



Institute of Information Theory
and Automation of the AS CR



FAKULTA
JADERNÁ
A FYZIKÁLNĚ
INŽENÝRSKÁ
ČVUT V PRAZE



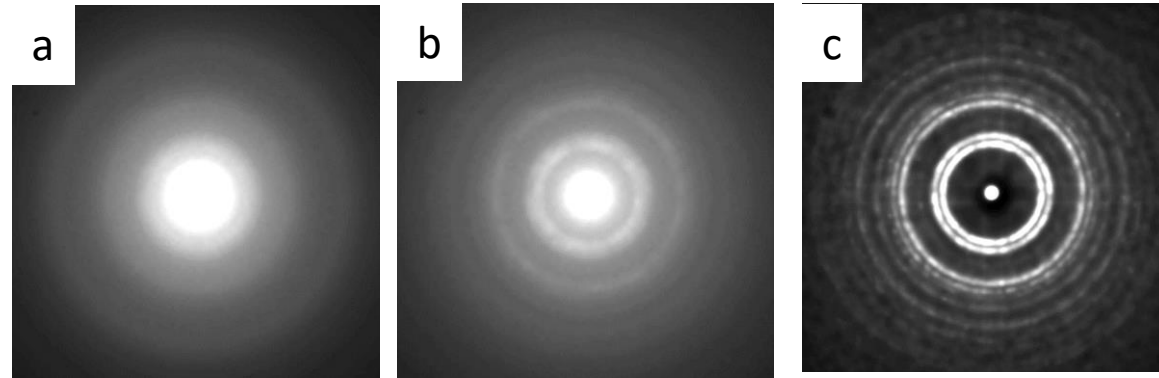
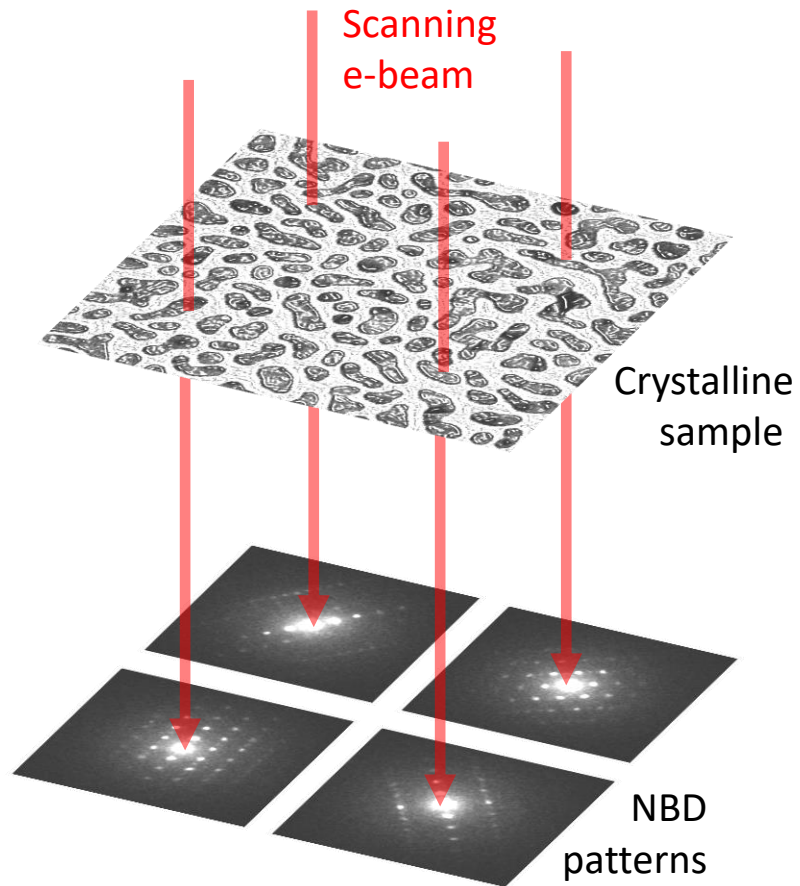
ÚSTAV
MAKROMOLEKULÁRNÍ
CHEMIE
AKADEMIE VĚD ČESKÉ REPUBLIKY

Problematika práškové difrakce v SEM

David Rendl

Doc. Ing. Filip Šroubek, Ph.D. DSc., doc. RNDr. Miroslav Šlouf, Ph.D.

Princip metody



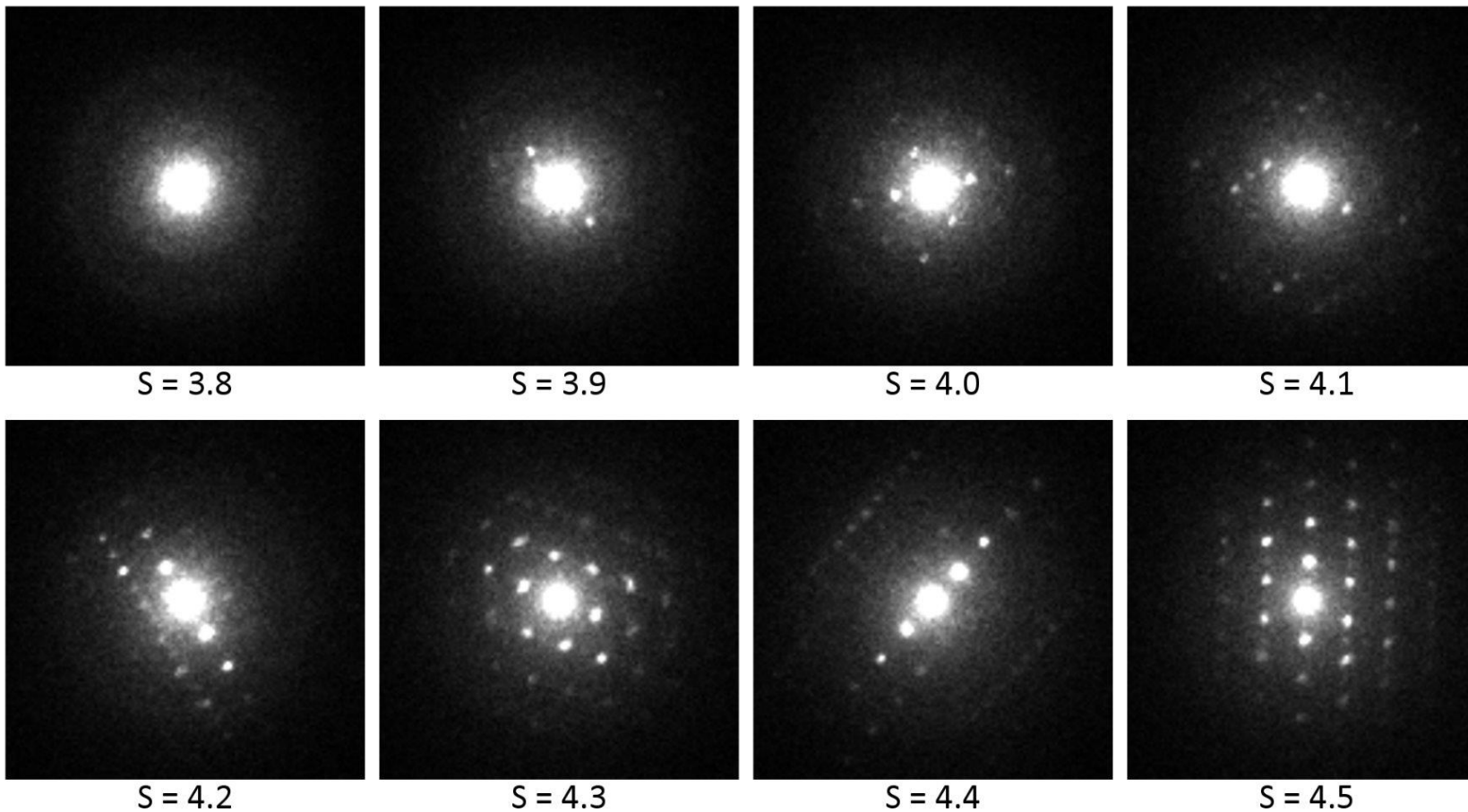
Final powder diffractogram.

