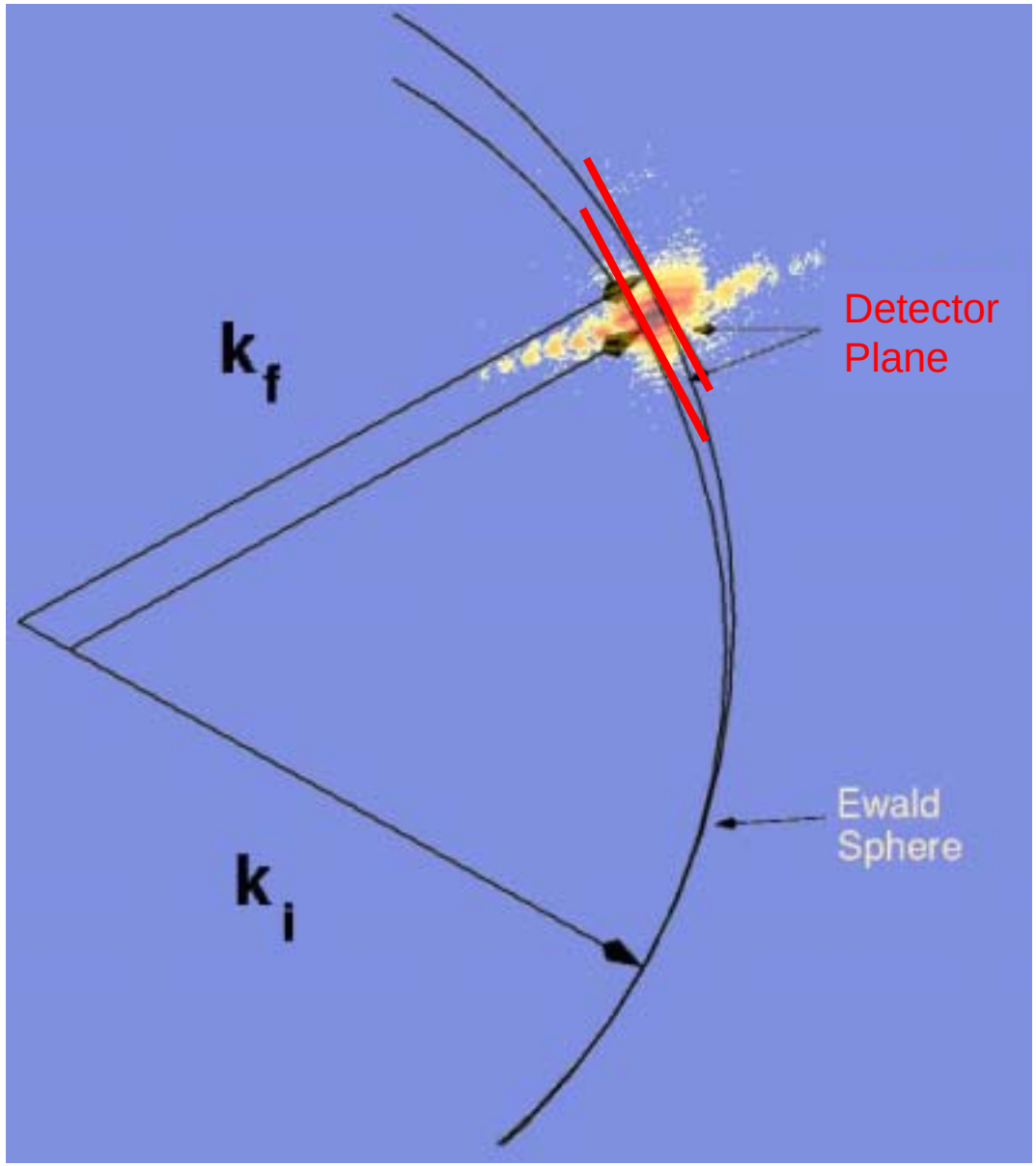
Reconstructed amplitudes in real space (10050 iterations)



ER-HIO

Since the X-ray beam penetrates the sample
=> three-dimensional reconstruction desired

For a **three-dimensional reconstruction** we need the three dimensional intensity in reciprocal space:



http://groups.mrl.uiuc.edu/Robinson/~gjwillms/research.html

Energy scan of the (001) superstructure peak of $Fe_{65}Al_{35}$ (UNICAT 34 ID, APS)

Pixel size 22.5 ◈ 22.5 μm^2; 401 pixels in *y* direction

ΔQ ◈ 2.9 ◈ 10^{-5} Å^{-1} ◈ 21.5 μm ◈ 54 nm resolution

Summary

- Detrended Fluctuation Analysis is a proper method for analysing XPCS data of slow dynamics.

- Non-compact phase objects, e.g., antiphase domains, can be reconstructed using information on the illumination function?

Acknowledgements

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Thank you for your attention!