Institute of Information Theory and Automation of the AS CR

FAKULTA JADERNÁ A FYZIKÁLNĚ INŽENÝRSKÁ ČVUT V PRAZE

ÚSTAV MAKROMOLEKULÁRNÍ CHEMIE
AKADEMIE VĚD ČESKÉ REPUBLIKY

Problematika práškové difrakce v SEM

David Rendl

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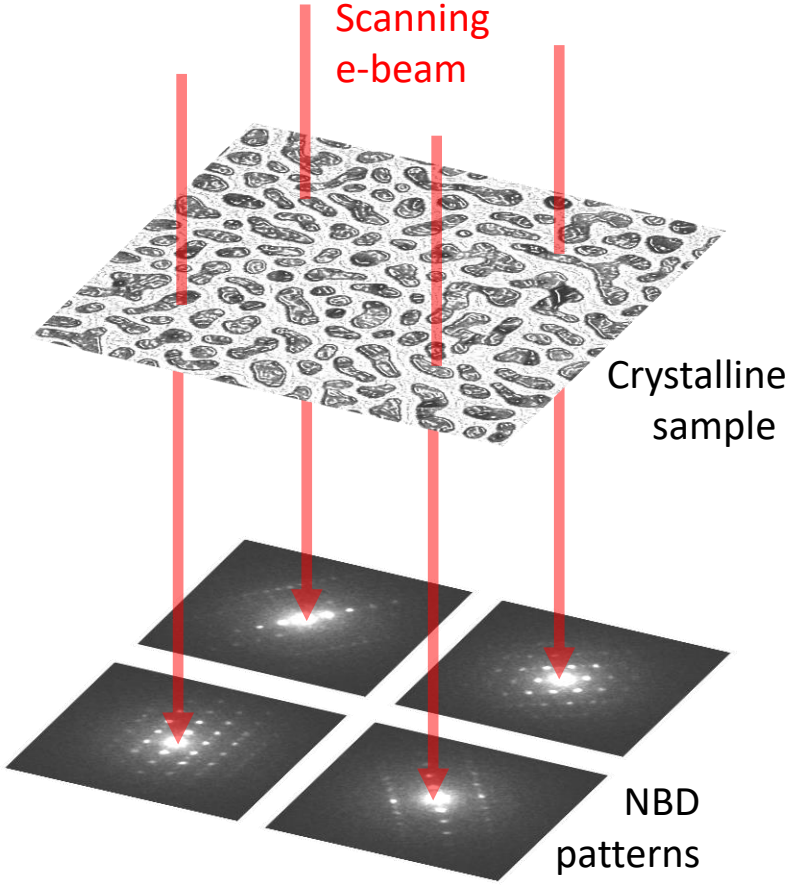
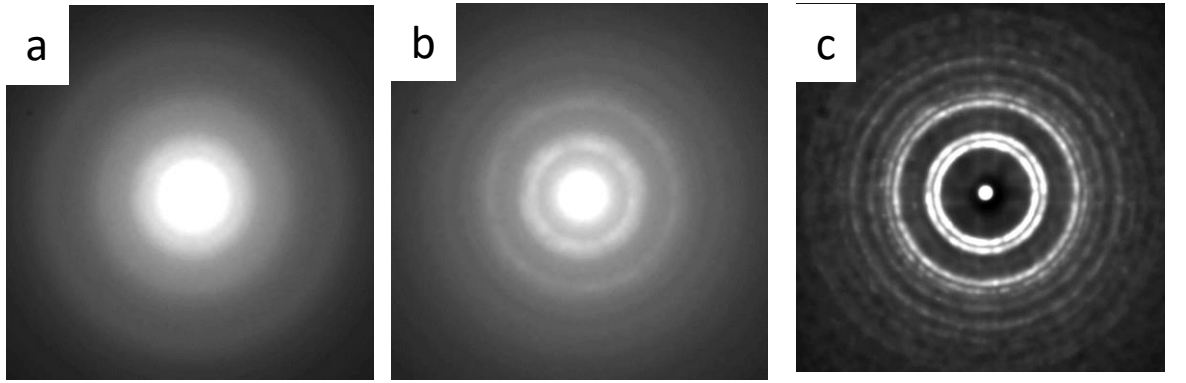
Princip metody





