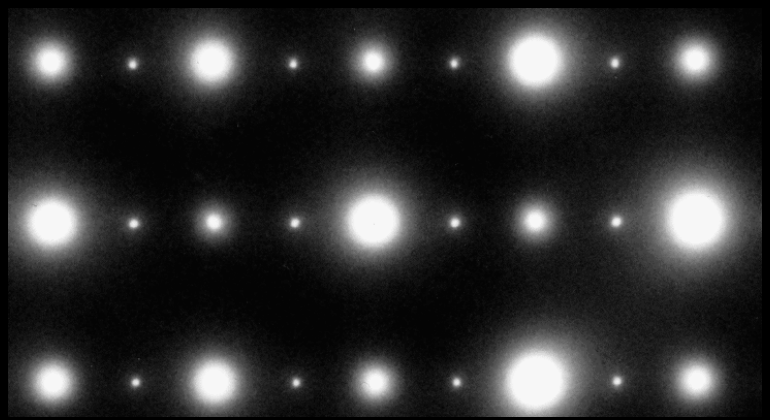
Accurate extraction of reciprocal space information from transmission electron microscopy images

Edward Rosten and Susan Cox

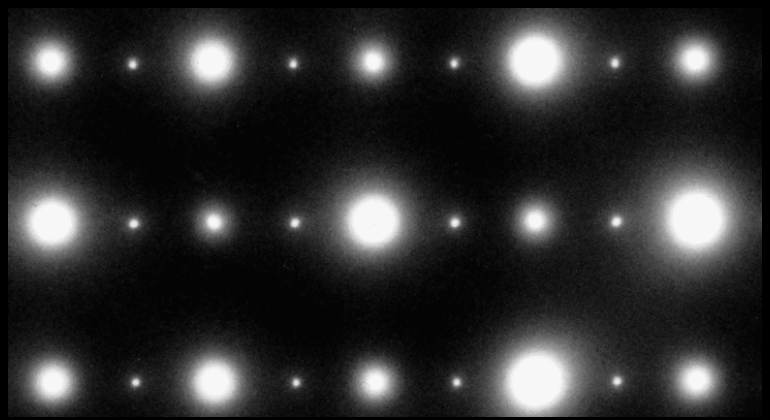
LA-UR-06-8287

Diffraction patterns



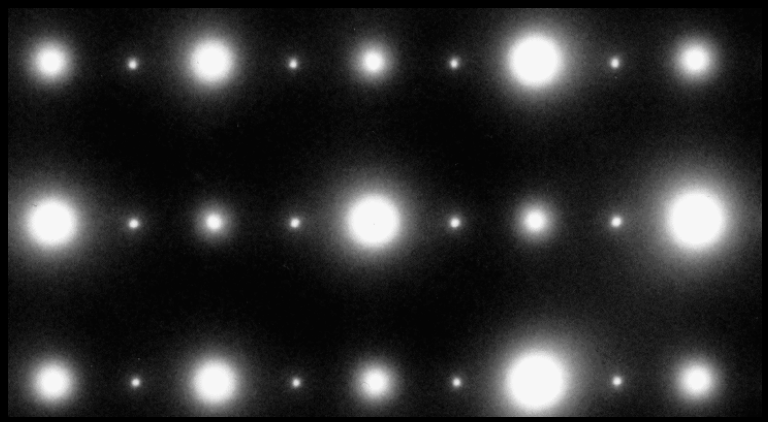
Diffraction pattern is the *Power Spectral Density* of the crystal structure.

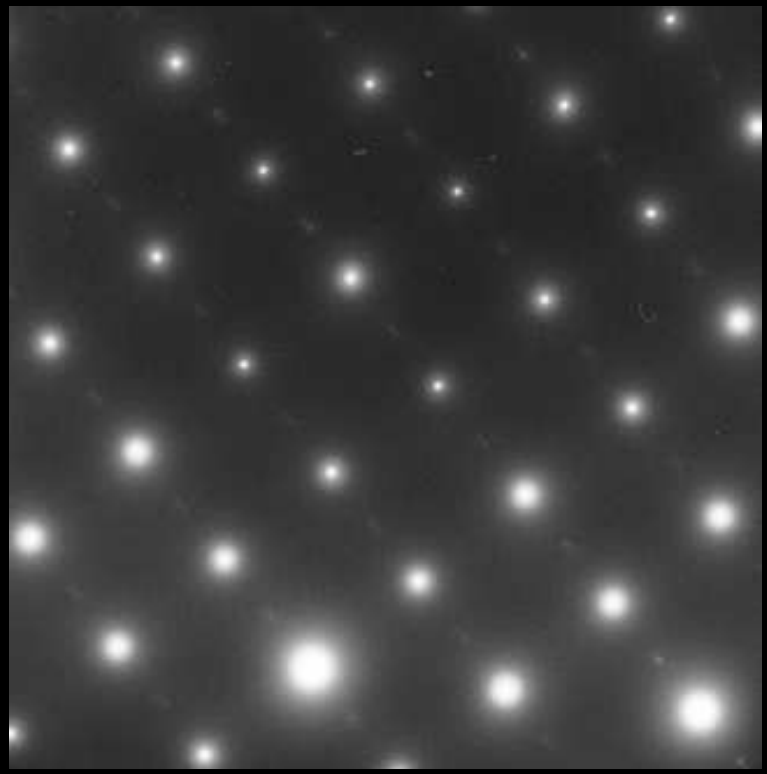
Diffraction patterns



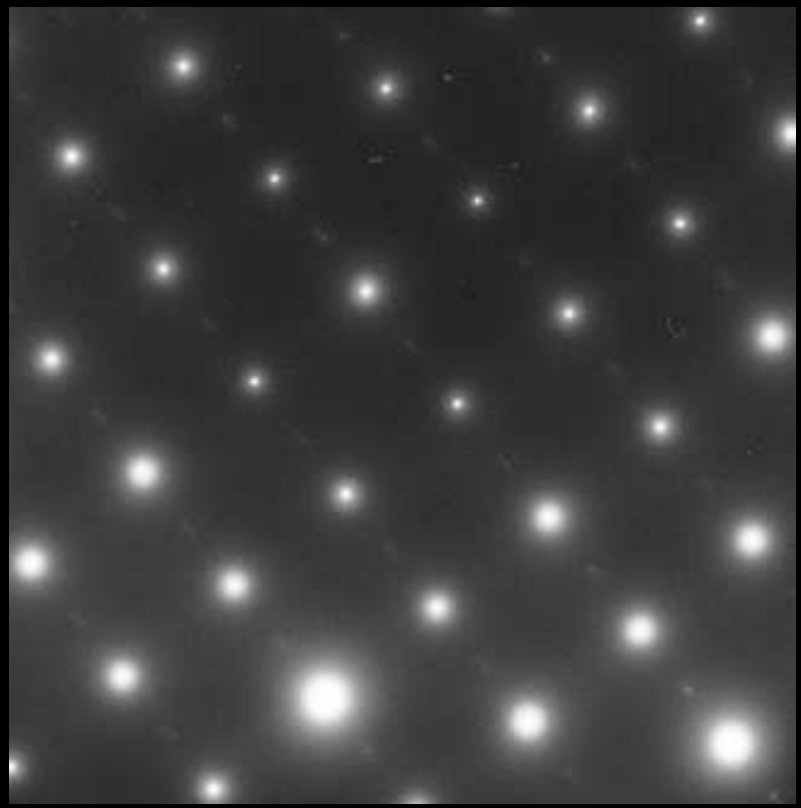
- TEM, X-ray diffraction, . . .
- Manganites, Uranium, Nicklates, Cuprates, . . .

Diffraction patterns

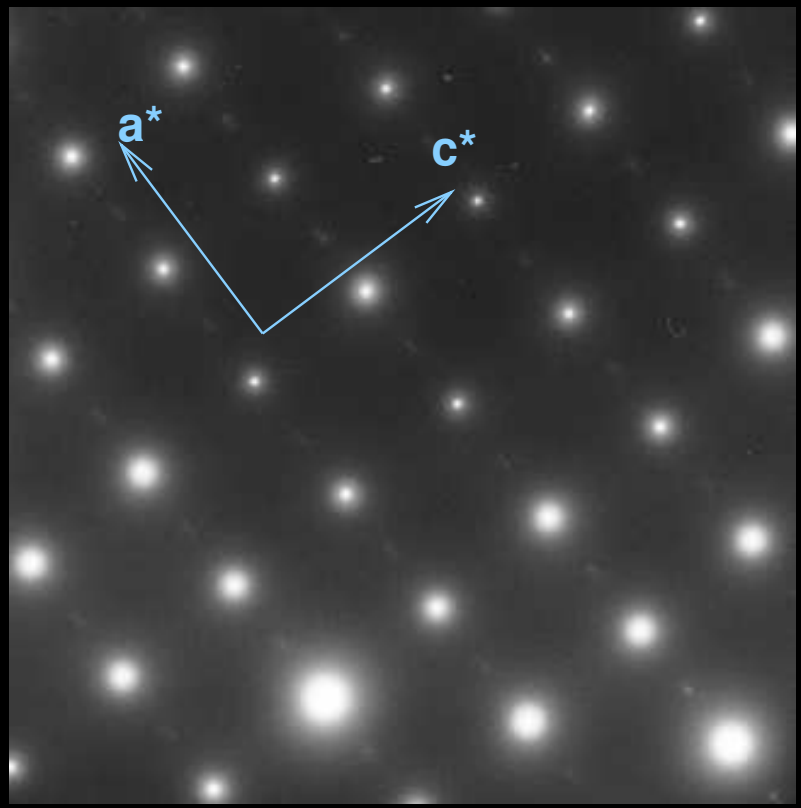




Diffraction patterns



Diffraction patterns



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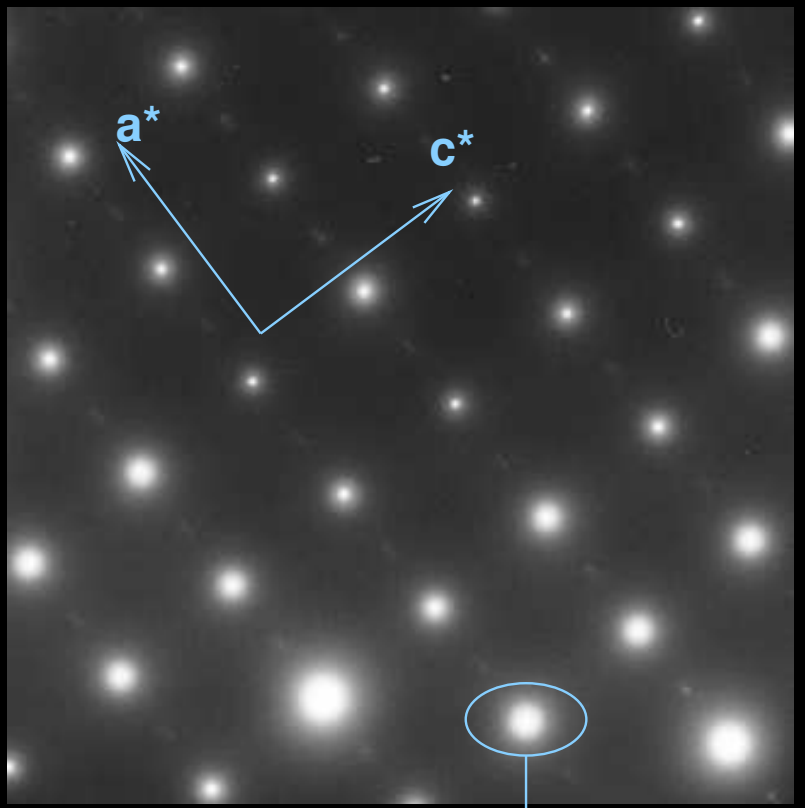

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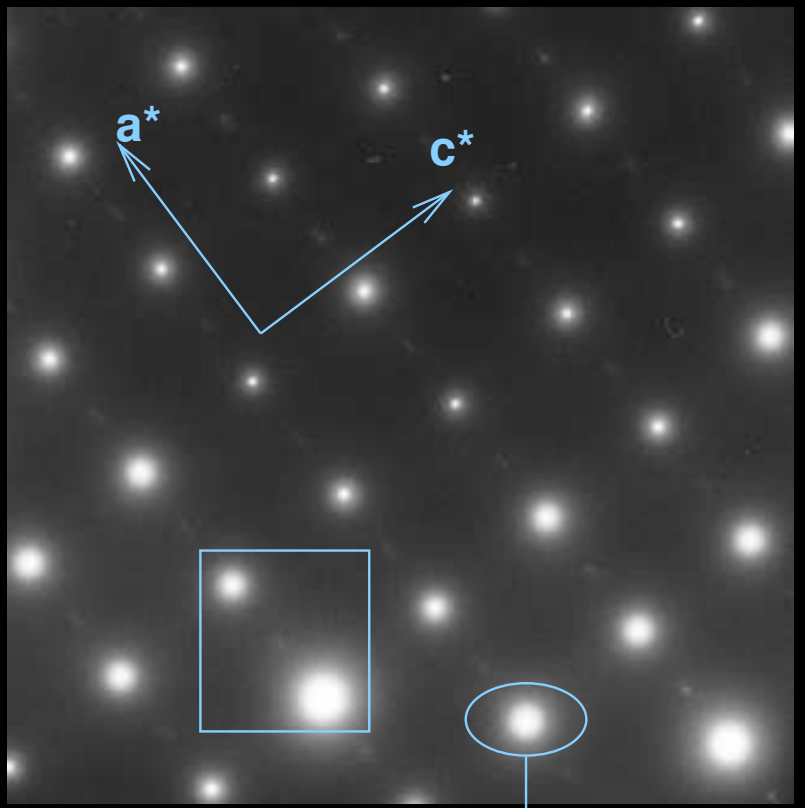

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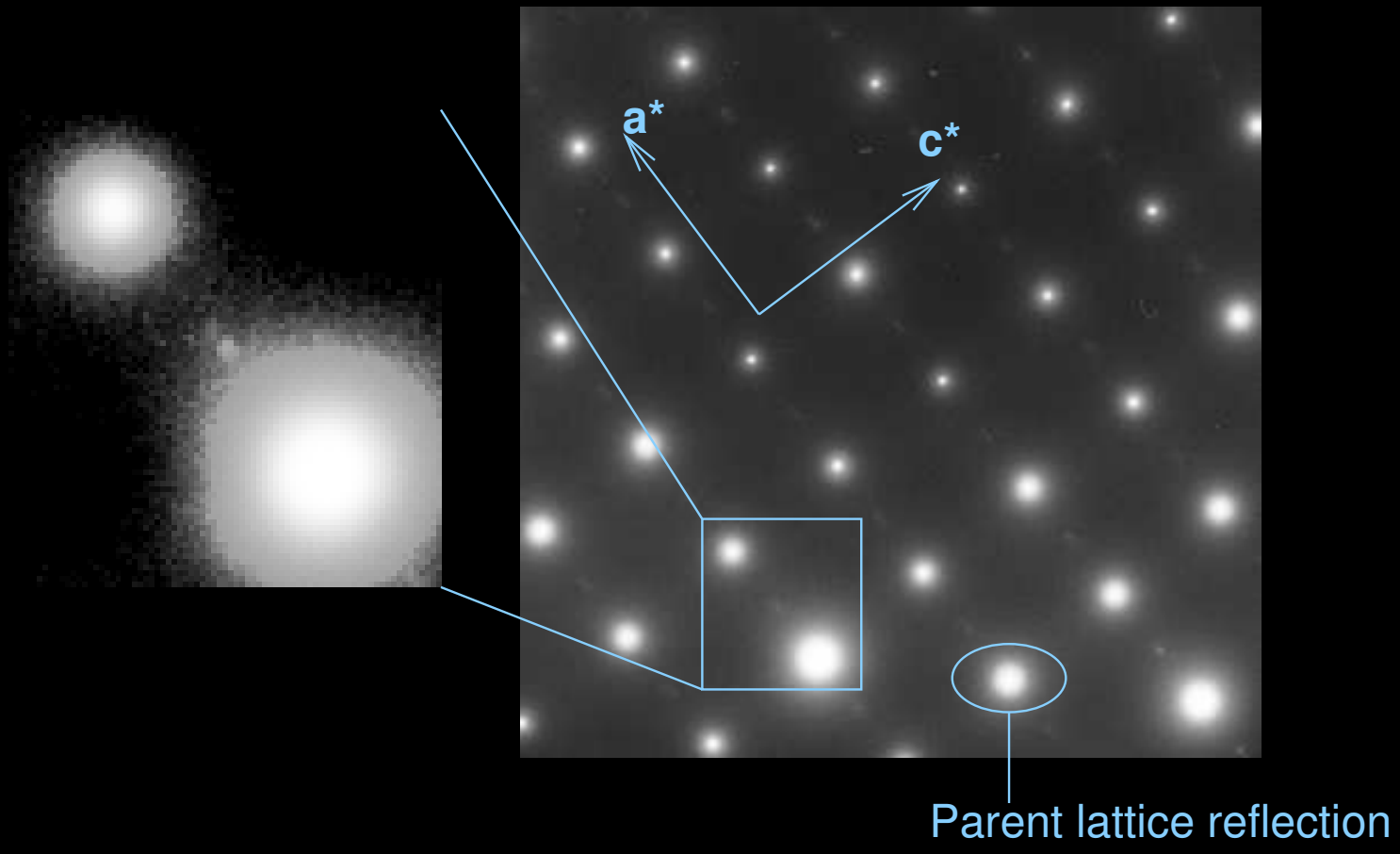
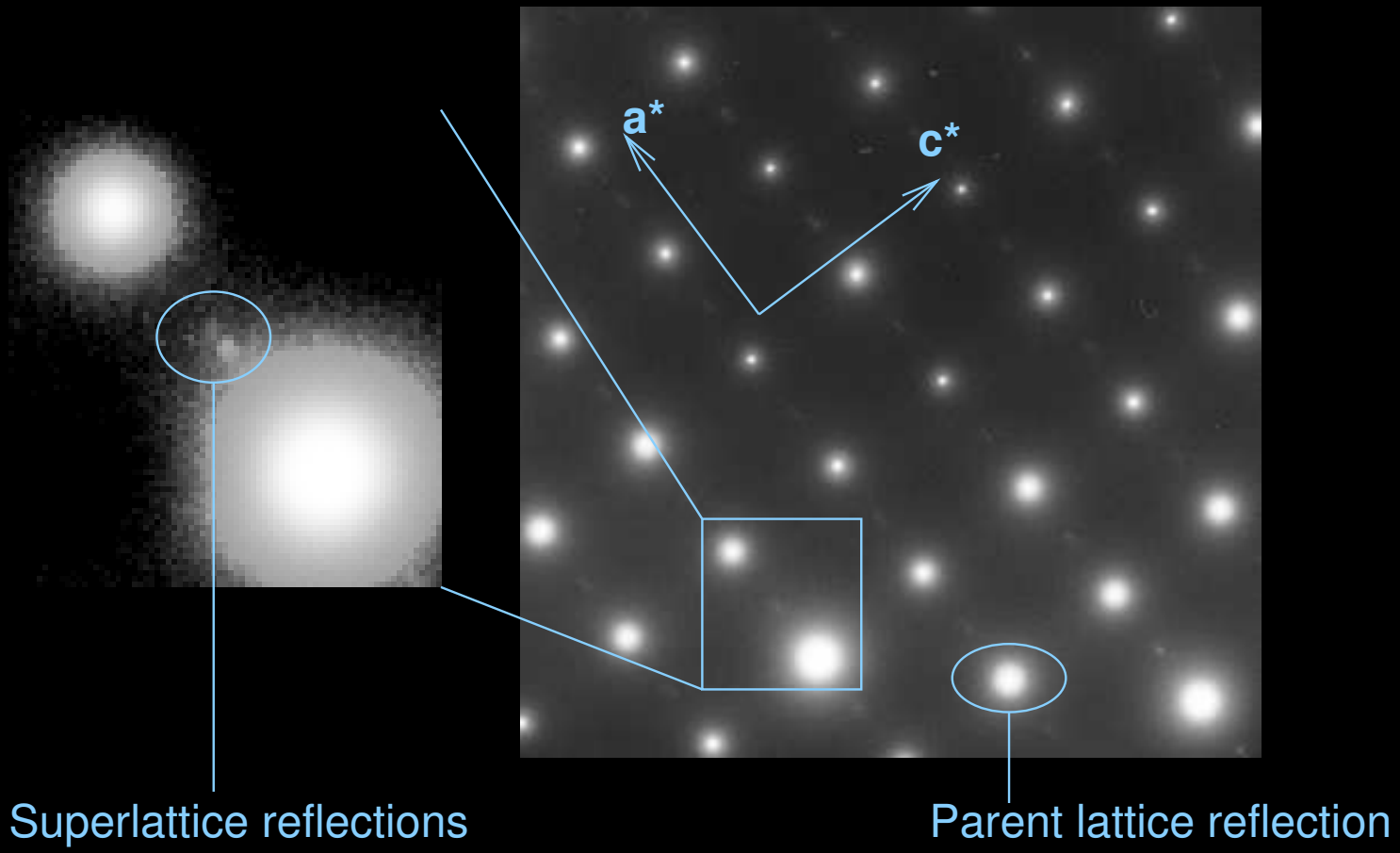
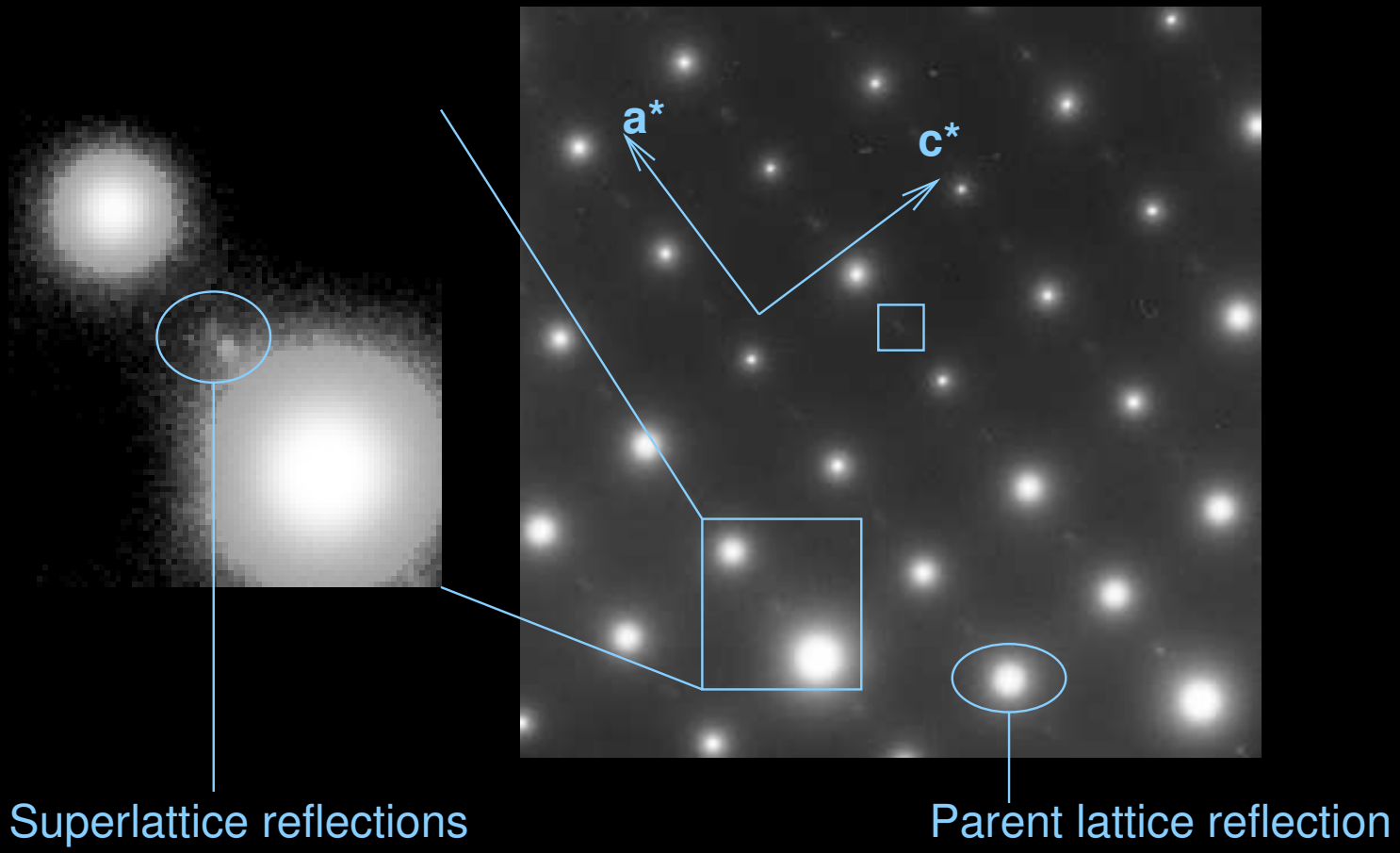