(a) Sum all files.

(b) Sum only high-entropy files.

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

Filtrování difraktogramů



Dekonvoluce - Richardson-Lucy

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

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

Richardson-Lucy s regularizací

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

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



Snímek rozmazaný Gaussovskou PSF s přidaným šumem



Dekonvoluce RL algoritmem bez regularizace



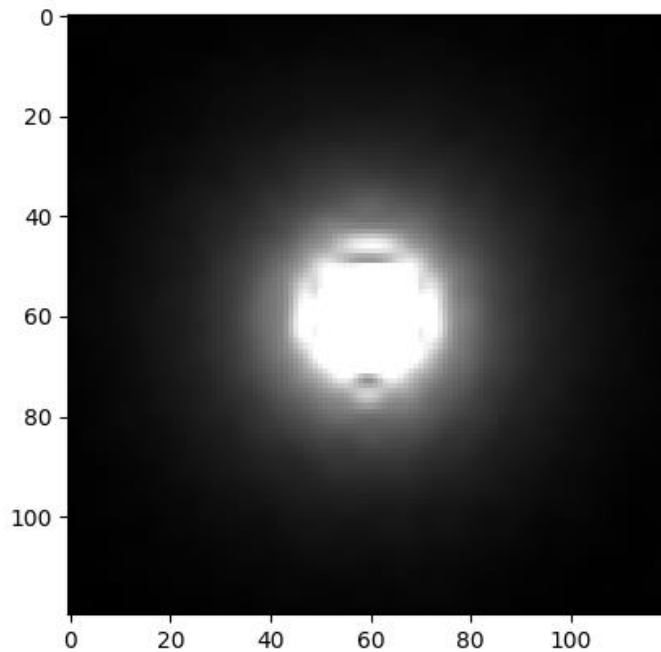
Dekonvoluce RL algoritmem s TM regularizací



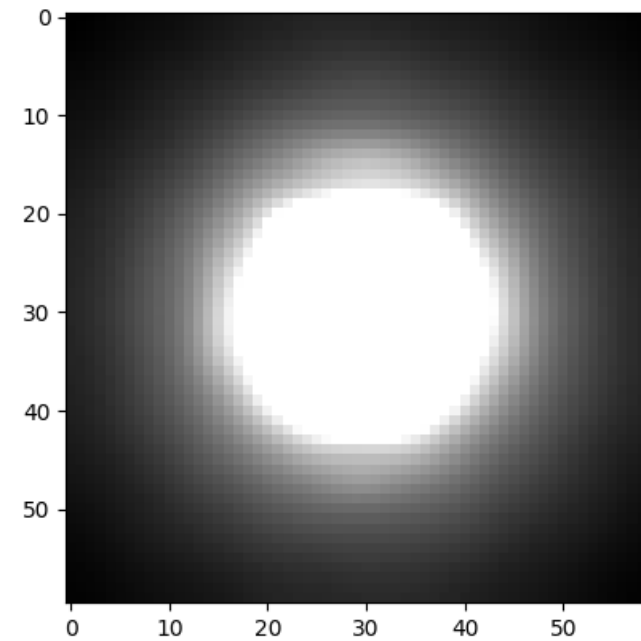
Dekonvoluce RL algoritmem s TV regularizací

Odhady PSF

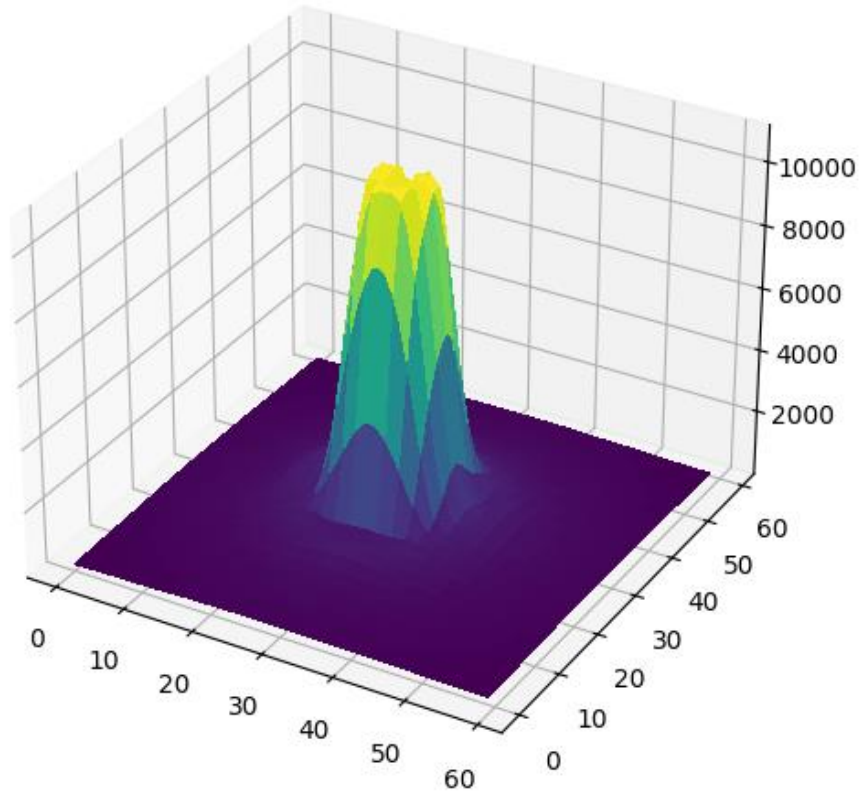
Odhad PSF z centrálního maxima difraktogramu