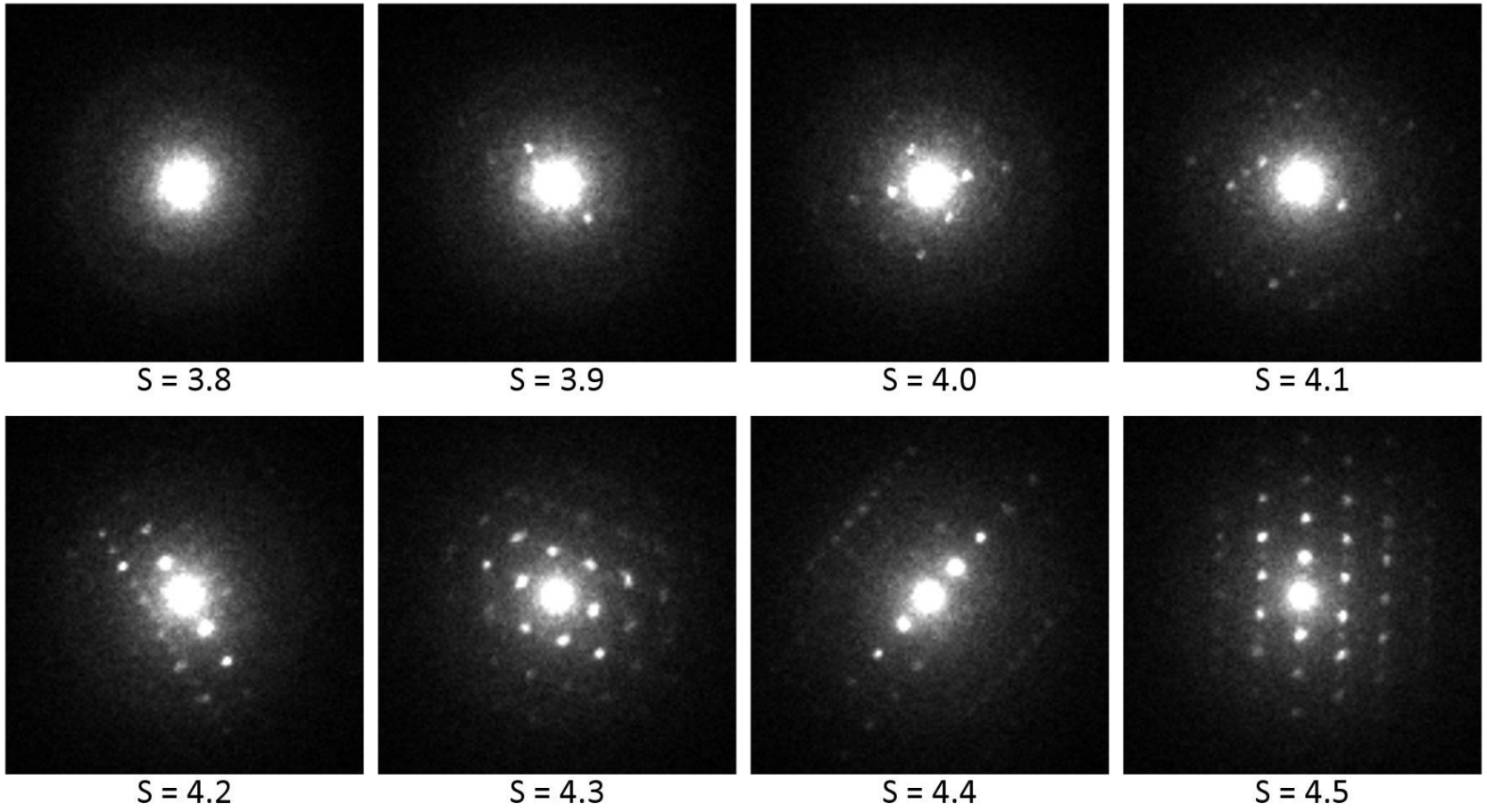
Final powder diffractogram.

(a) Sum all files.

(b) Sum only high-entropy files.

(c) Sum high-entropy files with the PSF deconvolution.

Filtrování difraktogramů



Dekonvoluce - Richardson-Lucy

$$p(I|O) = \prod_x \frac{[(P * O)(x)]^{I(x)} \cdot e^{-(P*O)(x)}}{I(x)!} \quad \Rightarrow \quad L(O) = \int_x (P * O)(x) - I(x) \ln[(P * O)(x)] dx$$

$$P(-x) * \frac{I(x)}{(P * O)(x)} = 1. \quad \Rightarrow \quad O_{k+1} = O_k \left[P^T * \frac{I}{(P * O)} \right]$$

Richardson-Lucy s regularizací

$$L(O) = \int_x (P * O)(x) - I(x) \ln[(P * O)(x)]dx + \lambda_{TM} \int_x |\nabla O(x)|^2 dx \quad \Rightarrow \quad O_{k+1} = \left[P^T * \frac{I}{(P * O)}\right] \cdot \frac{O_k}{1 + 2\lambda_{TM} \triangle O_k}$$

$$L(O) = \int_x (P * O)(x) - I(x) \ln[(P * O)(x)]dx + \lambda_{TV} \int_x |\nabla O(x)|dx \quad \Rightarrow \quad O_{k+1} = \left[P^T * \frac{I}{P * O}\right] \frac{O_k}{1 - \lambda_{TV} div\left(\frac{\nabla O_k}{|\nabla O_k|}\right)}$$

Snímek rozmazaný Gaussovskou PSF s přidaným šumem

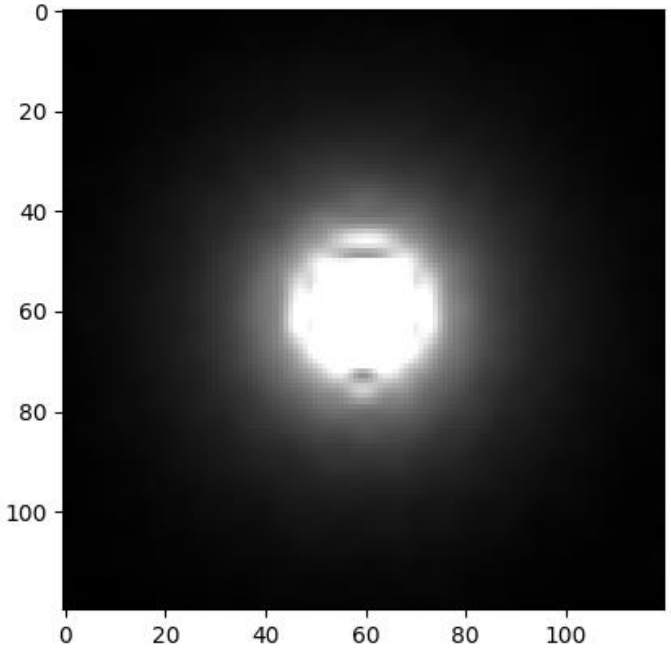
Dekonvoluce RL algoritmem bez regularizace

Dekonvoluce RL algoritmem s TM regularizací

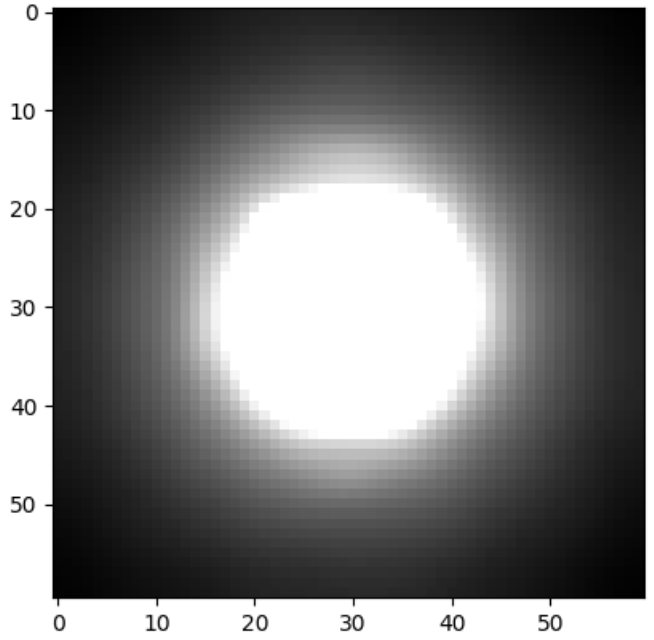
Dekonvoluce RL algoritmem s TV regularizací

