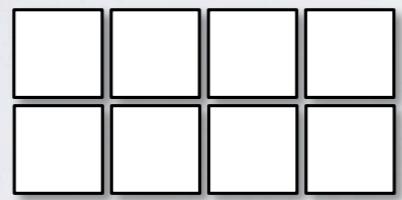


UNBENDING

Image Processing of 2D Crystals

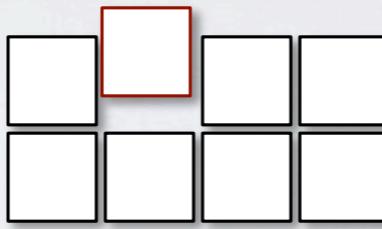
CRYSTAL DISTORTION

Perfect Crystal

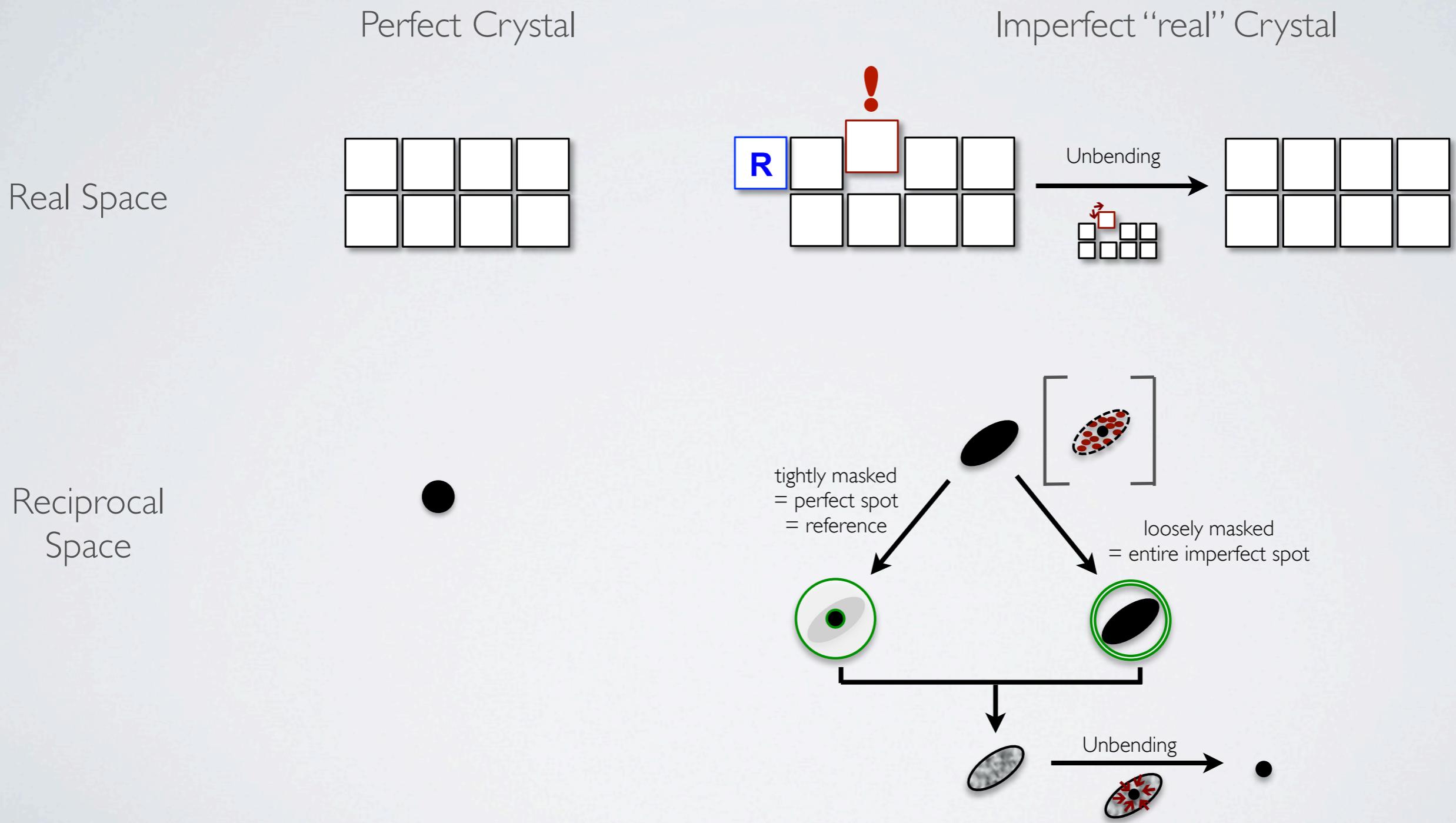


Real Space

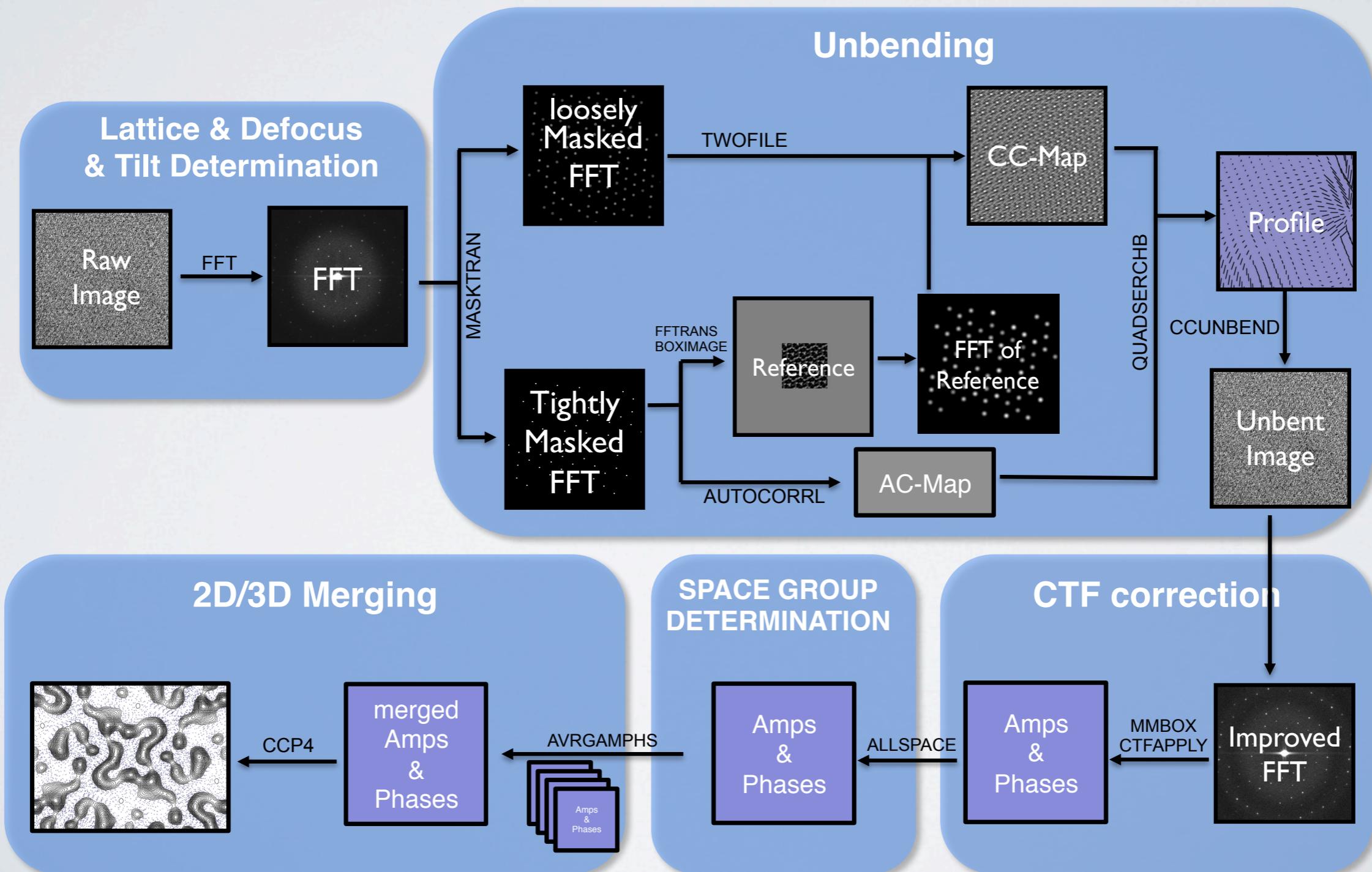
Imperfect “real” Crystal



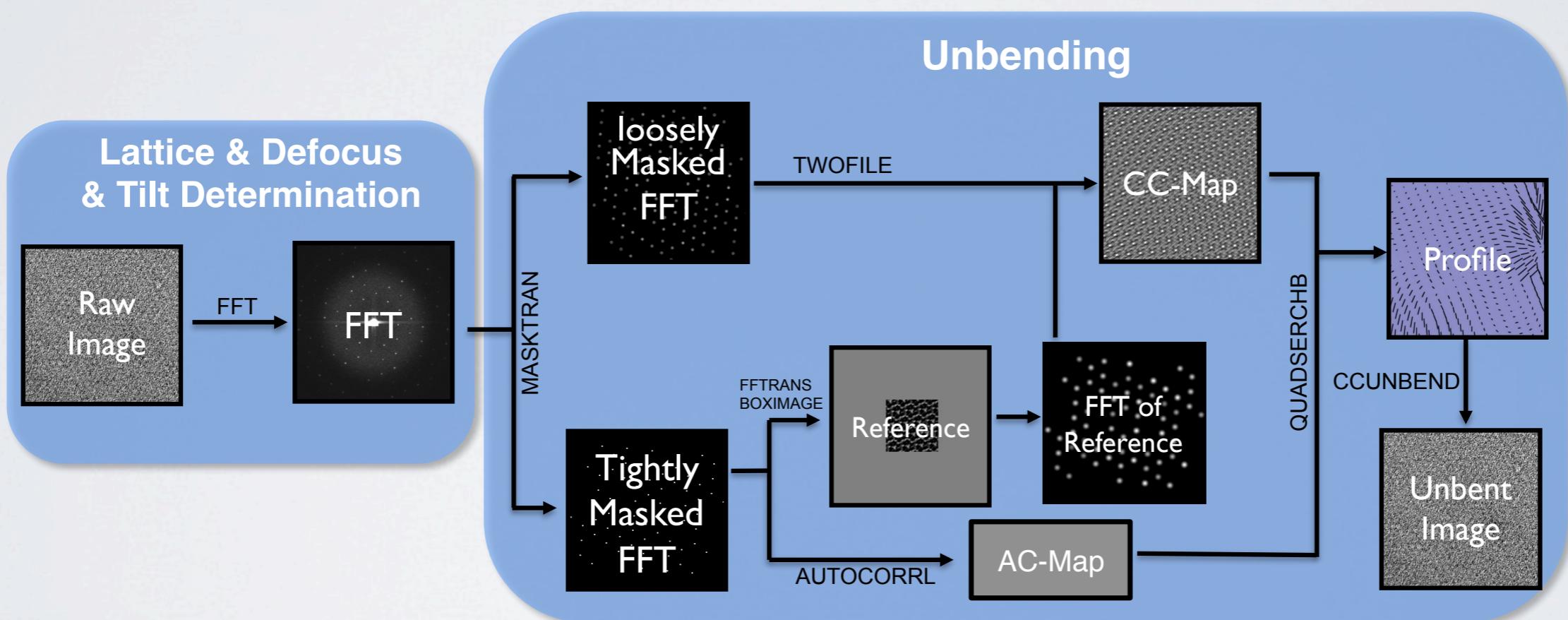
CRYSTAL DISTORTION



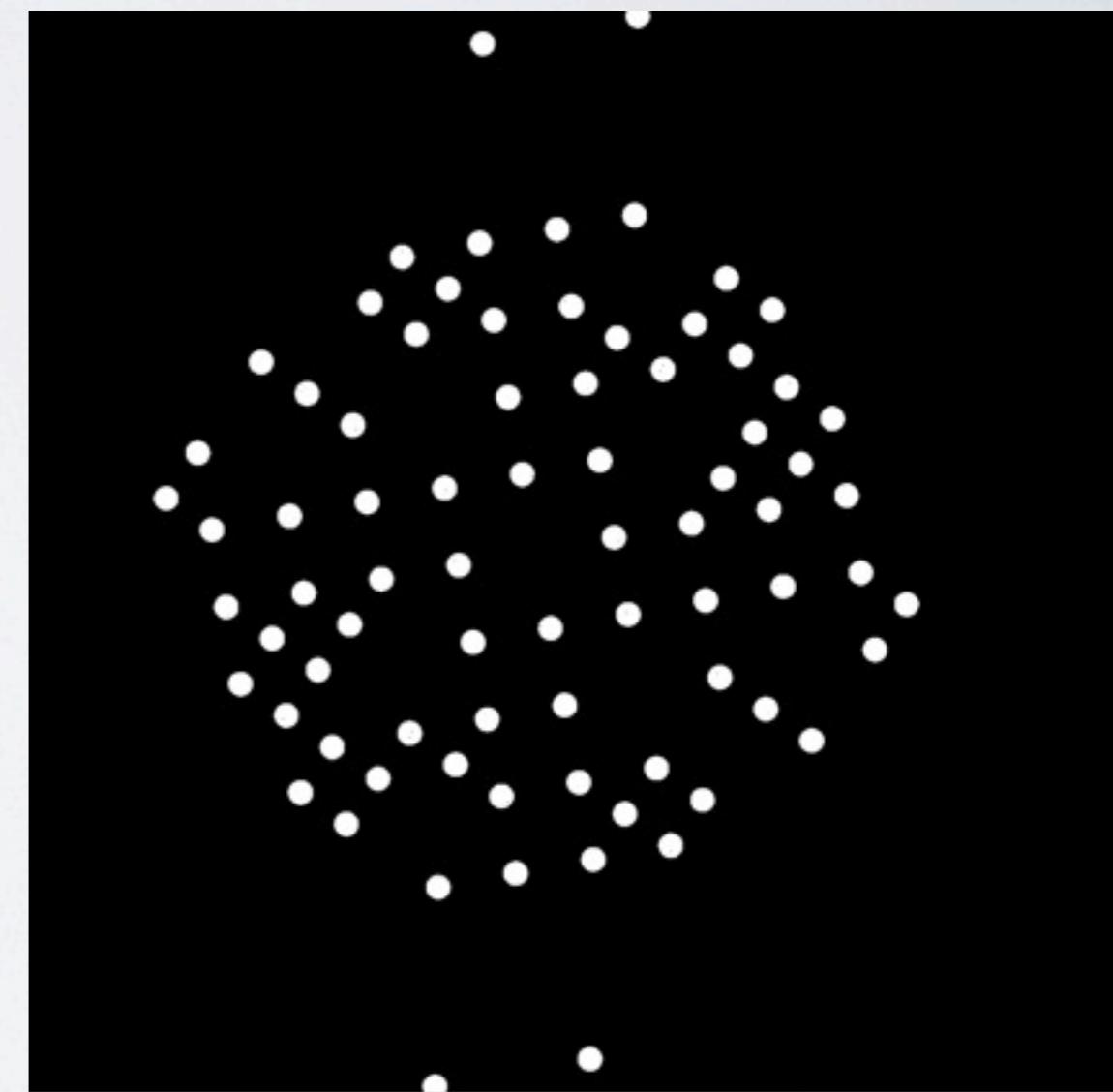
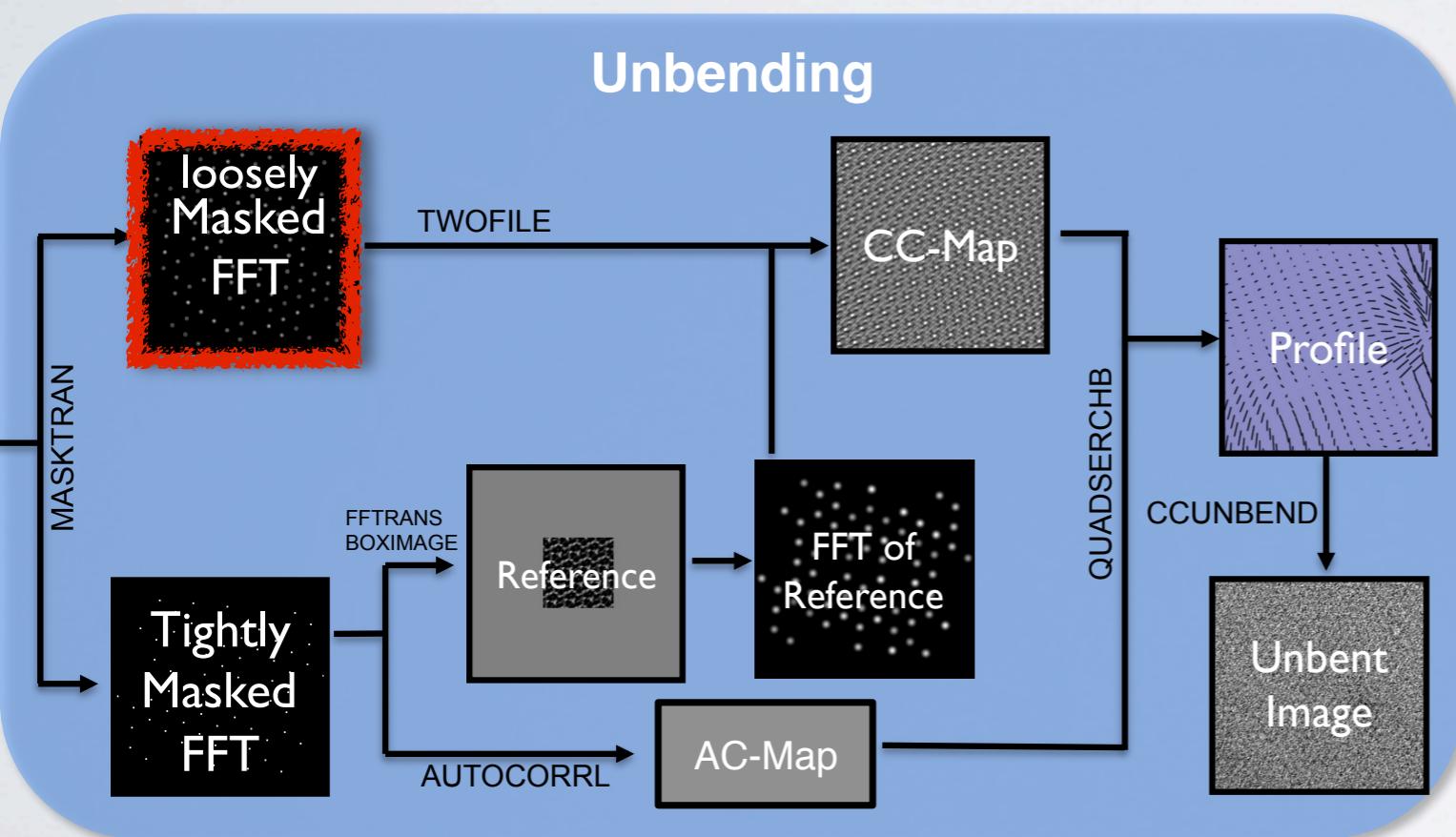
SINGLE IMAGE PROCESSING OF 2D CRYSTALS