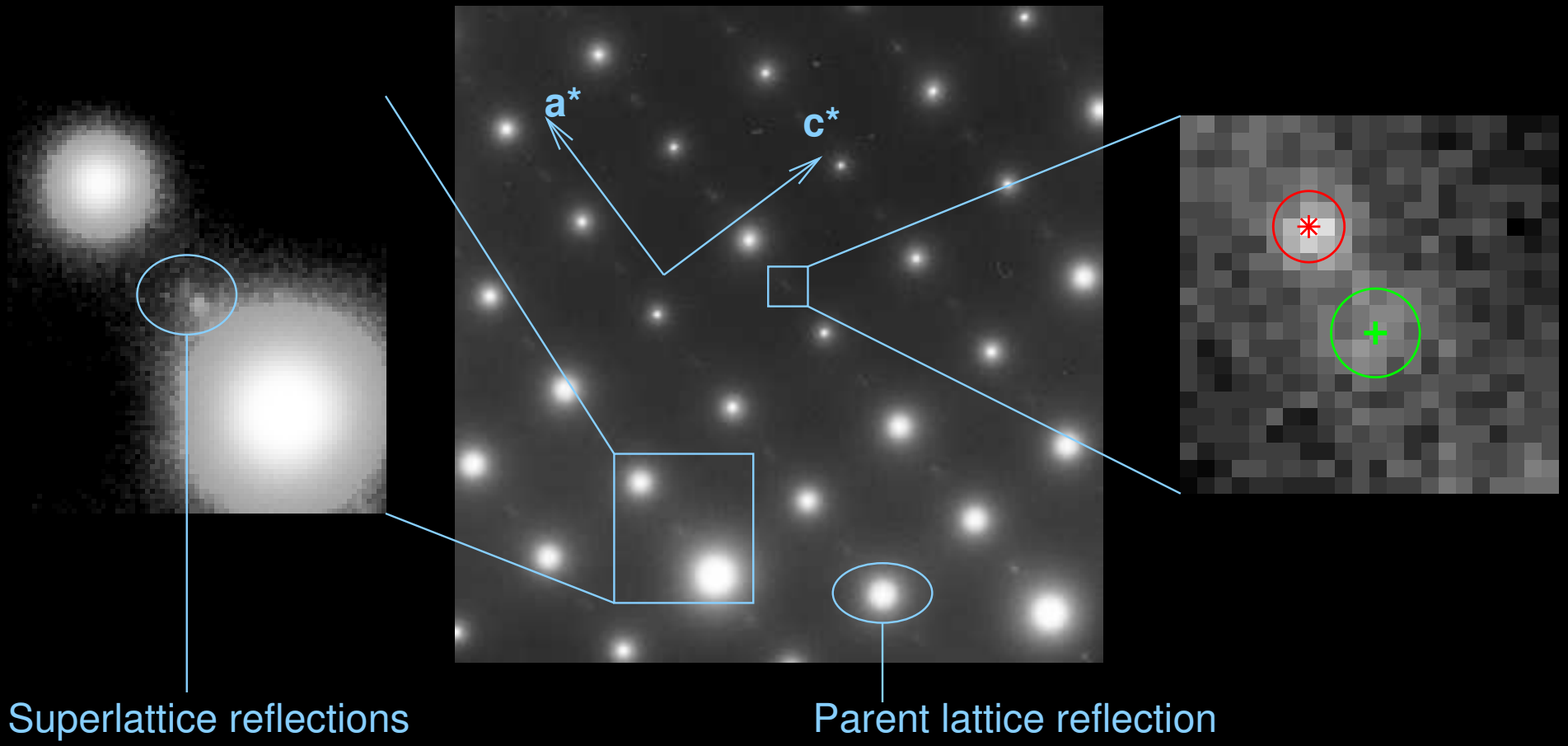
Diffraction patterns



Diffraction patterns



Diffraction patterns



TEM imaging

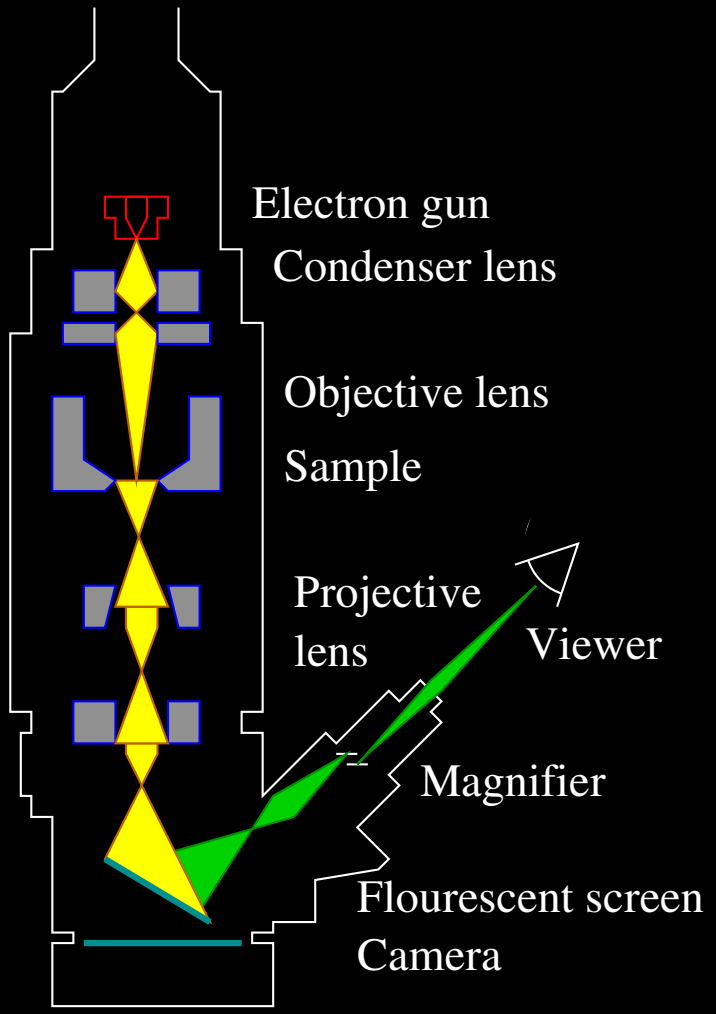


Image can be recorded on:

- CCD
  - Linear response
  - Not very robust
    - ⋆ Short exposure times only
- Film
  - Nonlinear response
    - ⋆ Response varies
  - Very robust
    - ⋆ Long exposure times possible

Images must be acquired on film.

Film response correction

- Noise is constant over the image
  - Shot noise is small
- Noise amplitide is small

$$\eta \approx \frac{\mathrm{d}f}{\mathrm{d}e}$$

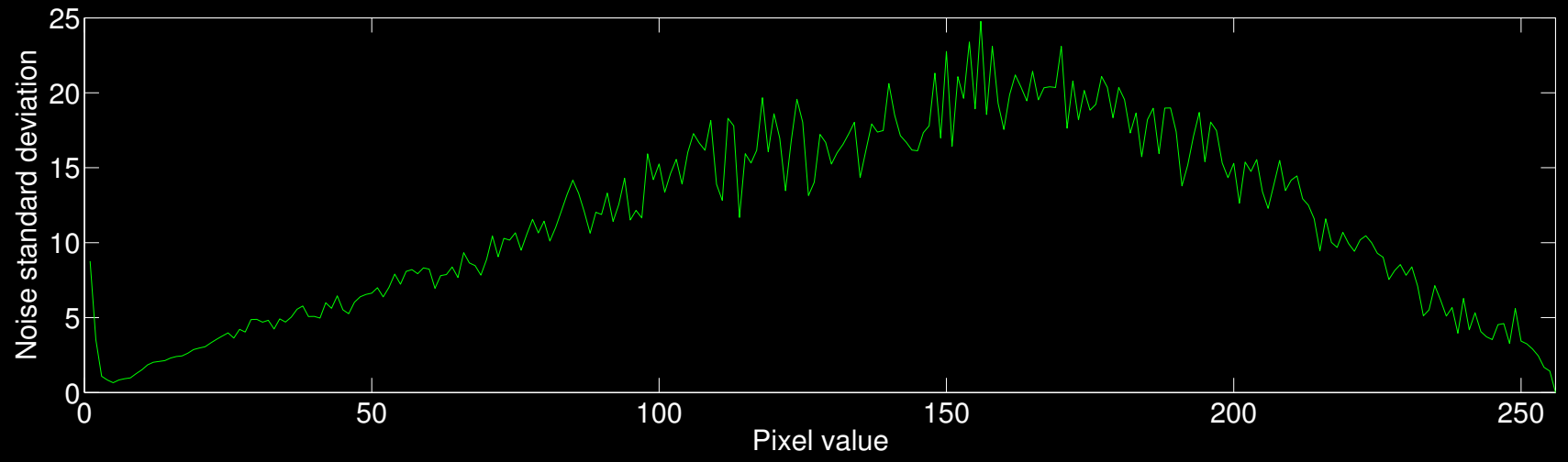
$f(e) =$ film intensity at electron intensity e

$\frac{\mathrm{d}f}{\mathrm{d}e} =$ film sensitivity

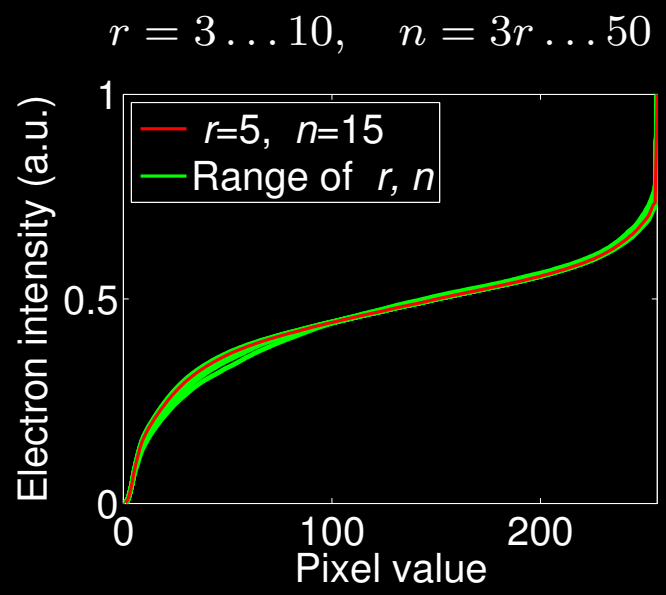
$\eta =$ noise intensity

Computing noise intensity

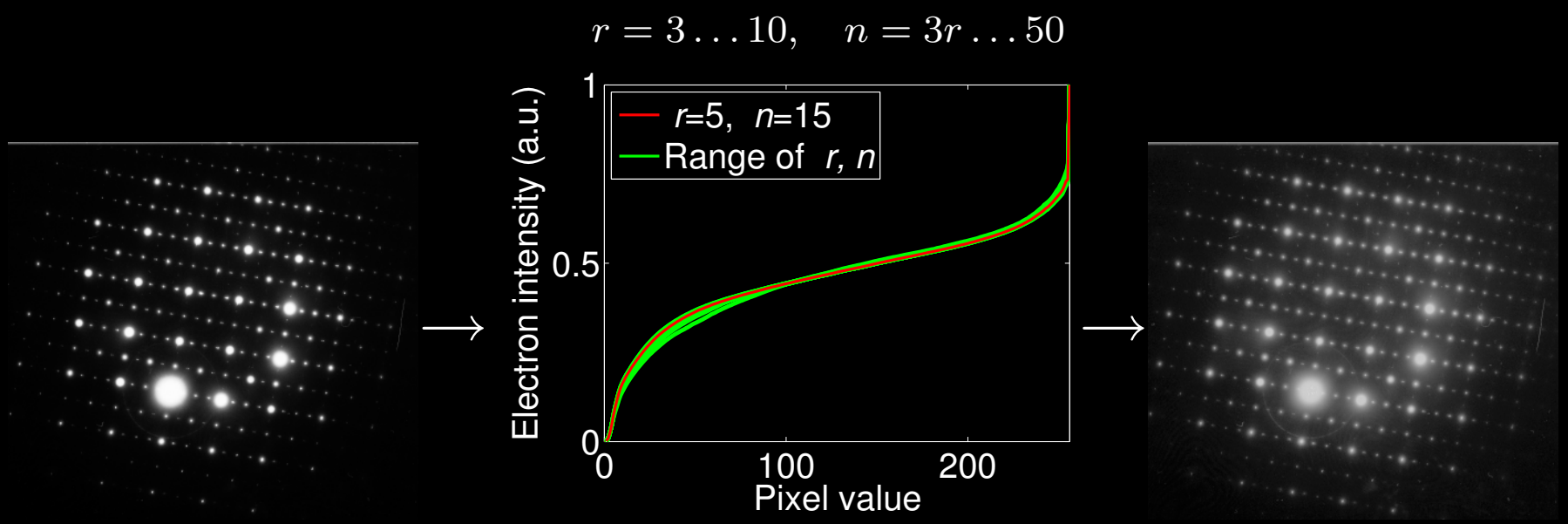
1. Smooth image
   - Horizontal smoothing by fitting local polynomial
   - Polynomial prevents spreading of spots
2. Smoothed image contains ‘true’ pixel values
3. Bin pixels according to ‘true’ intensity
4. $\eta_i = \sigma_i$



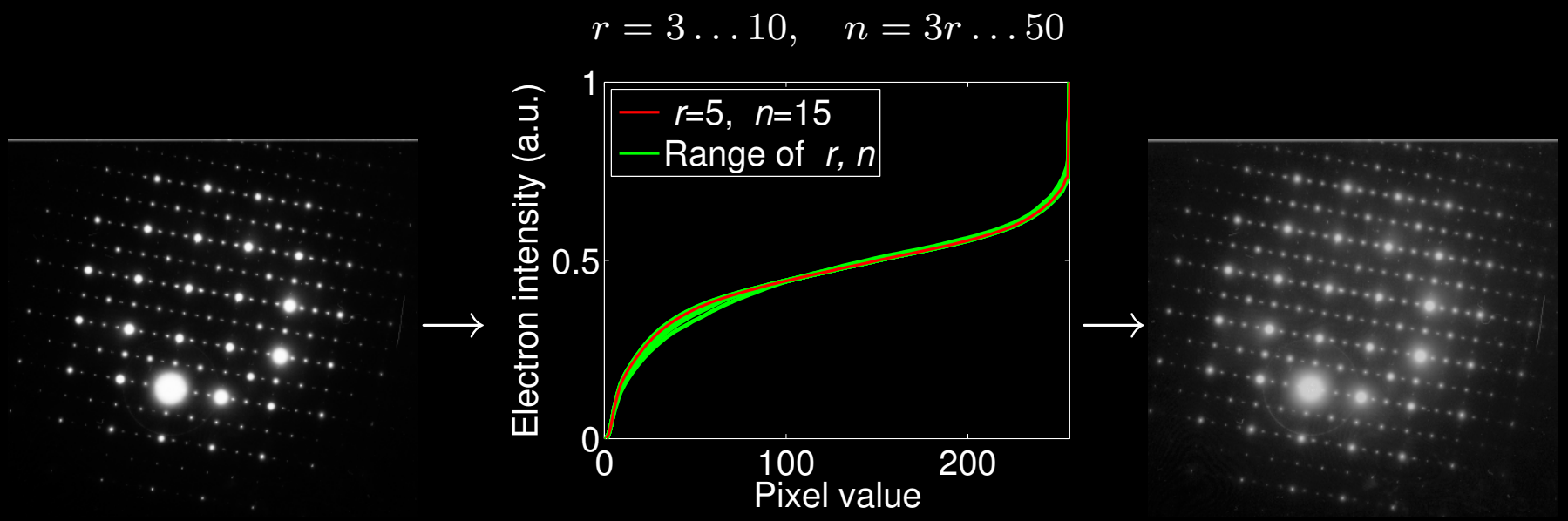
Film response

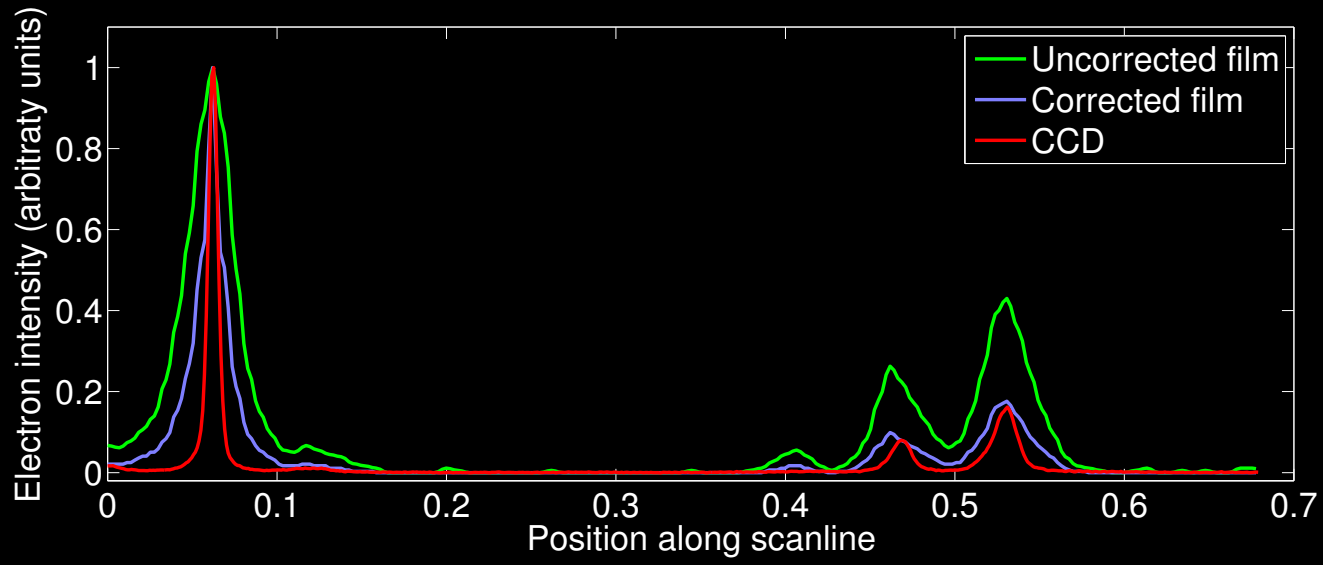


Film response



Film response

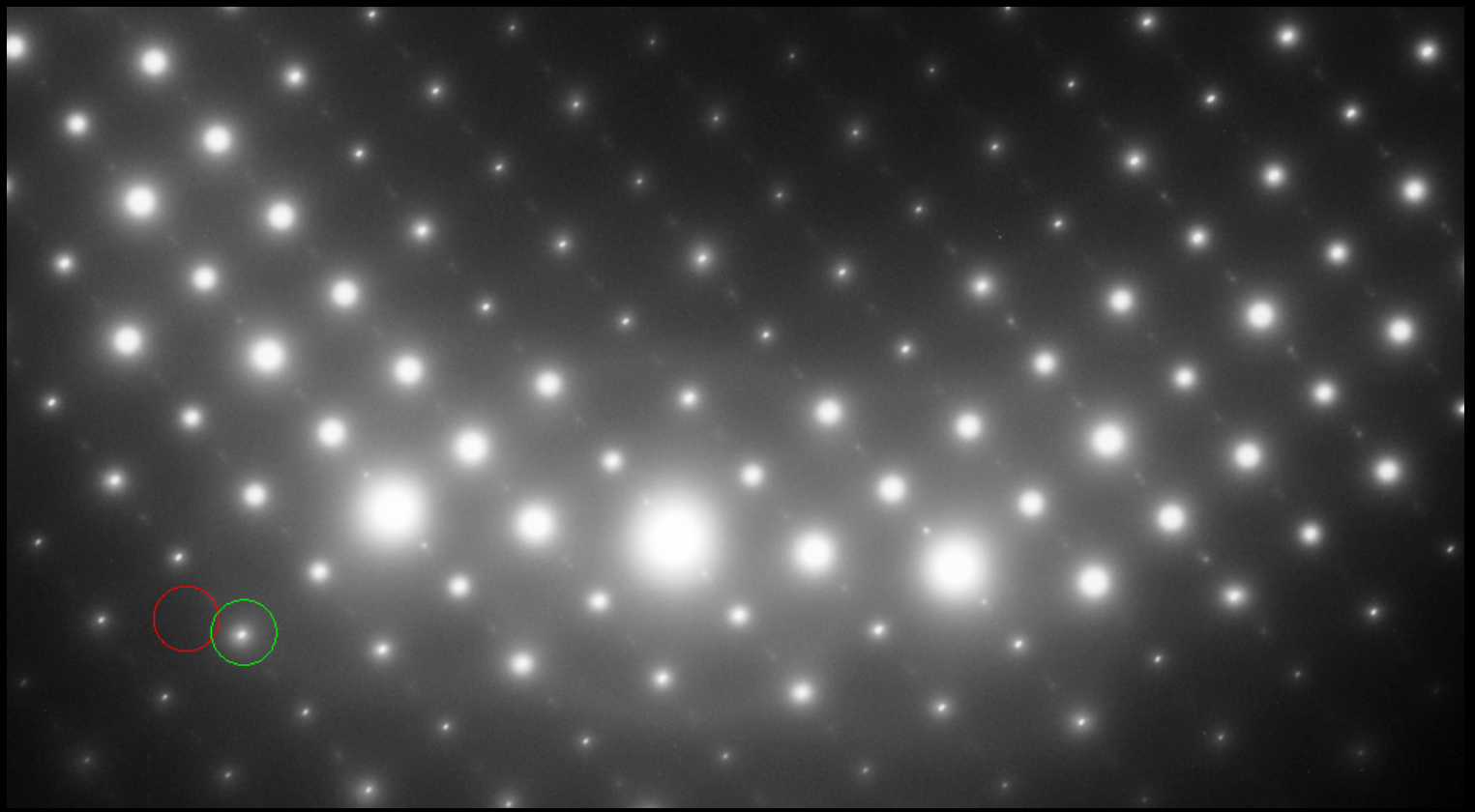




Parent lattice localisation

Mean shift:

