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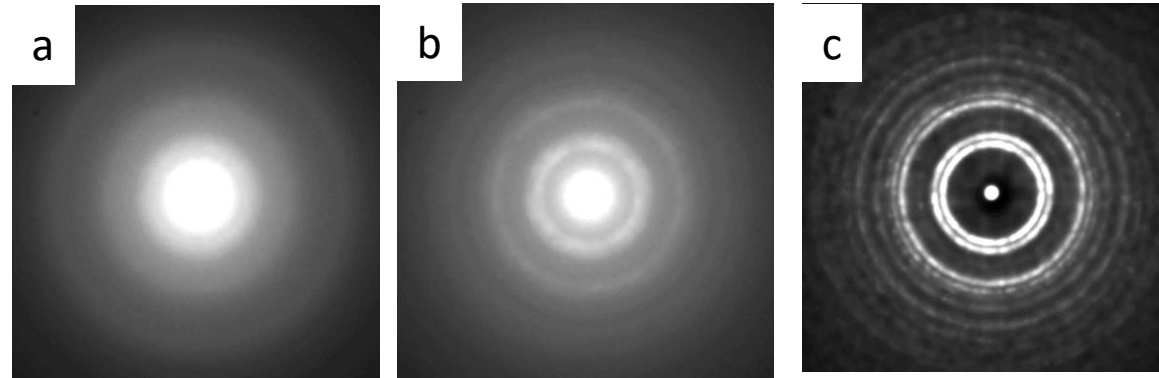
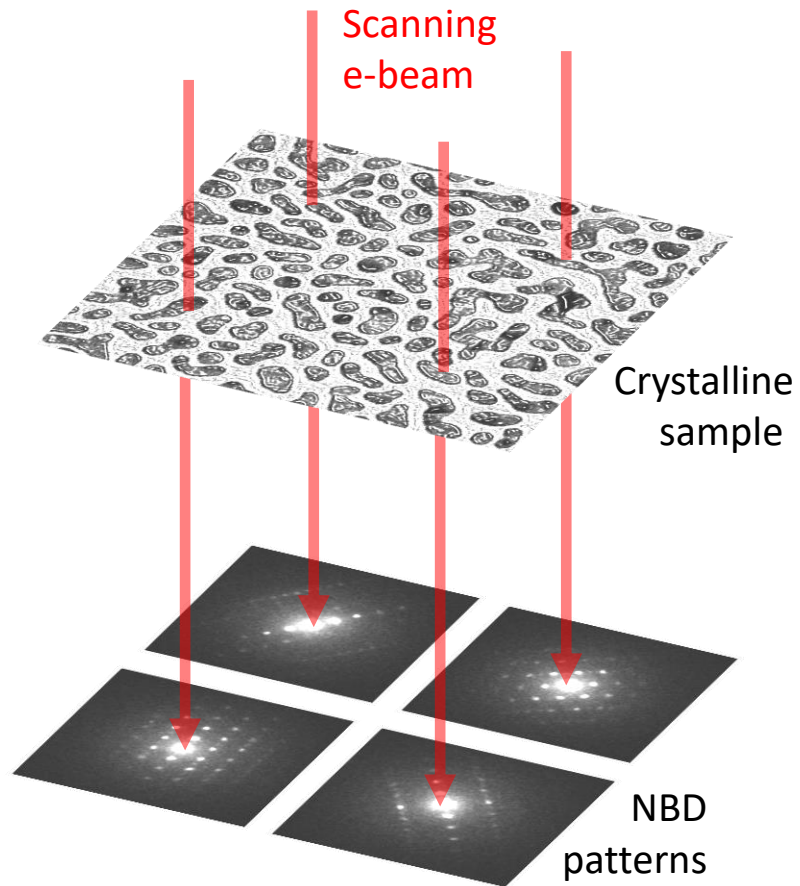
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Application of deconvolution in 4D STEM diffraction analysis

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4D-STEM PNBD



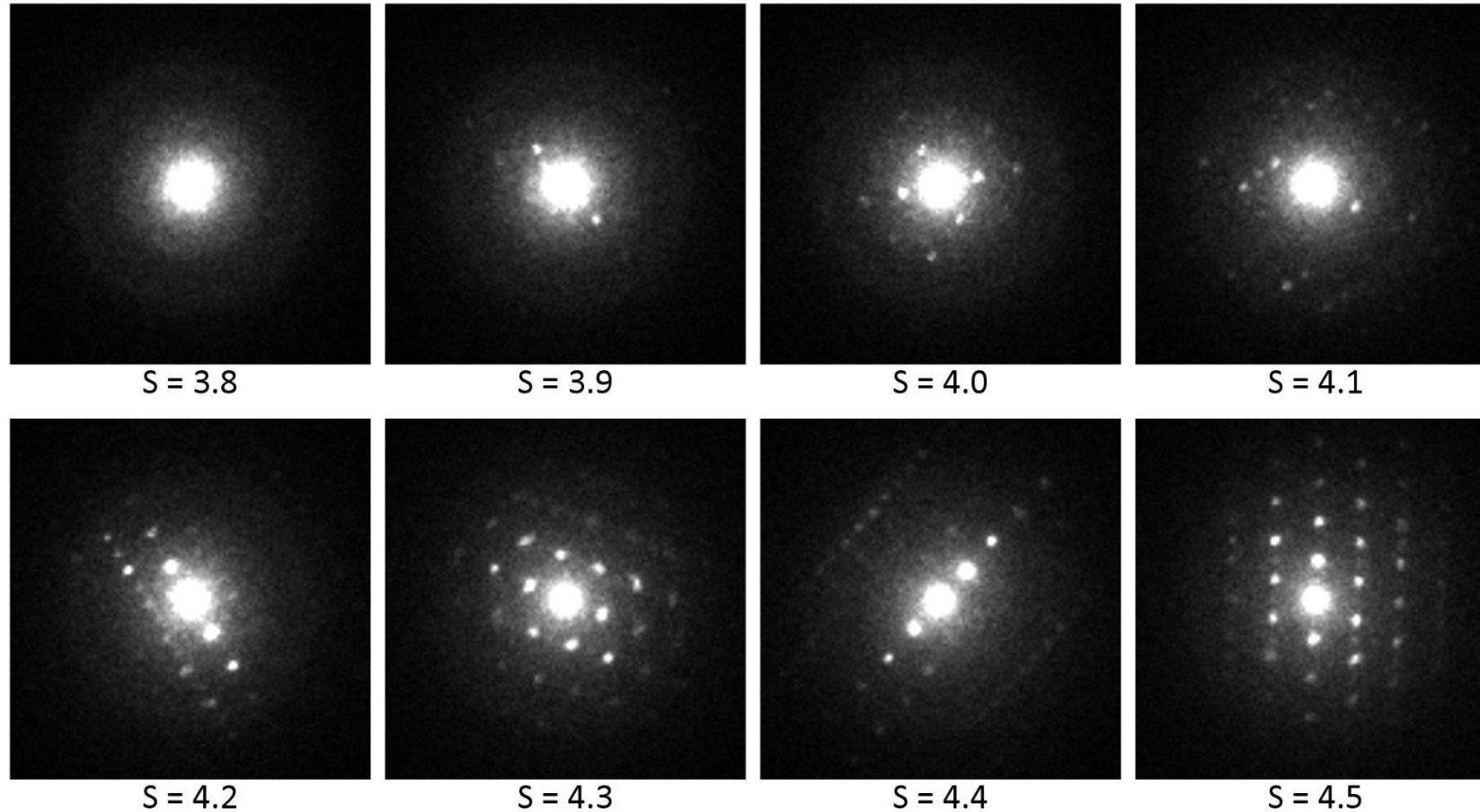
Final powder diffractogram.

