

Lattice Determination

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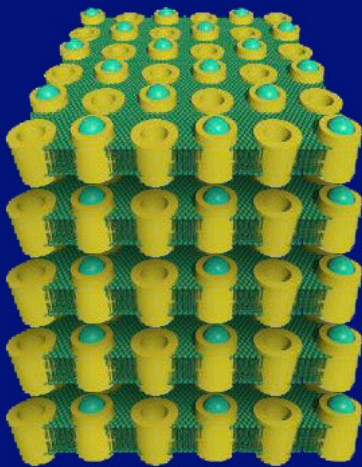
2dx Workshop
Basel, August 23–26, 2016

1

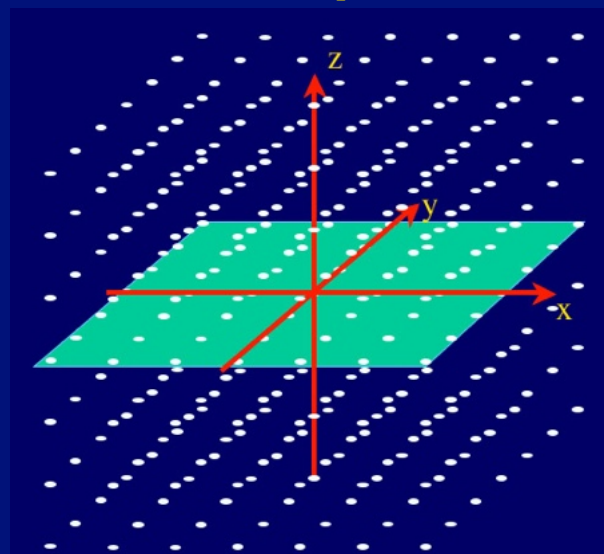
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The Third Dimension

Real Space



Fourier Space



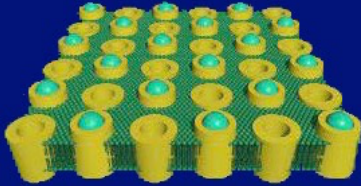
Diffraction Spots in 2D

2

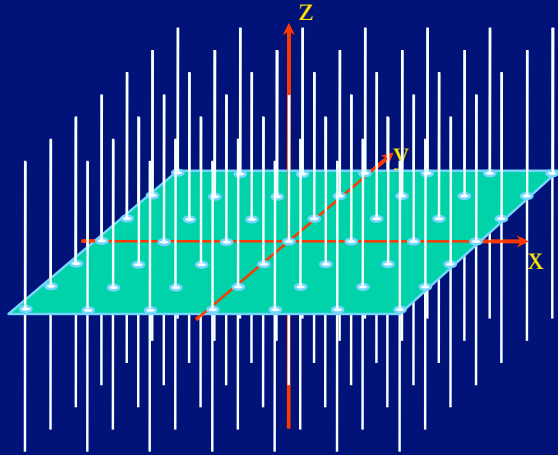
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The Third Dimension