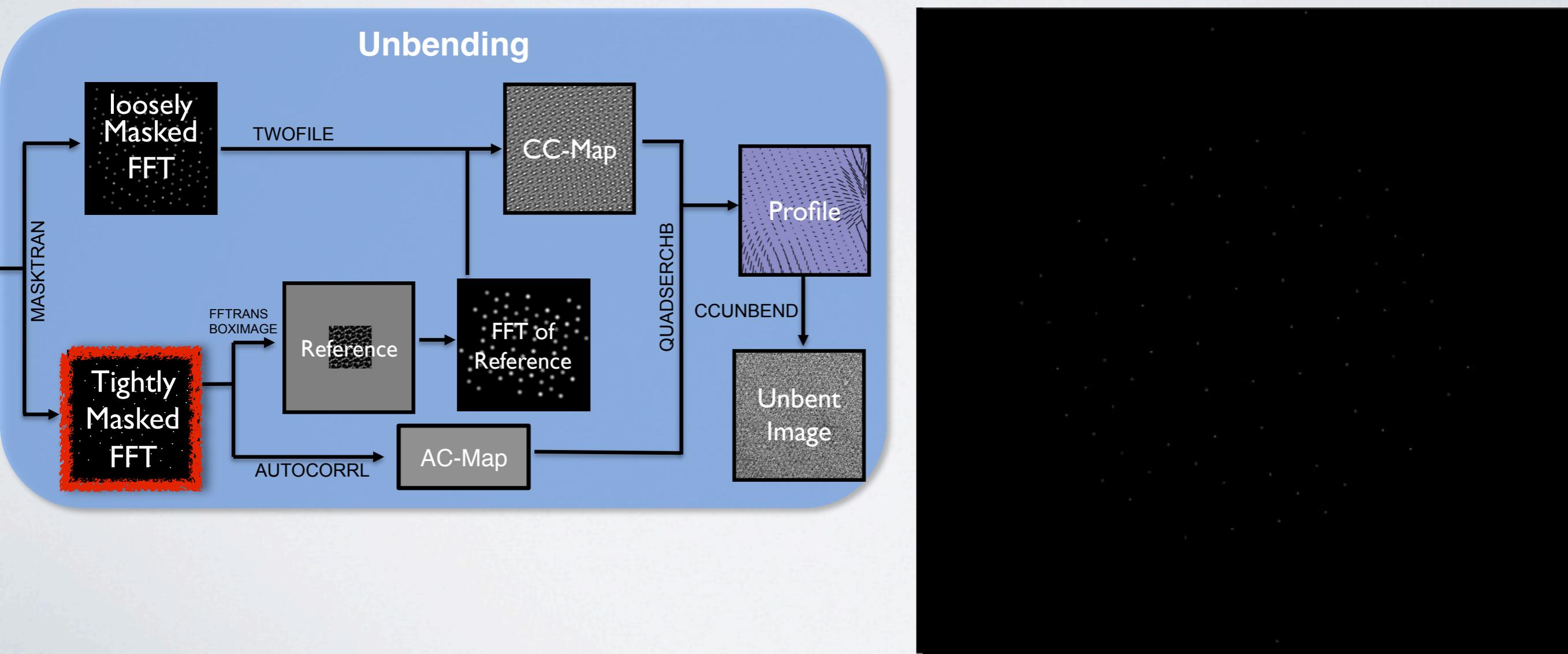
UNBENDING



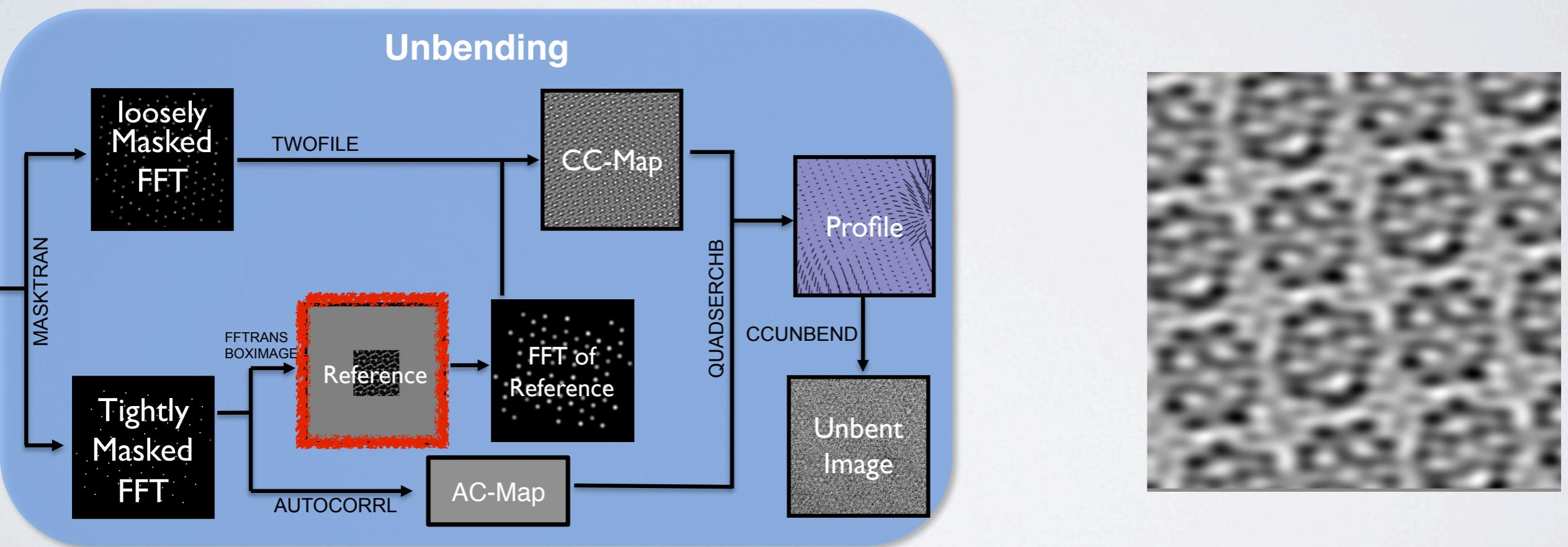
UNBENDING



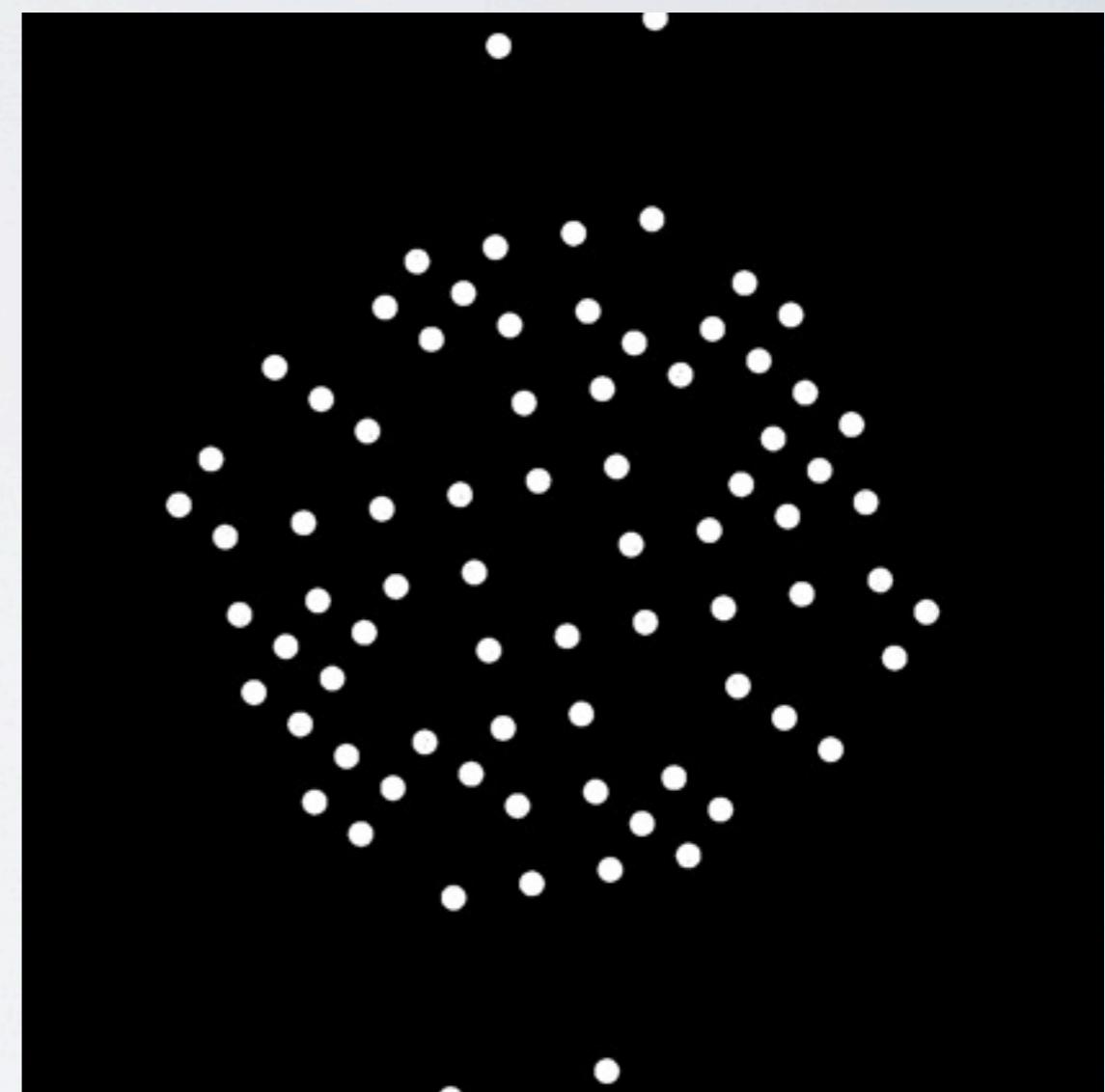