(a) Sum all files.

(b) Sum only high-entropy files.

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

Suitable diffractogram selection



Richardson-Lucy deconvolution

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

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

Regularized Richardson-Lucy

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

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



Image blurred with Gaussian PSF with additive noise



Richardson-Lucy deconvolution without regularization



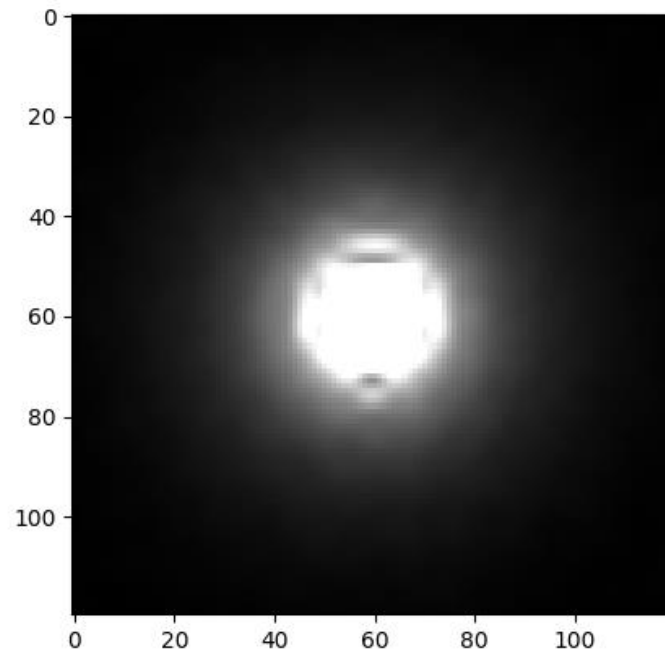
Richardson-Lucy deconvolution with L2 regularization



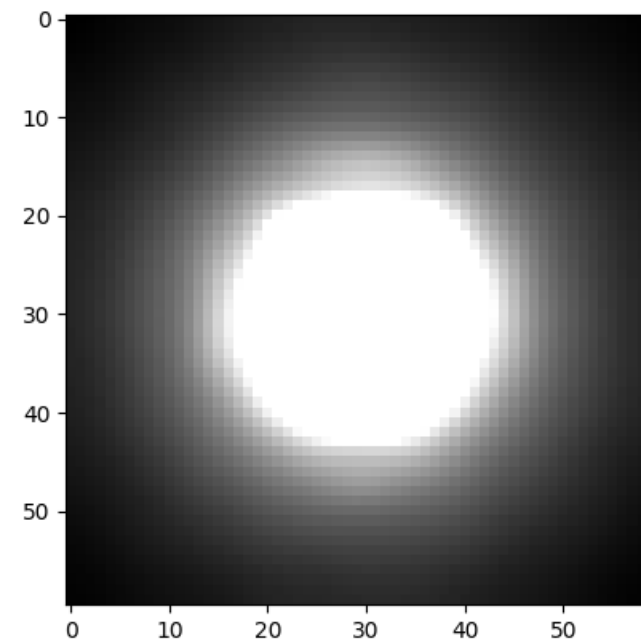
Richardson-Lucy deconvolution with L1 regularization

PSF estimation

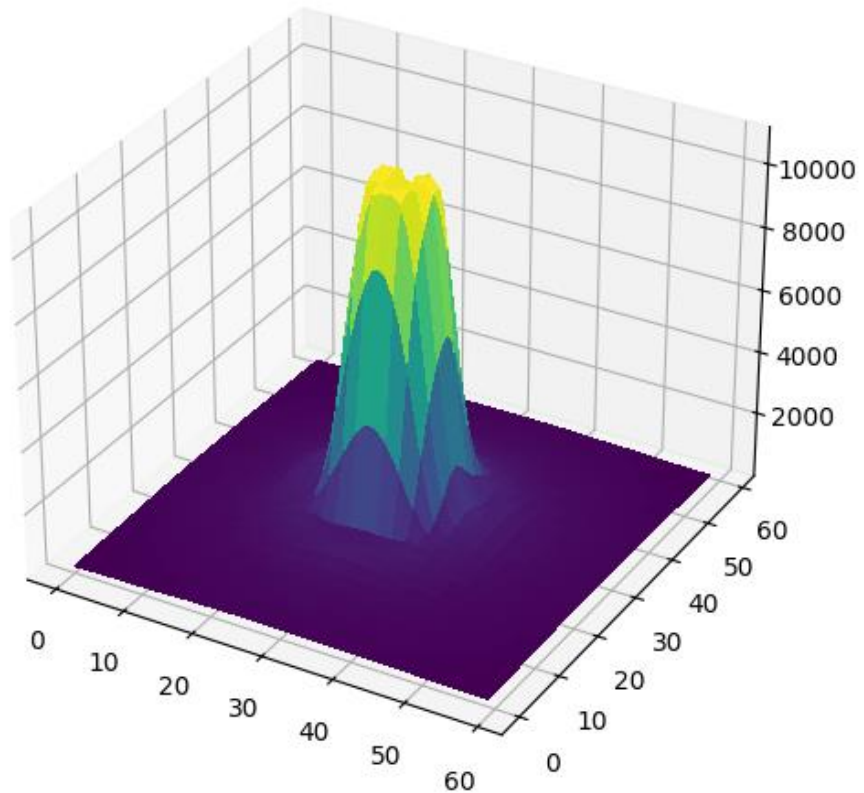
PSF estimate, central peak of diffractogram