- Compute centroid of pixels in window
- Move window centre to computed centroid



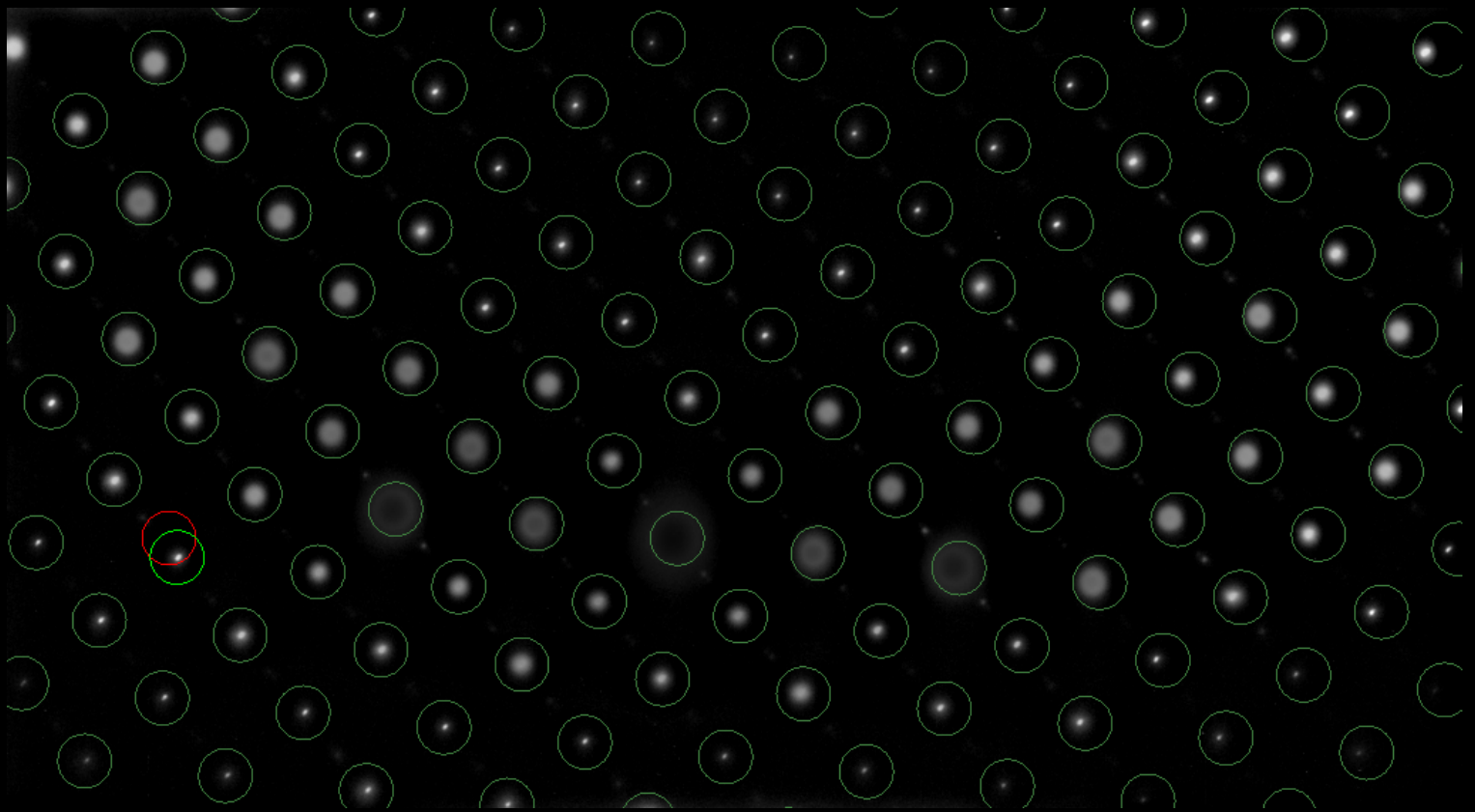
Parent lattice localisation

Mean shift:

- Removing background by filtering improves accuracy

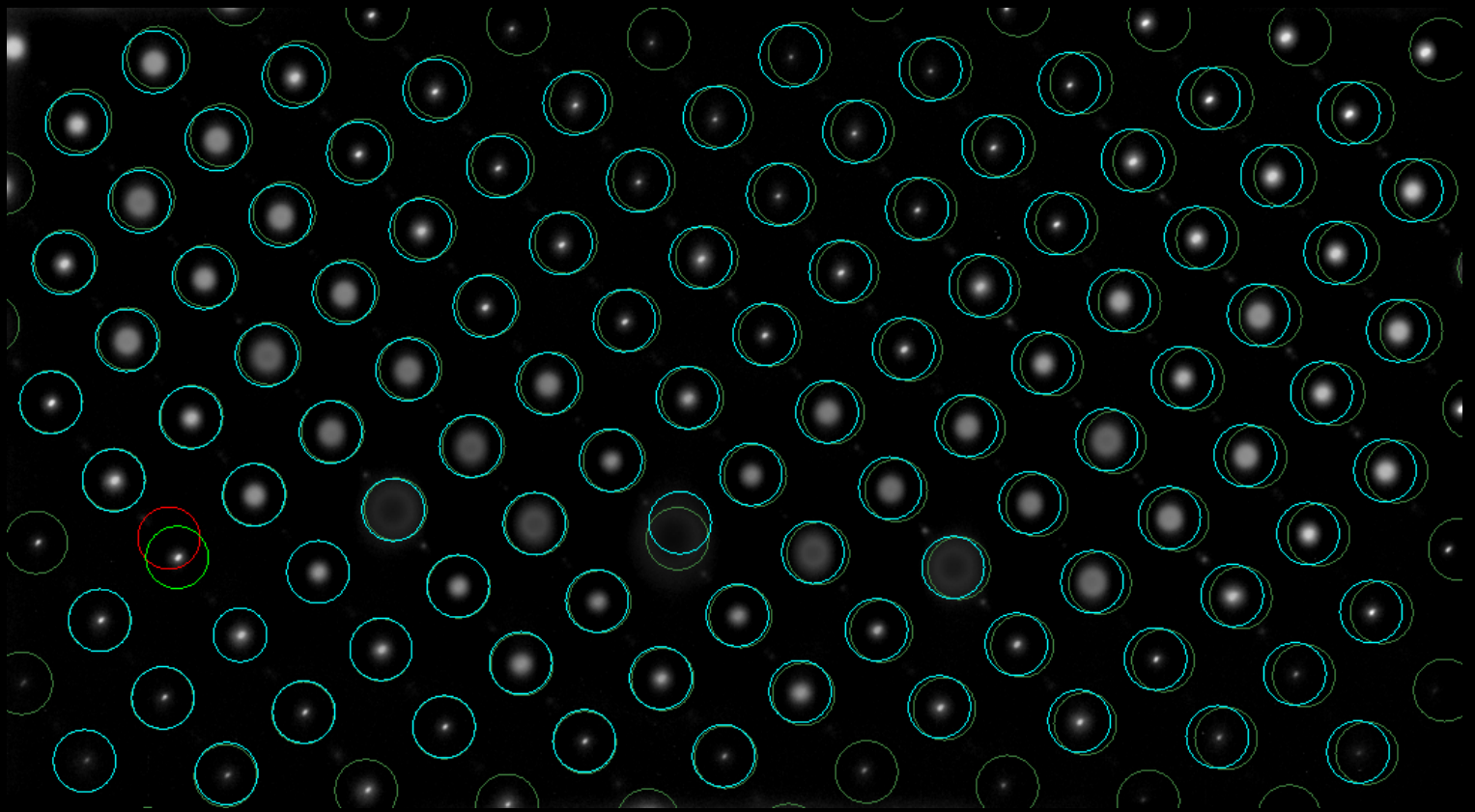
Parent lattice localisation

- Two points along $\mathbf{a}^*$ define grid
- Grid is inaccurate away from points



Parent lattice localisation

- Mean shift optimizes all points



Parent lattice refinement

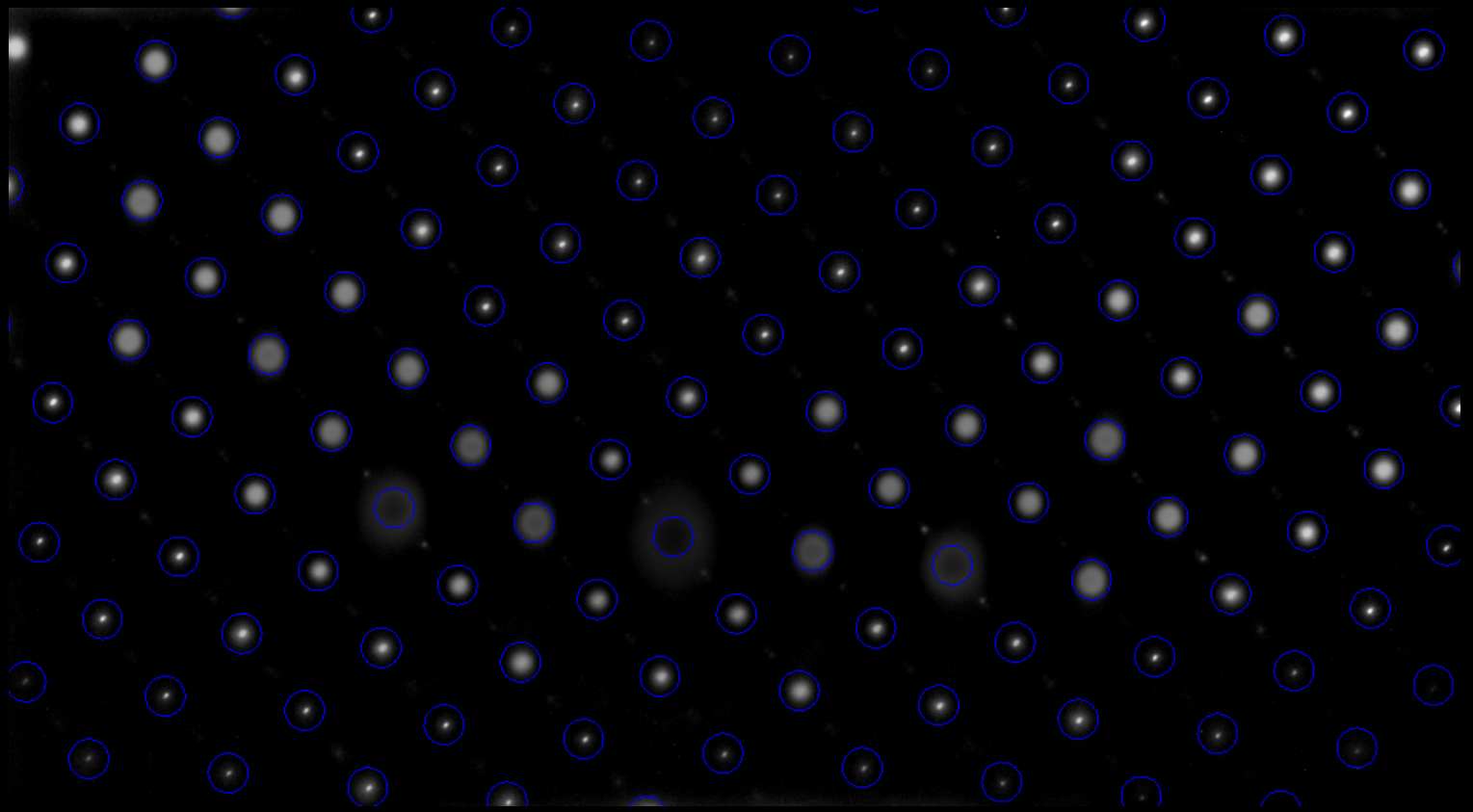
Model of imaging system:

$$\begin{pmatrix} sx \\ sy \\ s \end{pmatrix} = \begin{pmatrix} h_{1,1} & \dots & \dots & & & h_{1,2n+1} \\ h_{2,1} & \dots & \dots & & & h_{2,2n+1} \\ 0 & \dots & 0 & h_{3,2n-1} & h_{3,2n} & 1 \end{pmatrix} \begin{pmatrix} X^n \\ Y^n \\ \vdots \\ X \\ Y \\ 1 \end{pmatrix}$$

$$\begin{aligned} (X, Y) &= \text{pixel coordinate} \\ (x, y) &= \text{coordinate on grid} \end{aligned}$$

- Find $h_{1,1}, \dots, h_{3,2n}$ using reweighted least squares
- $n = 2$ is sufficient

Parent lattice refinement

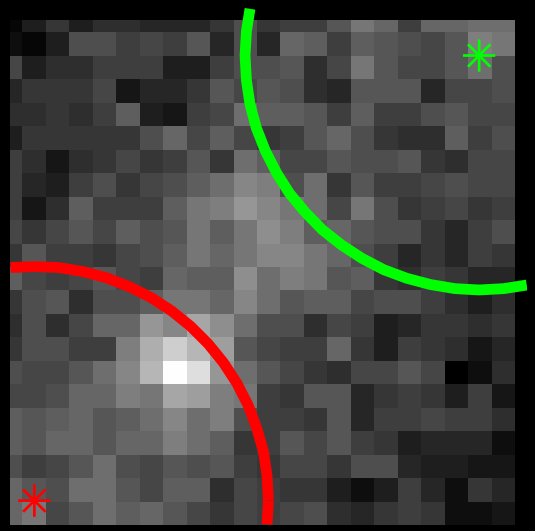


Super-lattice refinement

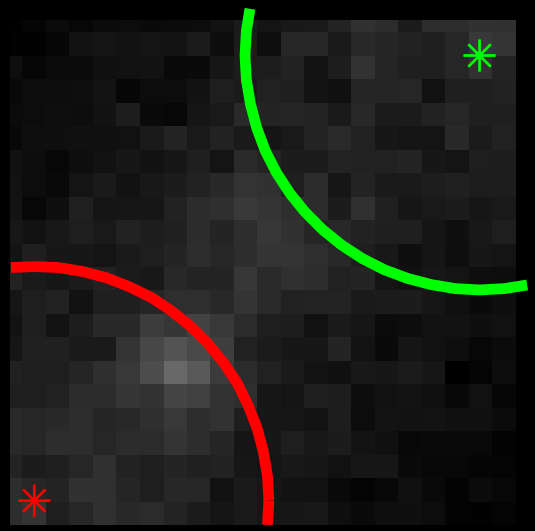
- Intensity is un-normalized probability distribution
- Spots are roughly Gaussian
- Background is roughly constant
  $\rightarrow$ Model as three component mixture model
- Fit mixture model with EM

Super-lattice refinement

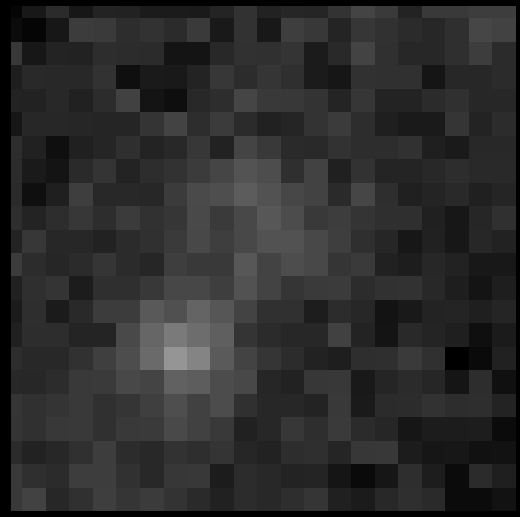
Image



Spots



Background



Super-lattice refinement

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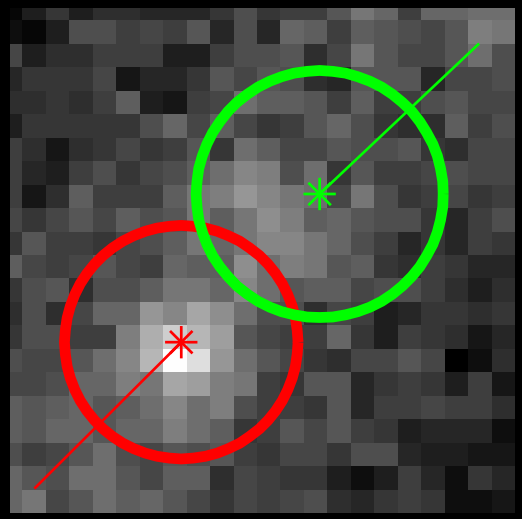

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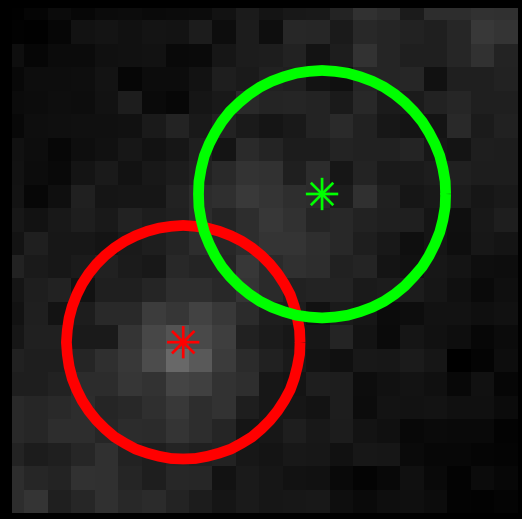

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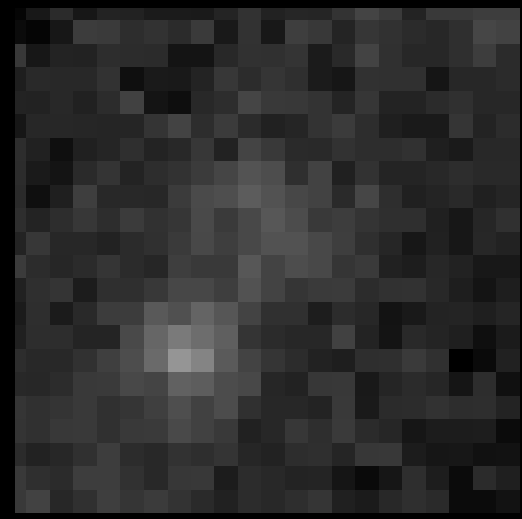

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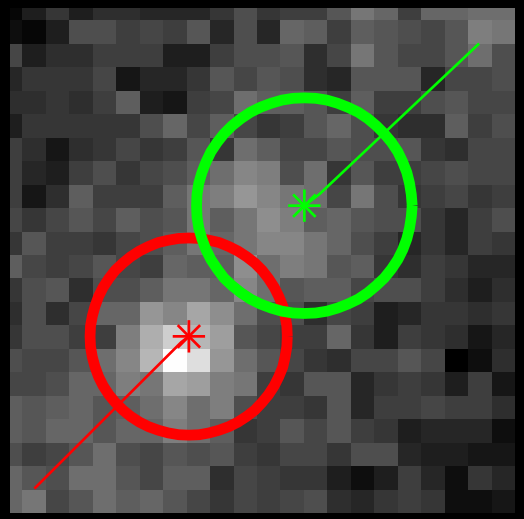

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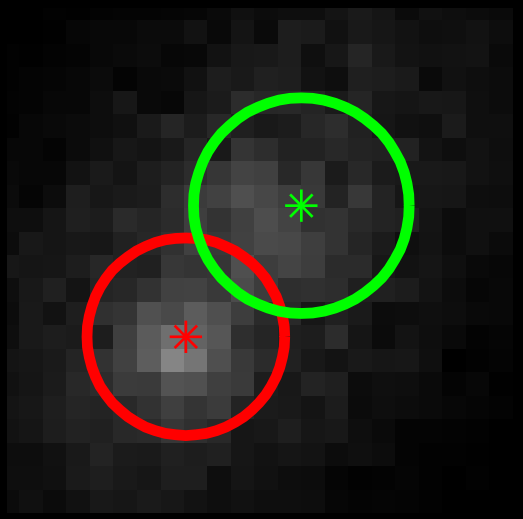

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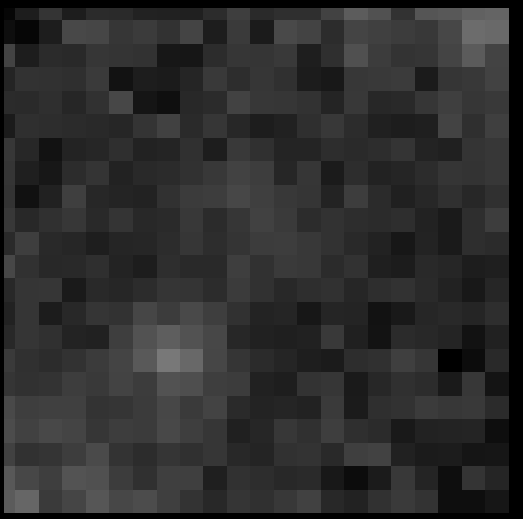