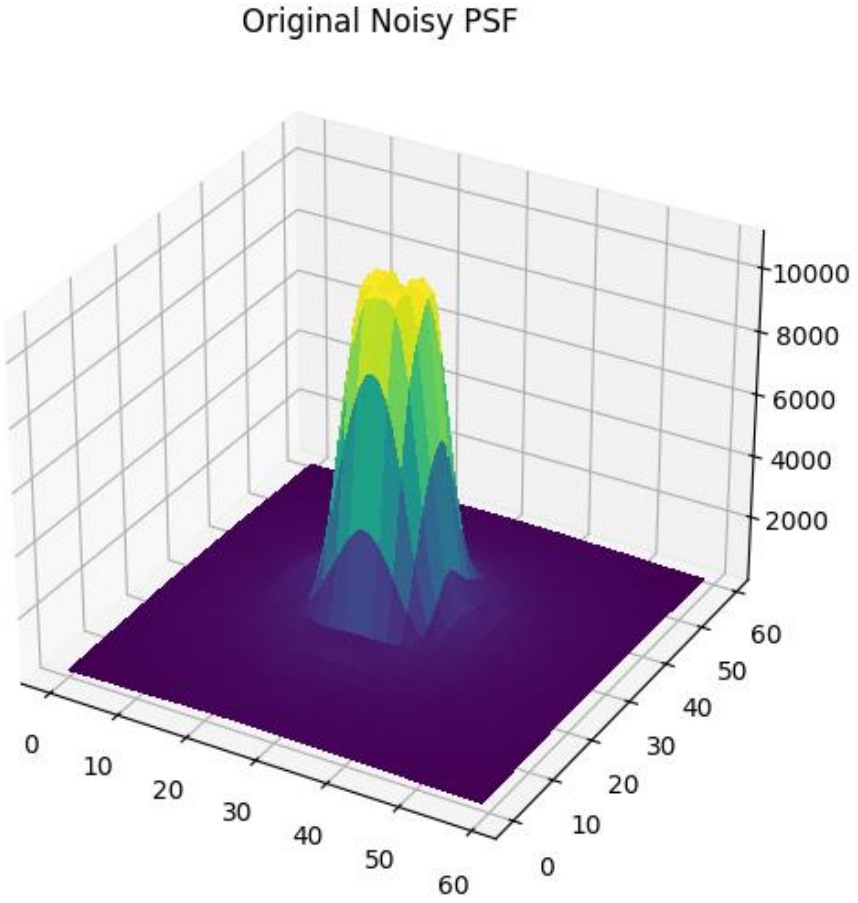
Odhady PSF

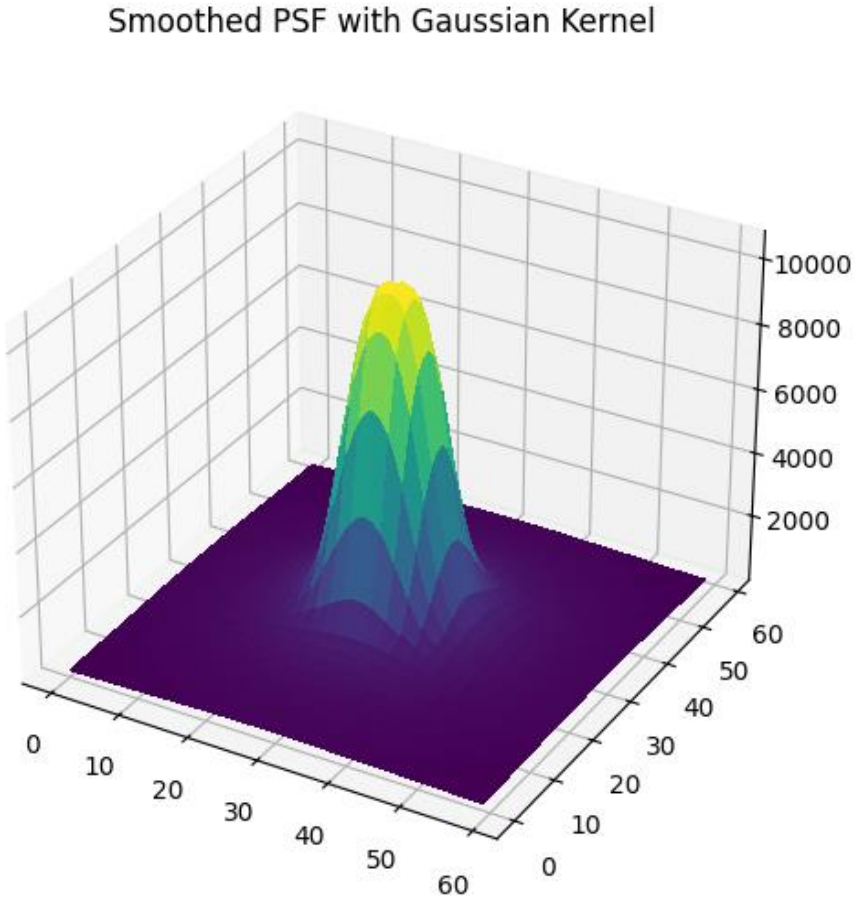
Odhad PSF z centrálního maxima difraktogramu