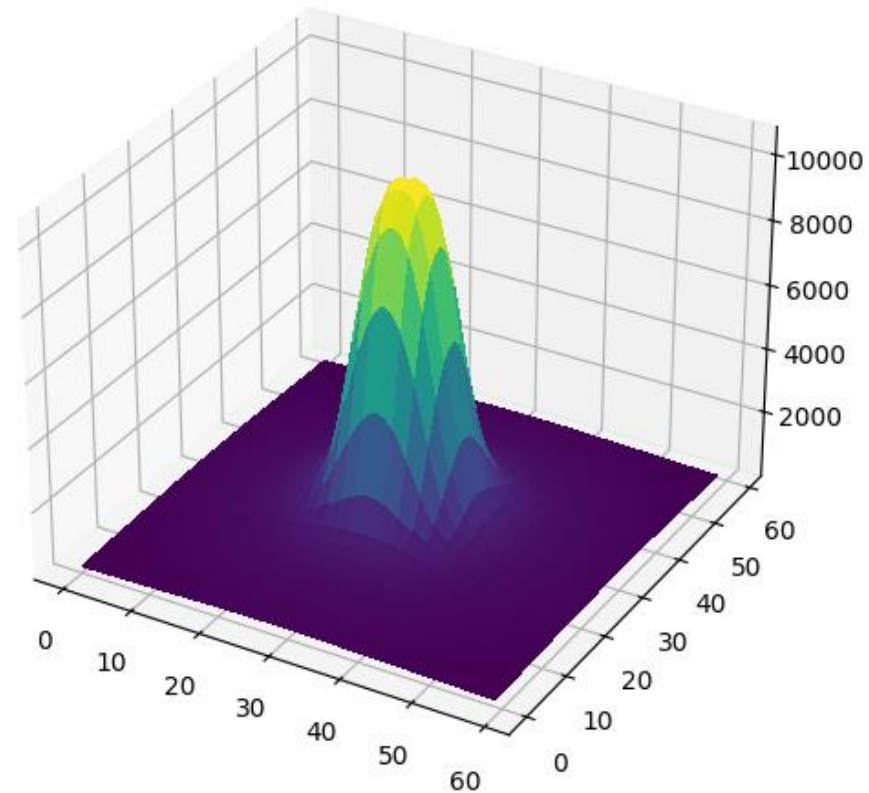
Kernel estimate of PSF based on central peak of diffractogram