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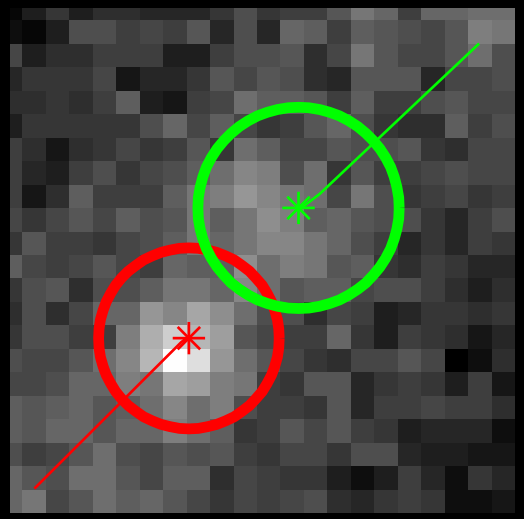
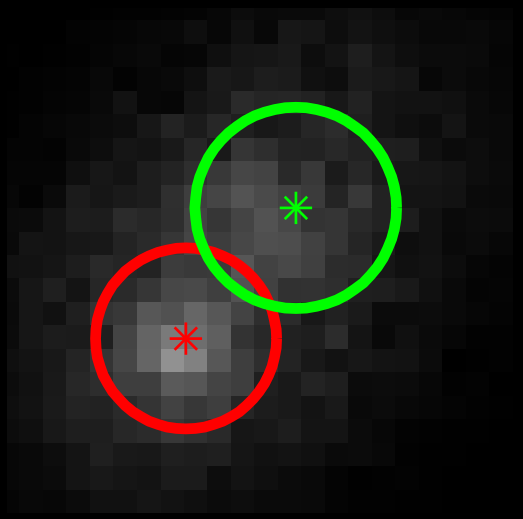


Spots



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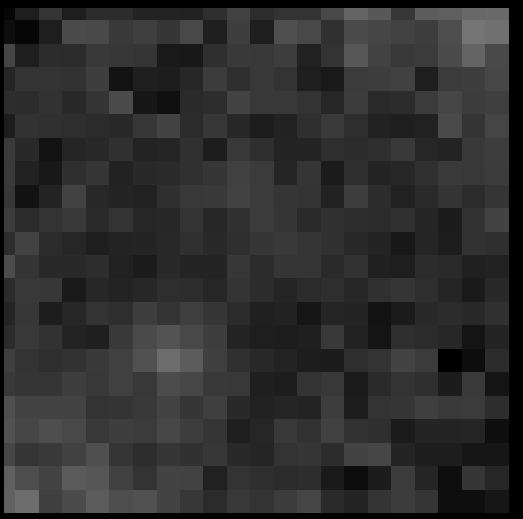

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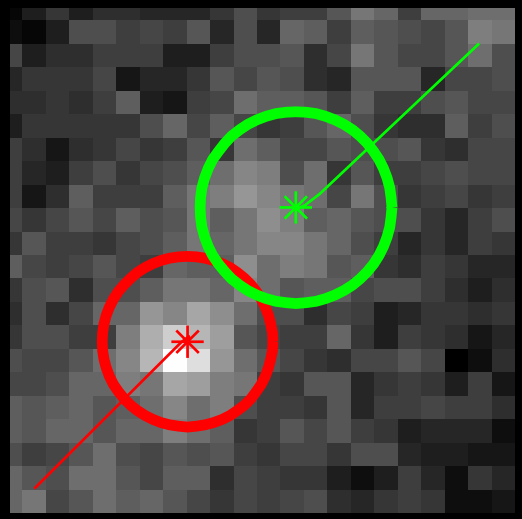
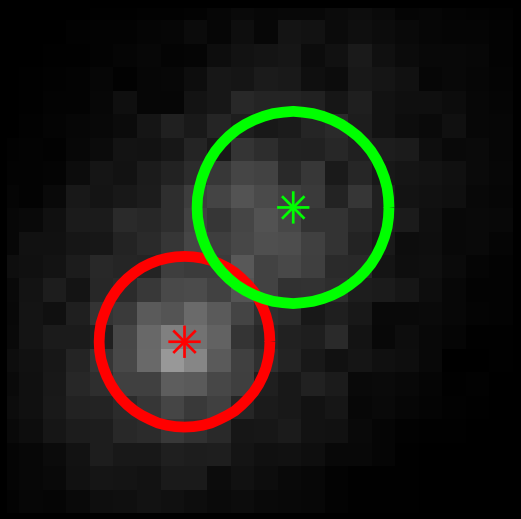


Spots



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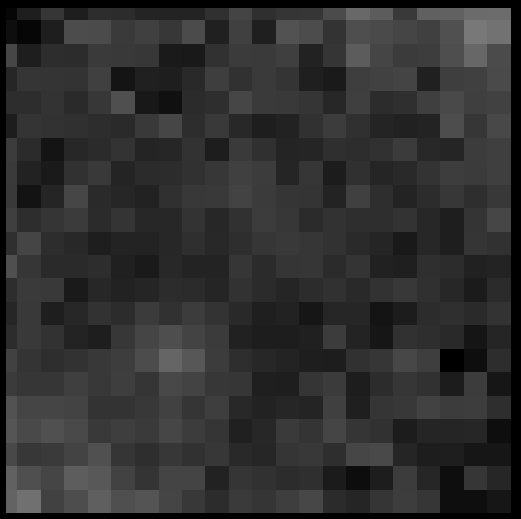

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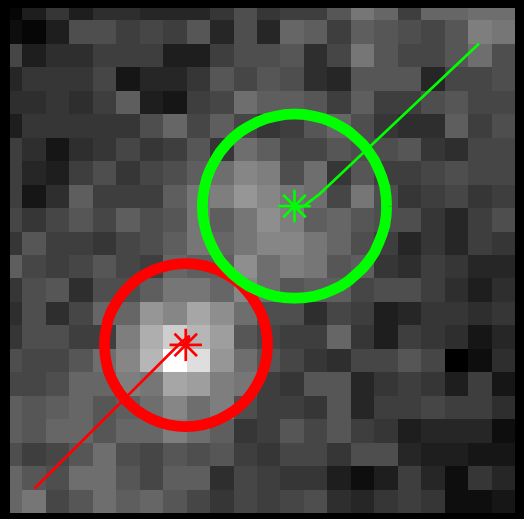
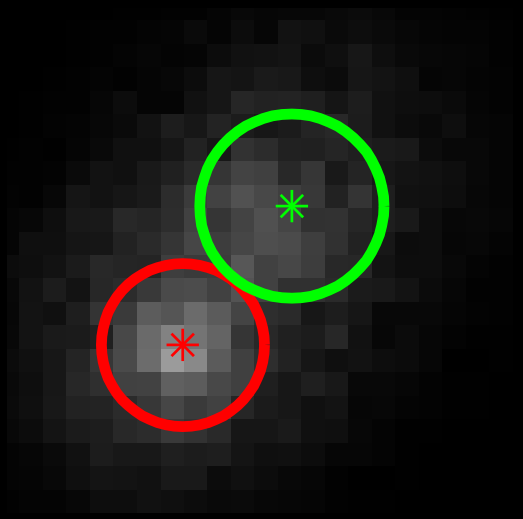


Spots



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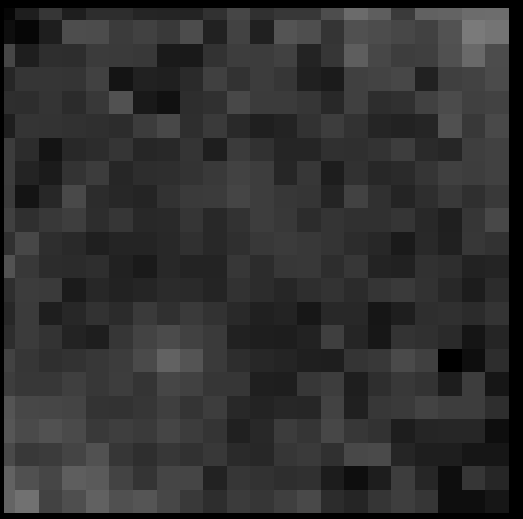

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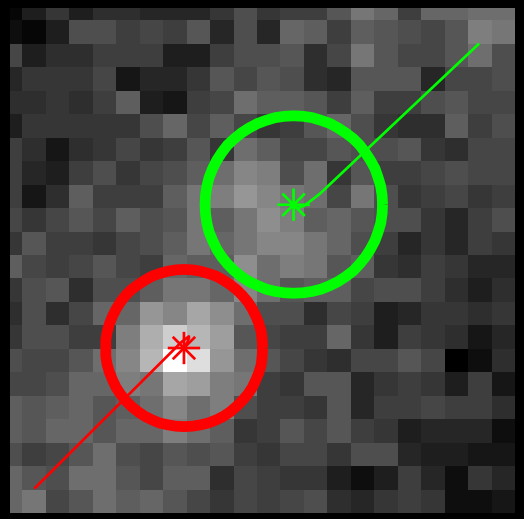

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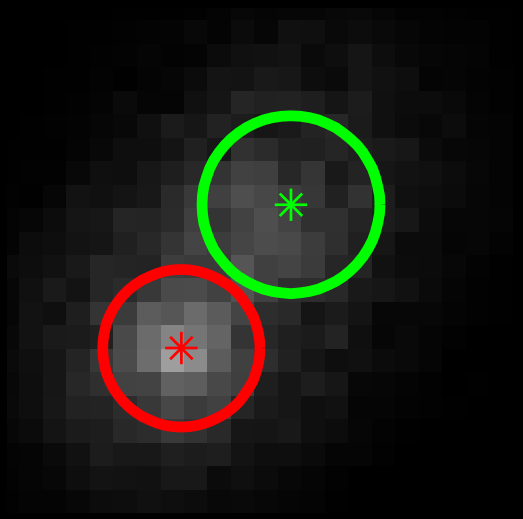

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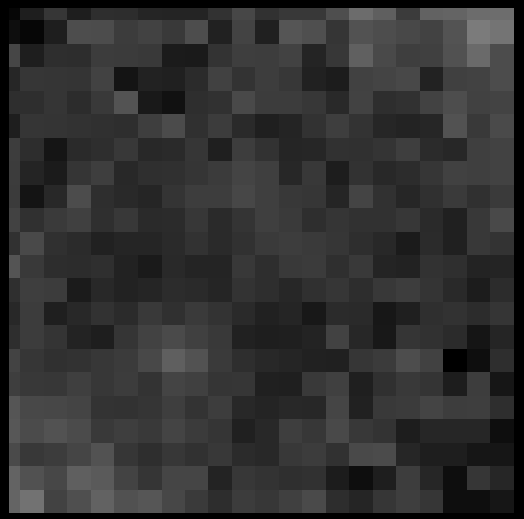

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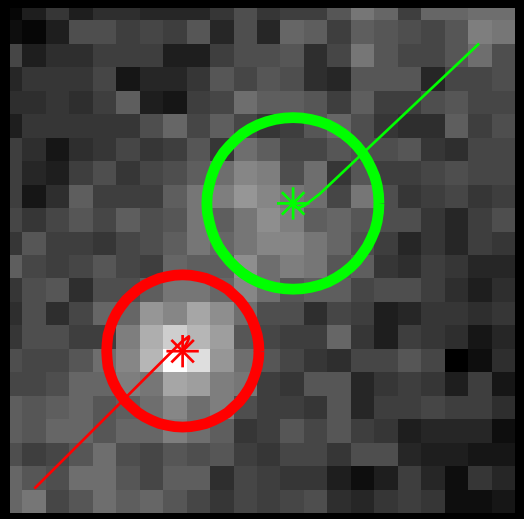
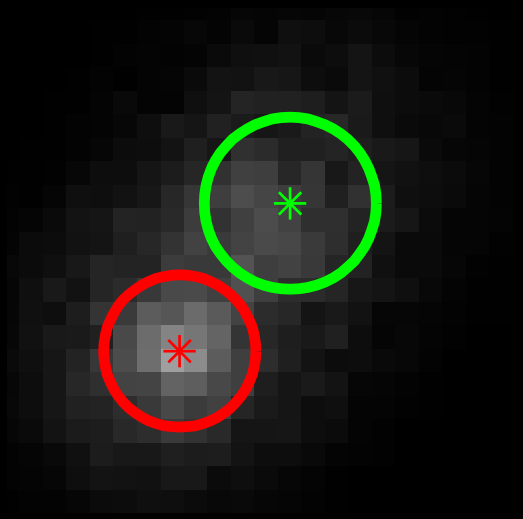


Spots



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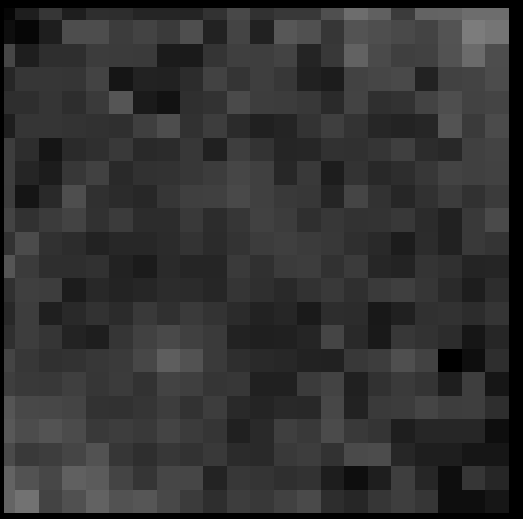

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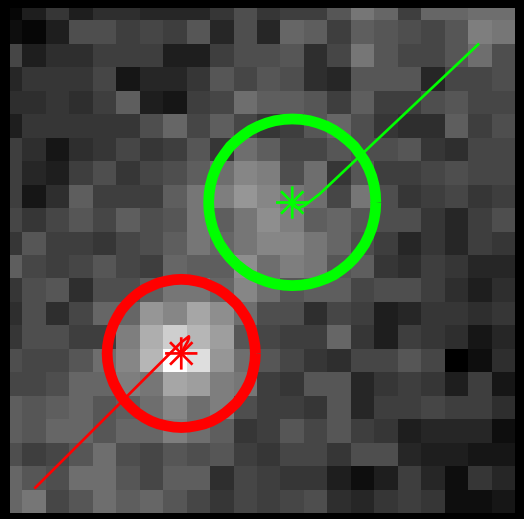

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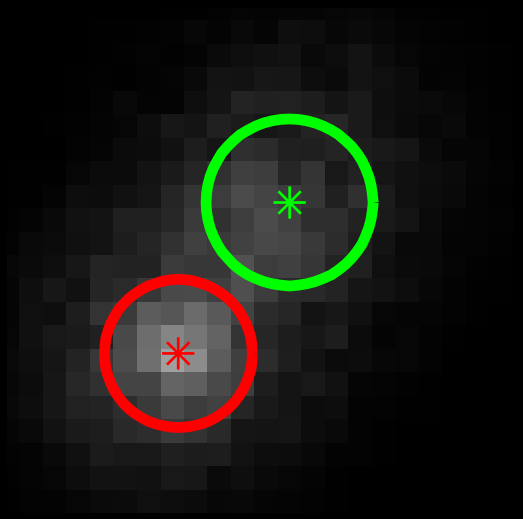

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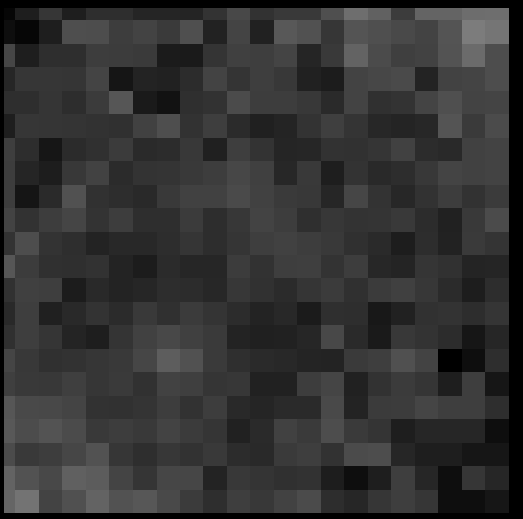

Super-lattice refinement

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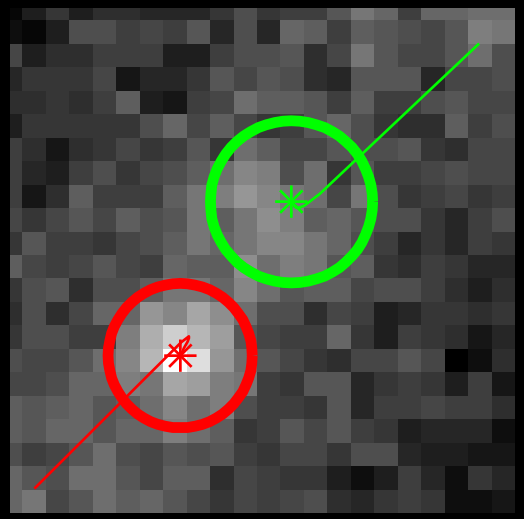
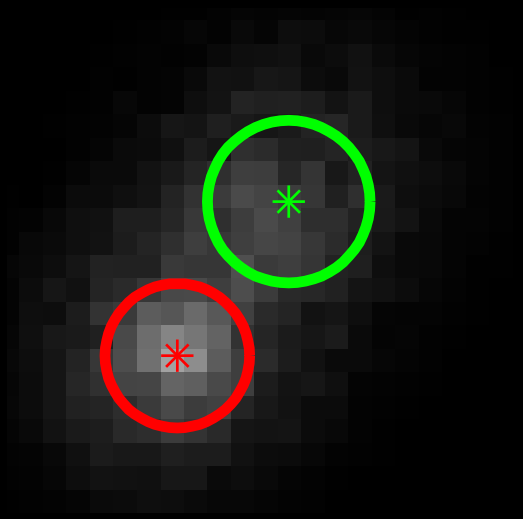


Spots



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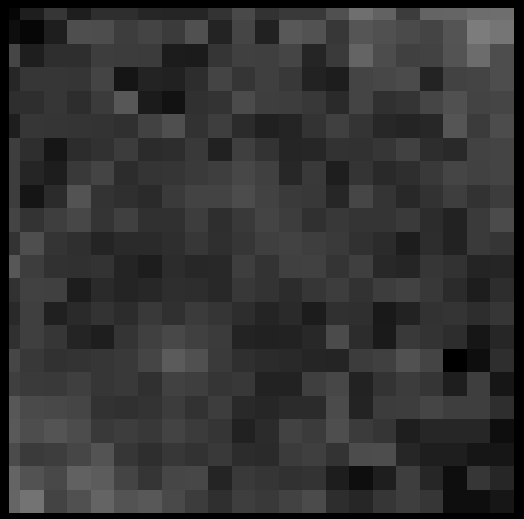

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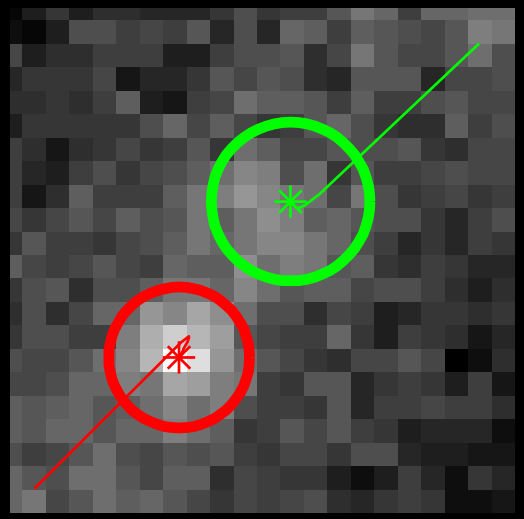
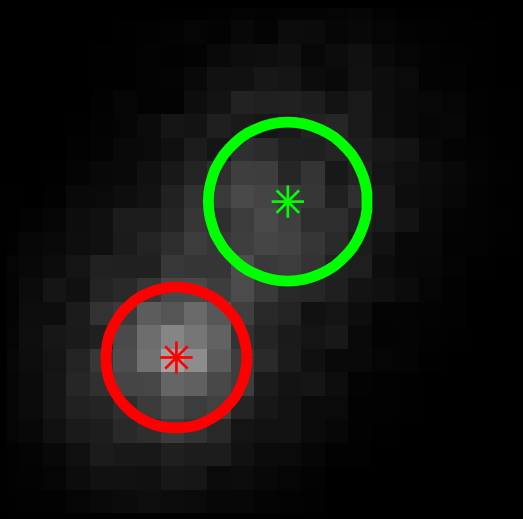
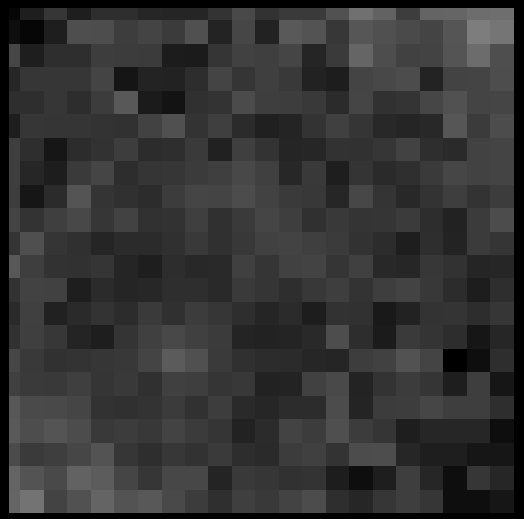


Spots

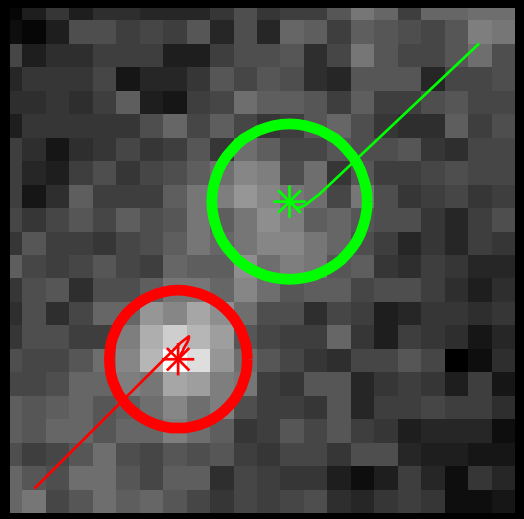


Background



Super-lattice refinement

Image



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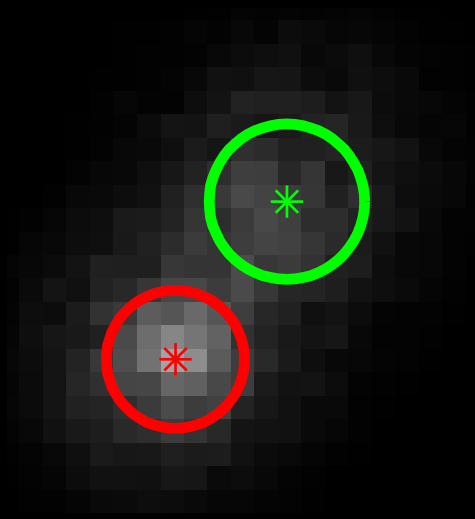