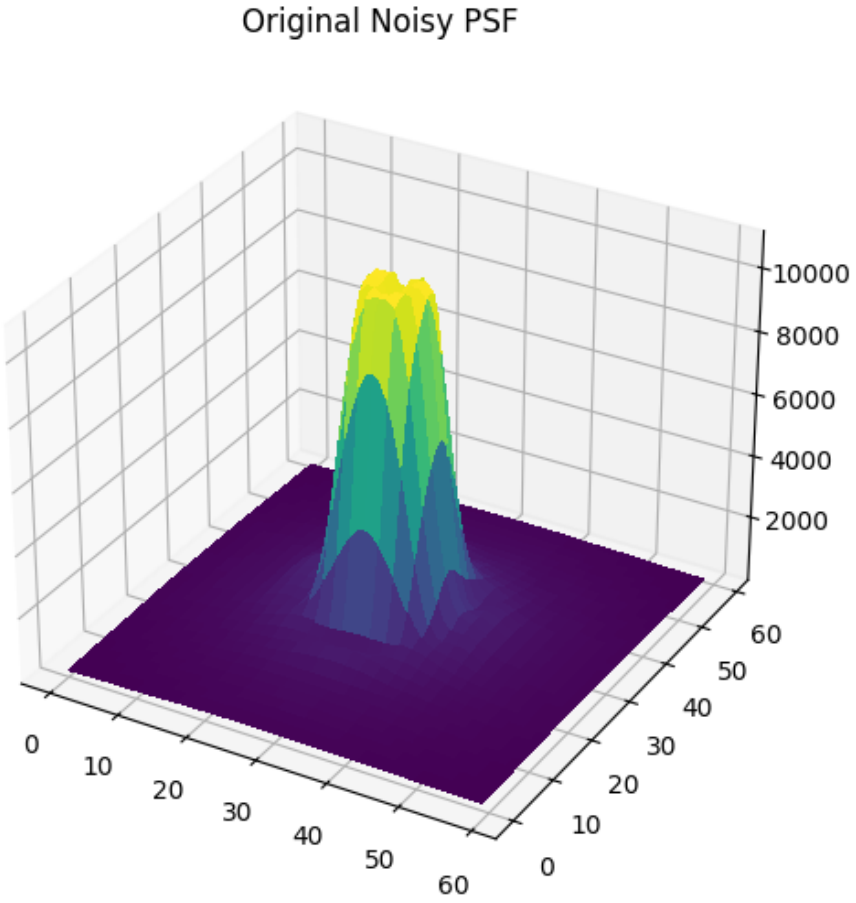


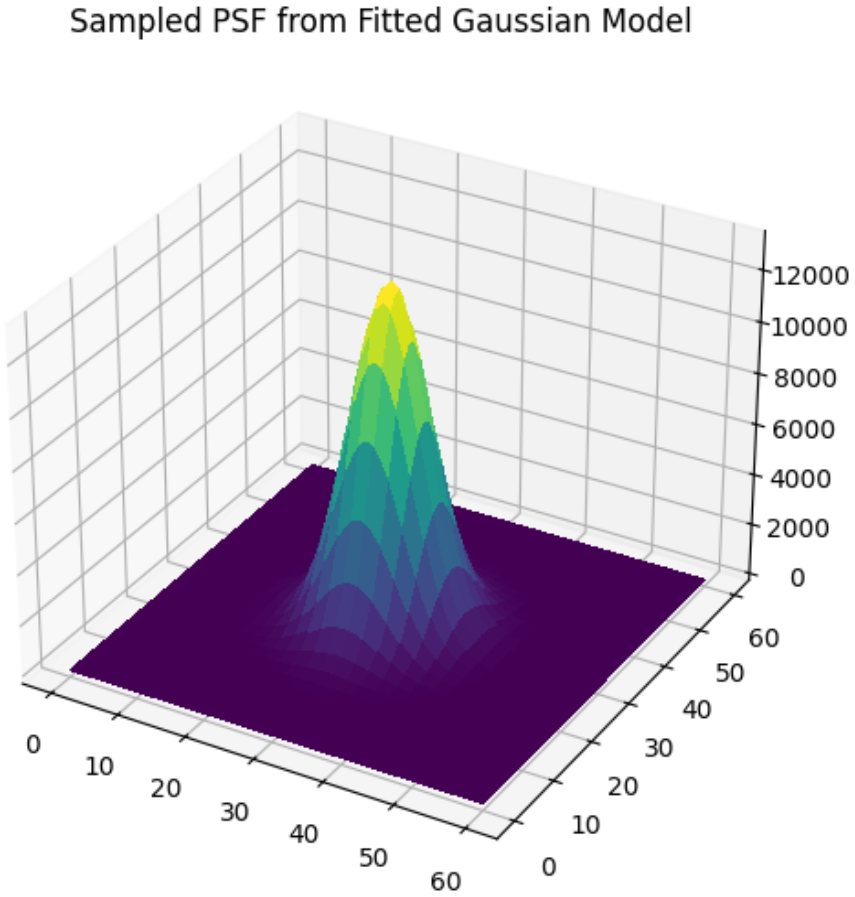
Jádrový odhad PSF z centrálního maxima difraktogramu