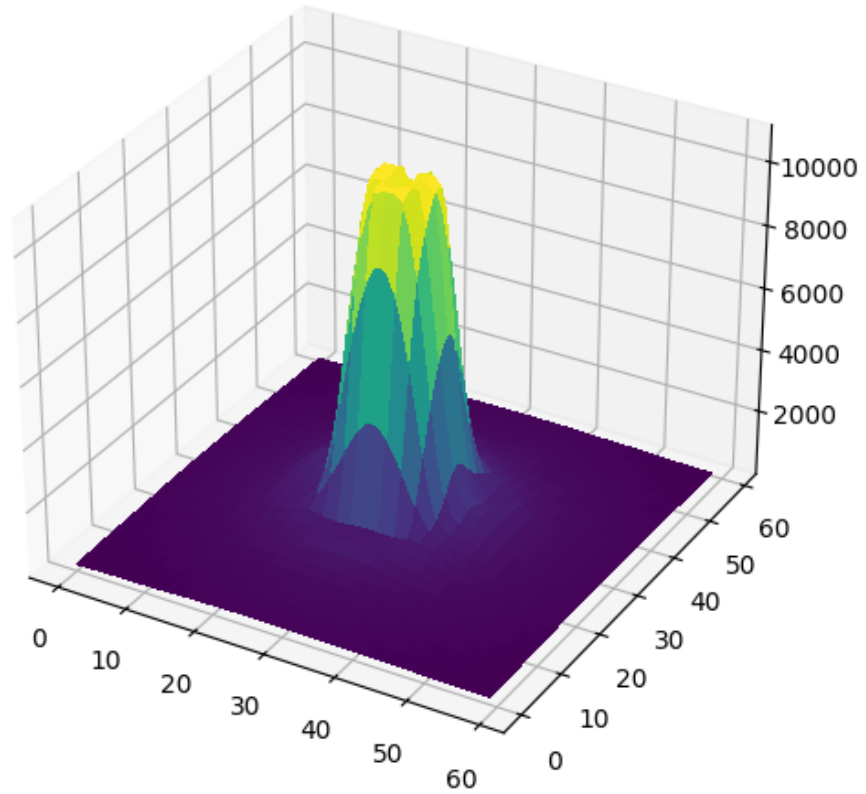
Original Noisy PSF



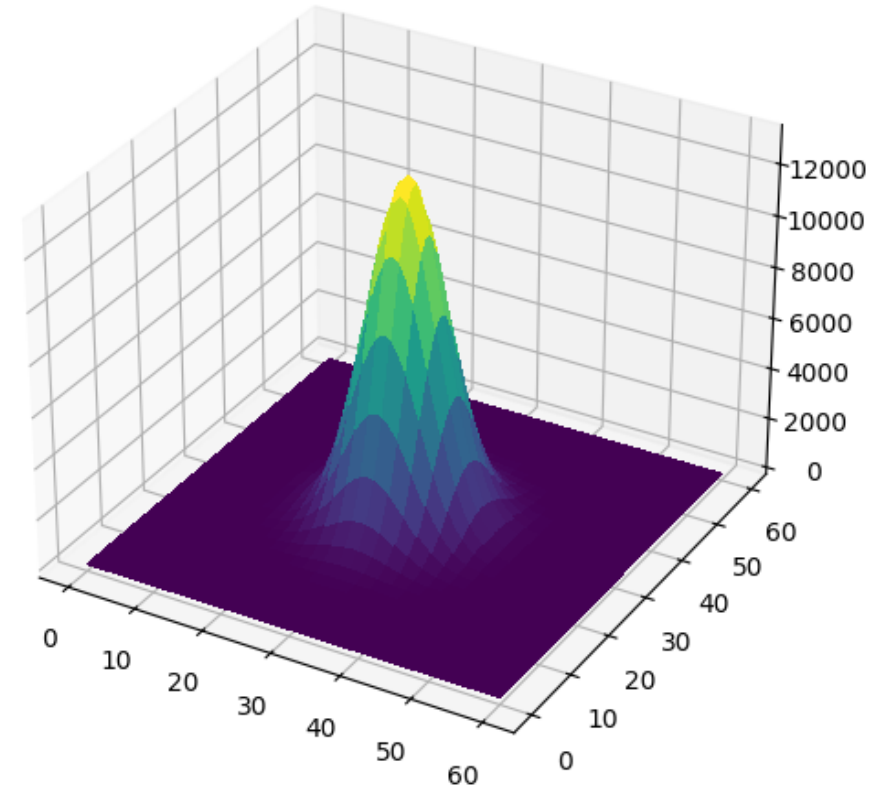
Smoothed PSF with Gaussian Kernel



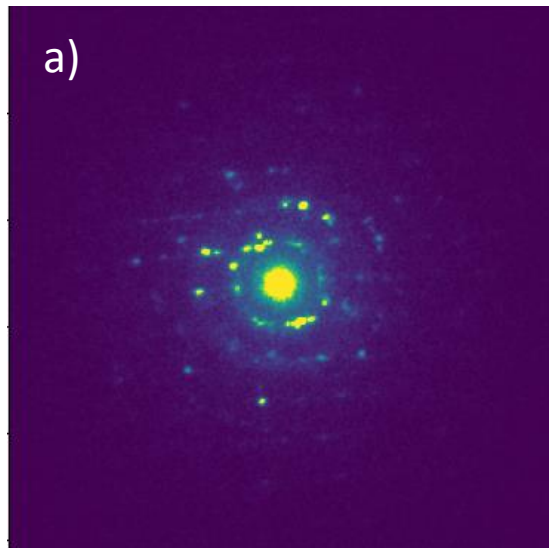
Original Noisy PSF



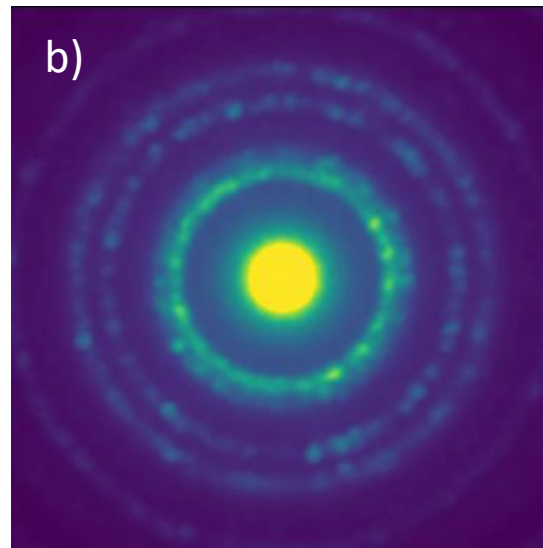