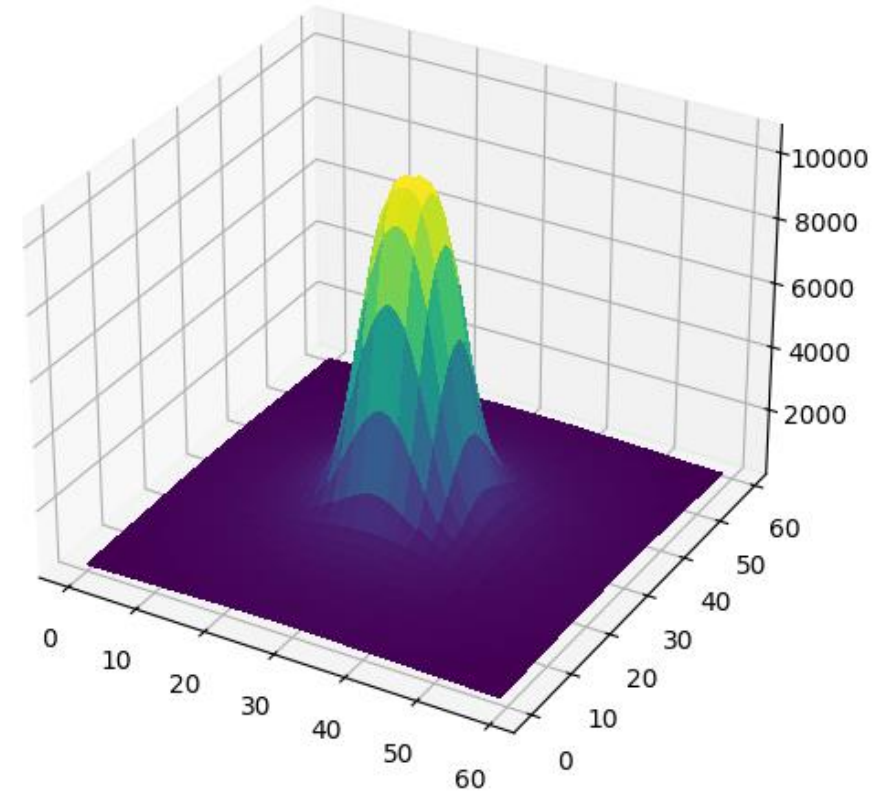
Jádrový odhad PSF z centrálního maxima difraktogramu