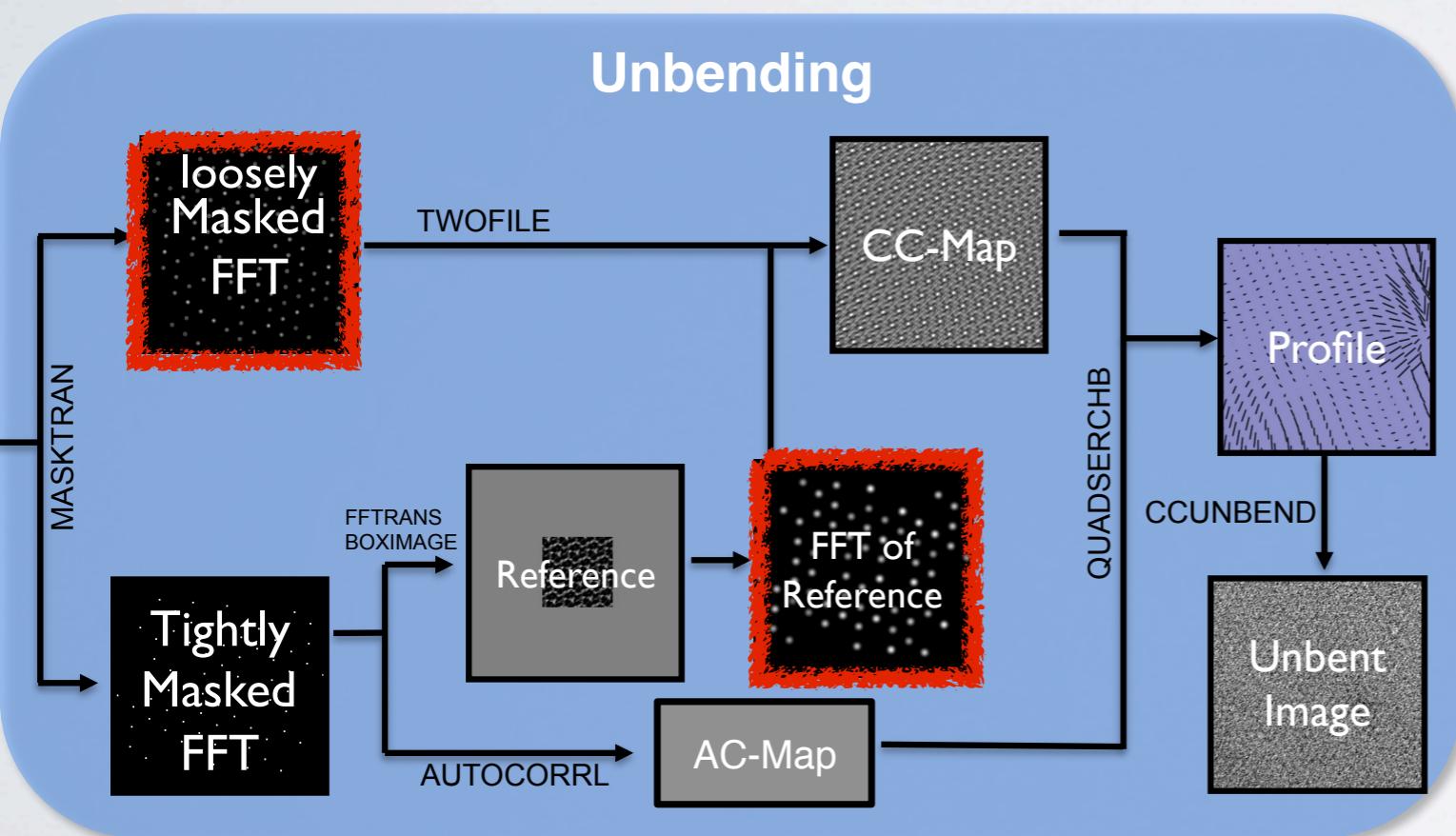
UNBENDING



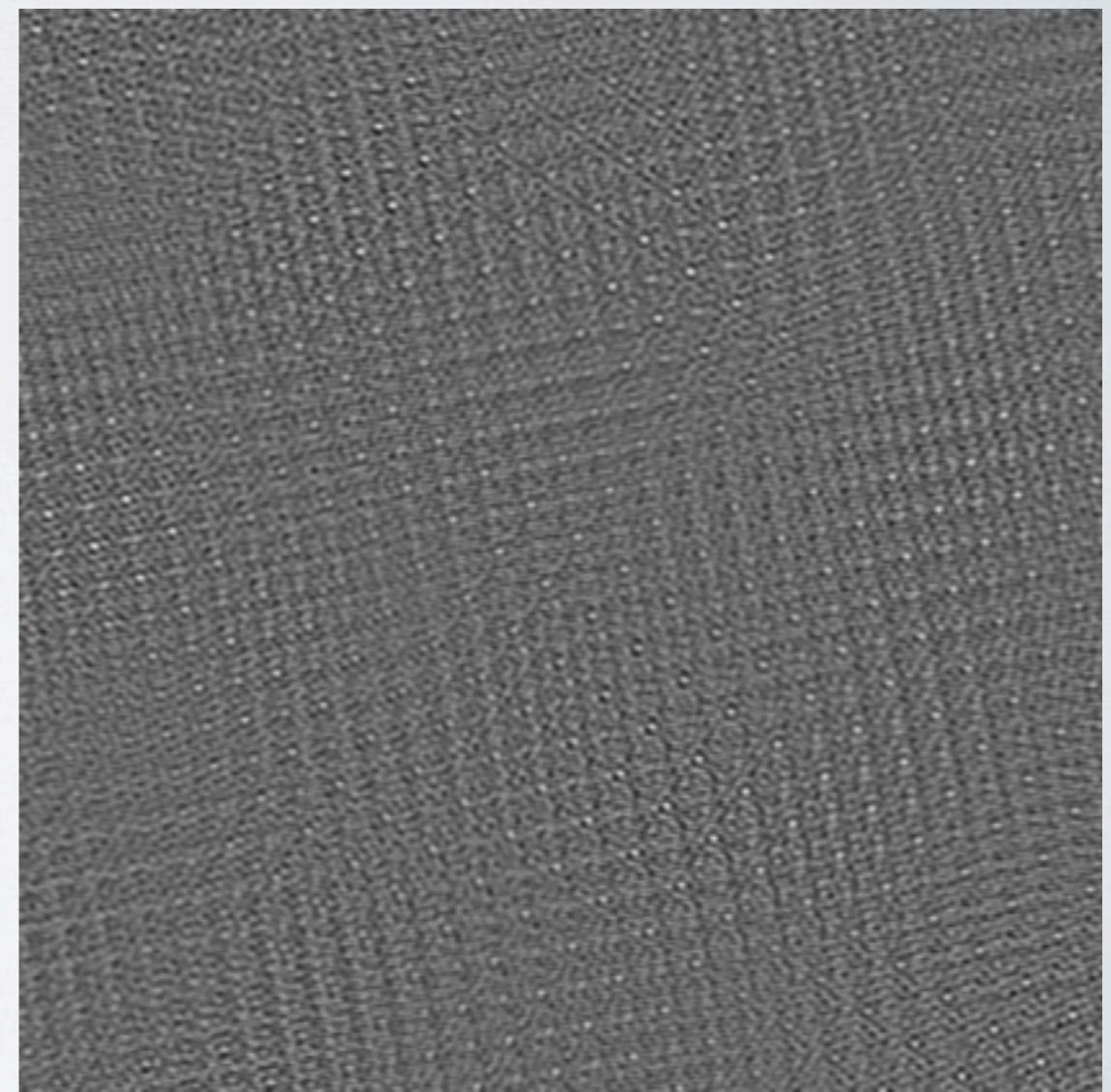
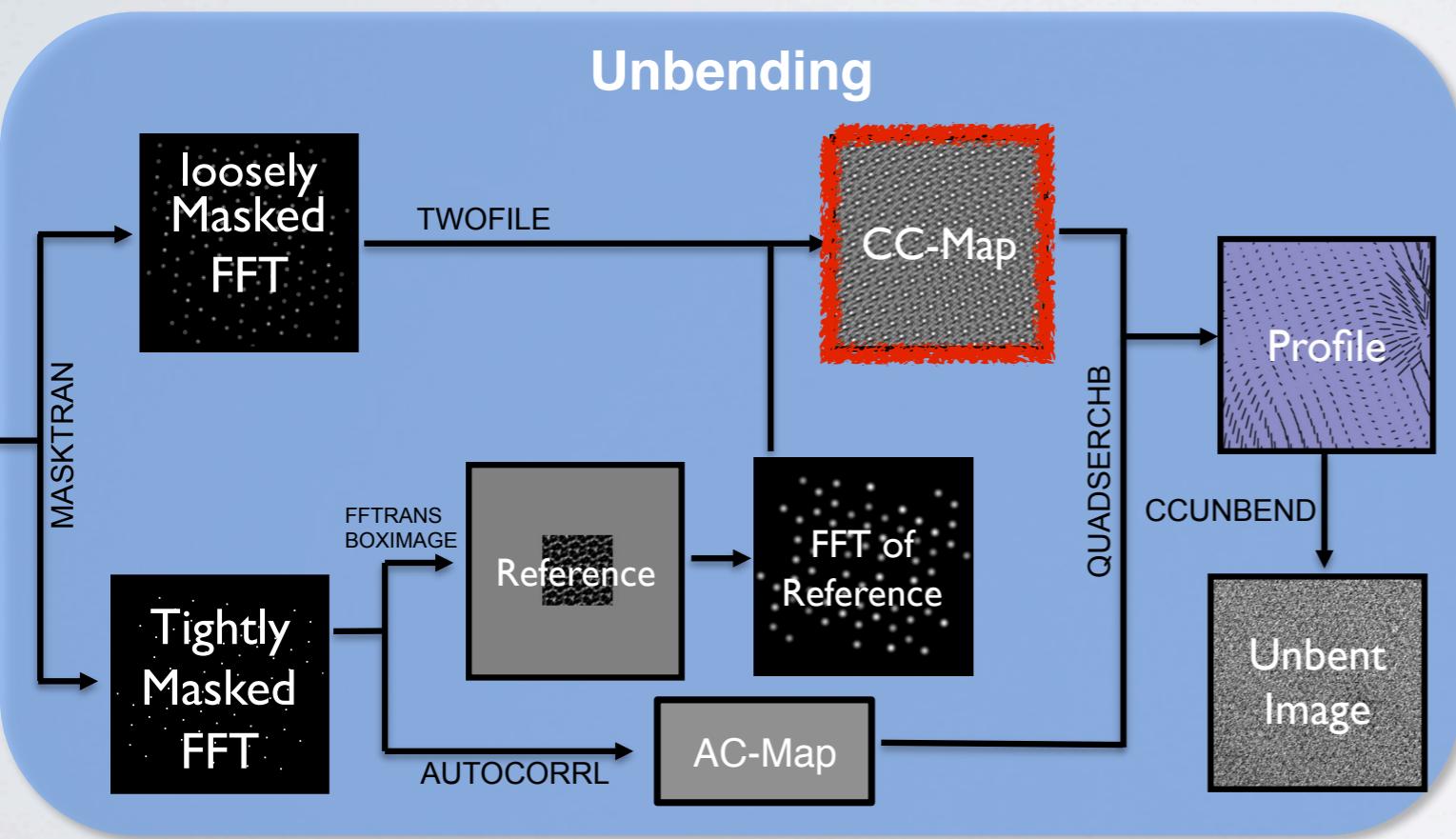
UNBENDING