Sampled PSF from Fitted Gaussian Model



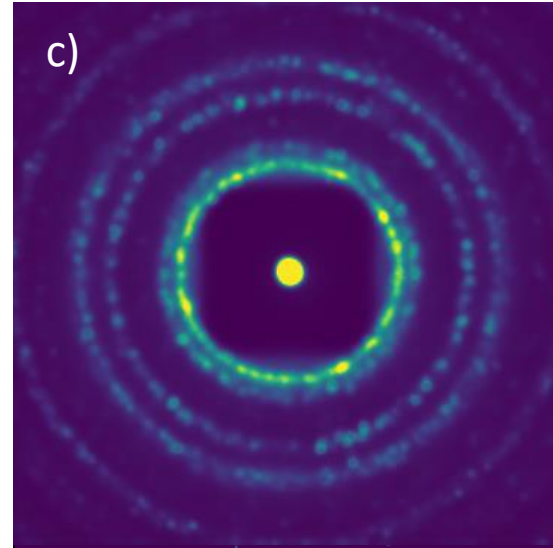
Diffractogram deconvolution



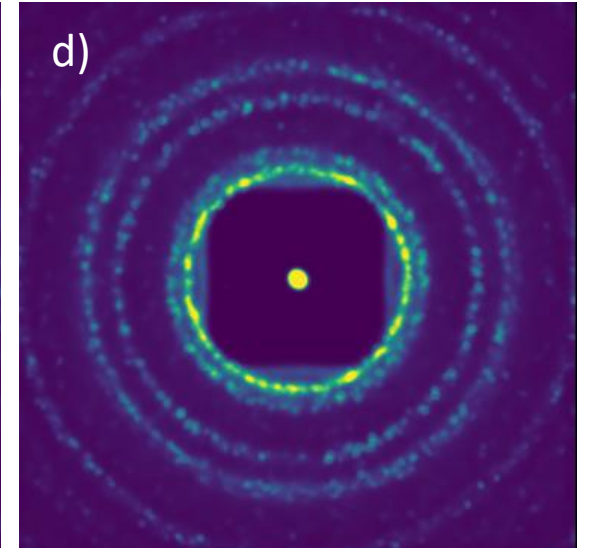
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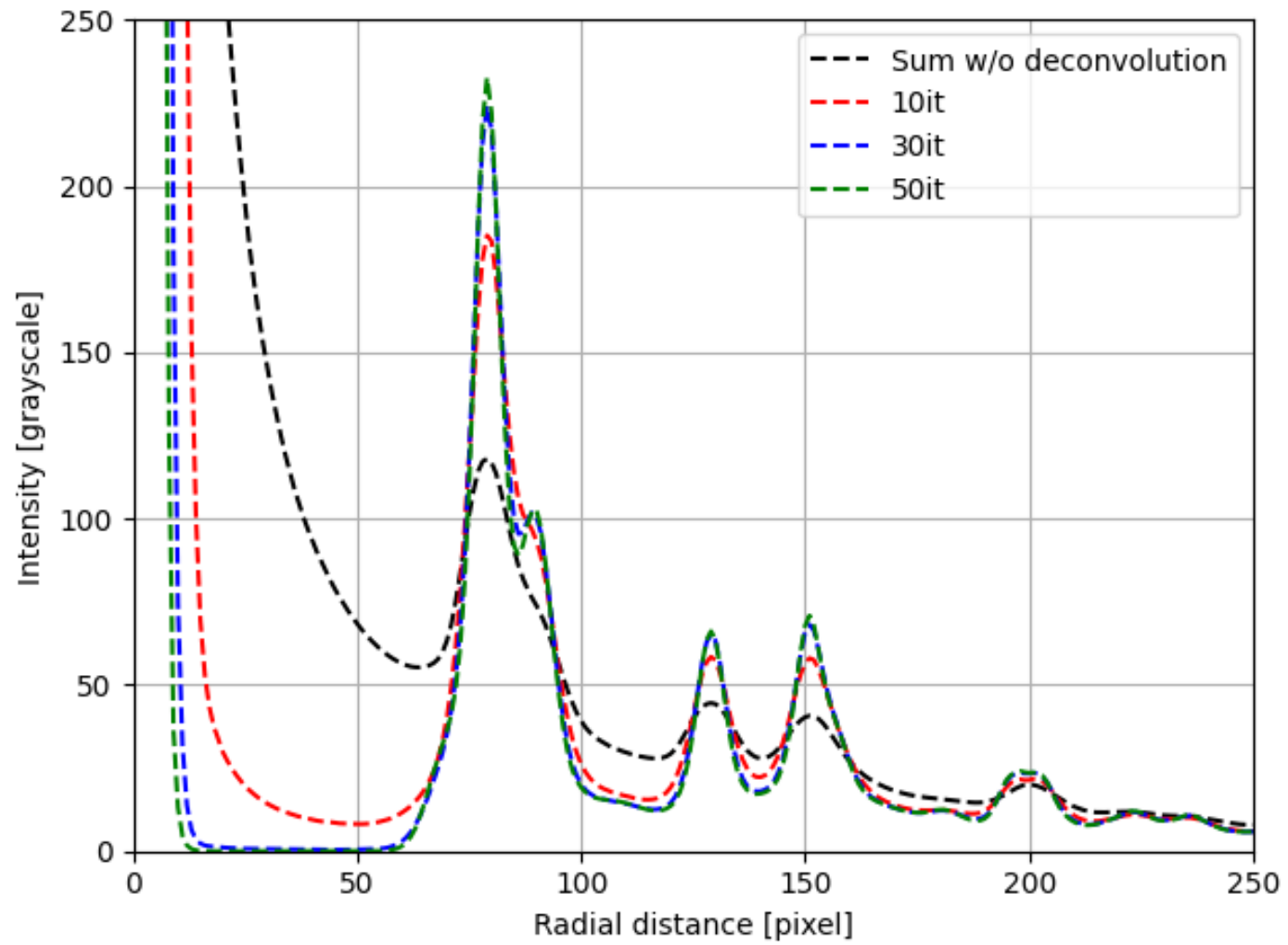
Součet bez dekonvoluce