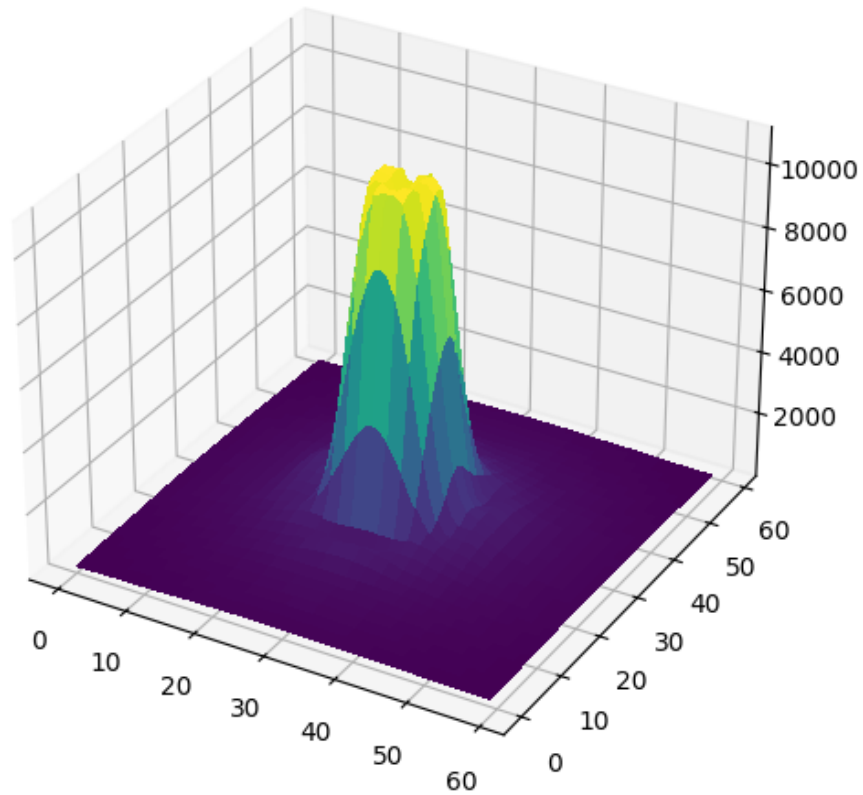
Original Noisy PSF



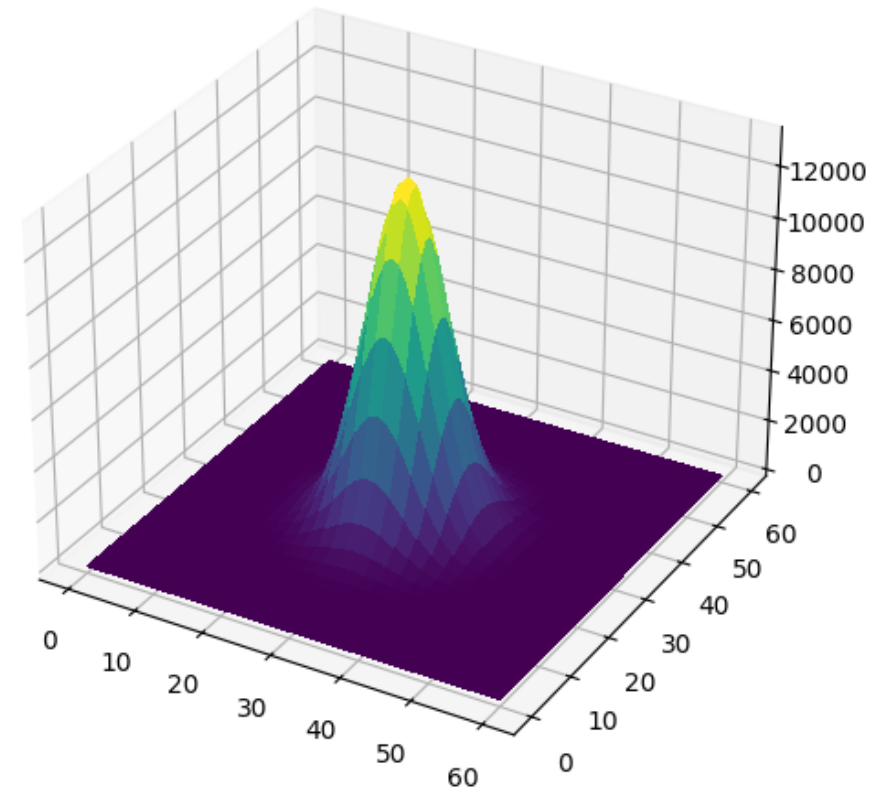
Smoothed PSF with Gaussian Kernel



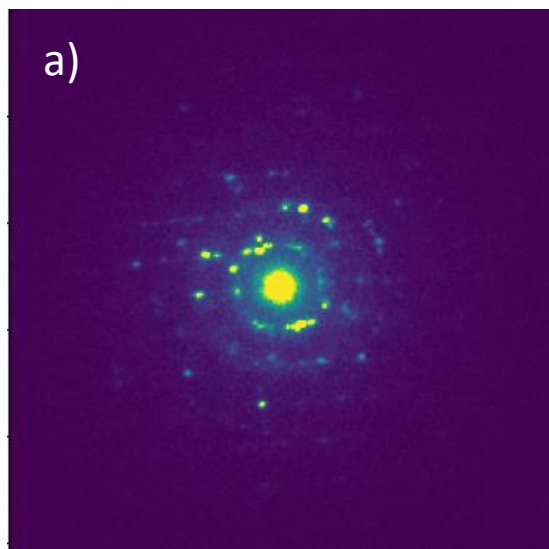
Original Noisy PSF



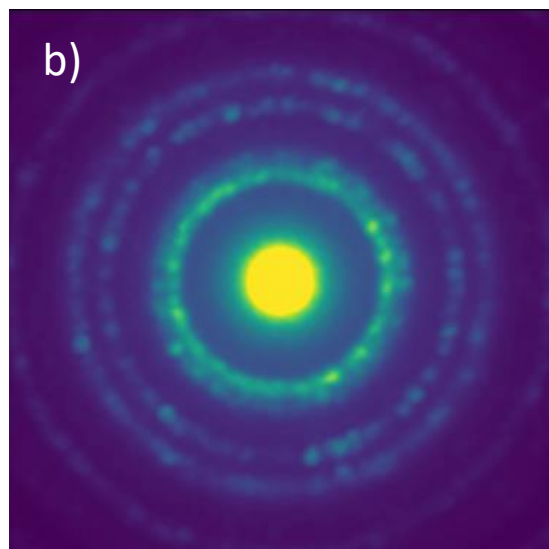