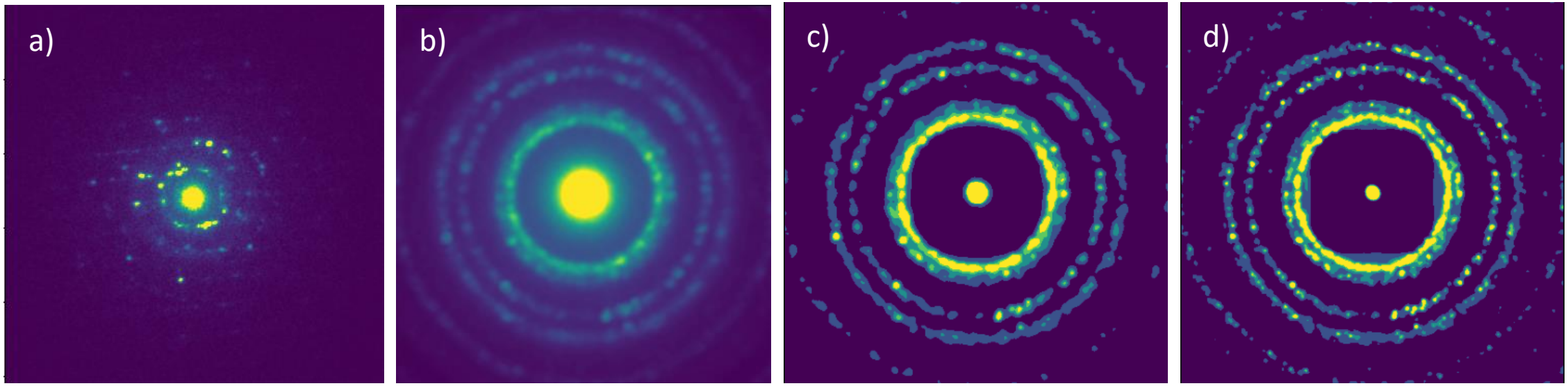

Original Noisy PSF
10000
8000
6000
4000
2000
0
10
20
30
40
50
60


Smoothed PSF with Gaussian Kernel
10000
8000
6000
4000
2000
0
10
20
30
40
50
60

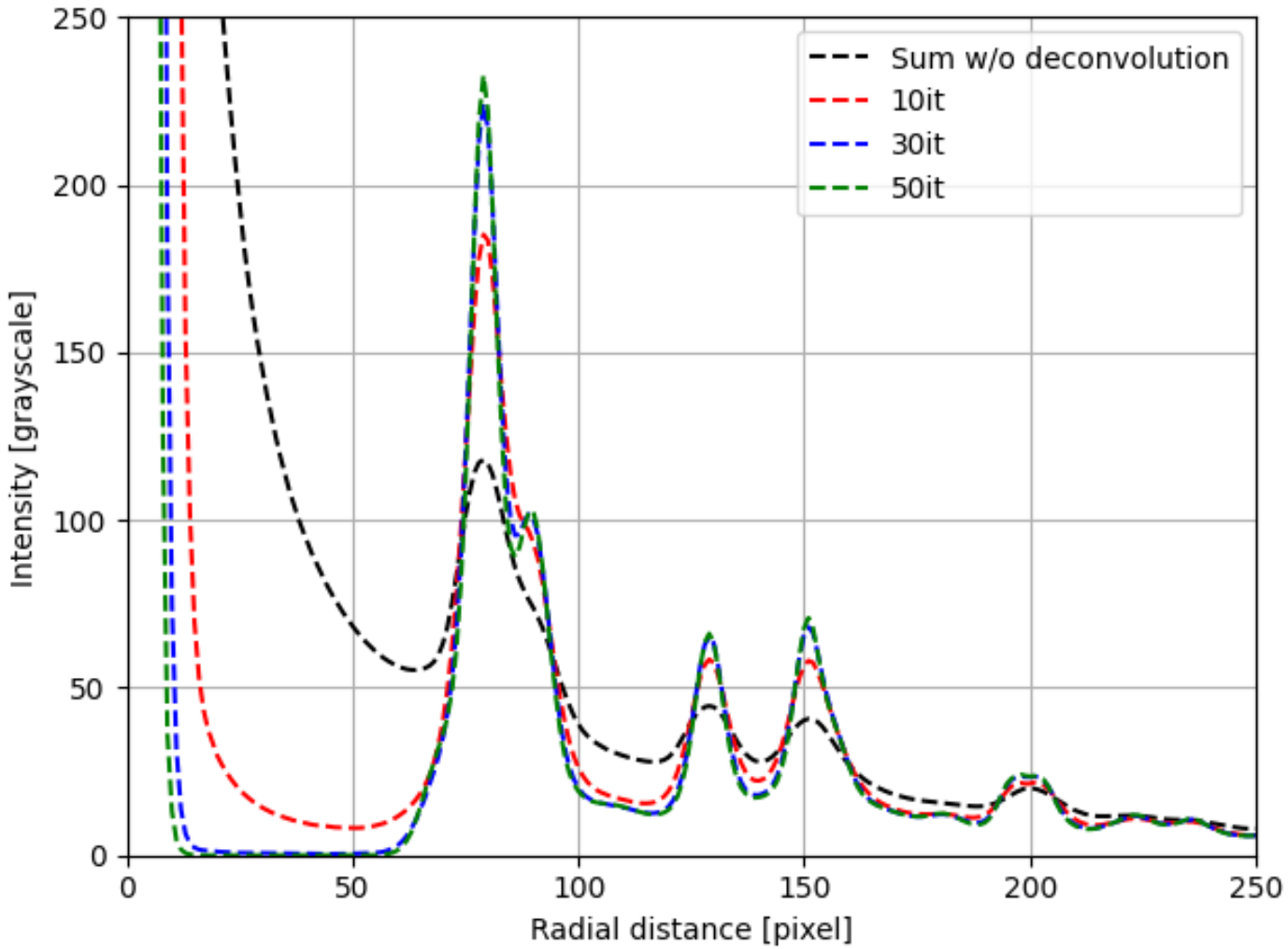