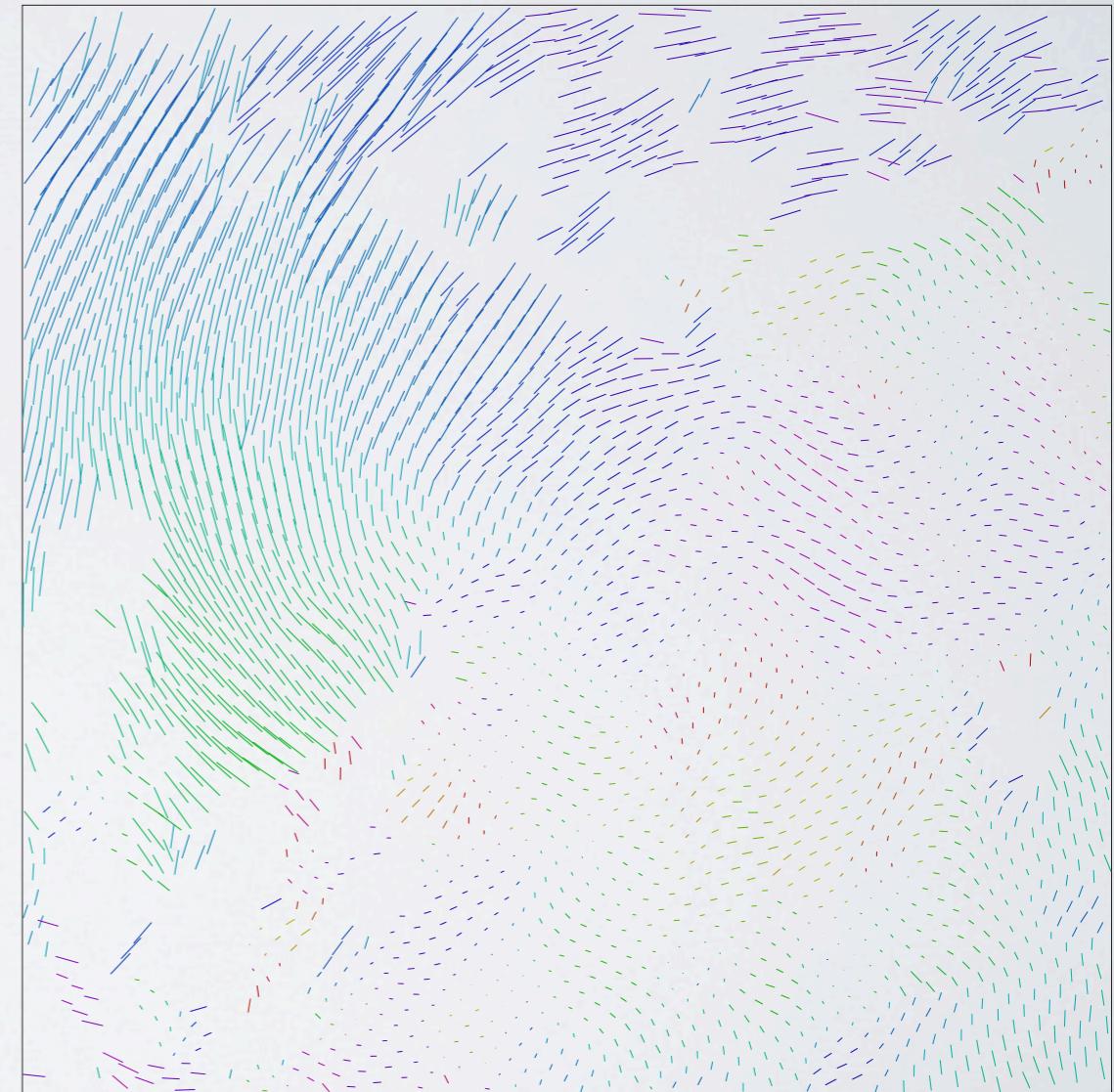
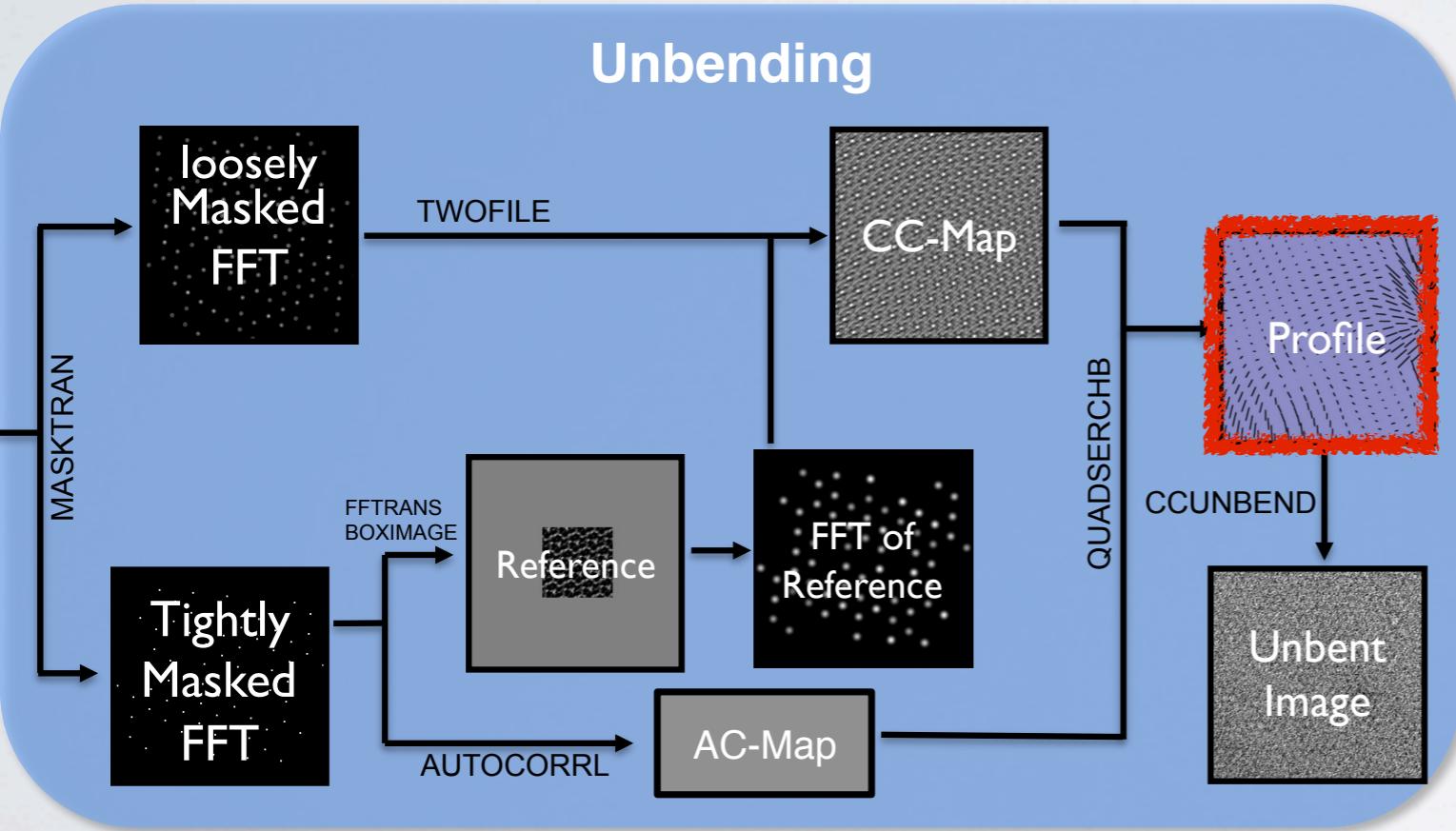
UNBENDING