Real Space



Fourier Space

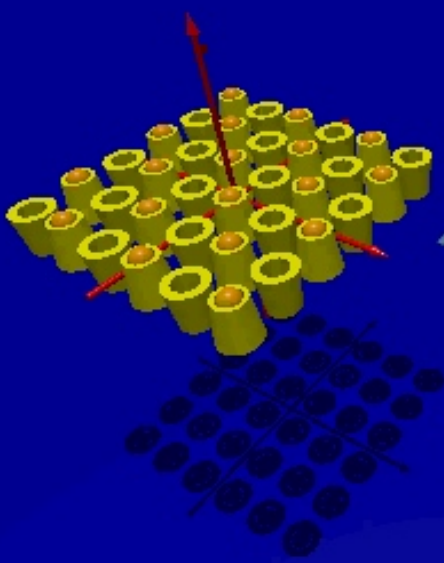


Diffraction Spots in 2D

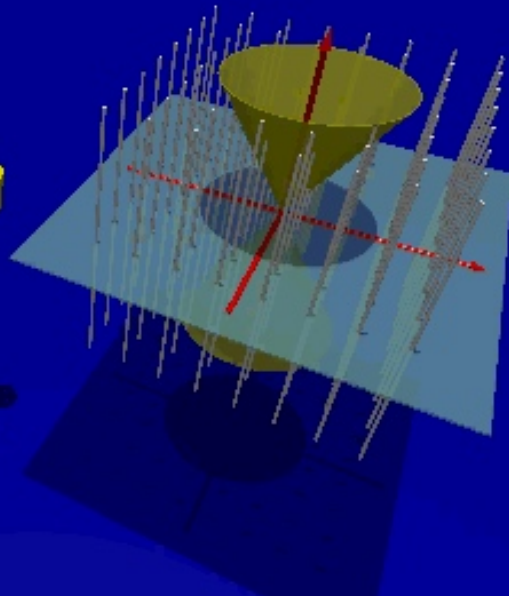
Lattice Lines in 3D

The Missing Cone

Real Space



Fourier Space

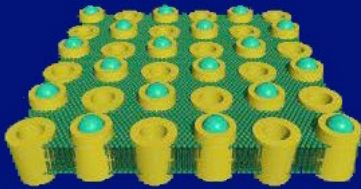


Diffraction Spots in 2D