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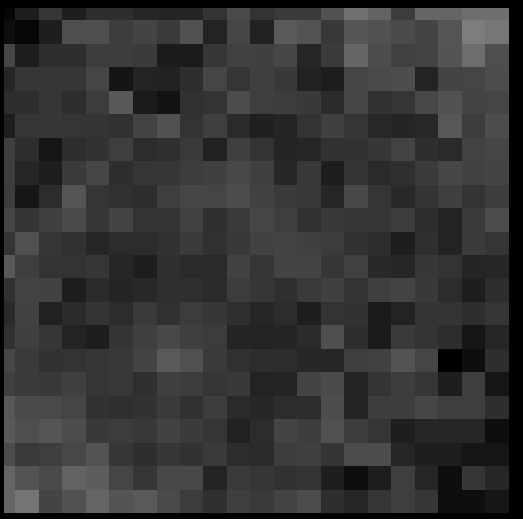

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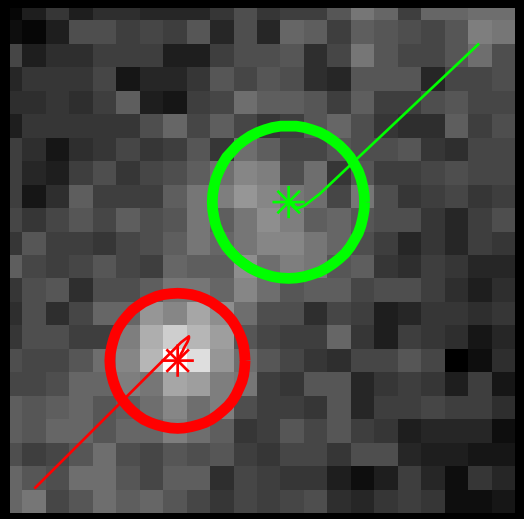

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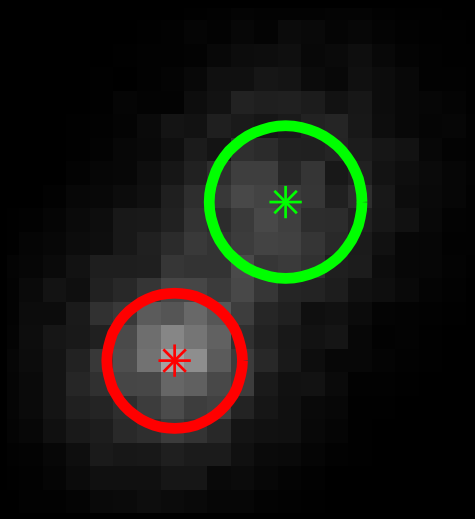

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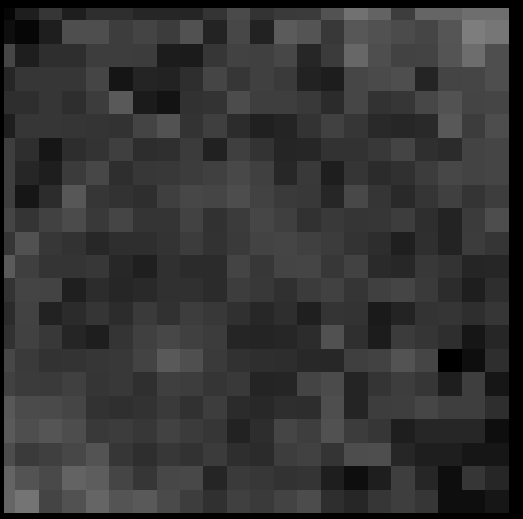

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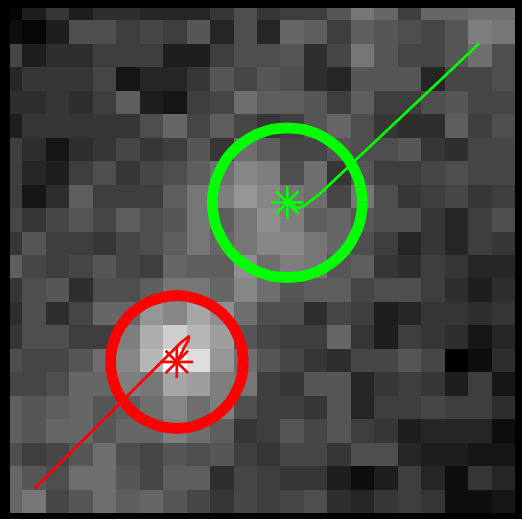

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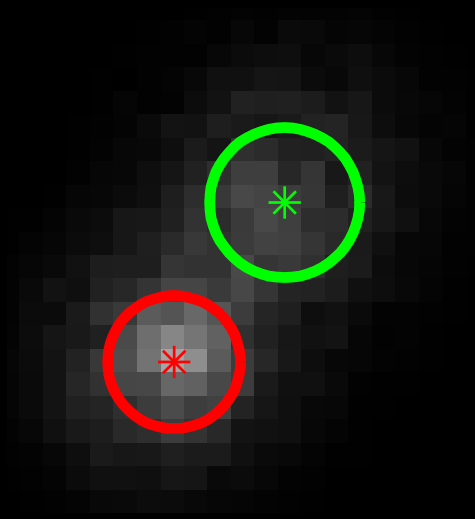

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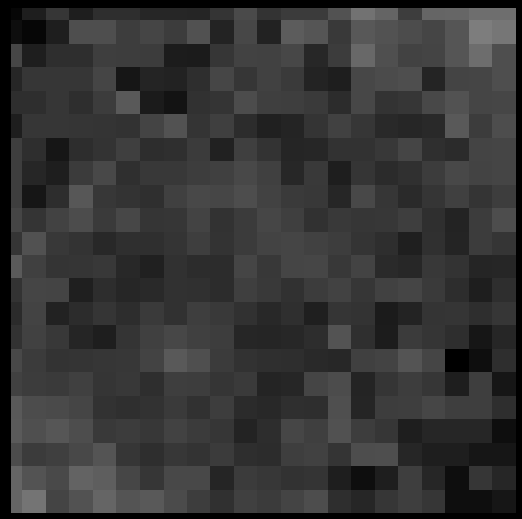

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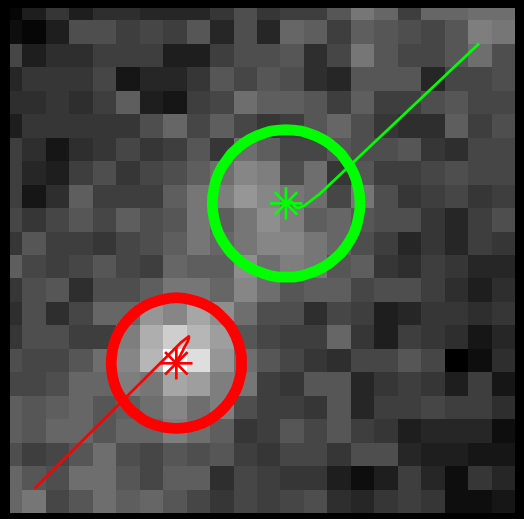

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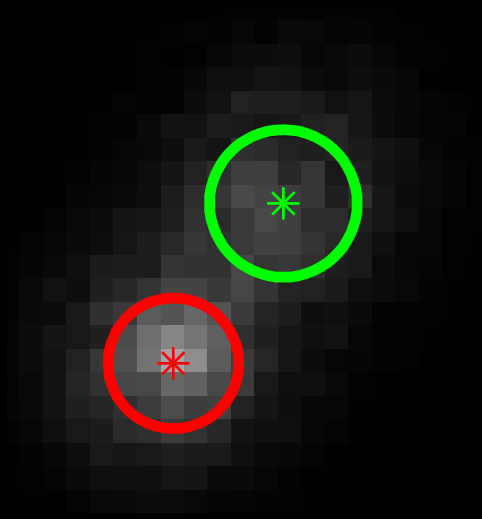

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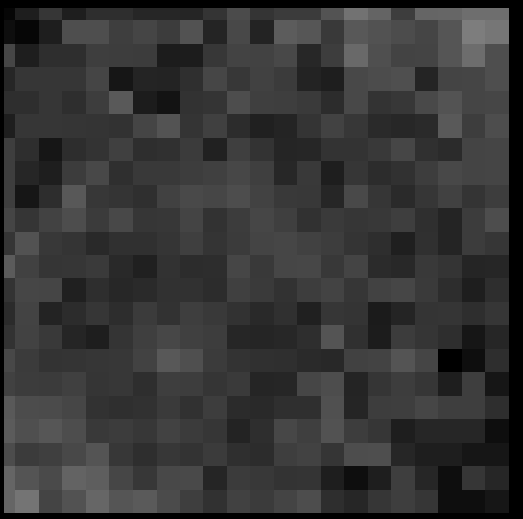

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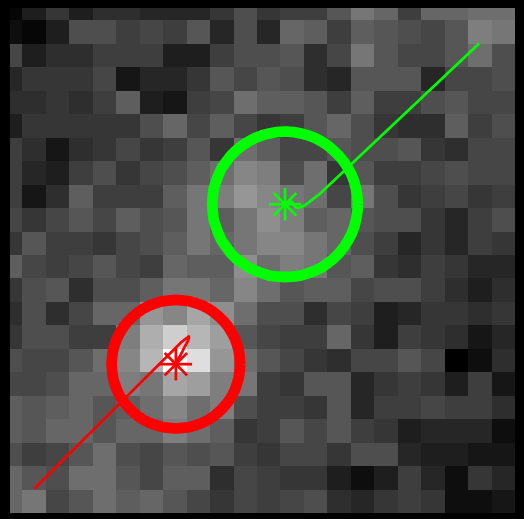

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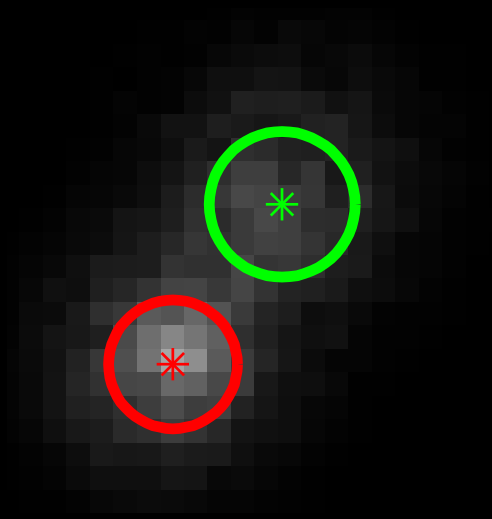

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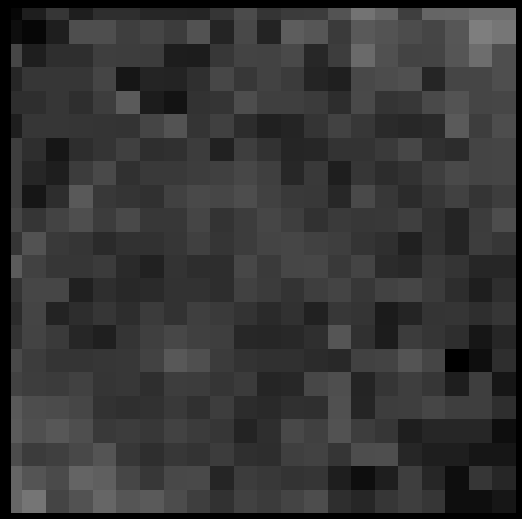

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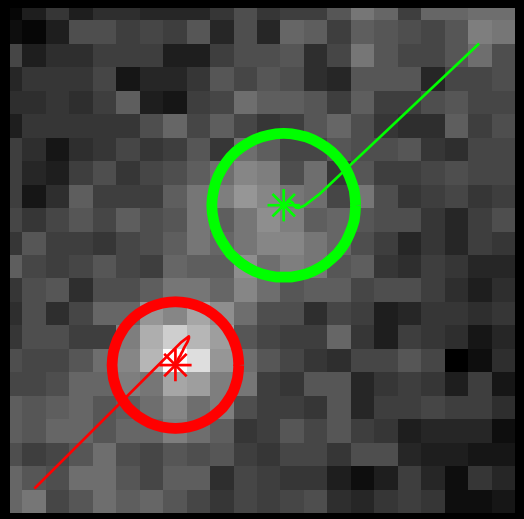

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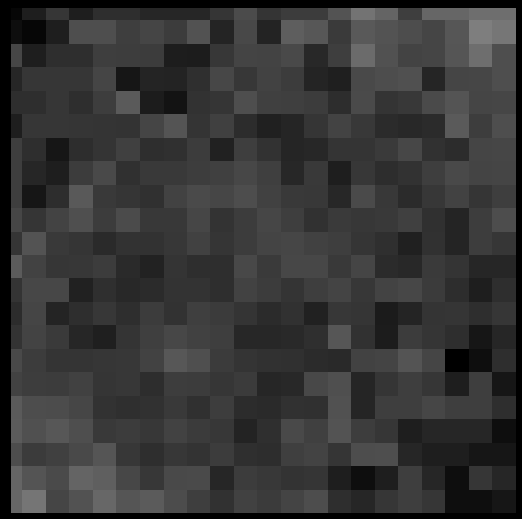

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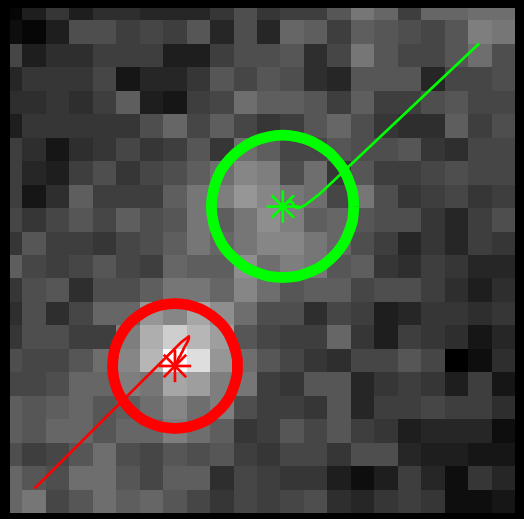

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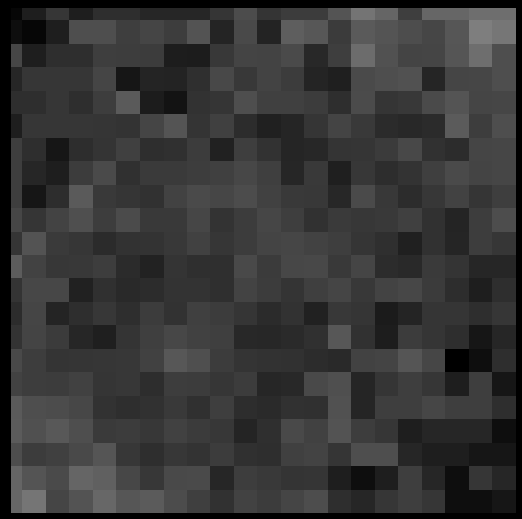

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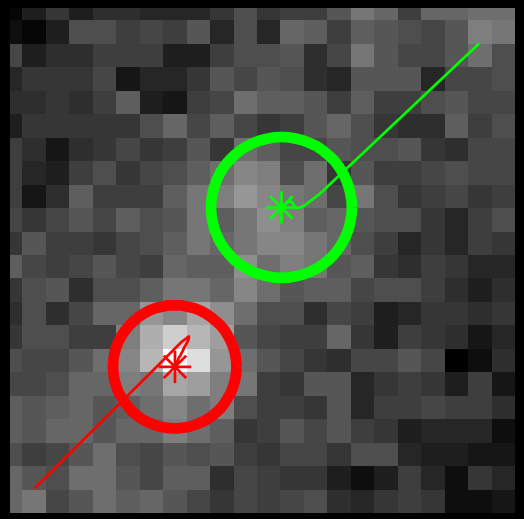

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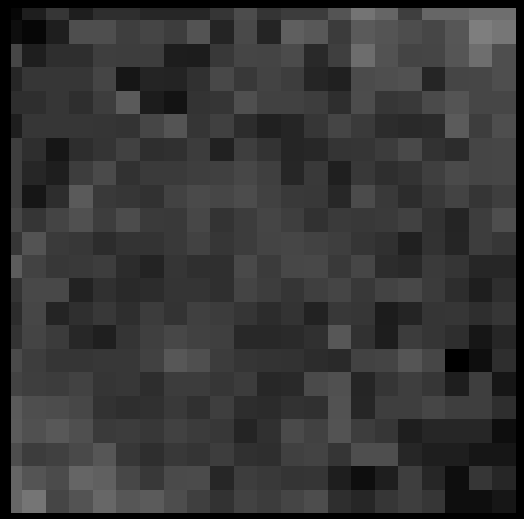

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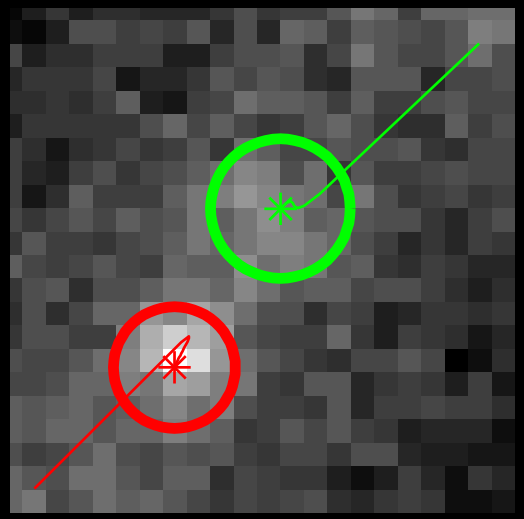

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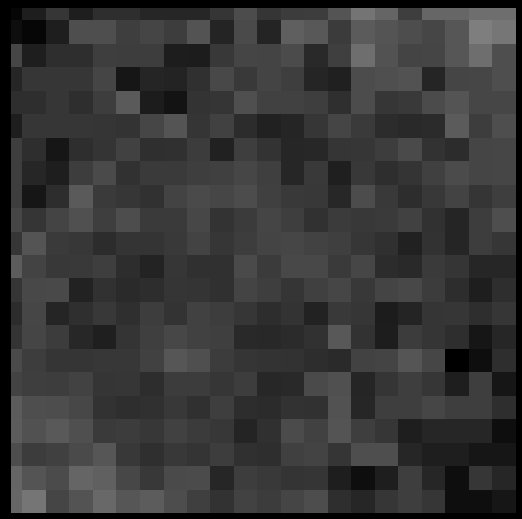

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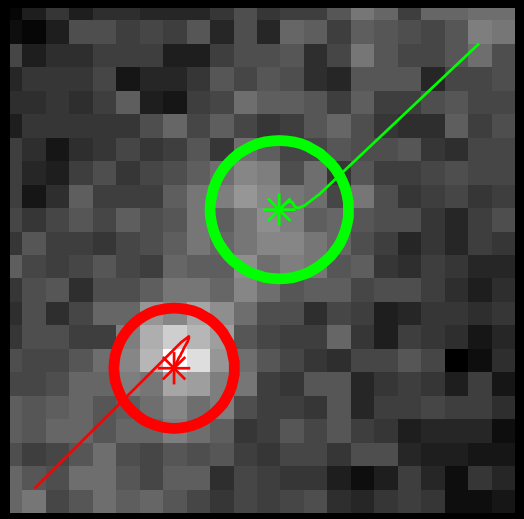

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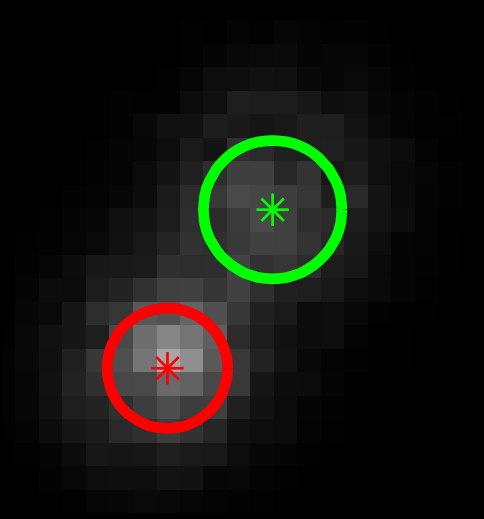

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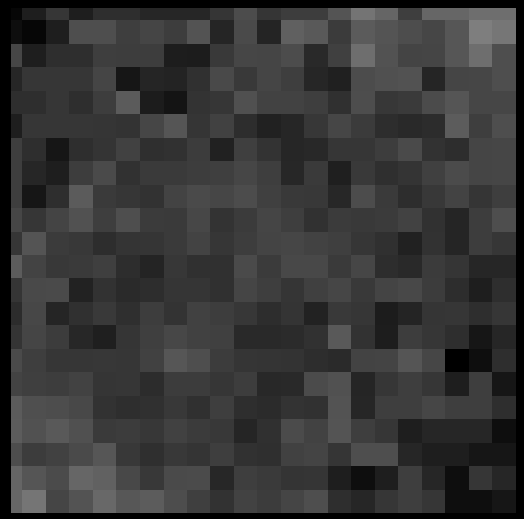

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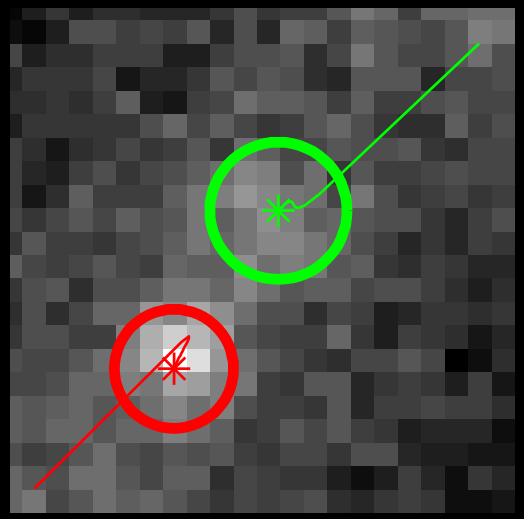