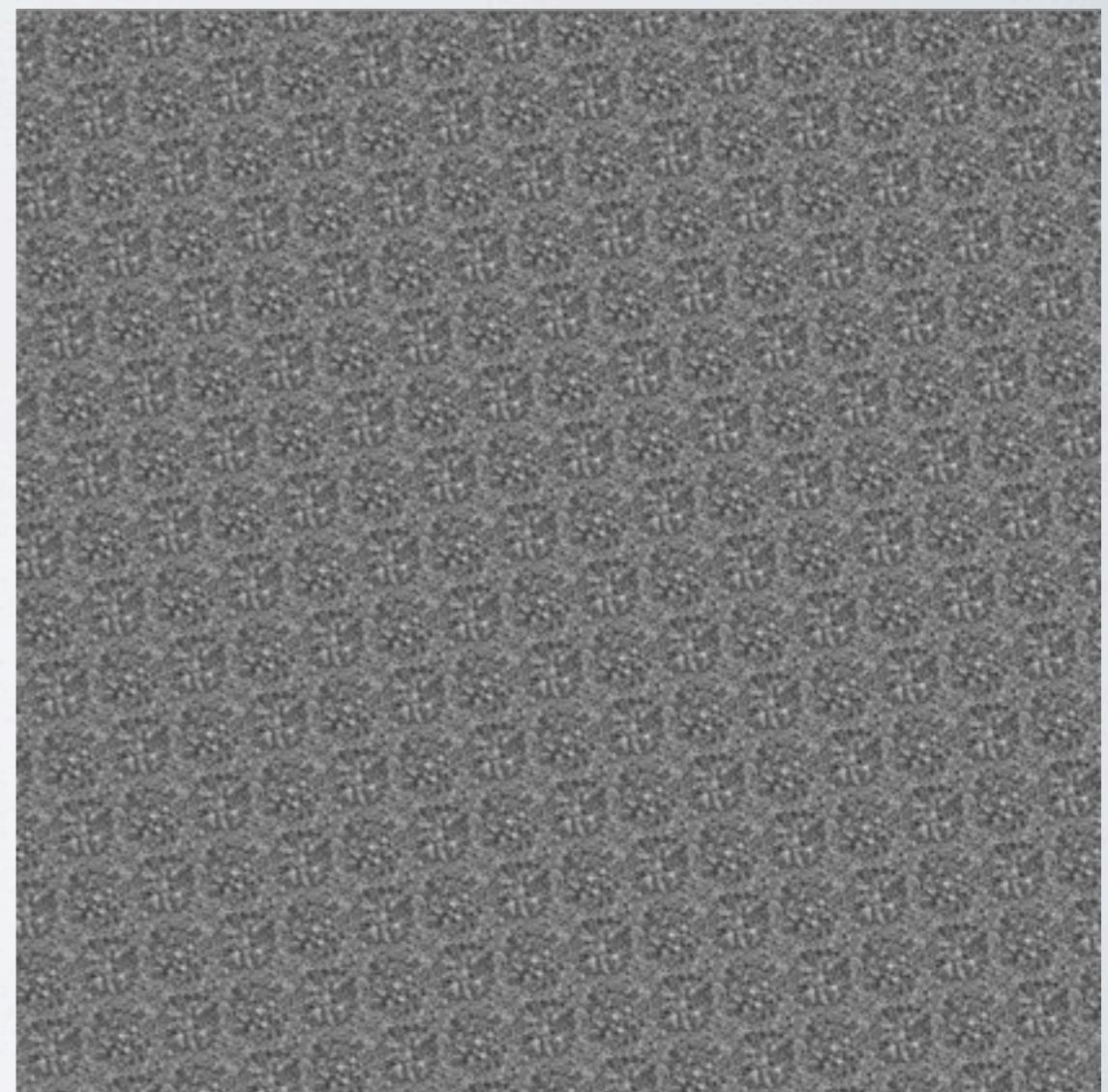
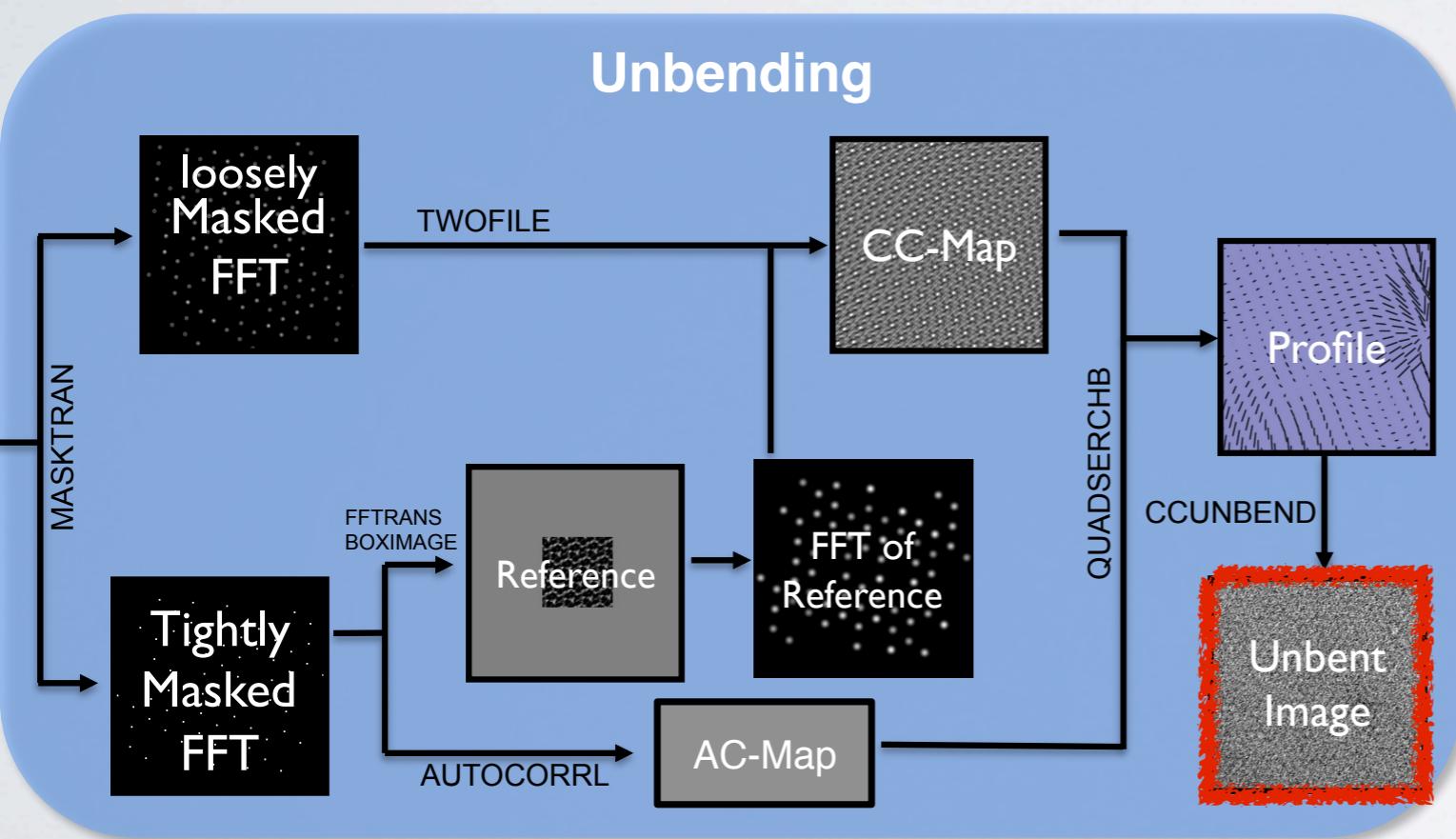
UNBENDING



UNBENDING

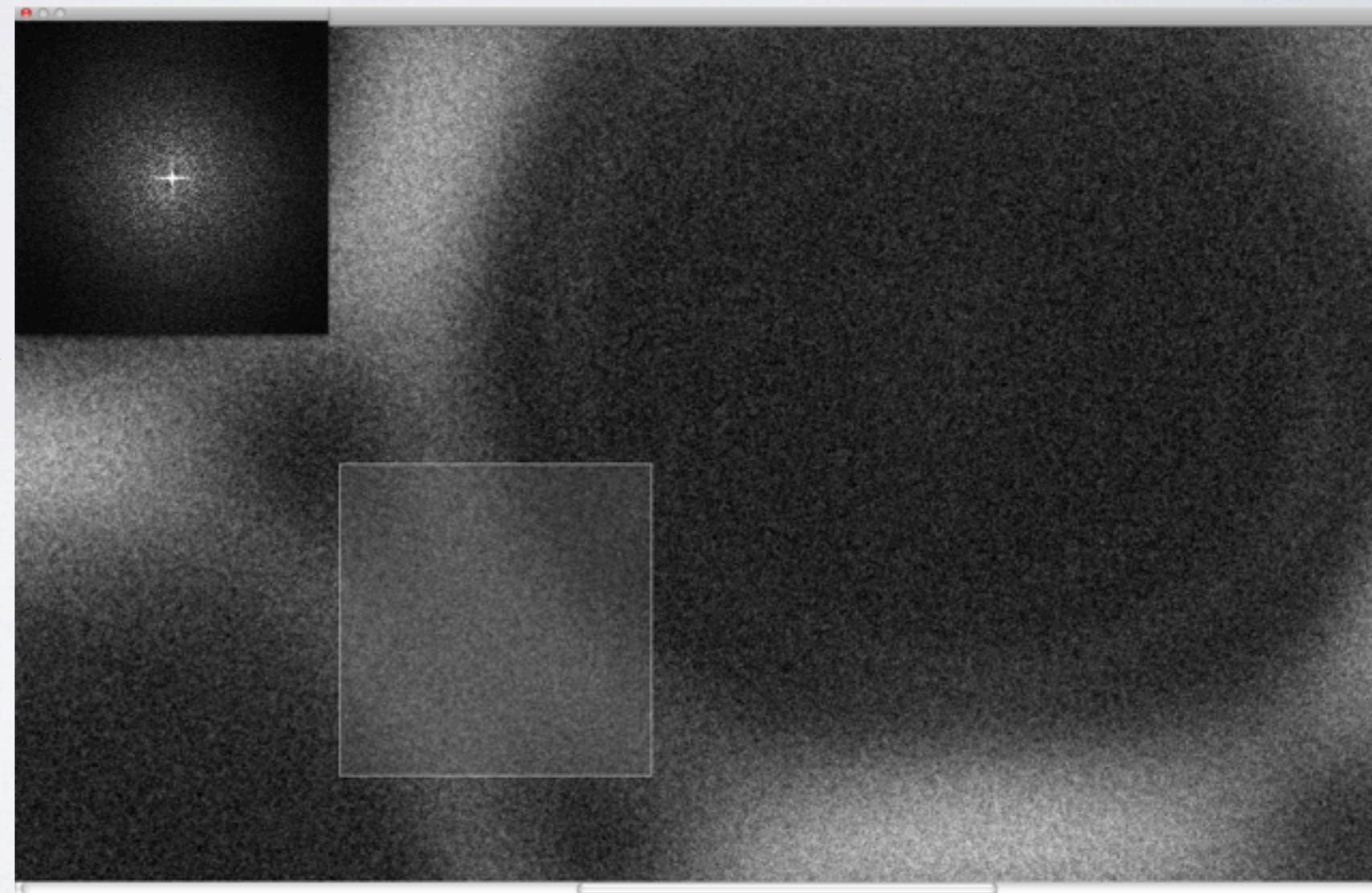


UNBENDING



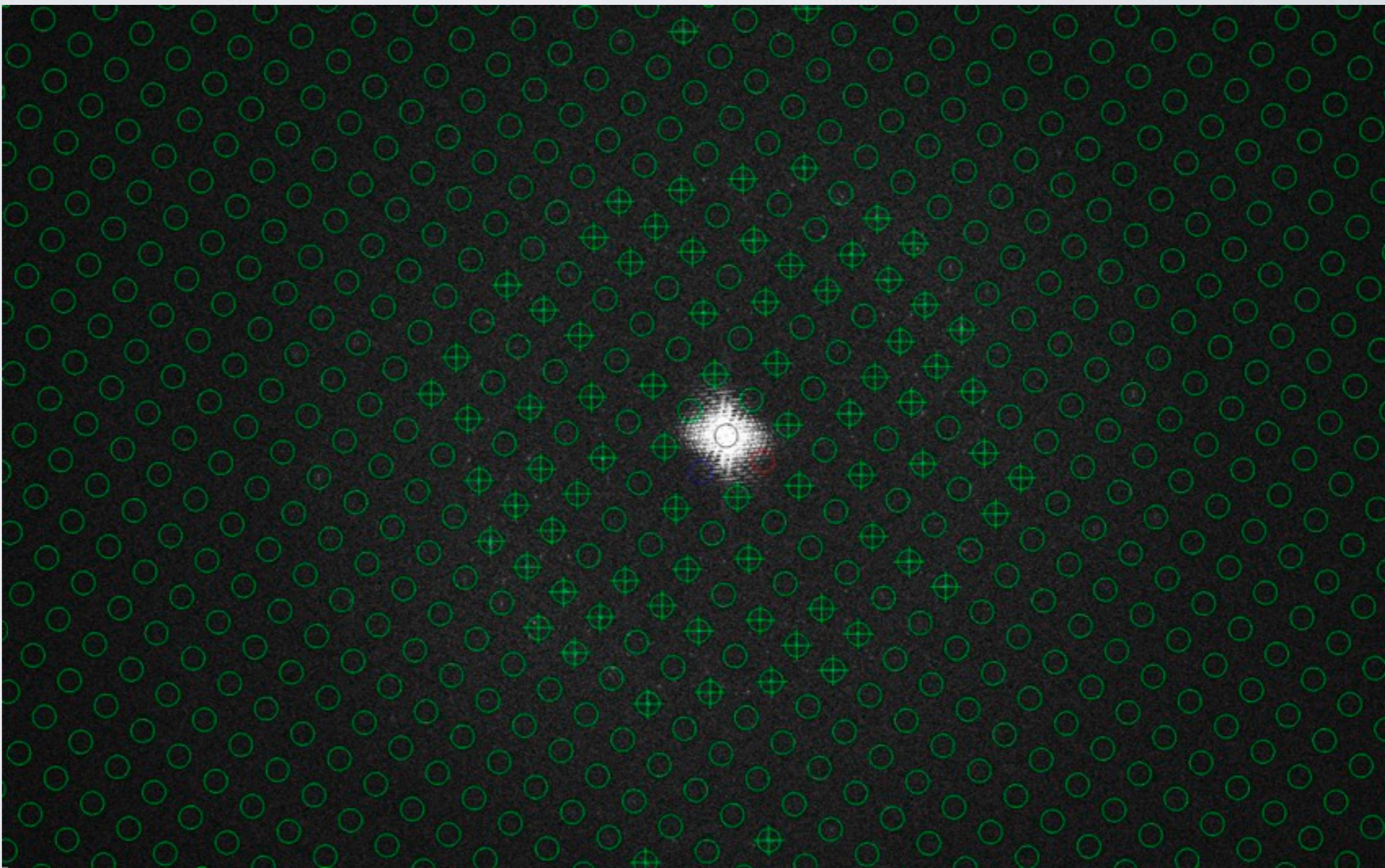
REFERENCE

- Default: Image Center
- Manual Selection

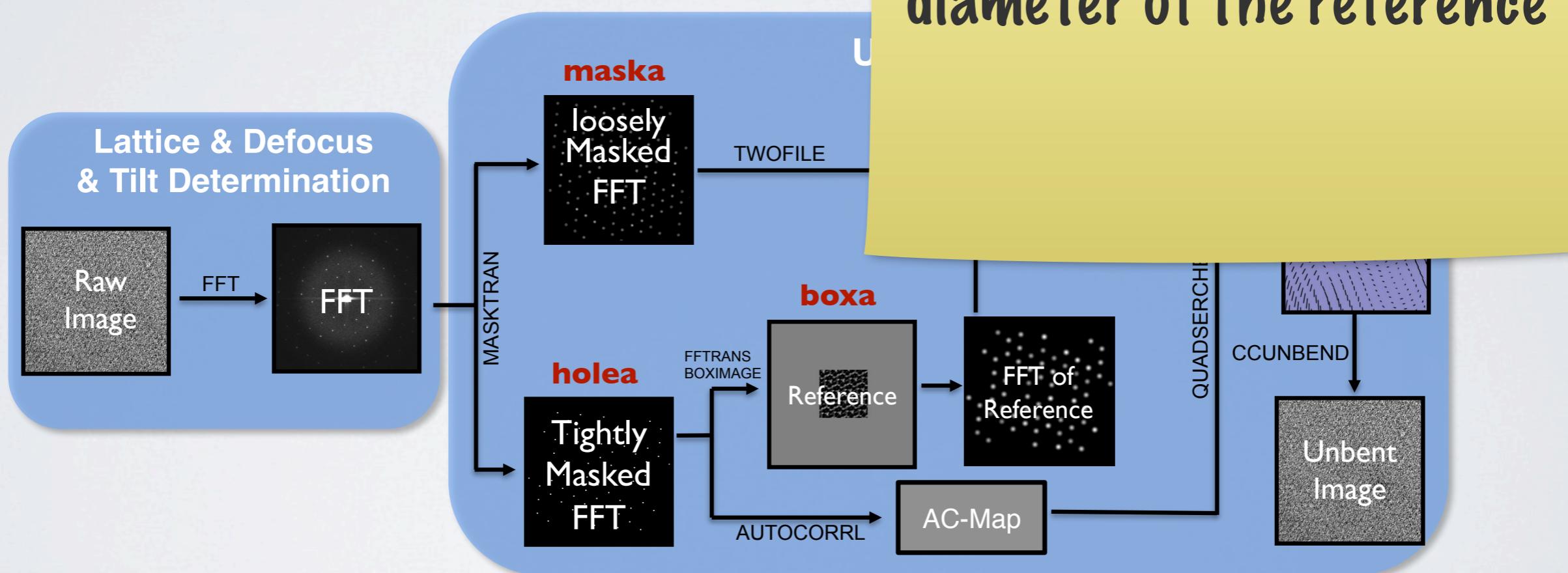


REFERENCE

- Spotlist



PARAMETERS



maska =

Fourier Filter radius

boxa =

diameter of the reference

QUALITY MEASURE

- IQ Values
 - The intensity ratio between the diffraction peak of and its local background