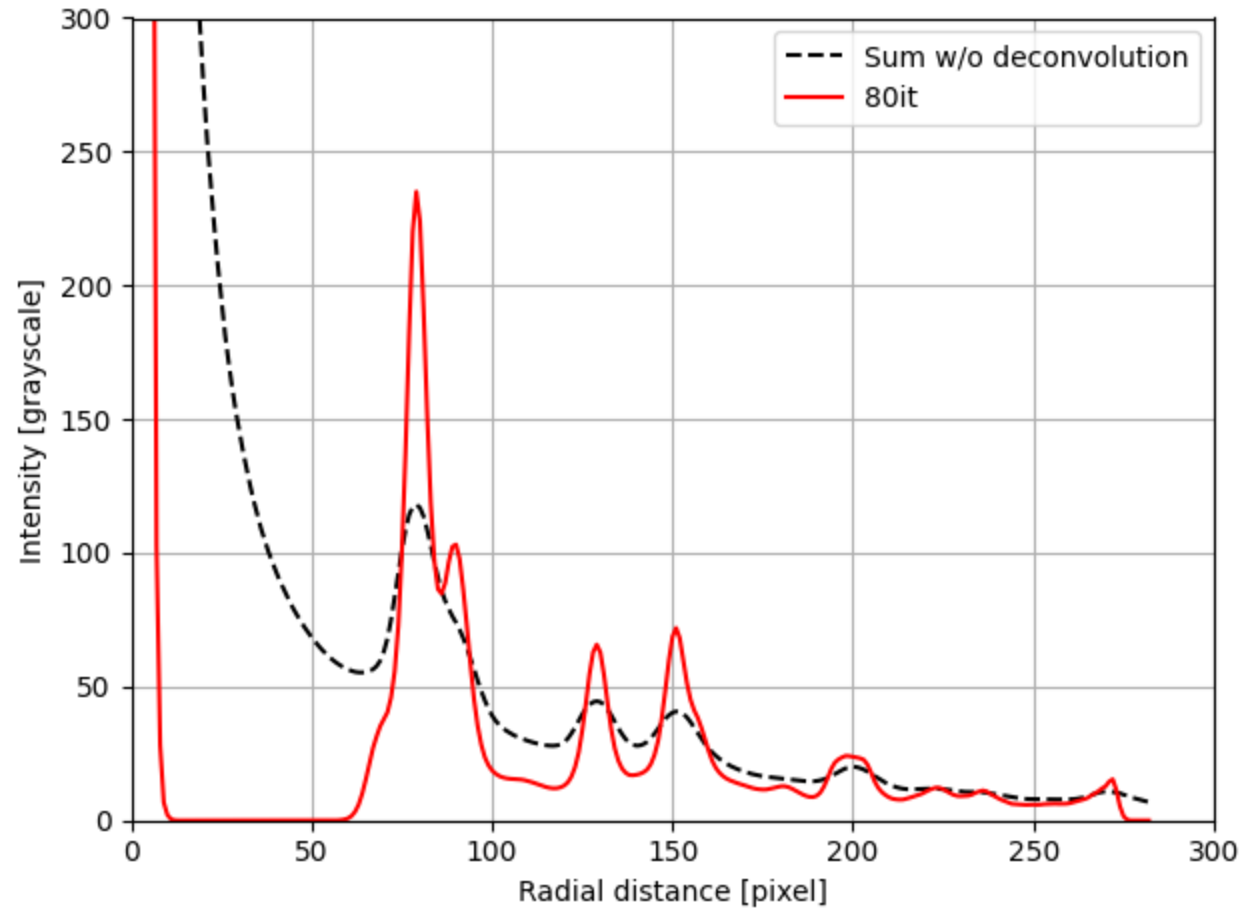


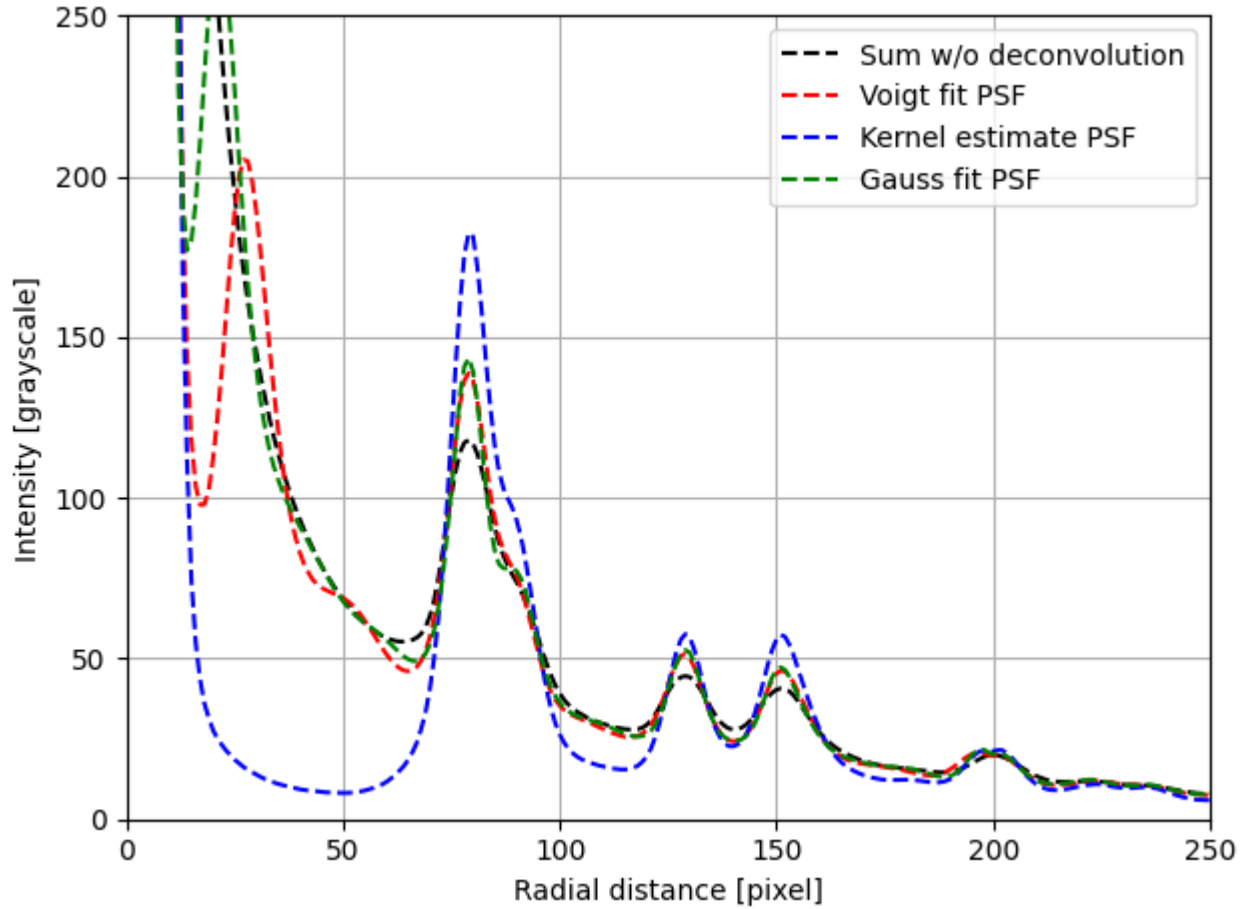
10 iterací RL algoritmu



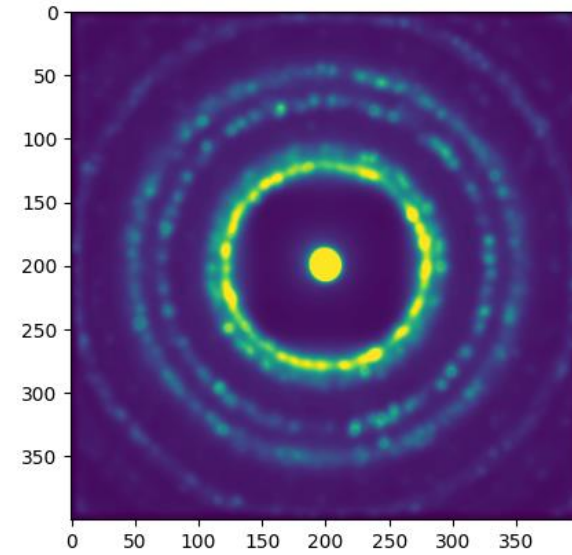
50 iterací RL algoritmu