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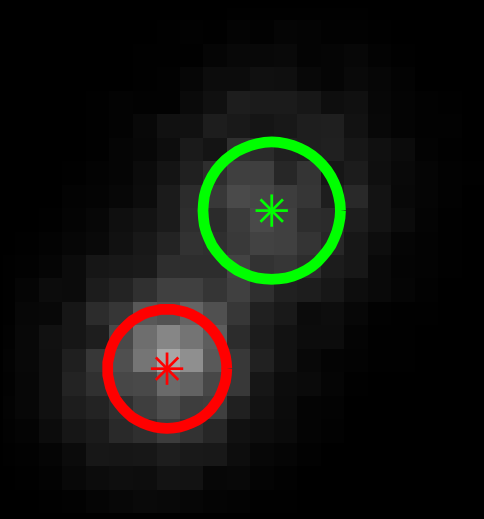

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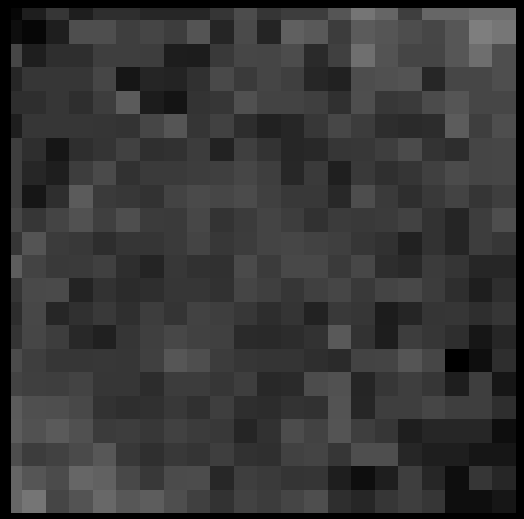

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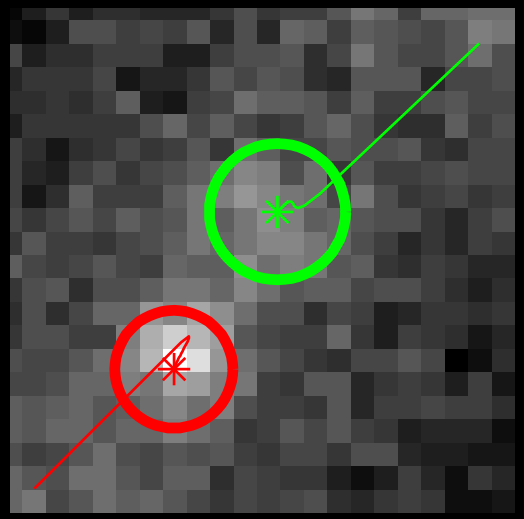

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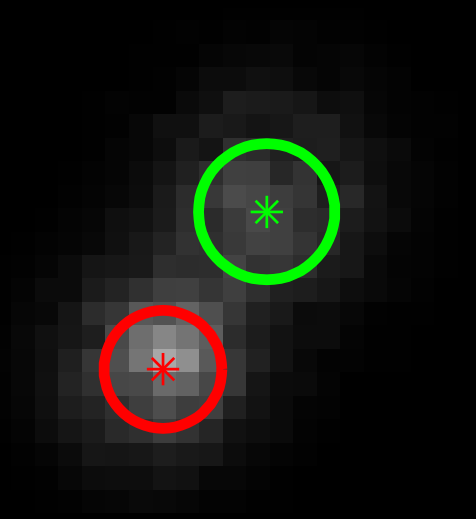

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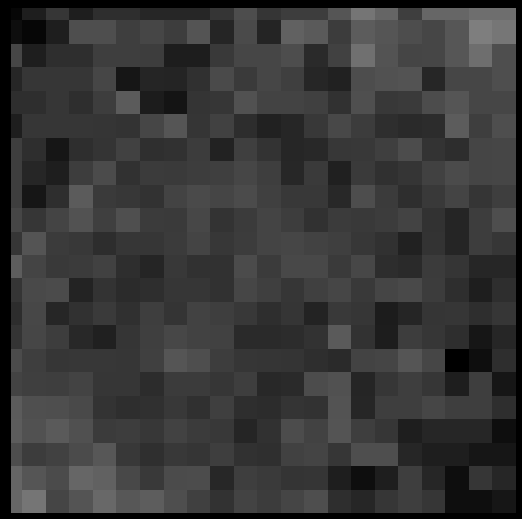

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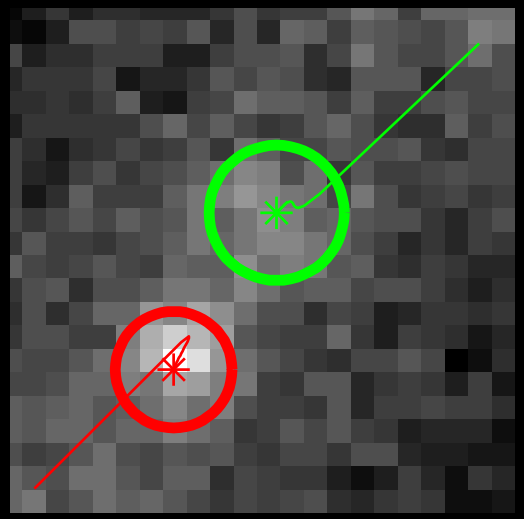

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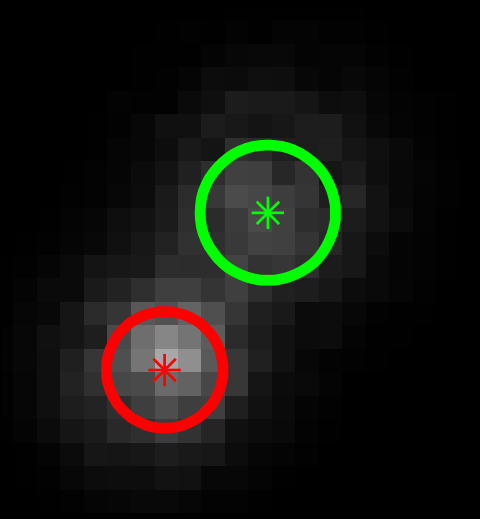

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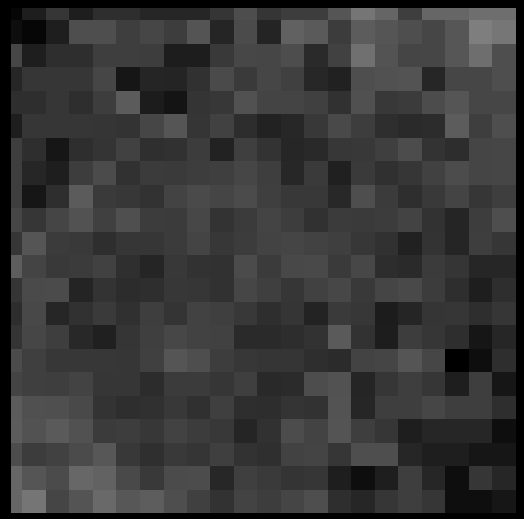

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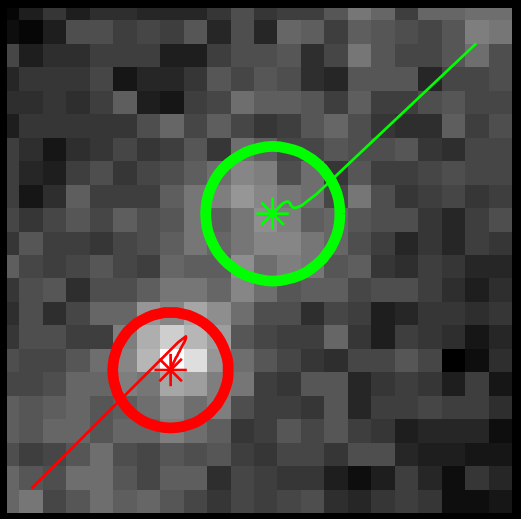

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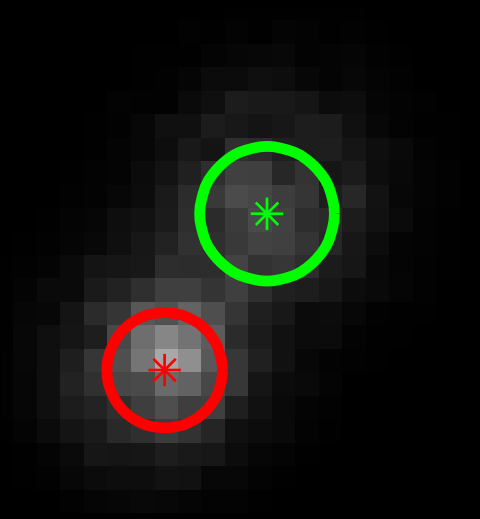

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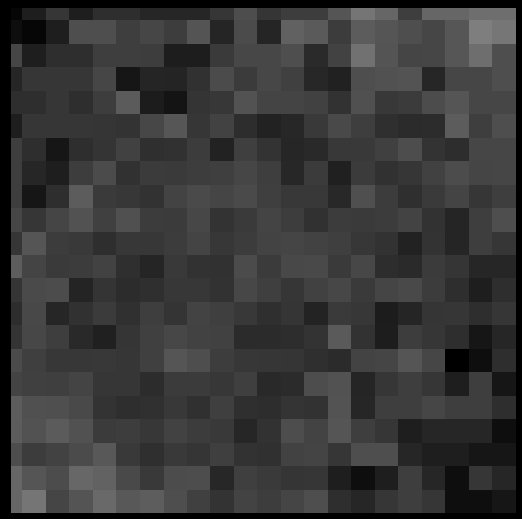

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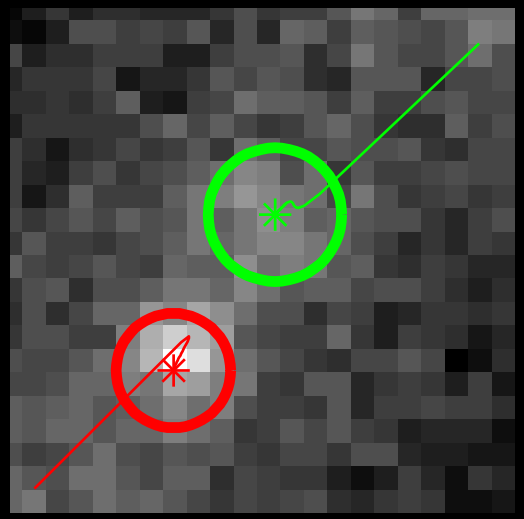

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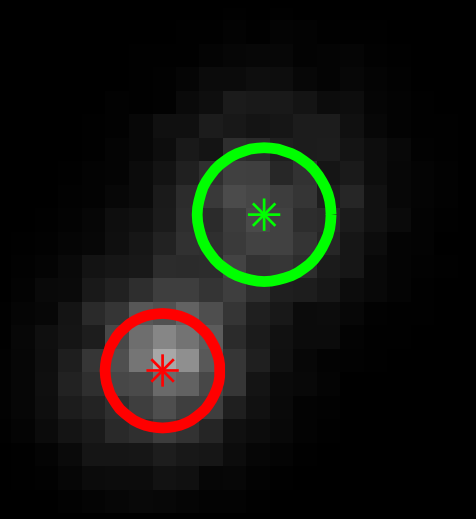

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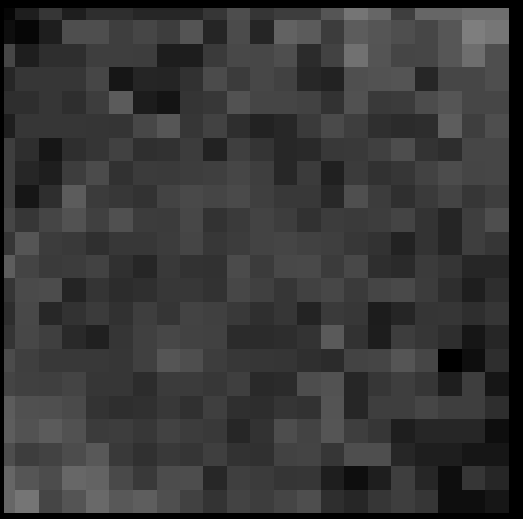

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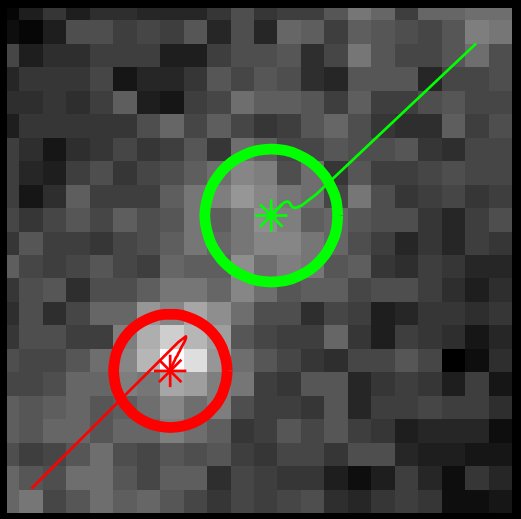

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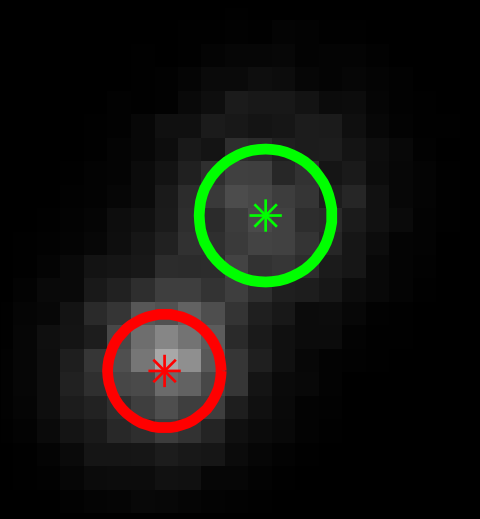

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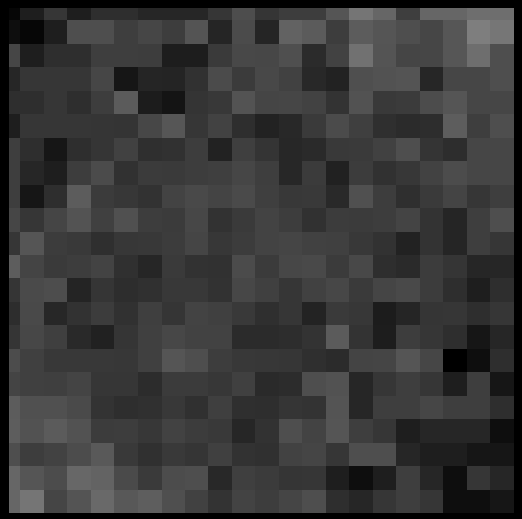

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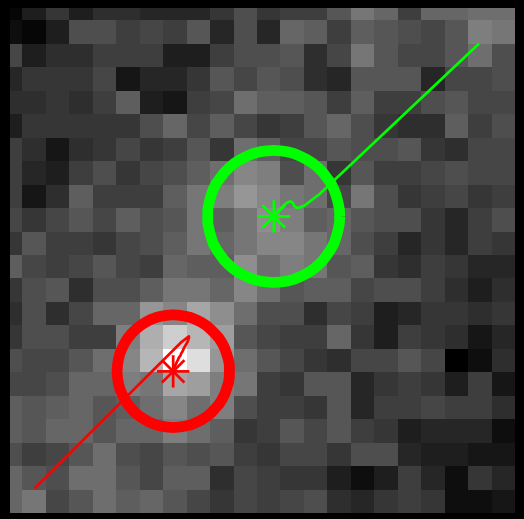

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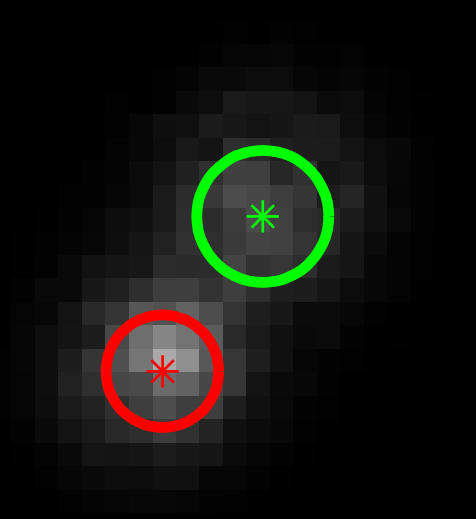

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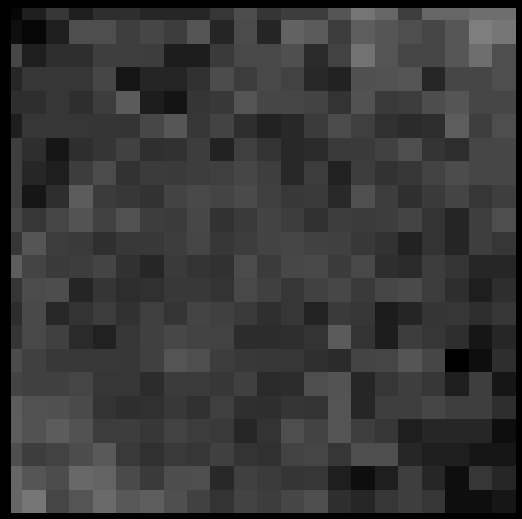

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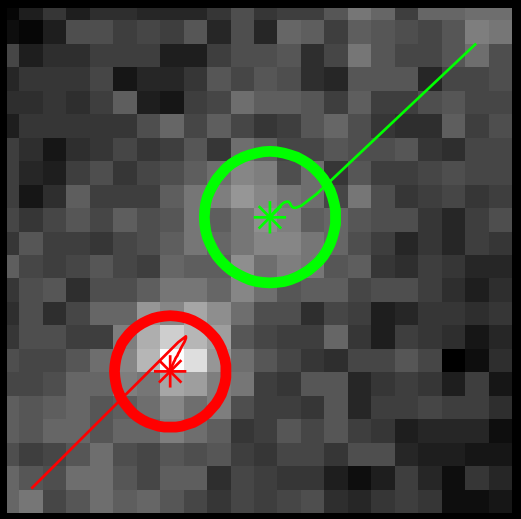

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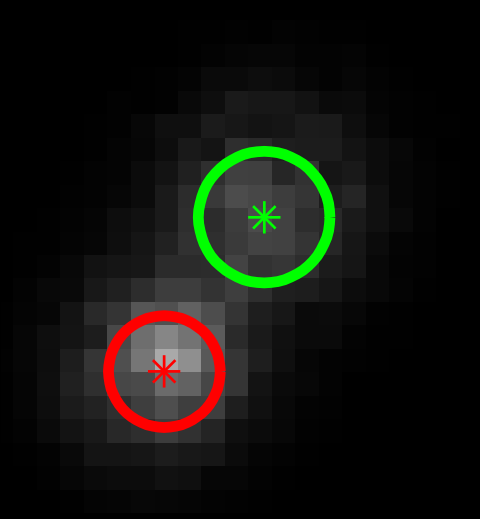

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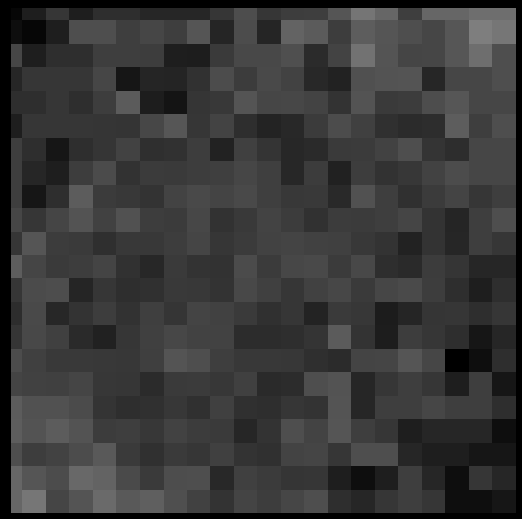

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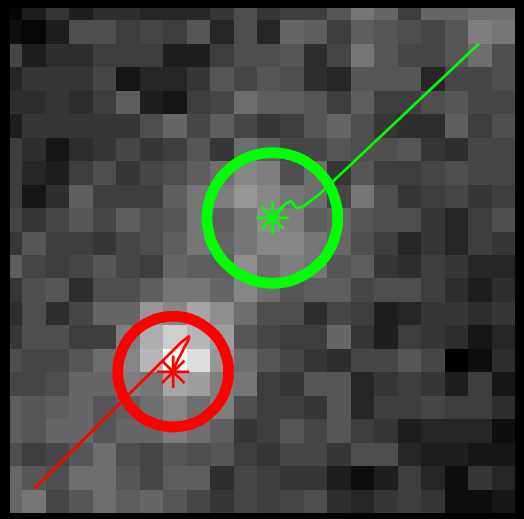

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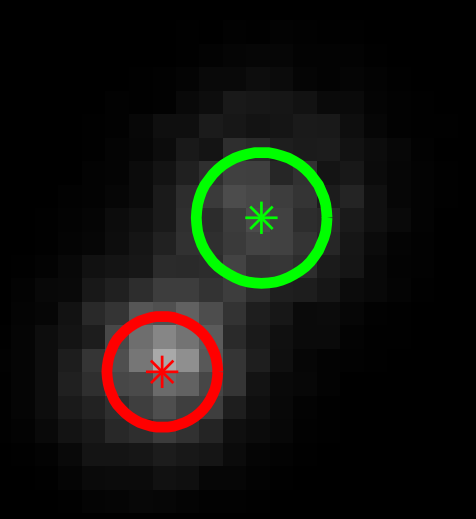

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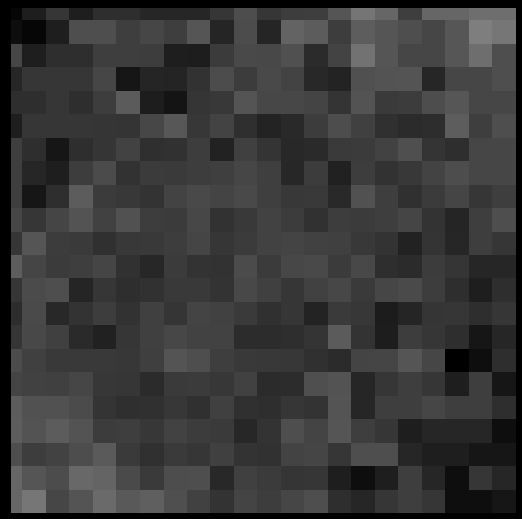