$$IQ = 1 + \text{int}\left(7 \cdot \frac{B}{P}\right)$$

- QVal

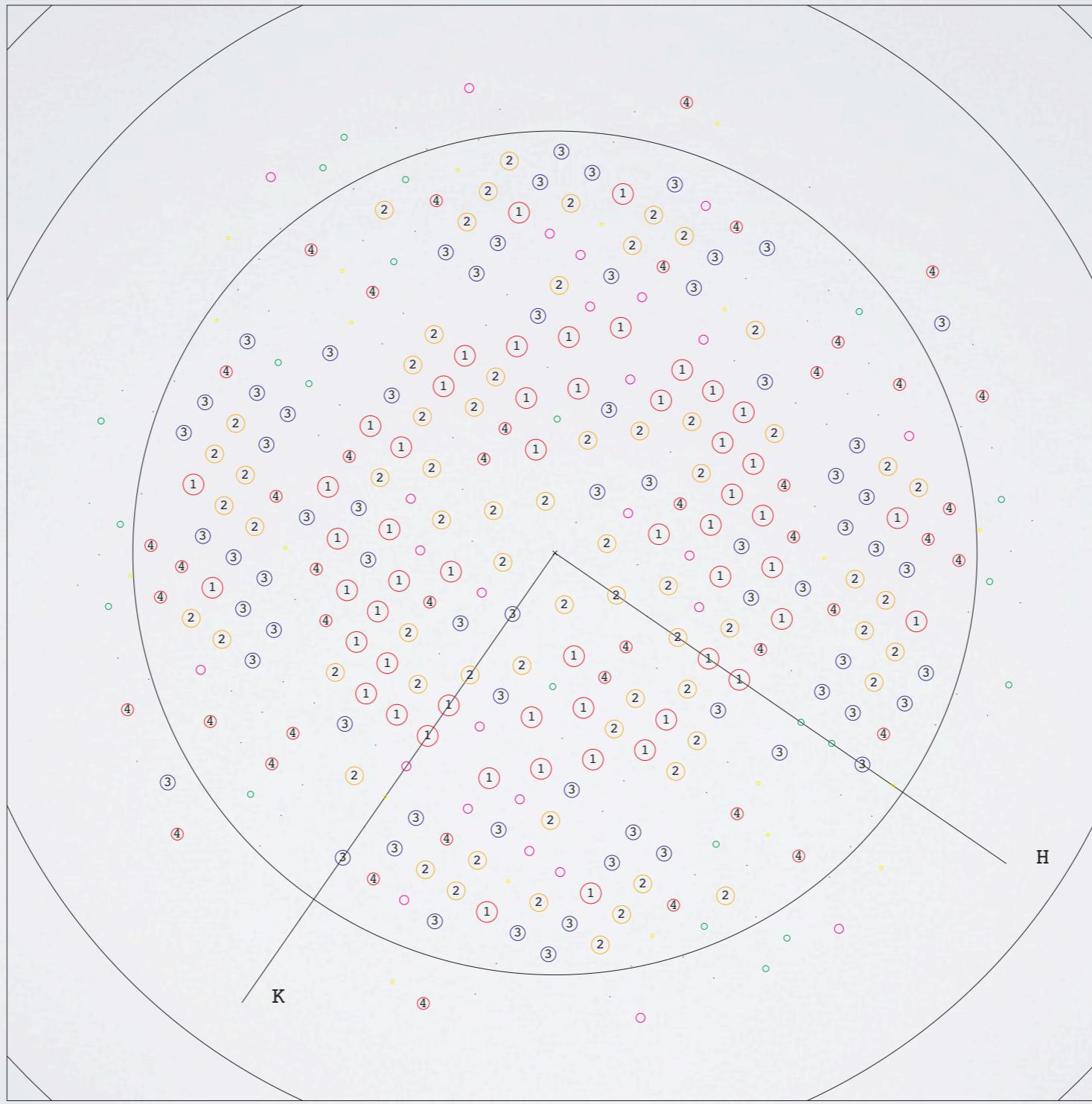
$$\frac{R}{500} \cdot (w_1 \cdot IQ1 + w_2 \cdot IQ2 + w_3 \cdot IQ3 + w_4 \cdot IQ4)$$