Sampled PSF from Fitted Gaussian Model



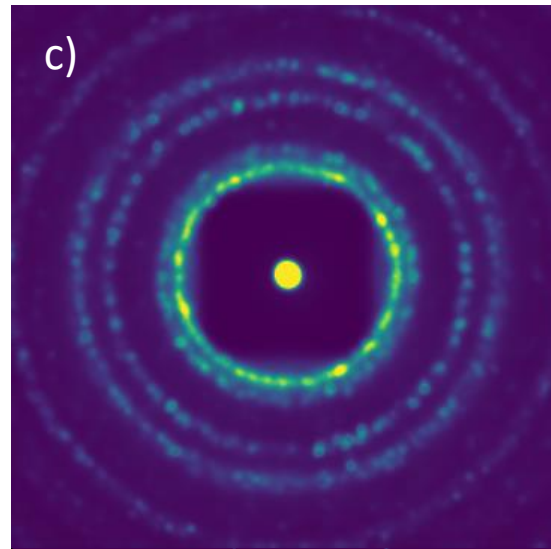
Dekonvoluce difraktogramů



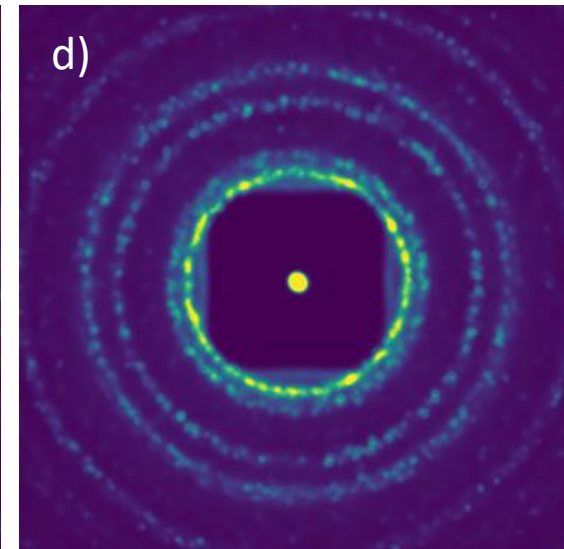
1 vzorek z datasetu



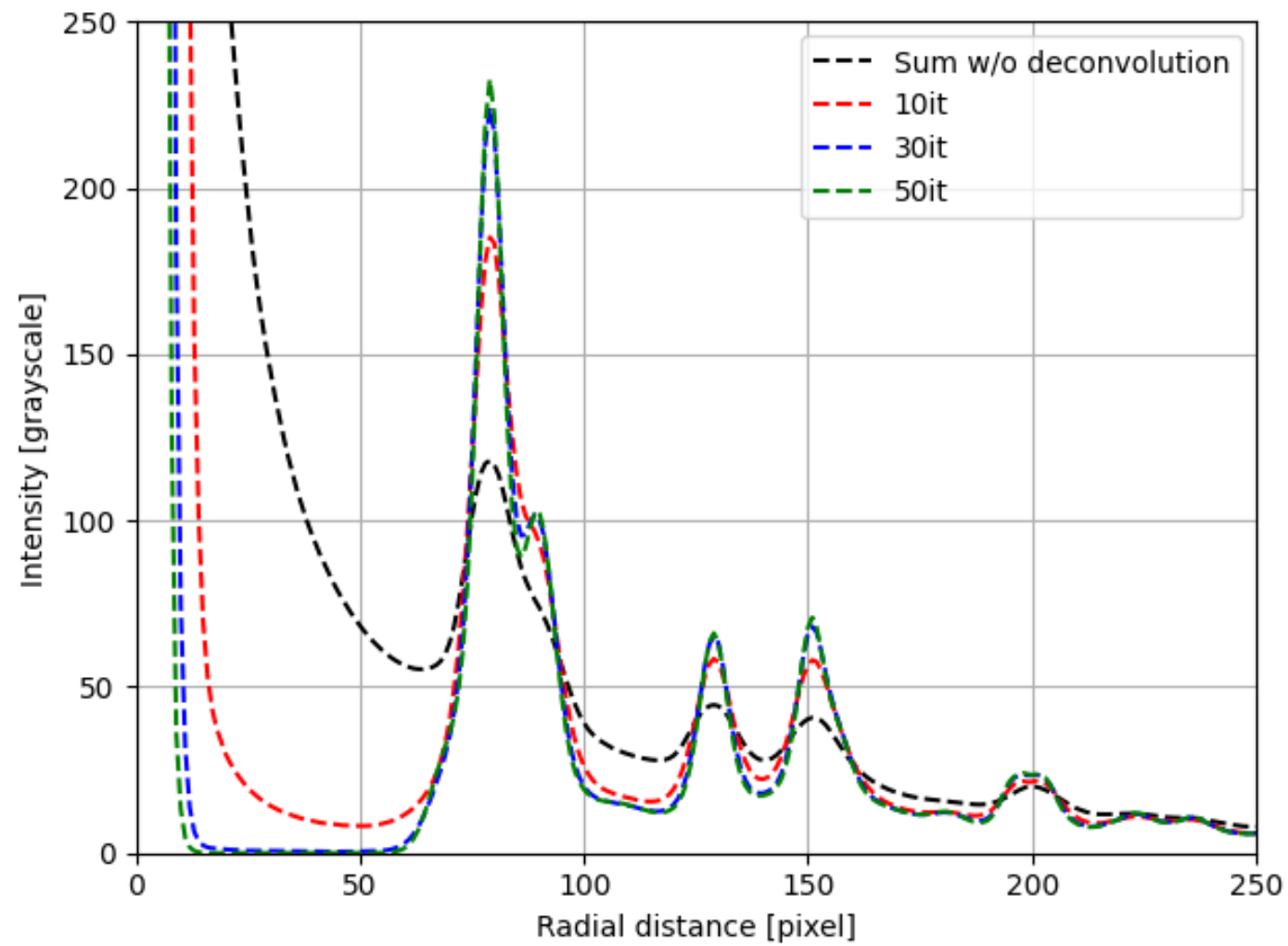
Součet bez dekonvoluce

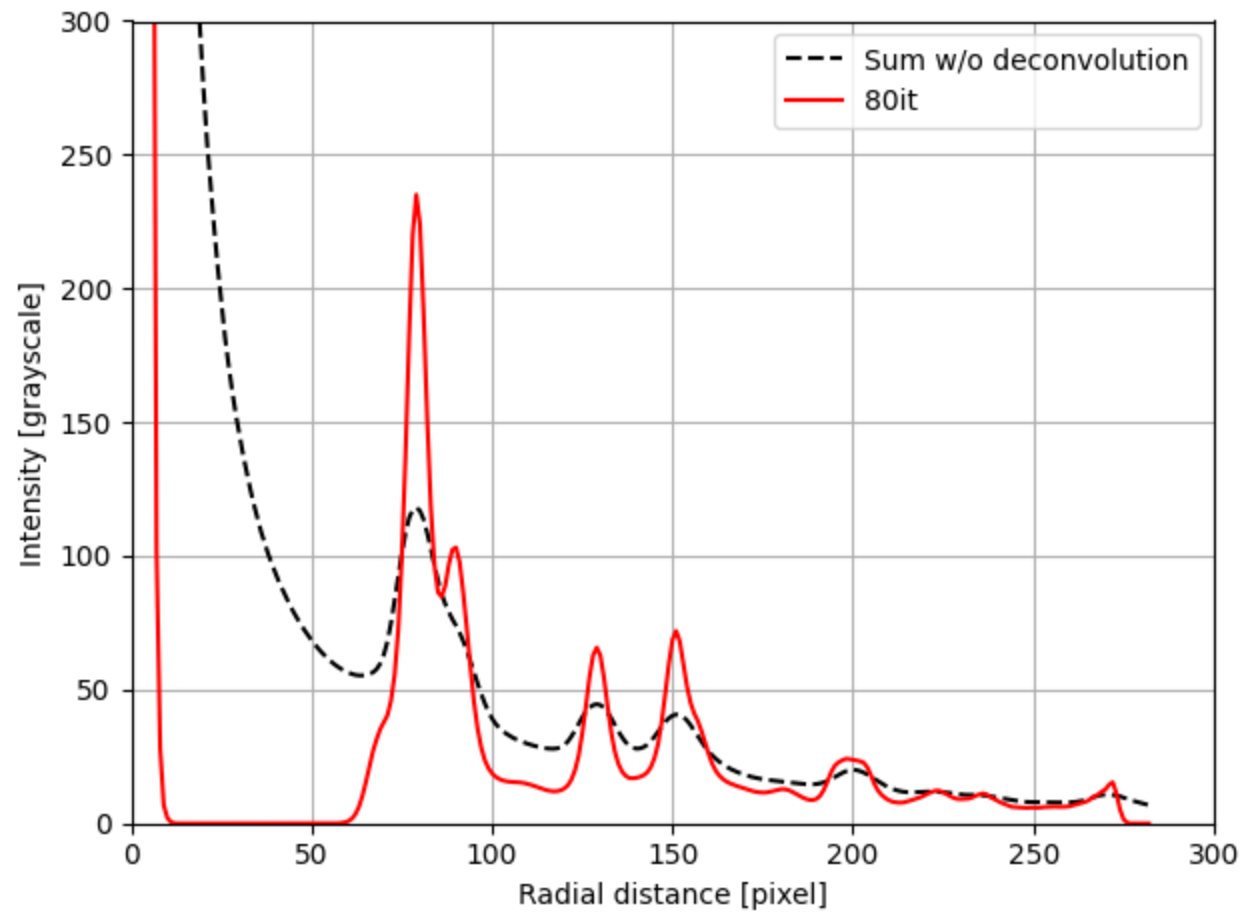