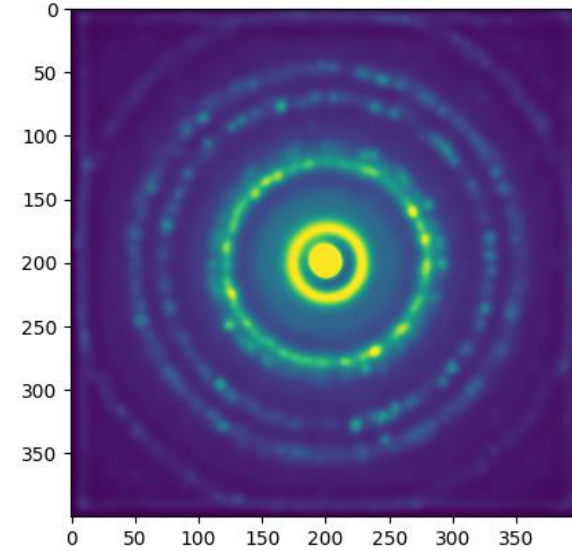


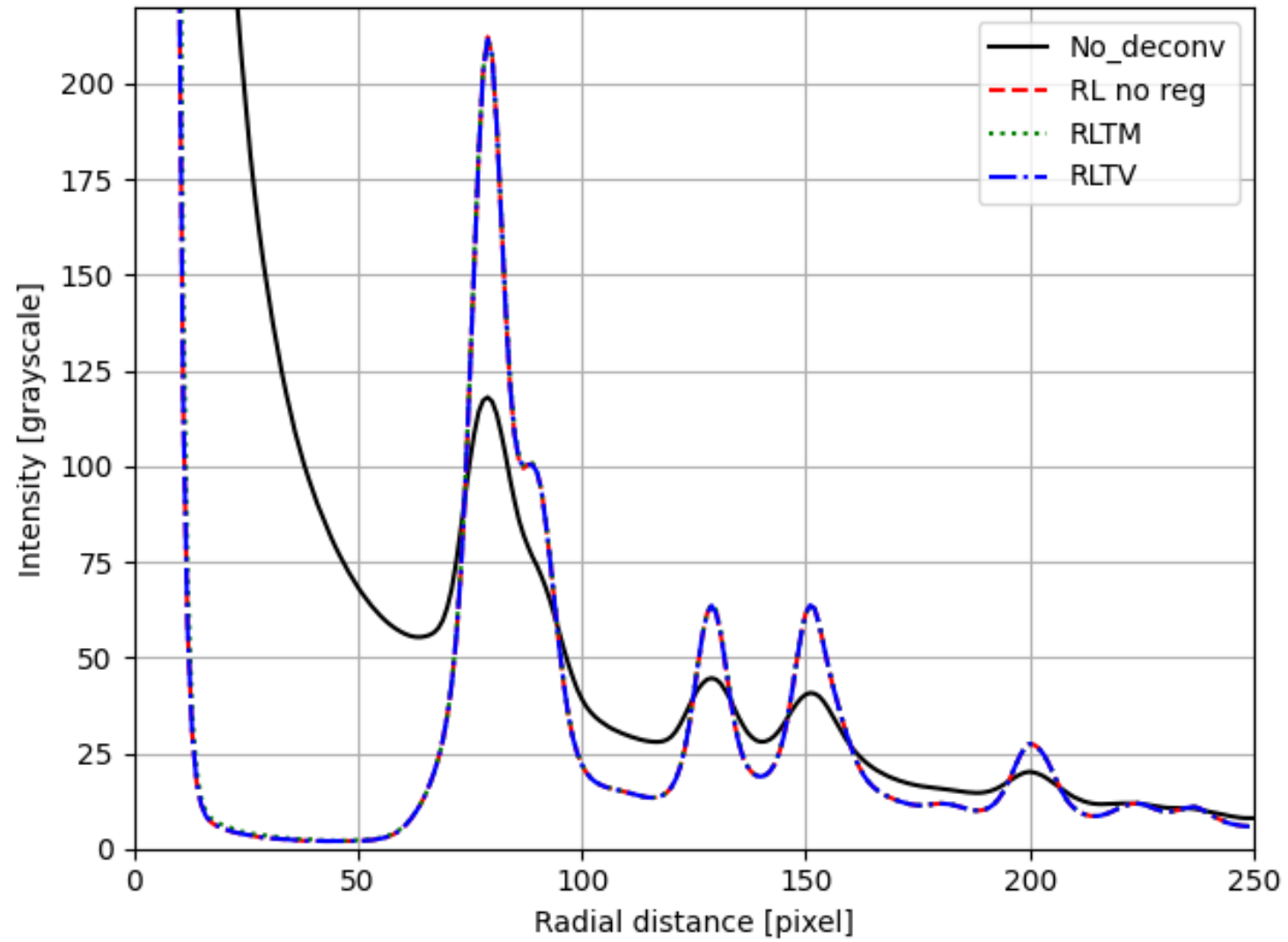


Kernel estimate of PSF



Voigt distribution fit





Synthetic training data

a)



Central peak

b)



Diffraction peaks

c)