R denotes the height of the central pixel of the averaged Fourier peak profiles

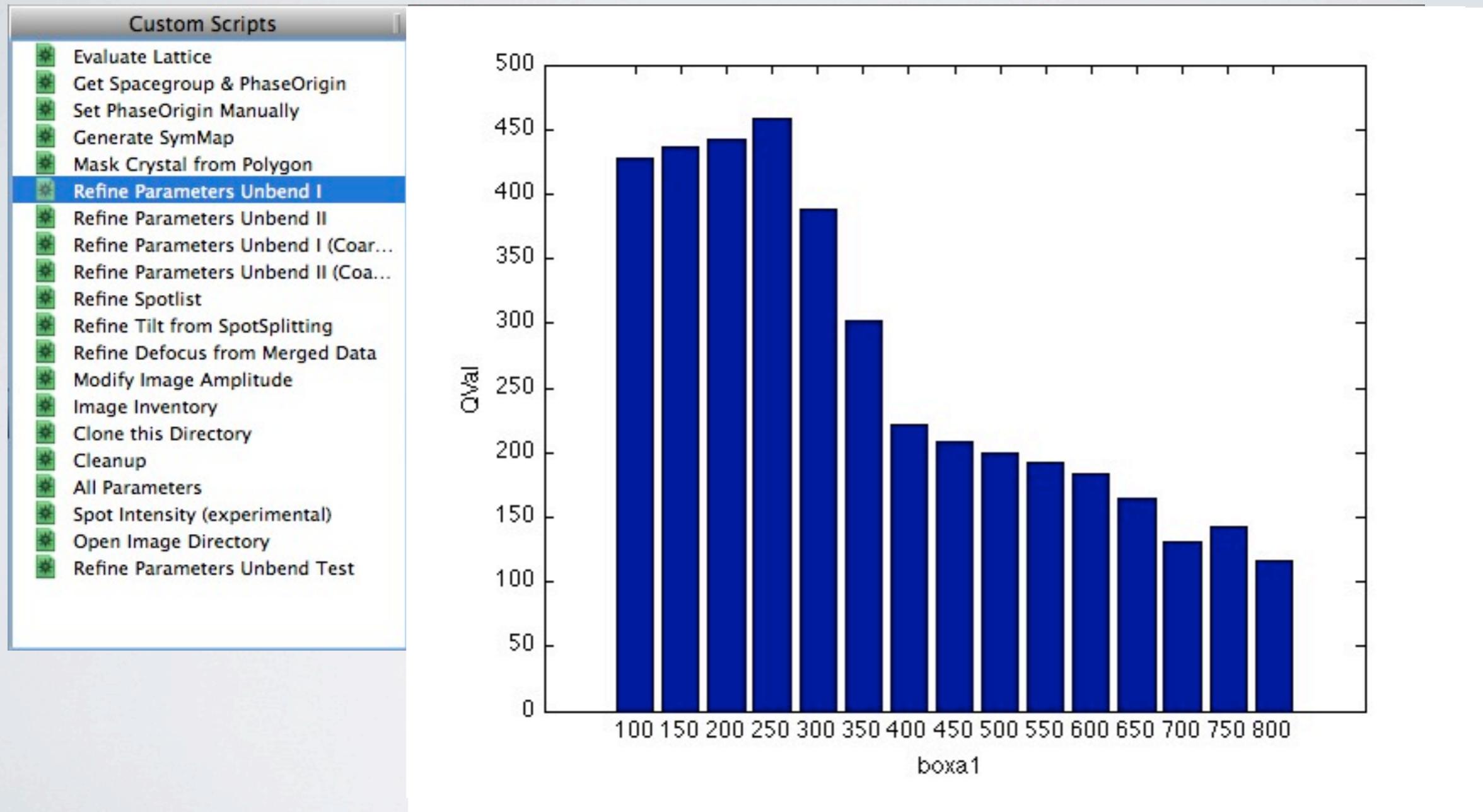
as calculated by mmbox

500 is the calibration factor

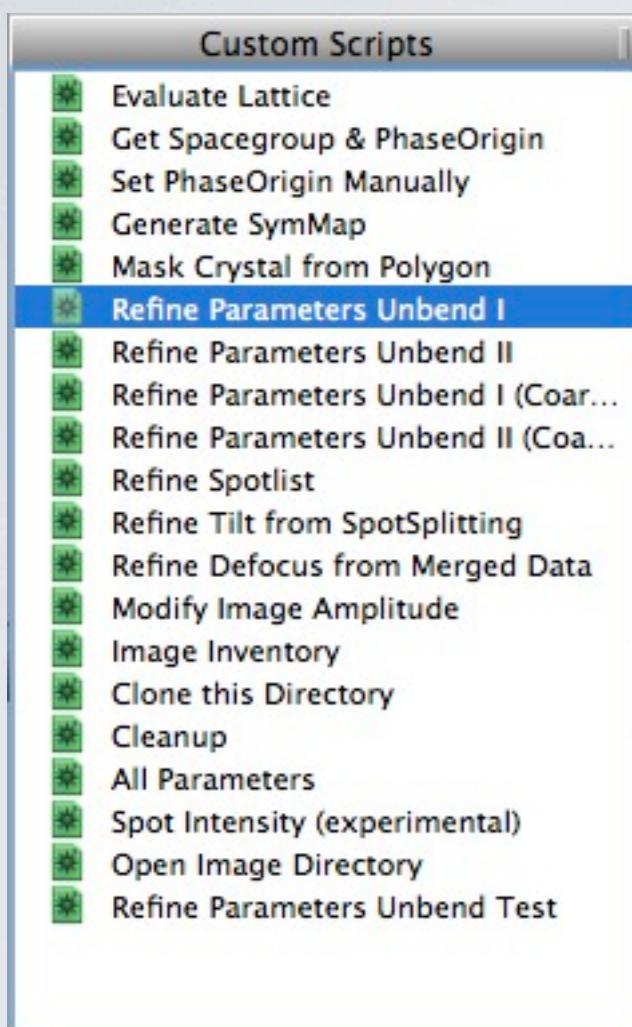
QUALITY MEASURE



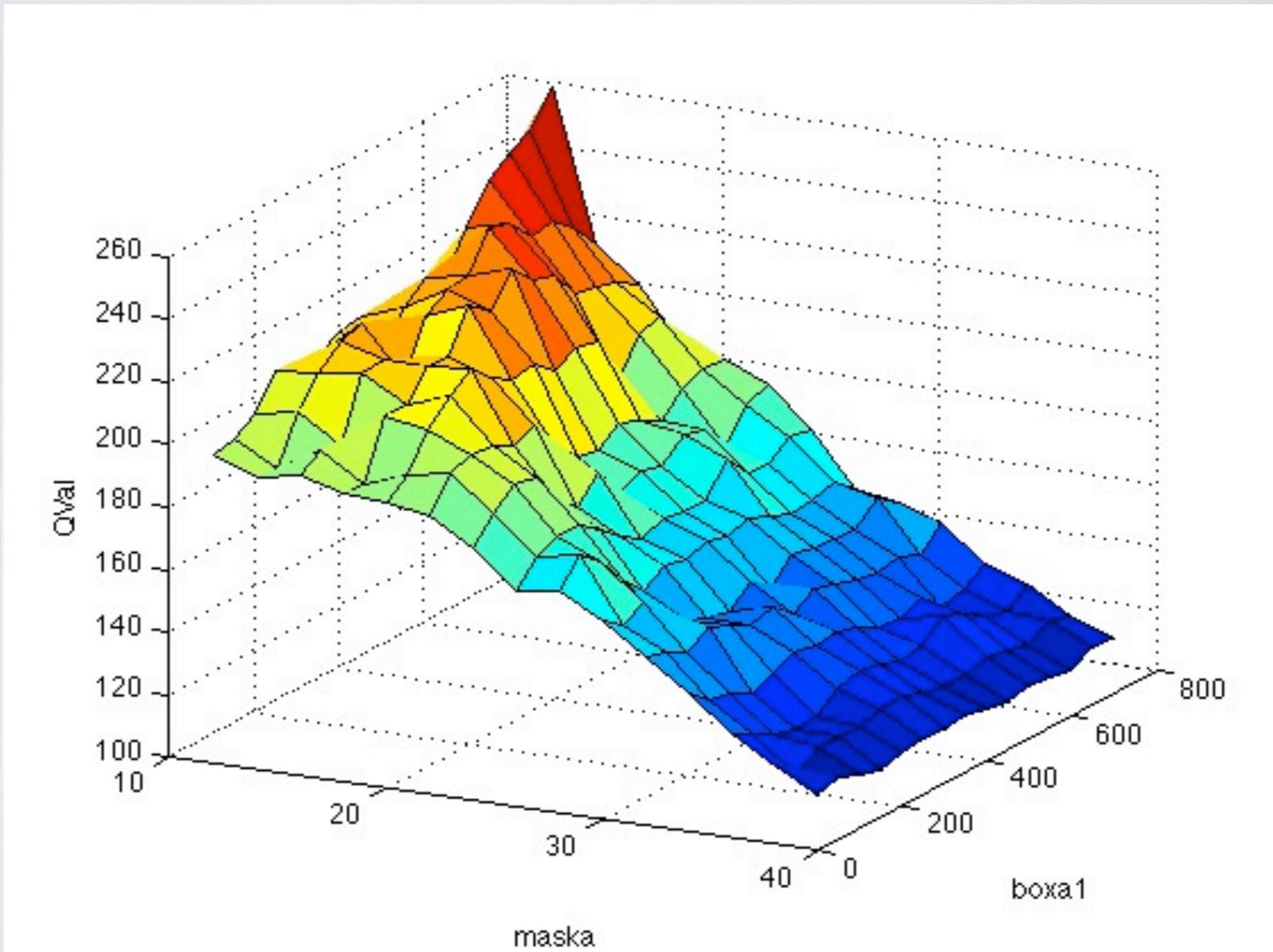
REFINE PARAMETERS FOR UNBENDING

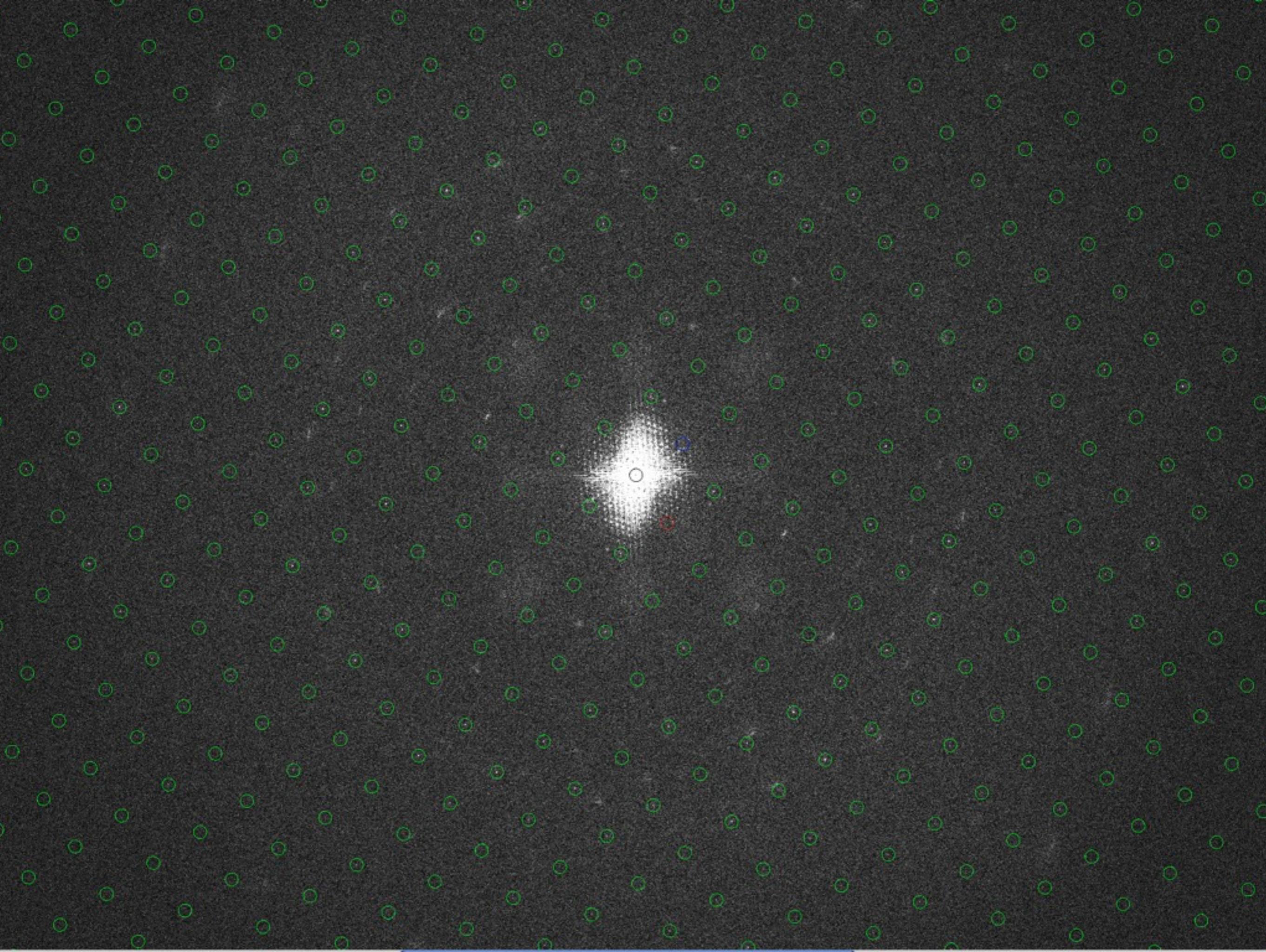


REFINE PARAMETERS FOR UNBENDING

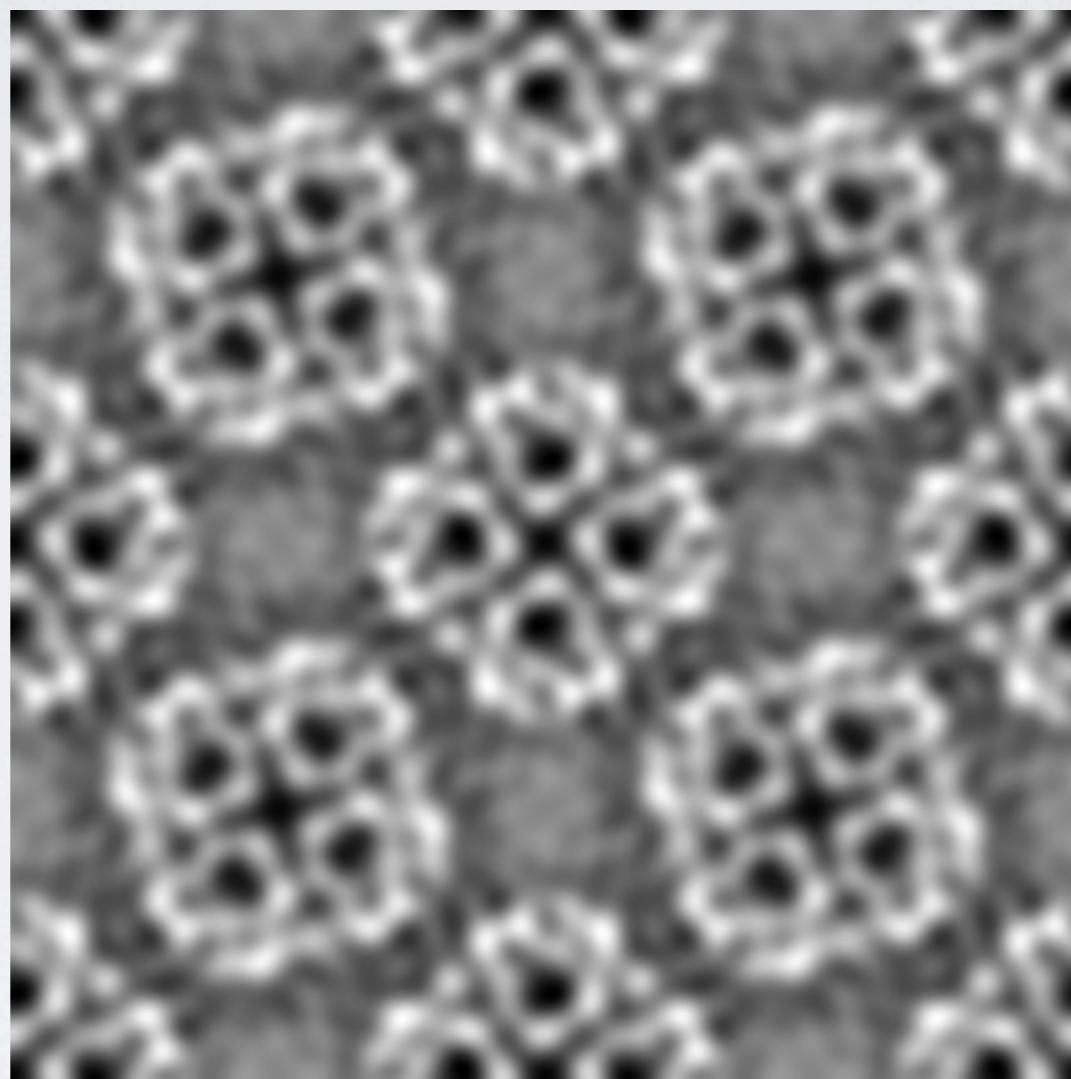


490 Iteration
35 s
286 min >4h





RESULTS



UNBENDING I & II

/Users/marheit/data/2dx/workshop/data2merge/glpf0000655301/

Unbend II

Standard Scripts

- Init Program
- Init Files and Parameters
- Calculate FFT
- Get Defocus & Tilt
- Get Lattice & Tilt
- Refine Lattice
- Calculate Crystal Tilt from...
- Get SpotList for Unbend I
- Unbend I**
- Get SpotList (complete)
- Unbend II**
- Synthetic Unbend
- Correct CTF
- ML-2D (for advanced us...)
- Generate Map

Custom Scripts

- Evaluate Lattice
- Get Spacegroup & Pha...
- Set PhaseOrigin Manu...
- Generate SymMap
- Mask Crystal from Pol...
- Refine Params Unbend I
- Refine Params Unbend II
- Refine Params Unben...
- Refine Params Unben...
- Refine Parameters Syn...
- Refine SpotList
- Refine Tilt from SpotS...
- Refine Defocus
- Refine Params (Only T...
- Modify Image Amplitu...