Original Noisy PSF
10000
8000
6000
4000
2000
0
10
20
30
40
50
60

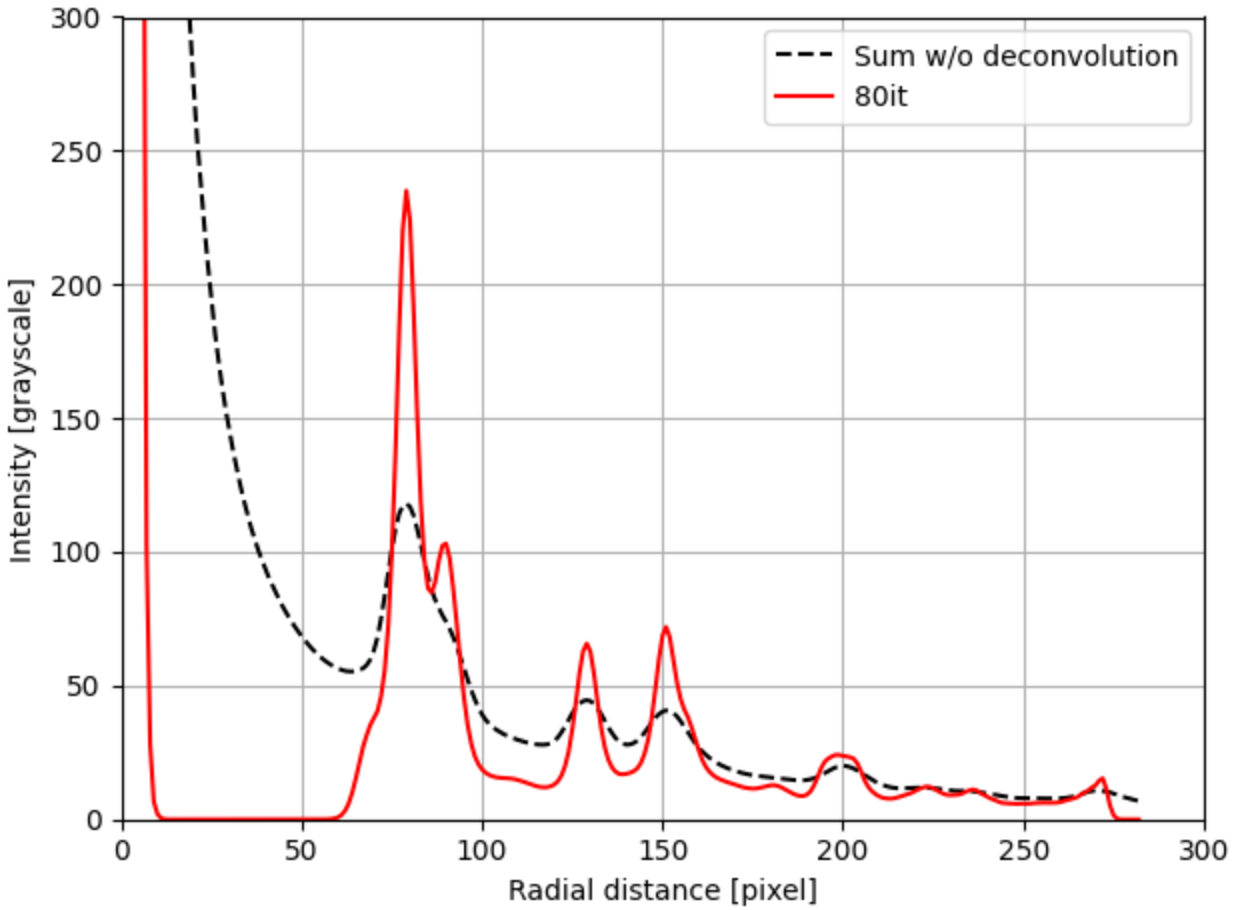

Sampled PSF from Fitted Gaussian Model
12000
10000
8000
6000
4000
2000
0
10
20
30
40
50
60