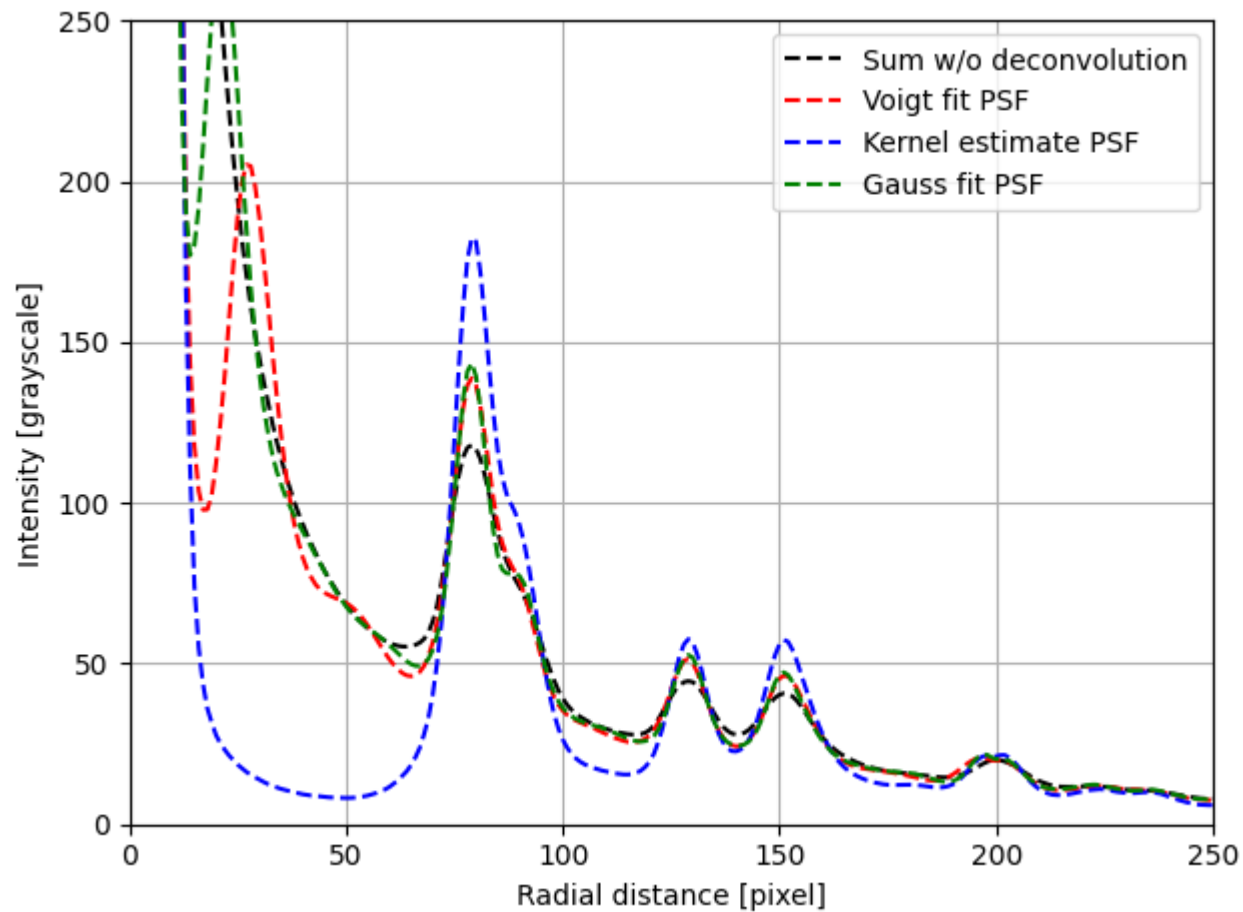
10 iterací RL algoritmu



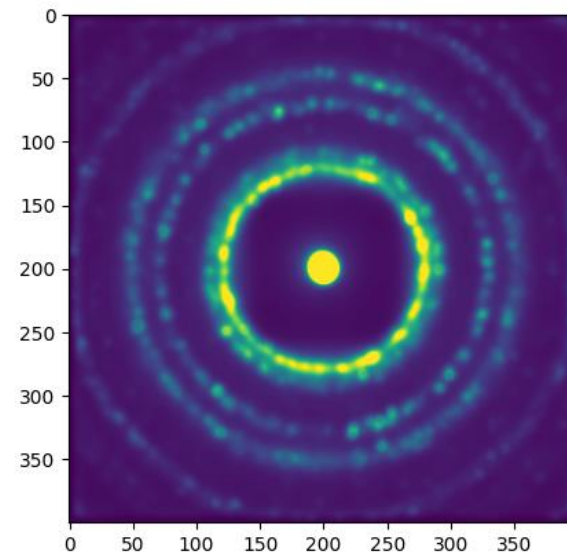
50 iterací RL algoritmu



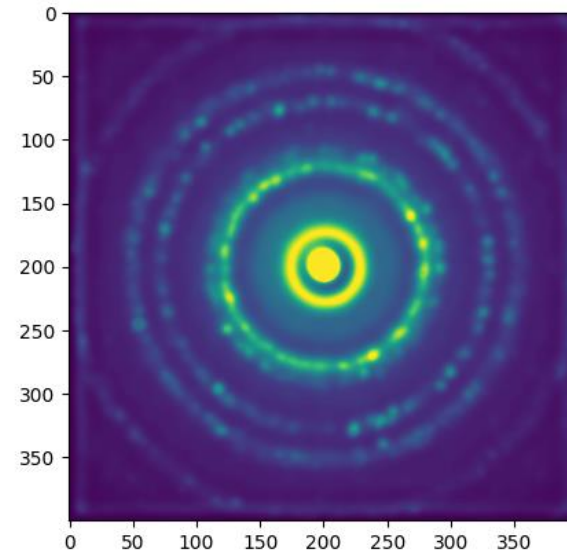


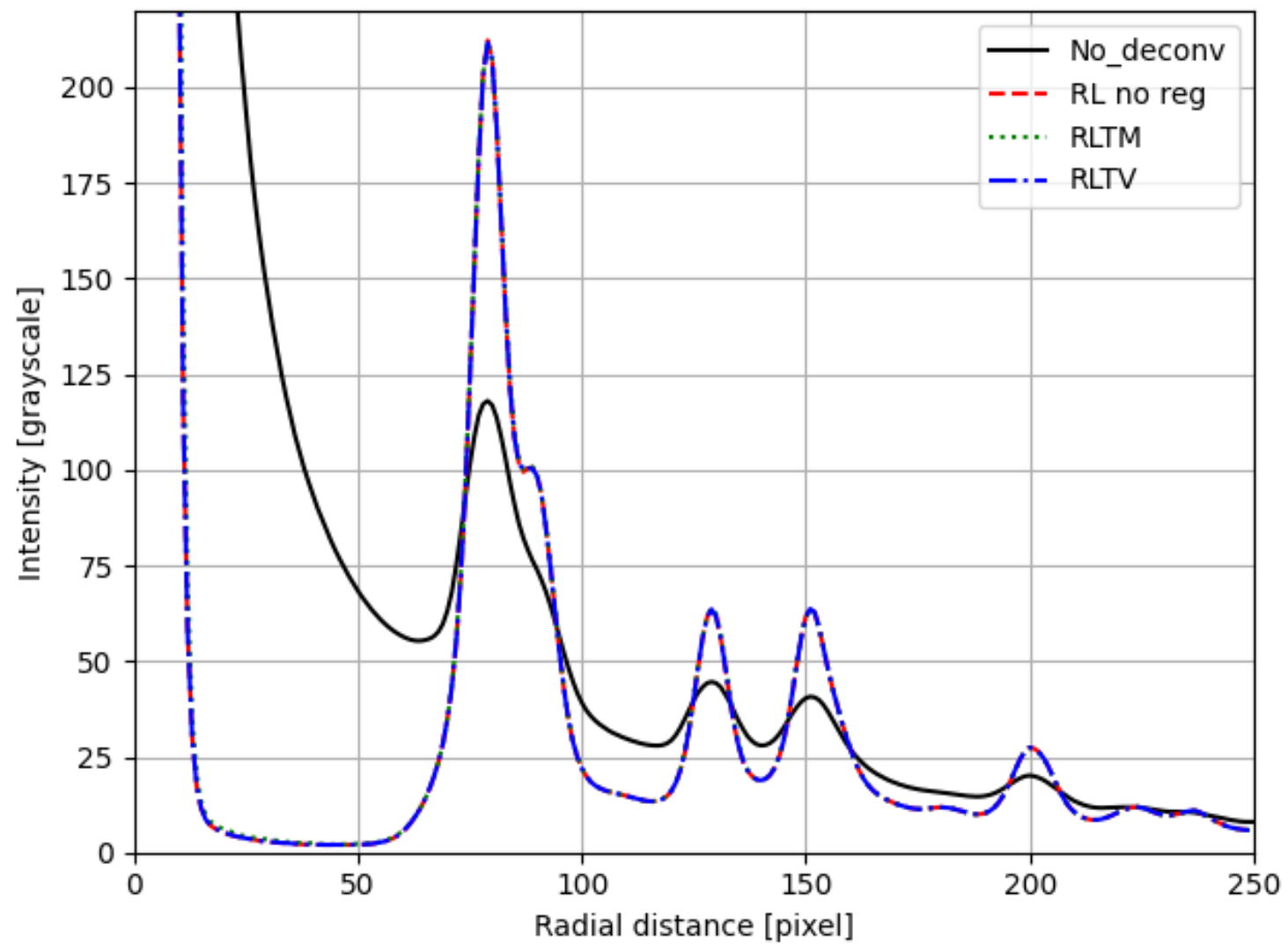


Jádrový odhad PSF