Processing Data – Standard

Image File

Image Name: glpf0000655301
 Image Side Length: 6000
 Comment:

Crystal Unbending

Use Synthetical Reference if possible?: Use Fourier Filtered reference: 15
 maskb01 (Fourier filter radius, later unbending): 0
 maskb02 (Fourier filter radius, later unbending): 3000 3000
 Reference location: 500
 boxb1 (Reference diameter later unbending): 0.17

Common Image Processing

Lower Resolution Limit (RESMIN): 200.0
 Upper Resolution Limit (RESMAX): 8.0
 ALAT (Z-dimension of unit cell to reconstruct): 200.0
 Choice of Unbending Program: 2dx_ccunbendk
 LCOLOR (Distortion plots in color?): Yes

Switches for Algorithm Selection

Do automatic masking of 2D crystal ?: No
 Generate information for manual masking ?: Yes

Program Technical Data

Keep Large Temporary Files ?: Yes

History - Low Verbosity

```
FFPETR/glpf0000655301.fft.wic
Unbend 1: maska=20, boxal=600: QVal= 189.3 ... IQ stat = 27 31 33 39 52 50 35 276 499
Unbend 2: maskb=22, boxb1=375: QVal= 198.8 ... IQ stat = 26 36 45 42 48 51 36 297 461
Unbend 2: maskb=24, boxb1=375: QVal= 201.9 ... IQ stat = 27 36 43 43 41 60 45 286 461
Defocus = 4397.94, 3874.12, 35.76
From EvaluateLattice:
RealCell= 103.0, 103.0
Real Ang= 90.0
Lattice = 48.089, -33.111, -33.193, -47.708
TLTAXIS = 32.17317
TLTANG = -6.62509
TLTXA = 66.72217
TAXA = 66.58259
TANGL = -6.62509
Unbend 1: maska=13, boxal=250: QVal= 237.8 ... IQ stat = 24 28 22 22 17 9 7 59 70
Unbend 2: maskb=15, boxb1=500: QVal= 317.3 ... IQ stat = 27 33 34 22 13 11 10 47 61
```

Results

QVAL_local	317.3
PSMAX	120
U2_IQ1	27
U2_IQ2	33
U2_IQ3	34
U2_IQ4	22
U2_IQ5	13
U2_IQ6	11
U2_IQ7	10
U2_IQ8	47
U2_IQ9	61
OVAL	317.3

Images

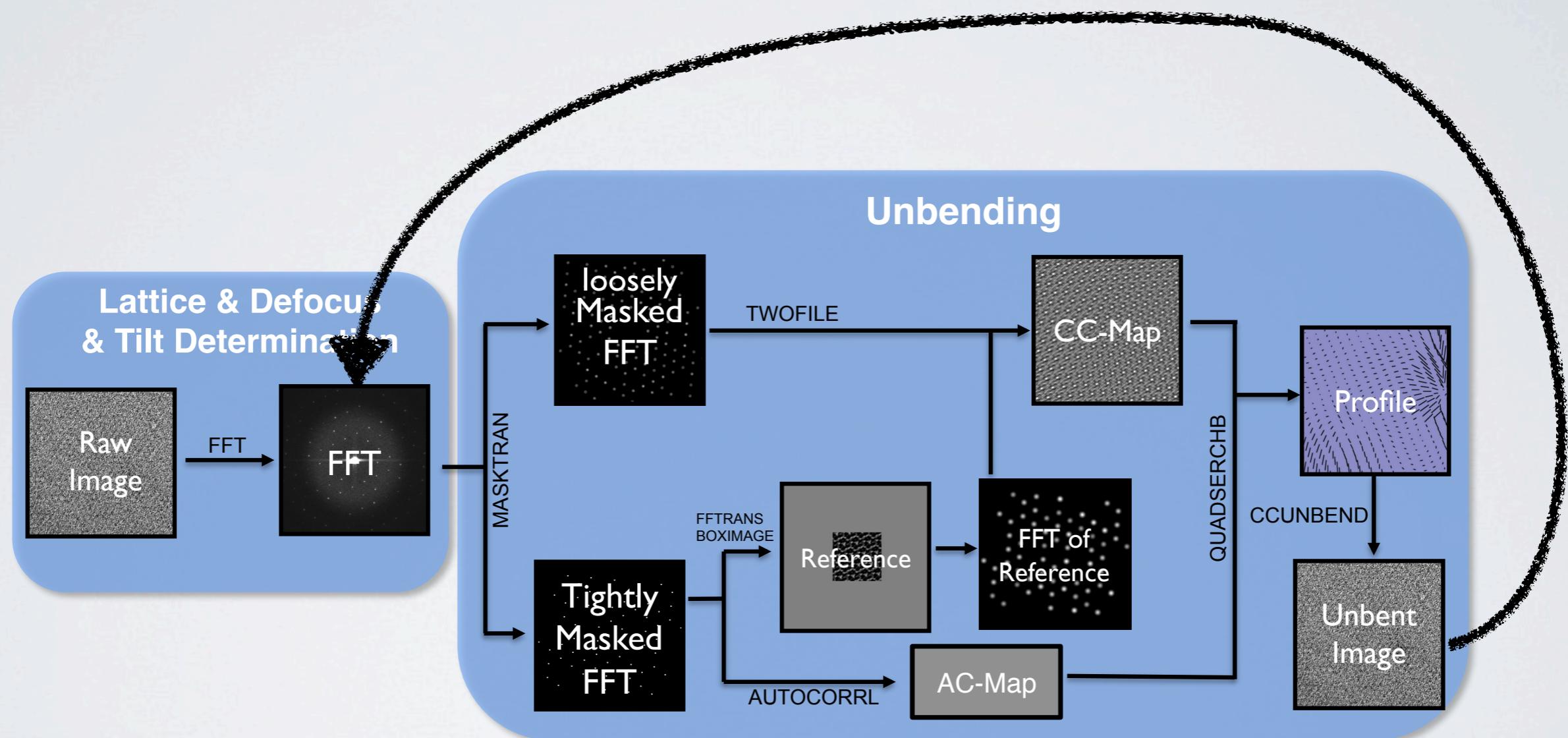
- FFT of Unbent Reference
- Reference Patch
- Center of Reference Patch
- Autocorrelation Function of Refere...
- Central Peak of Autocorrelation Fu...
- Filtered Image for Reference gener...
- Reference 1
- maskb-Masked FFT of Image (2)
- FFT of Reference 1
- XCF between Reference 1 and Image
- PS: Vector Plot of Distortion, Pas...
- xcf Map for Manual Masking

Status

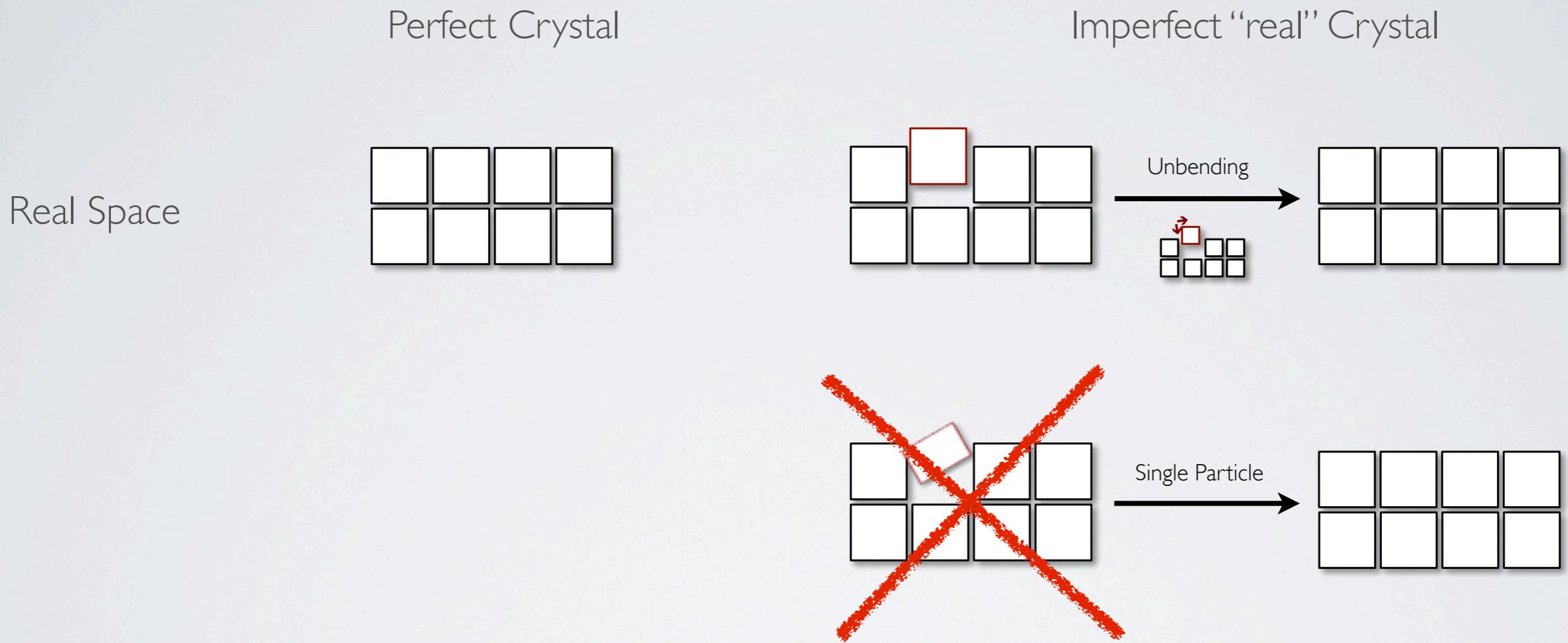
Th.Mag	70000.6	QVAL	317.3					
IQs.Unbl	-	QVal1	237.8					
24	28	22	17	9	7	59	70	
IQs.Unb.II	-	QVal2	317.3					
27	33	34	22	13	11	10	47	61
IQs.Unb.Syn	-	QValS	-					
PowerBins	[A]	15	12	9	7	5	3	
(noise=7)	#	228	38	67	12	7	7	
TiltInfo	Defoc.	Laz.	SpSplit	Merge	-	-	-	
Grd.TAxis	-	32.2	-	-	-	-	-	
Grd.TAng	-	-6.6	-	-	-	-	-	
Xst.TAxis	-	66.6	-	-	-	-	0.0	
Xst.TAng	-	-6.6	-	-	-	-	0.0	

FFT DEFOCUS LATTICE SPOTS UNBEND CTF MASK PHORI MERGE REPROCESS

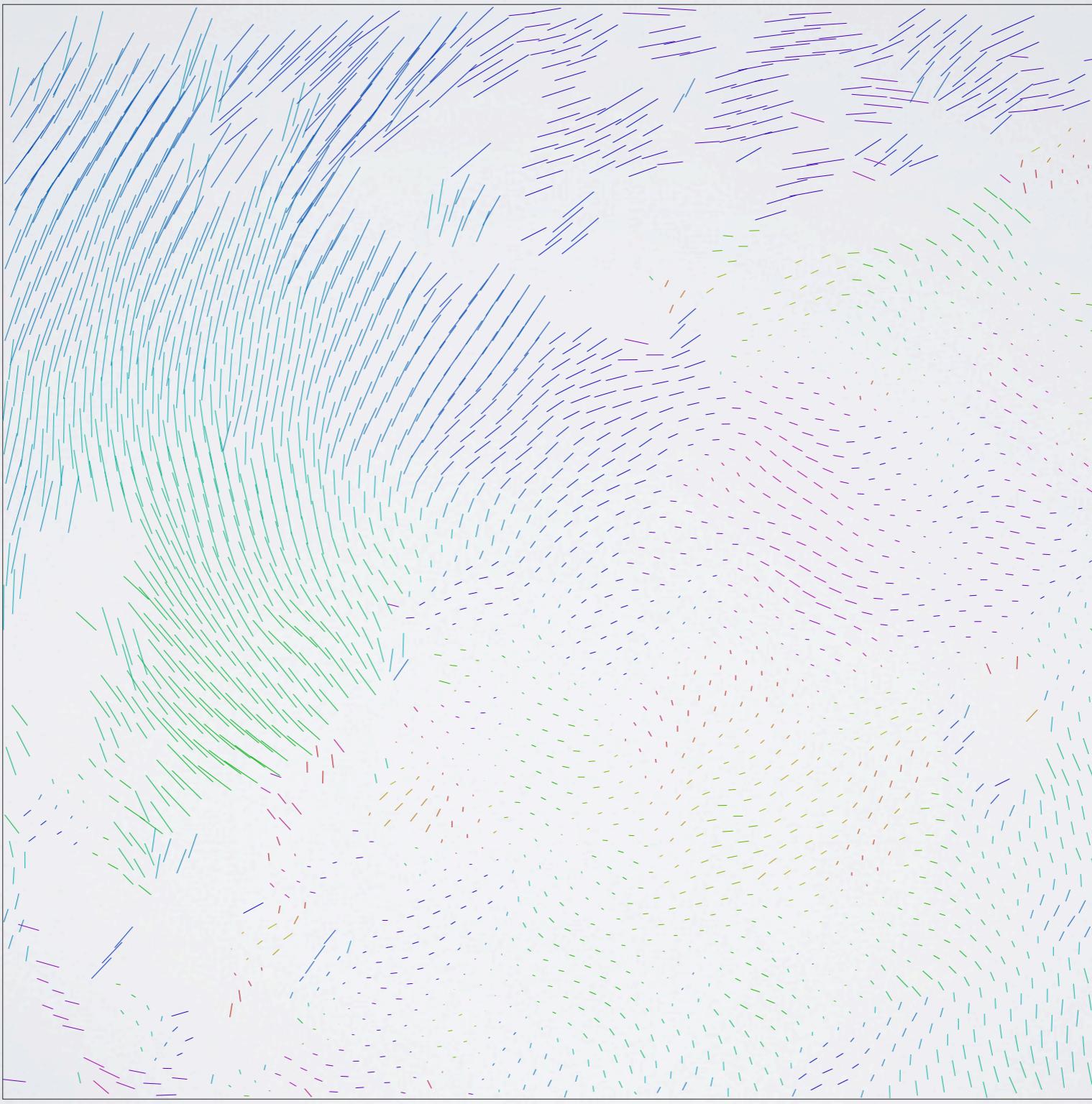
REUNBEND CRYSTAL



DRAW BACKS



MASKING



QUESTIONS?