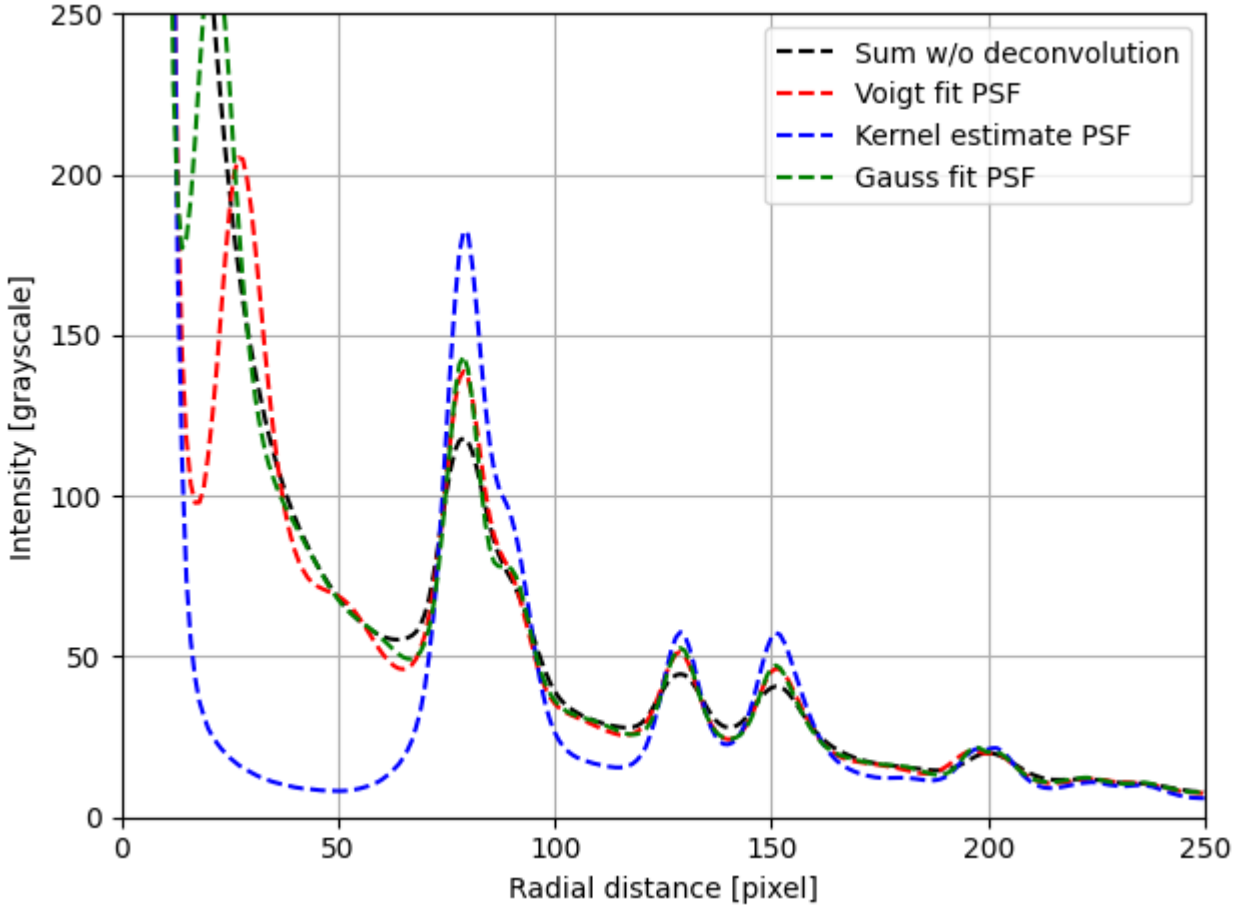
Dekonvoluce difraktogramů



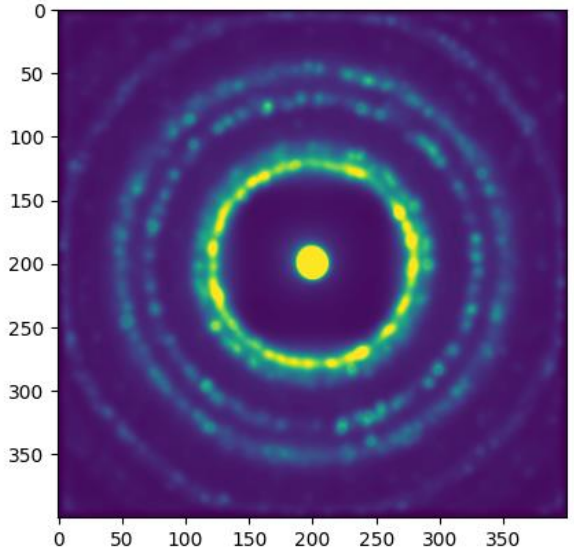
1 vzorek z datasetu | Součet bez dekonvoluce | 10 iterací RL algoritmu | 50 iterací RL algoritmu


Sum w/o deconvolution
10it
30it
50it
Intensity [grayscale]
Radial distance [pixel]
0
50
100
150
200
250

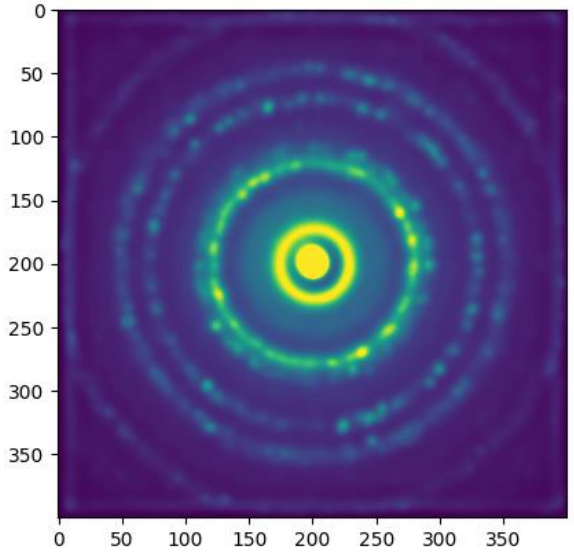

Sum w/o deconvolution
80it
Intensity [grayscale]
Radial distance [pixel]
0
50
100
150
200
250
300