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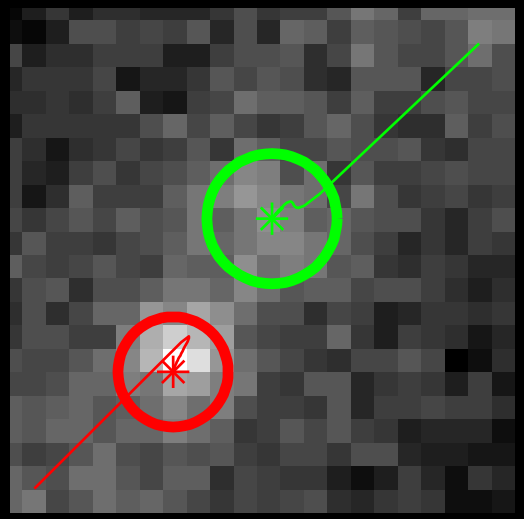

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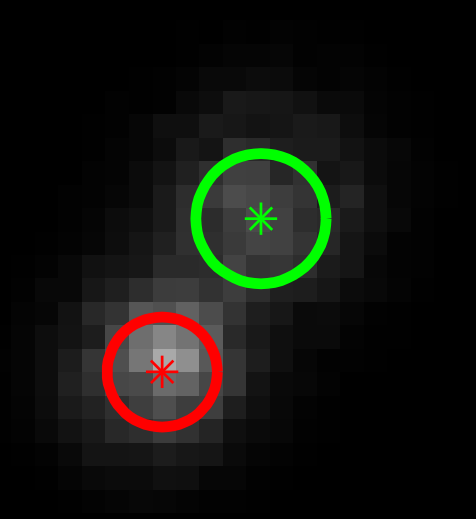

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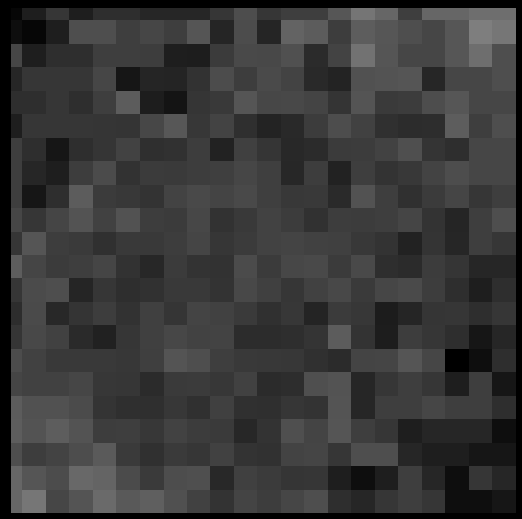

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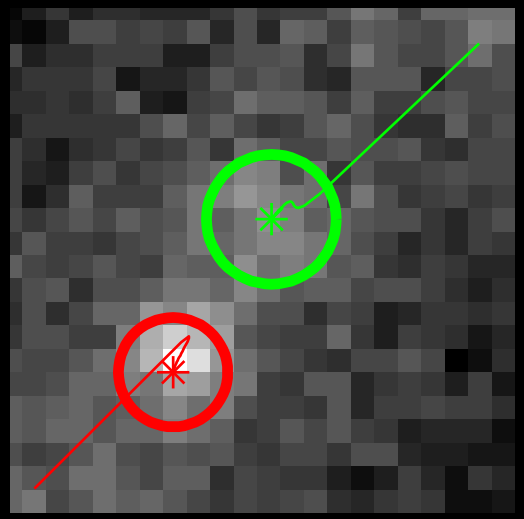

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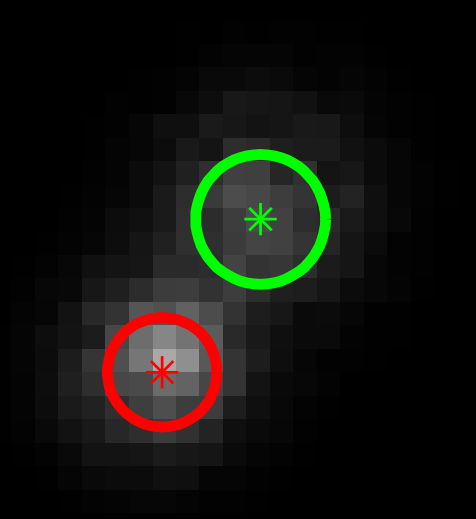

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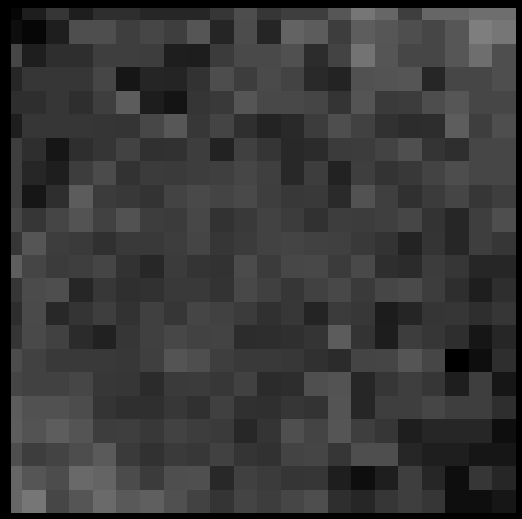

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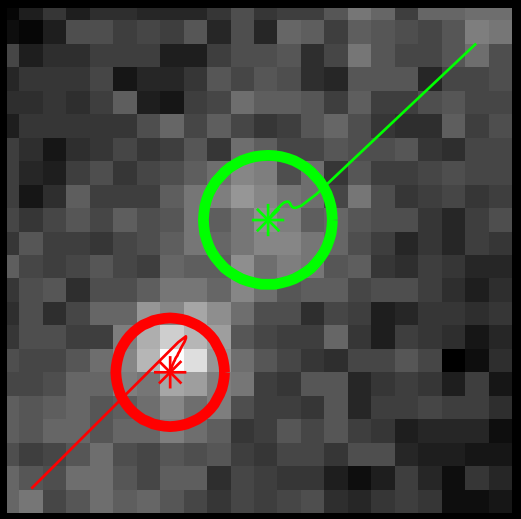
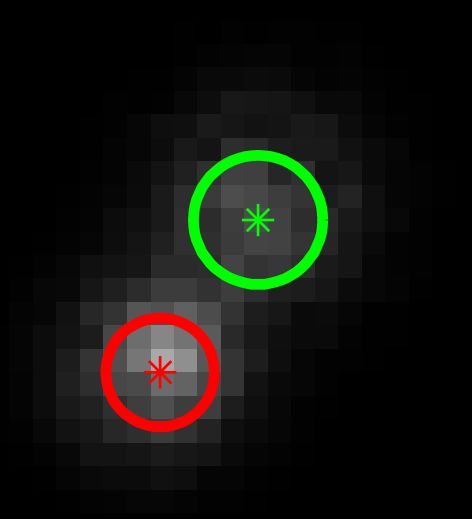


Spots



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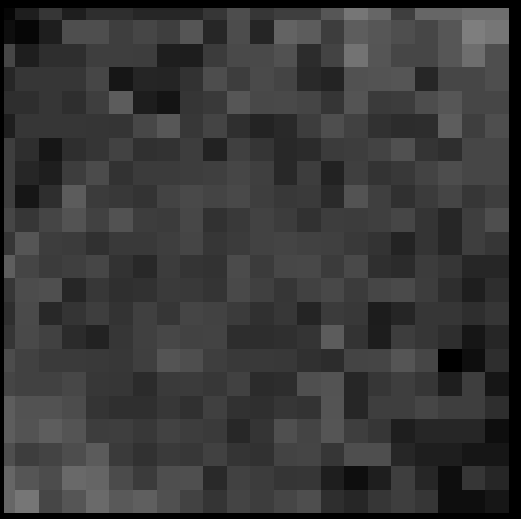
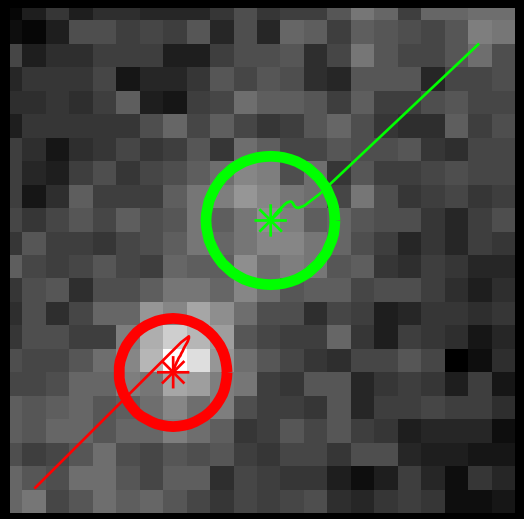


Super-lattice refinement

Image



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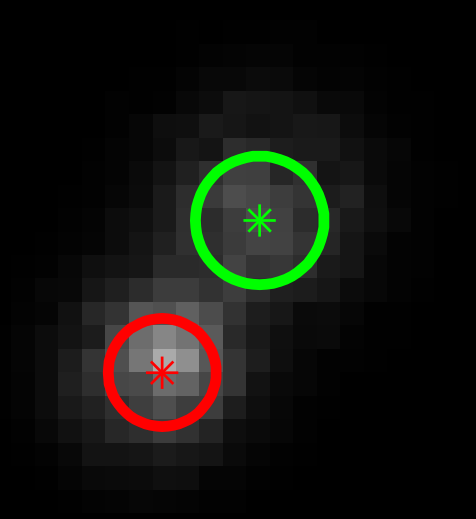

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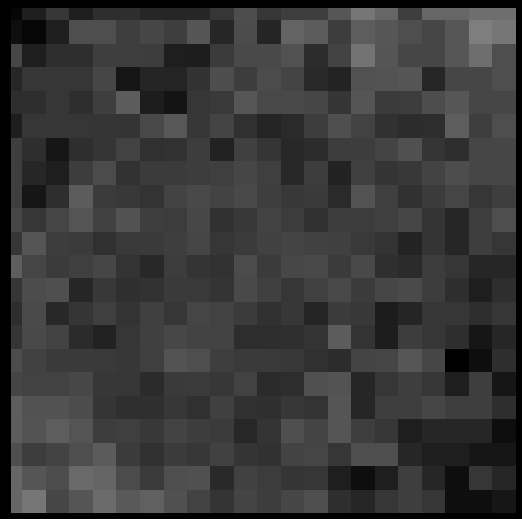
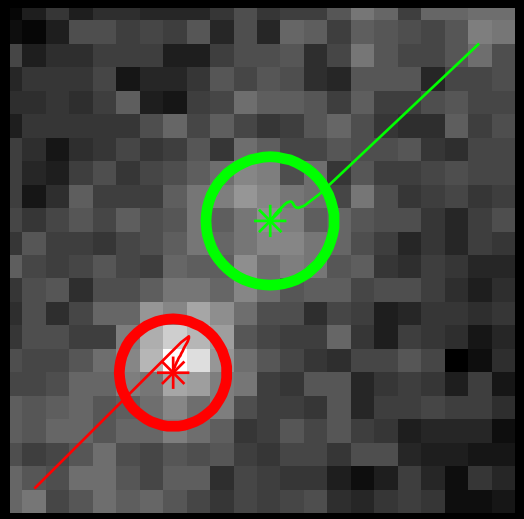


Super-lattice refinement

Image



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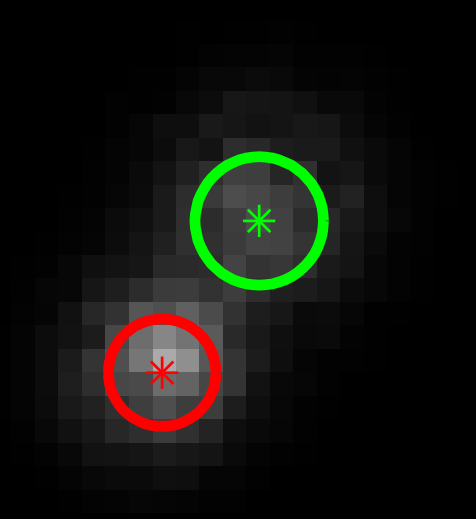

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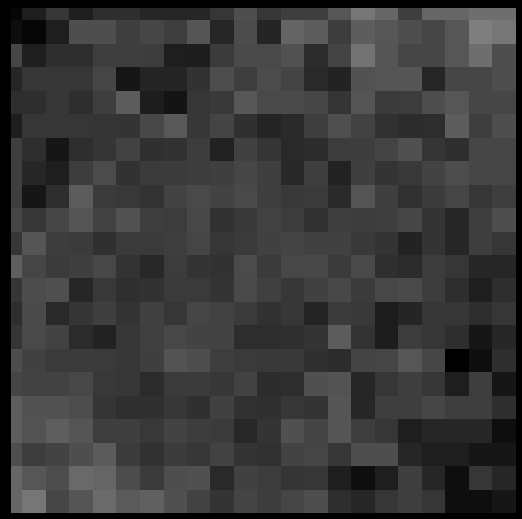

Super-lattice refinement

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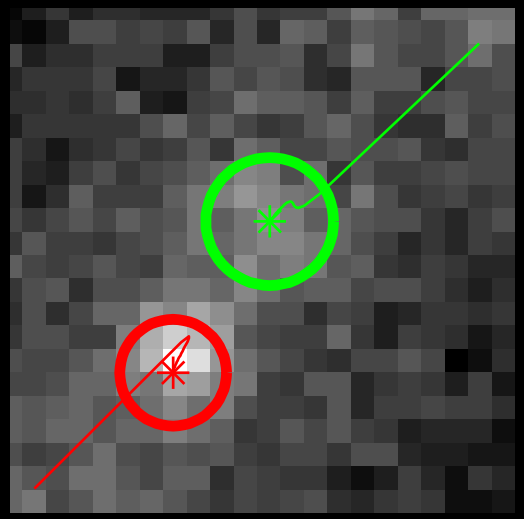

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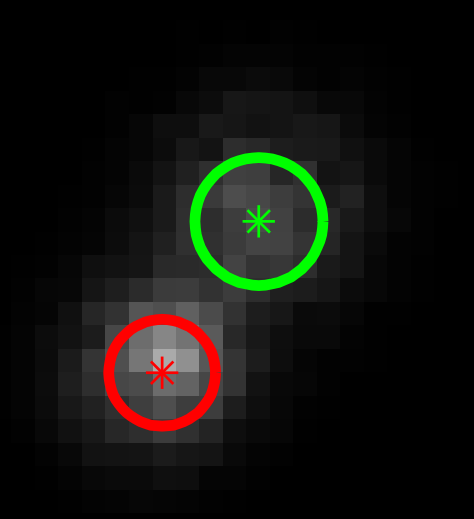

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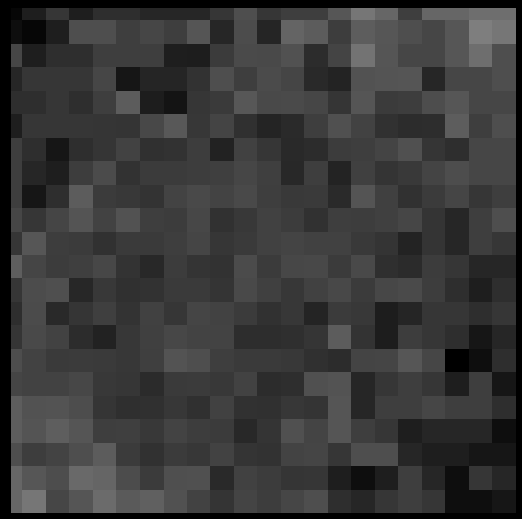

Super-lattice refinement

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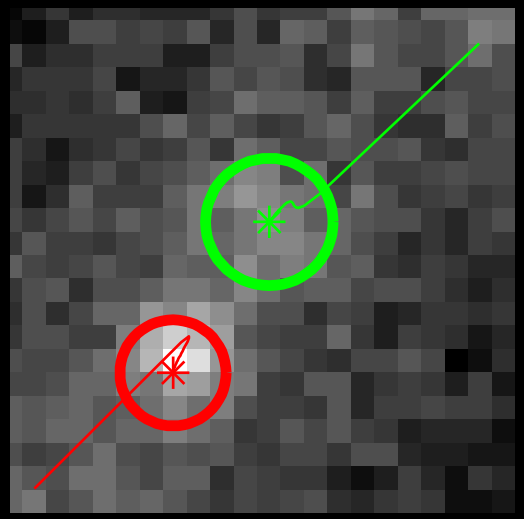

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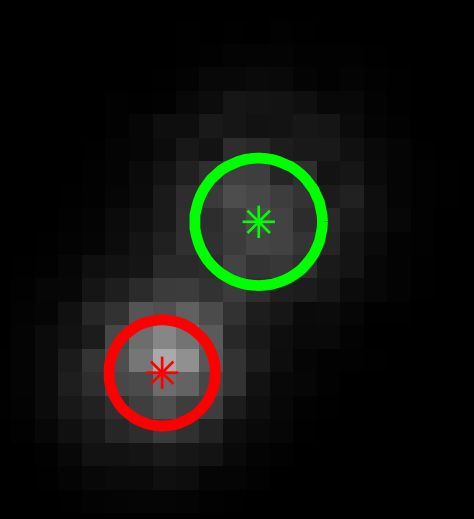

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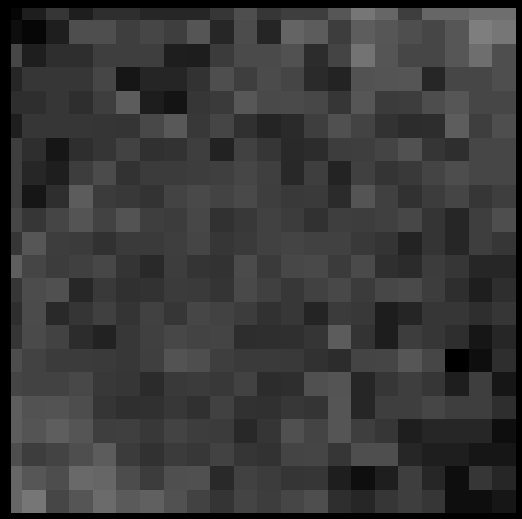

Super-lattice refinement

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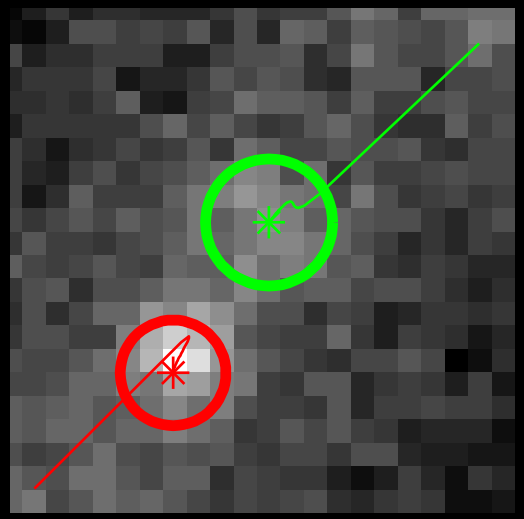
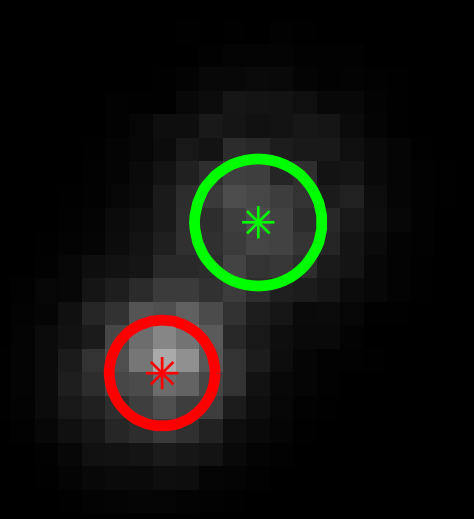


Spots



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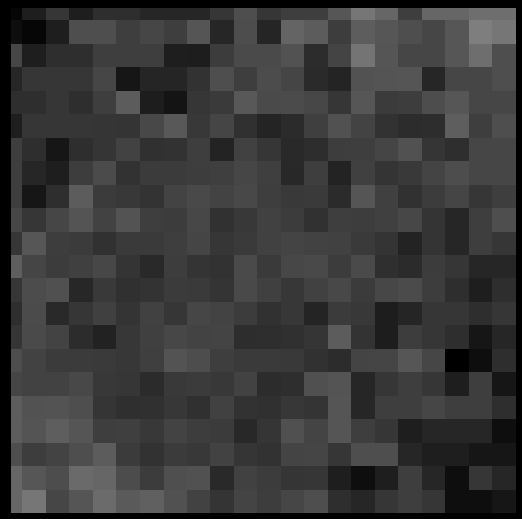

Super-lattice refinement

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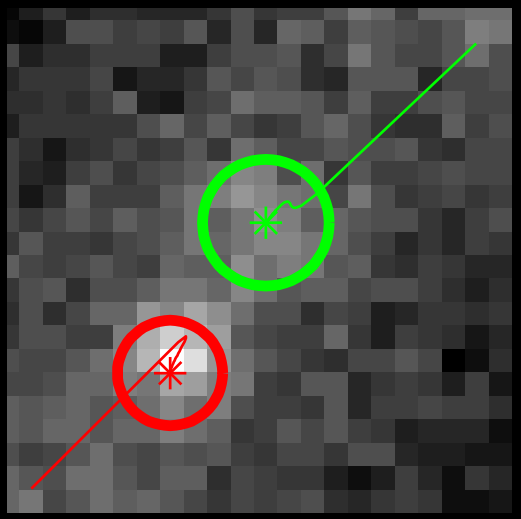

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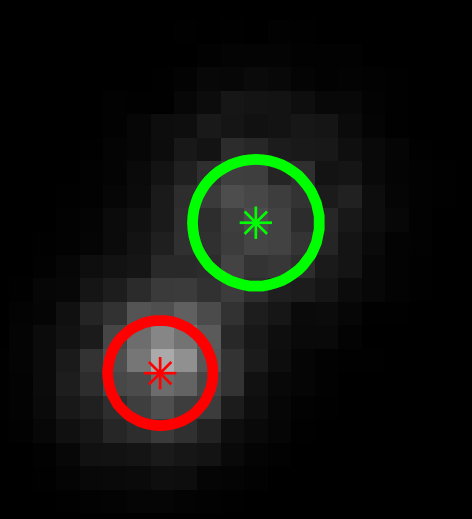

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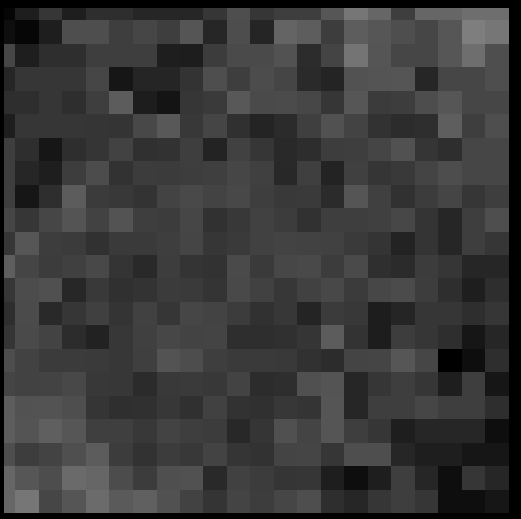