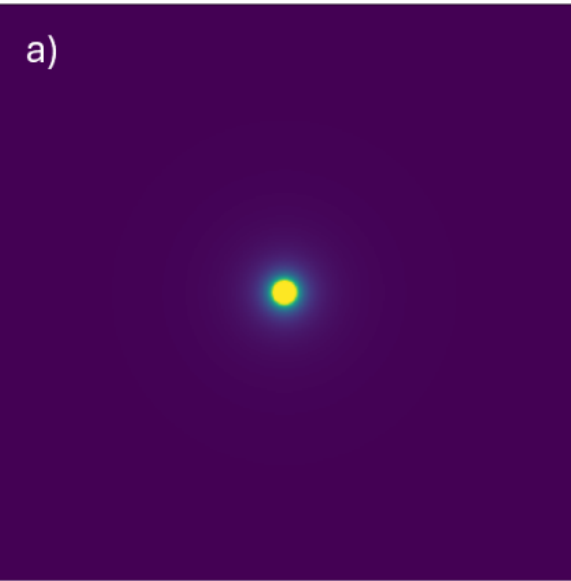
Fit Voigtovy distribuce





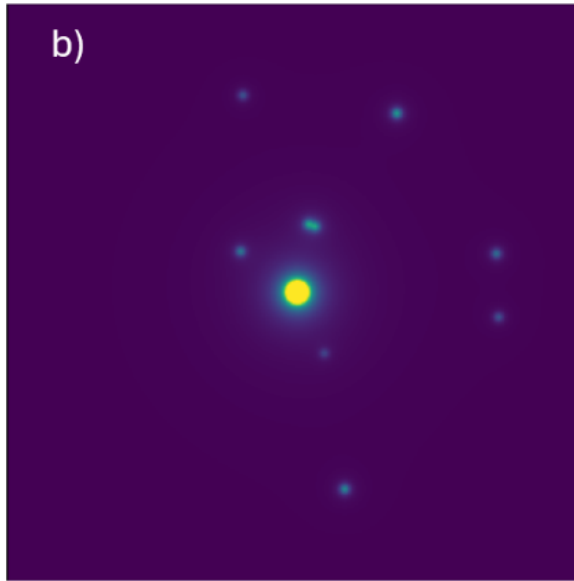
Simulace syntetických dat

a)



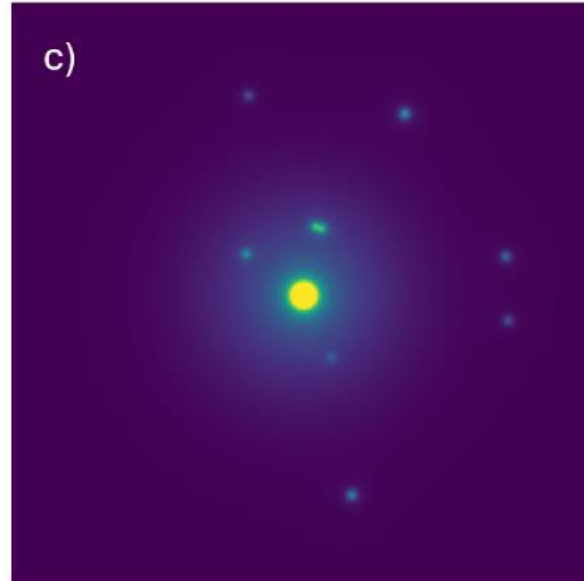
Centrální maximum

b)



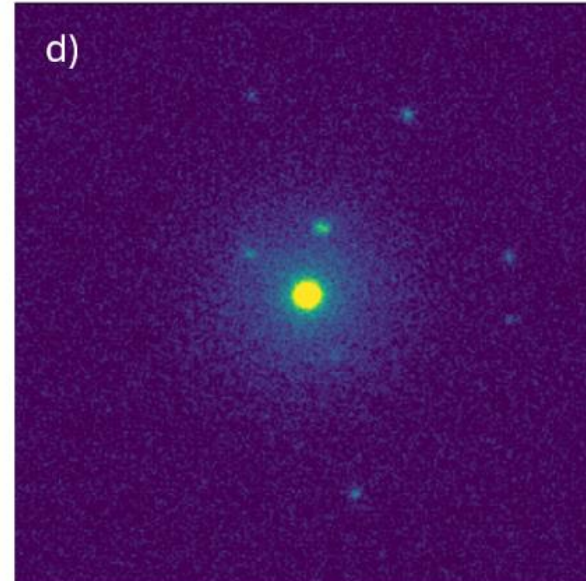
Difrakční maxima

c)