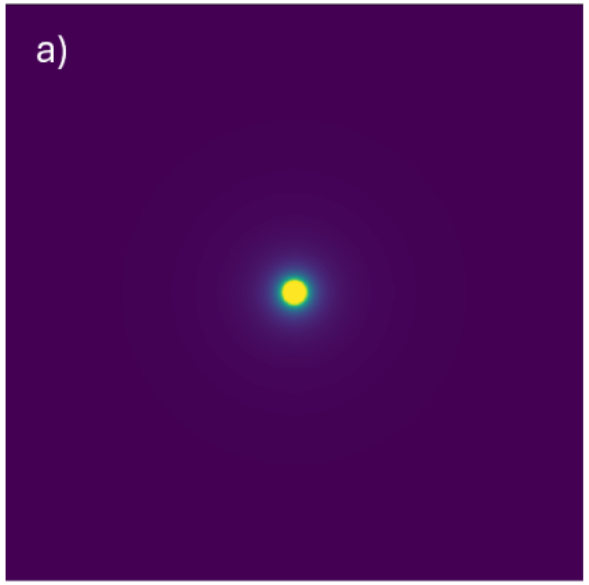
Jádrový odhad PSF



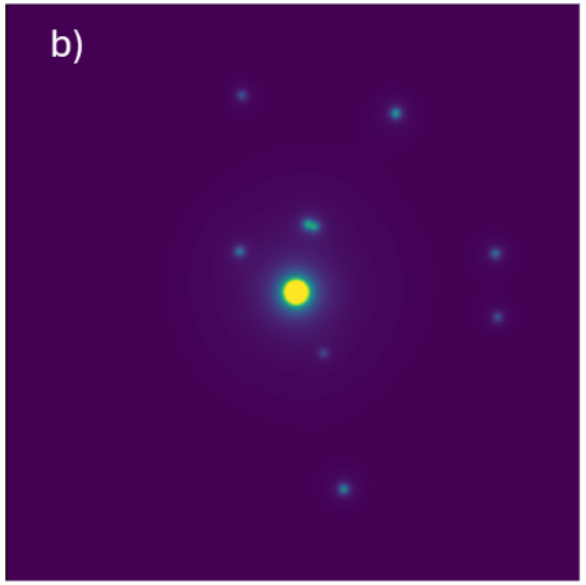
Fit Voigtovy distribuce



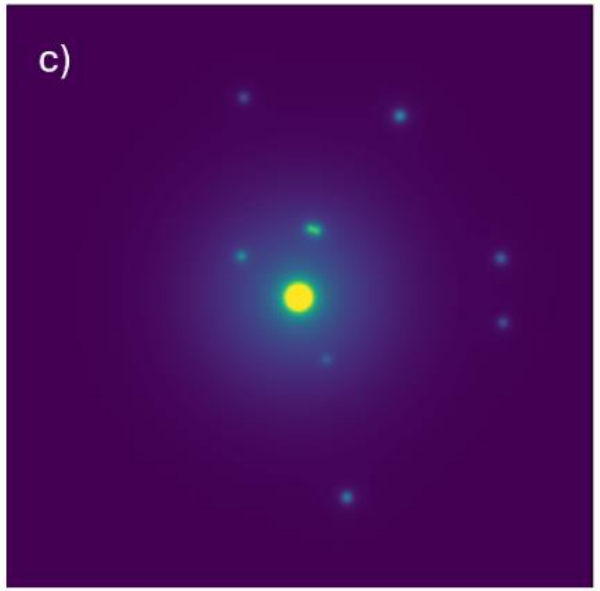
Simulace syntetických dat



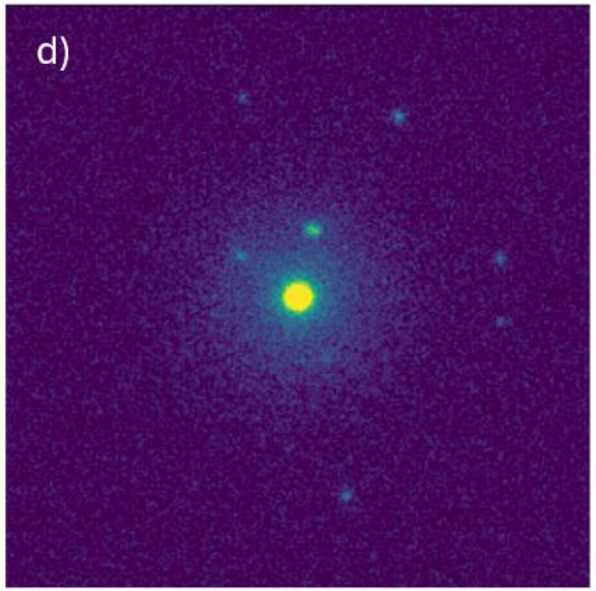
Centrální maximum



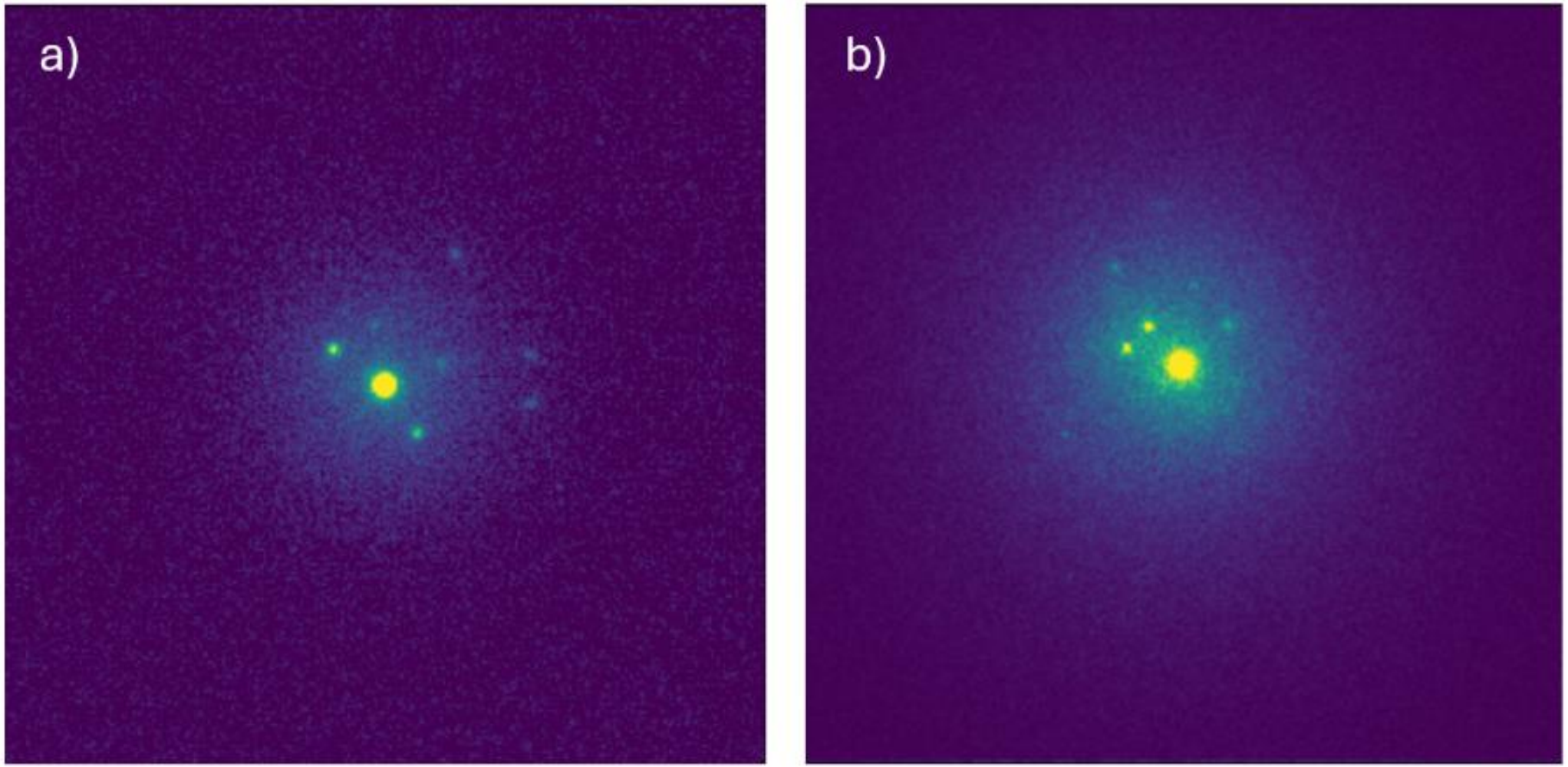
Difrakční maxima



Neuniformní pozadí



Přičtení šumu


a)
b)

Výhled do budoucna