Super-lattice refinement

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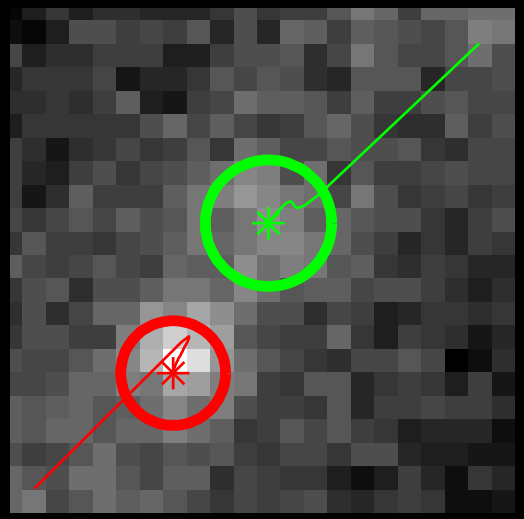

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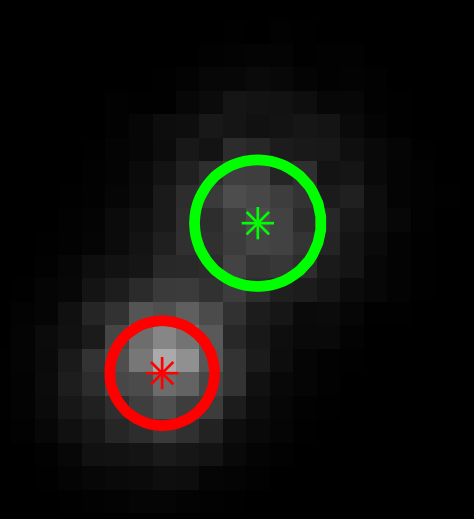

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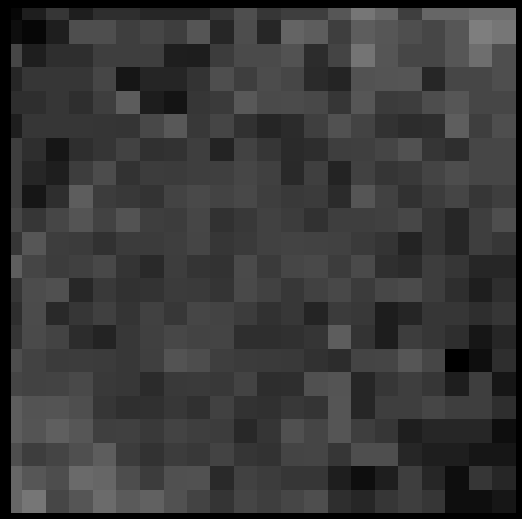
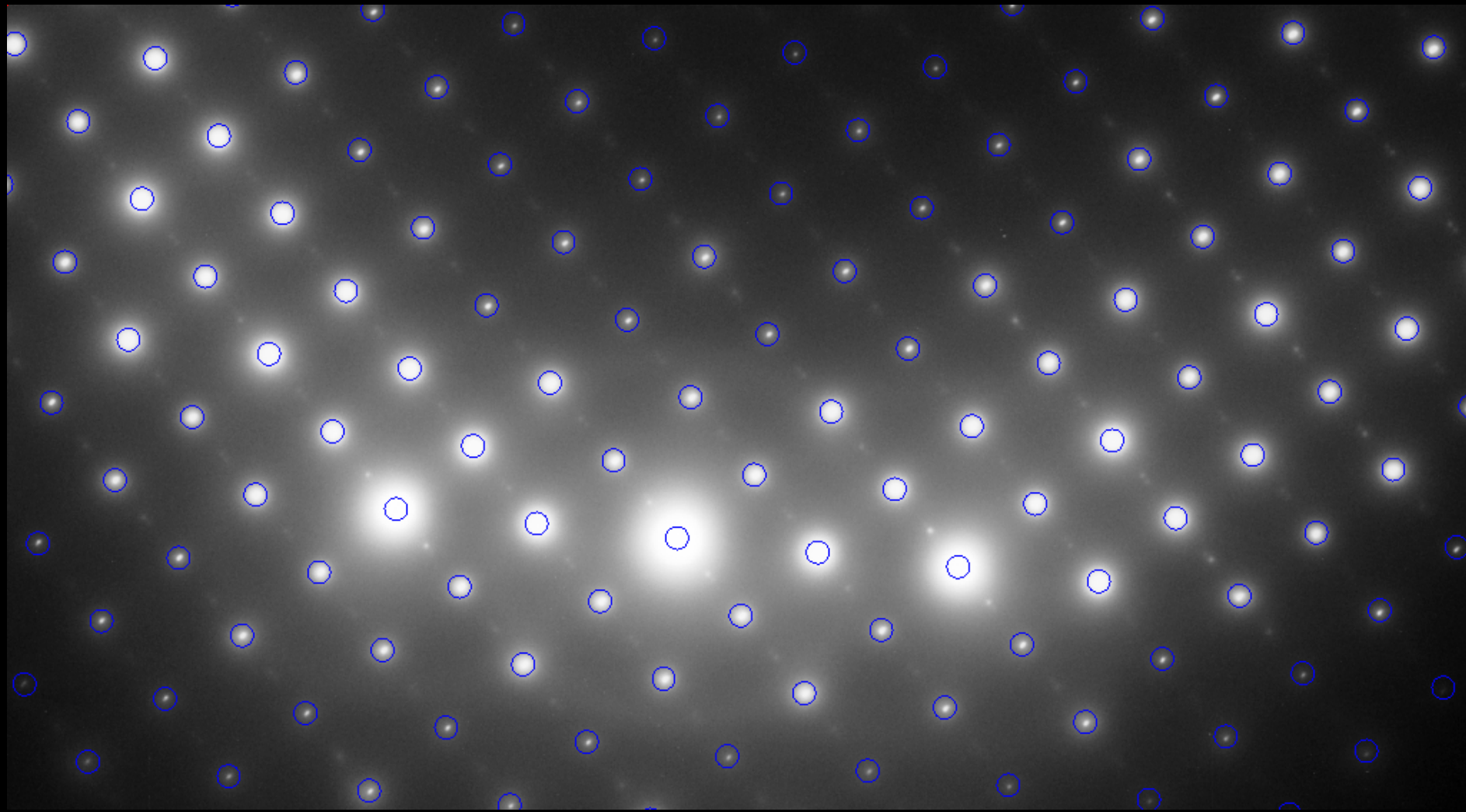
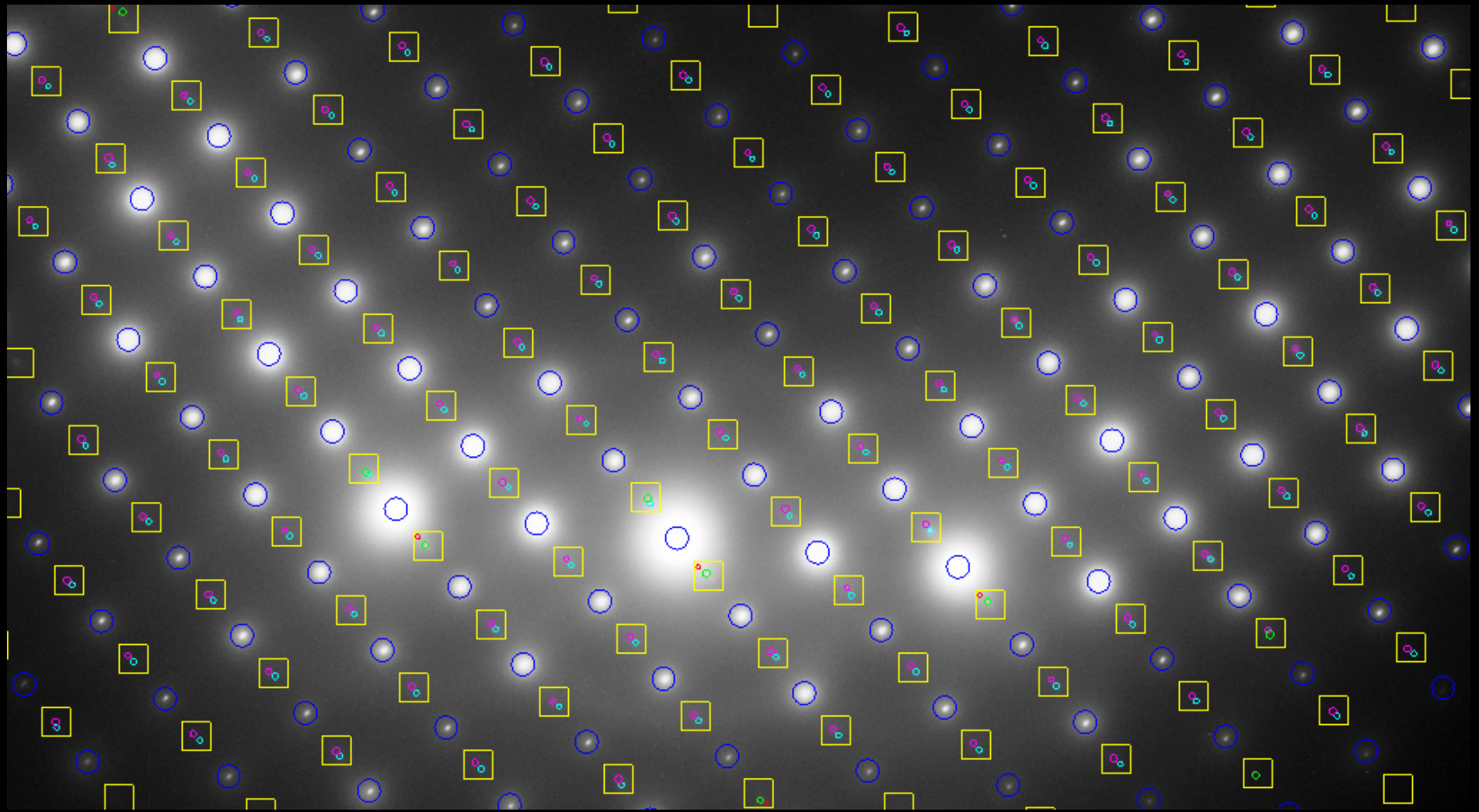


Robust mean computation

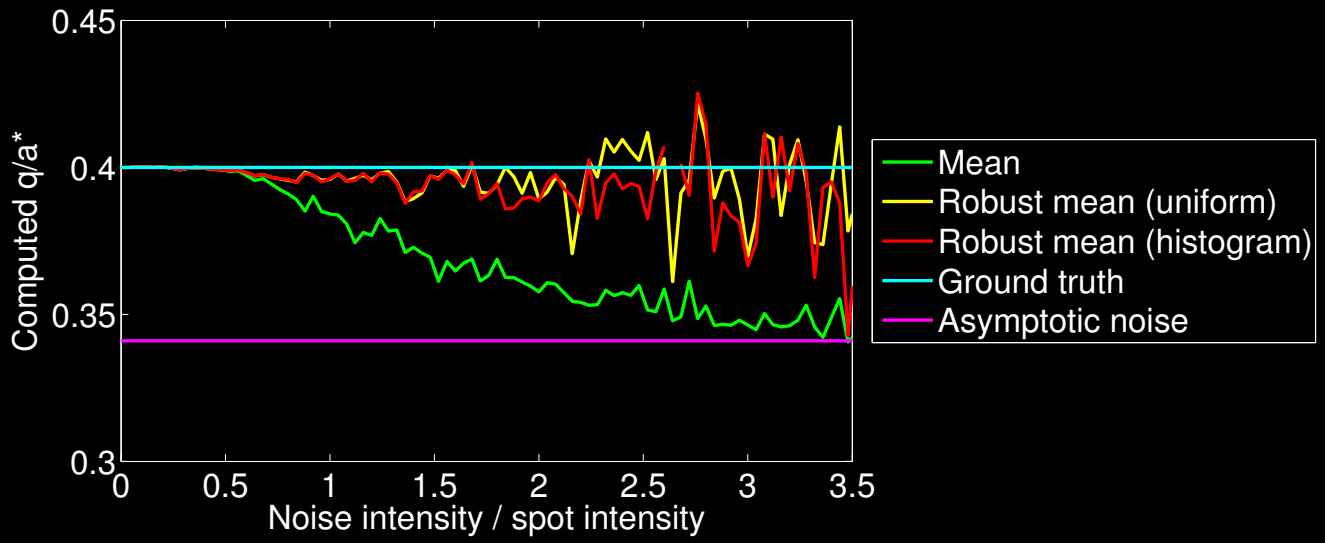


Robust mean computation

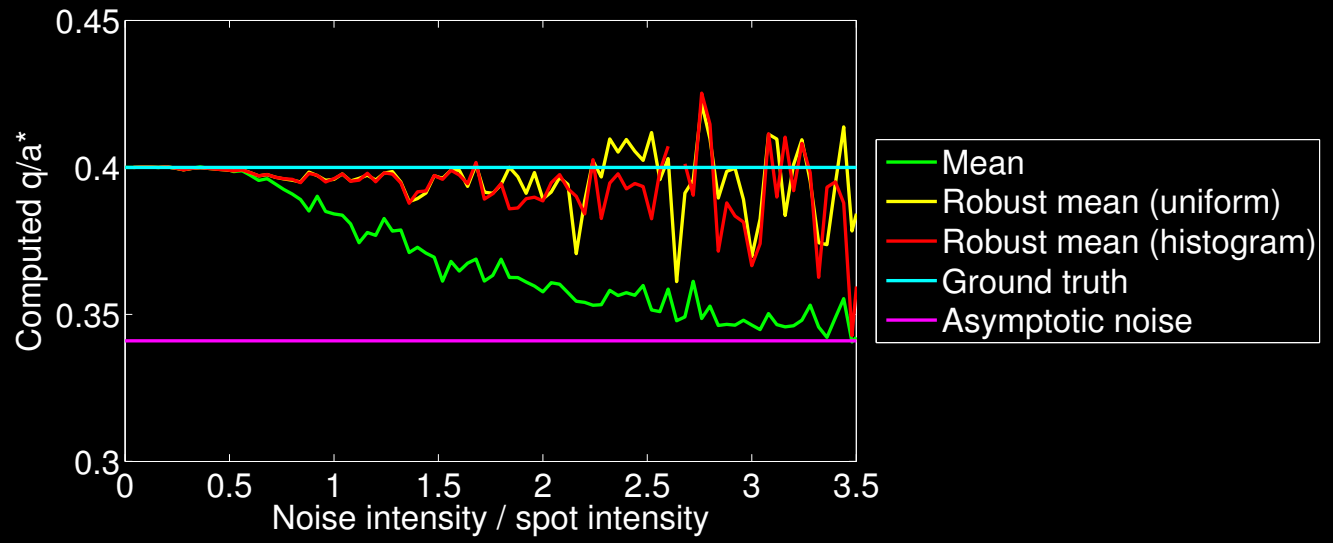


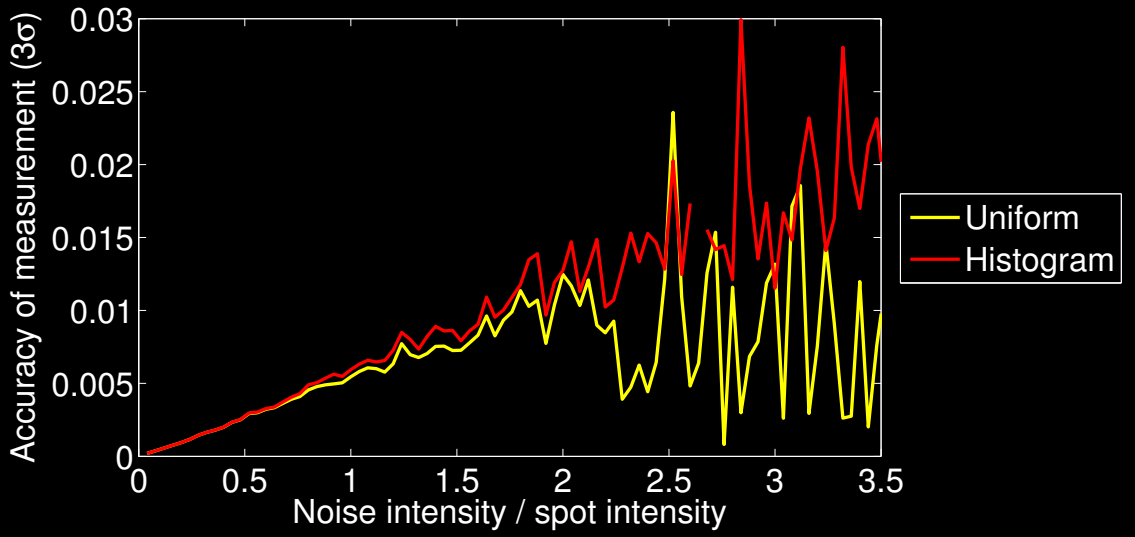
Use EM to compute the mean

Evaluation: Uncorrelated noise

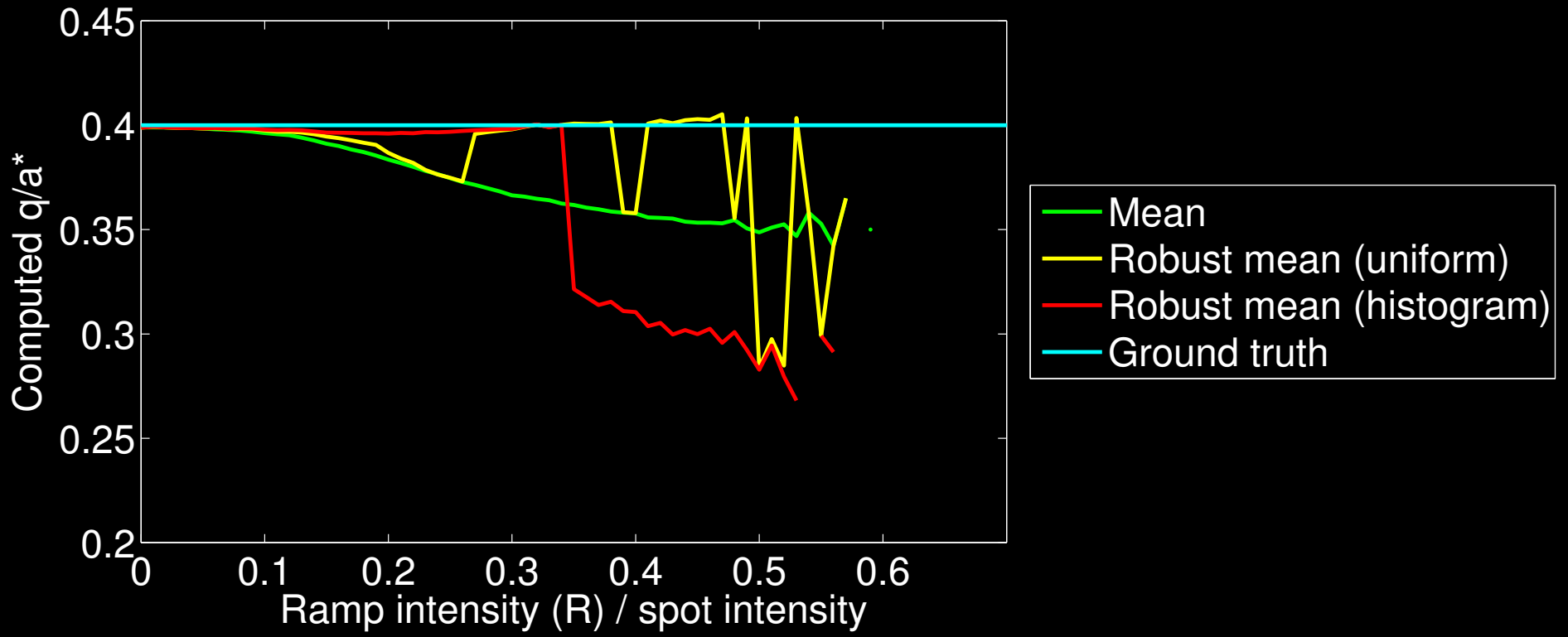


Evaluation: Uncorrelated noise

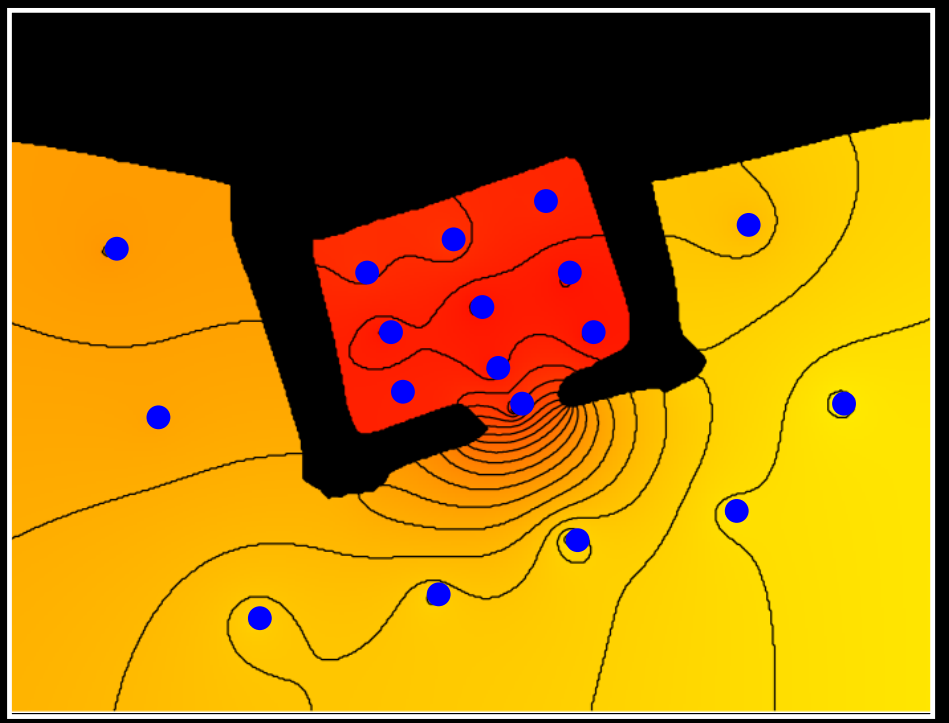




Evaluation: Correlated noise



Results on $La_{0.5}Ca_{0.5}MnO_3$



$3\sigma = 0.02$ pixels

Any Questions?