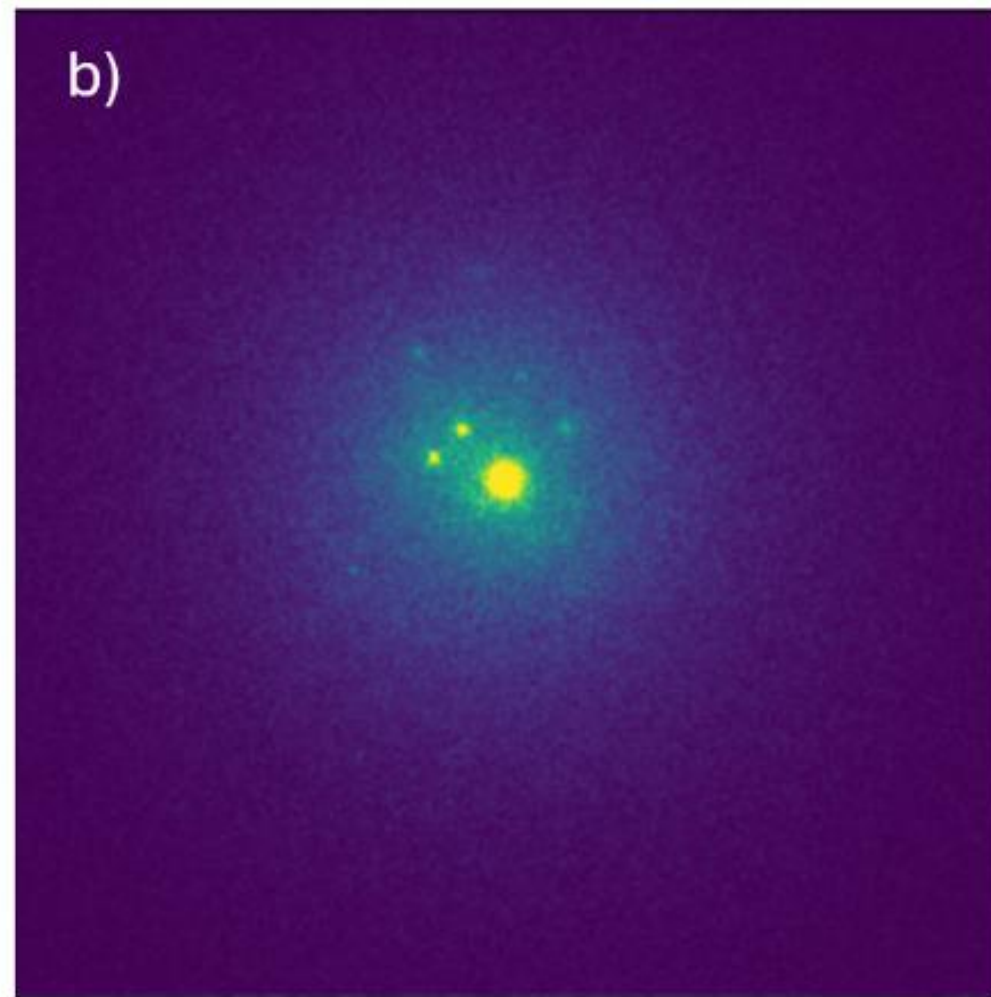
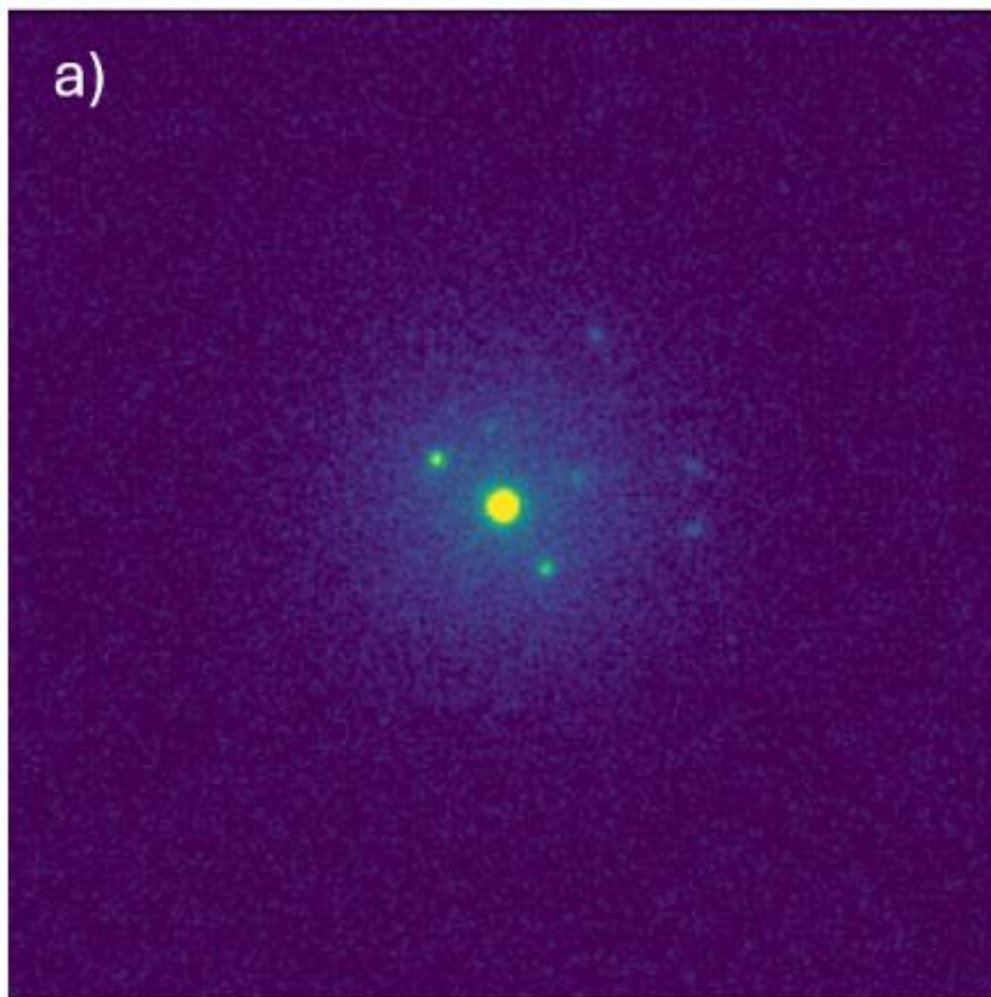


Neuniformní pozadí

d)



Přičtení šumu



Výhled do budoucna