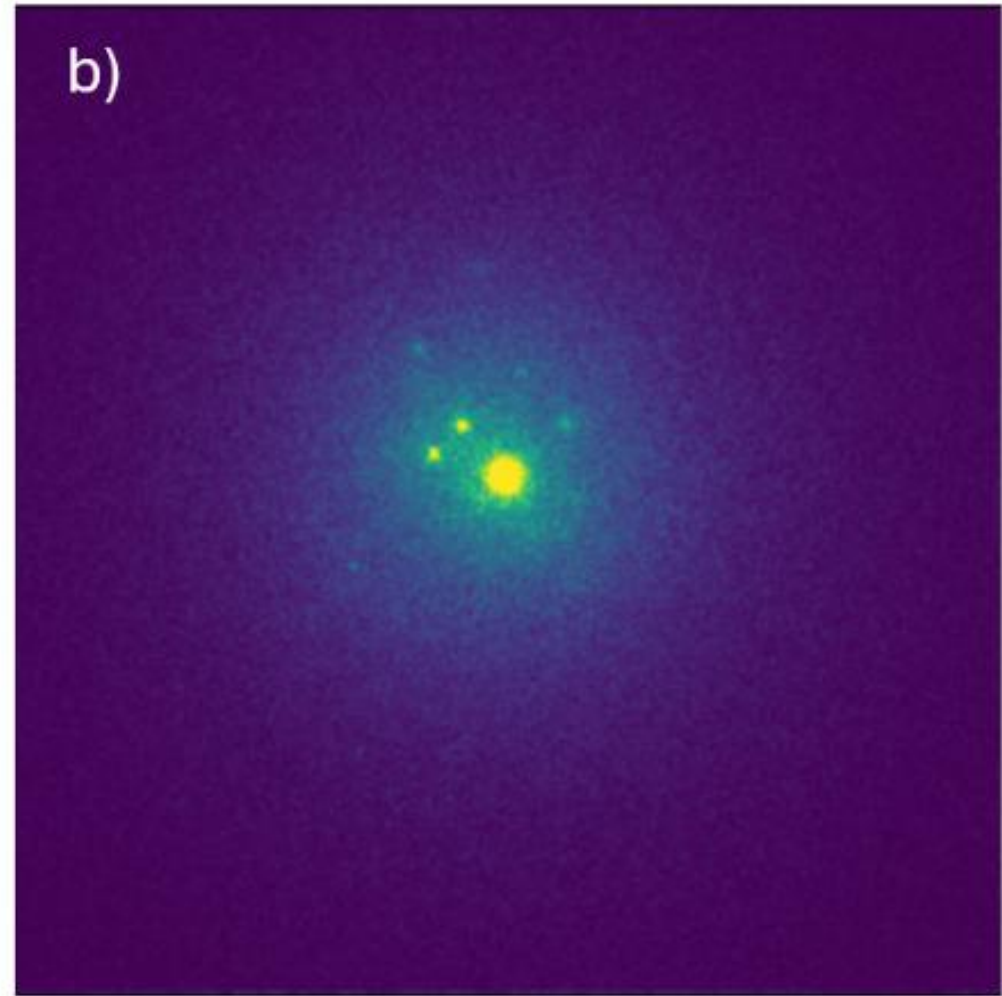
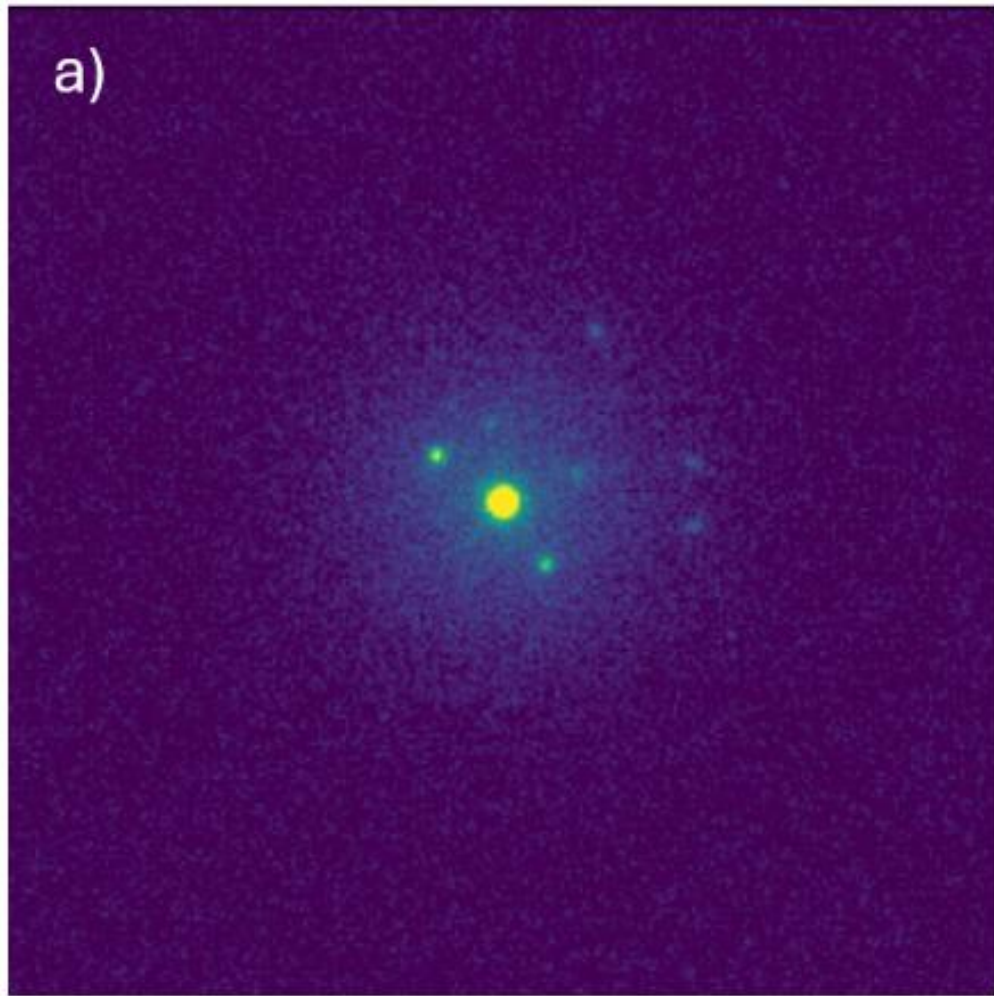


Gaussian background

d)



Additive noise



Future plans