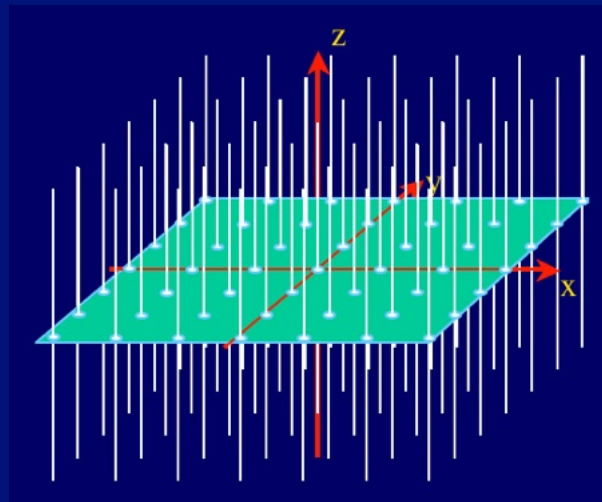
Lattice Lines in 3D

The Third Dimension

Real Space



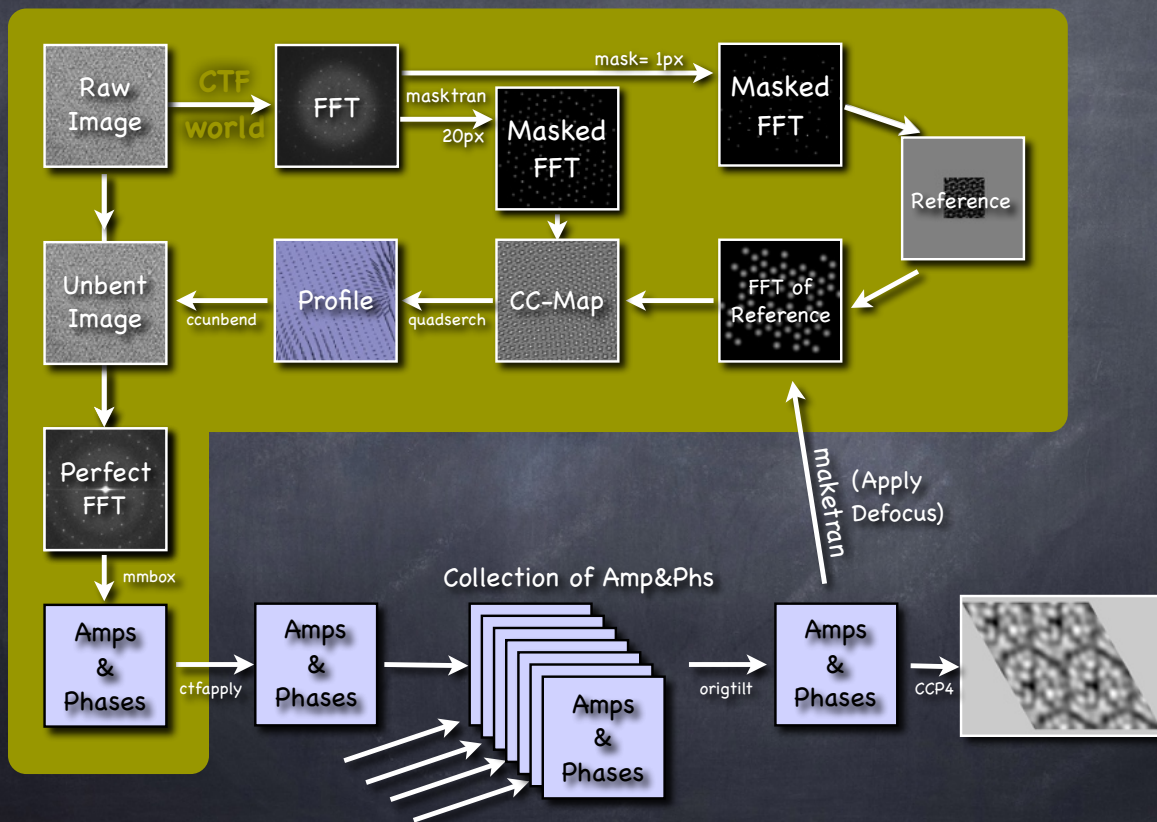
Fourier Space



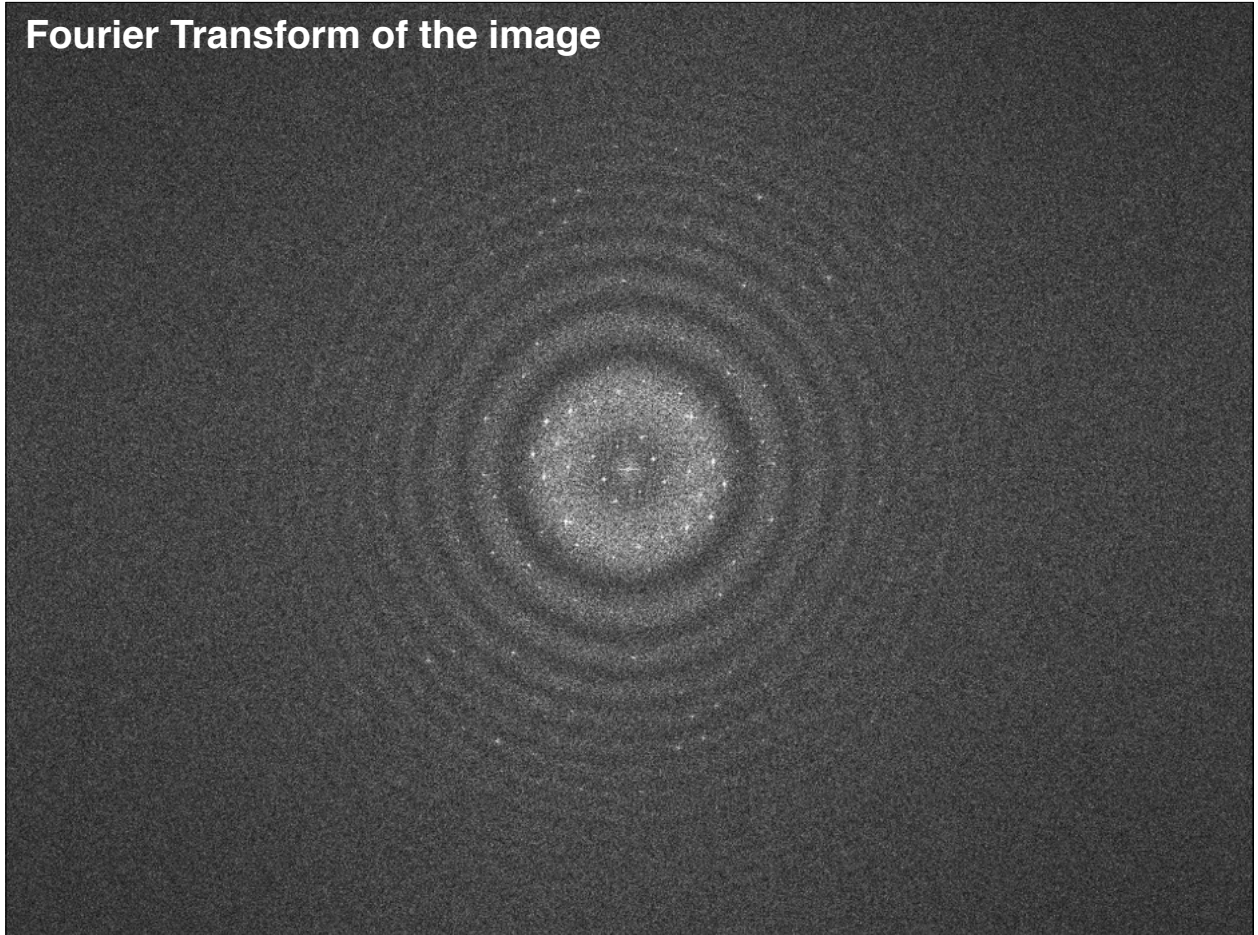
Diffraction Spots in 2D

Lattice Lines in 3D

Algorithm Non-tilted



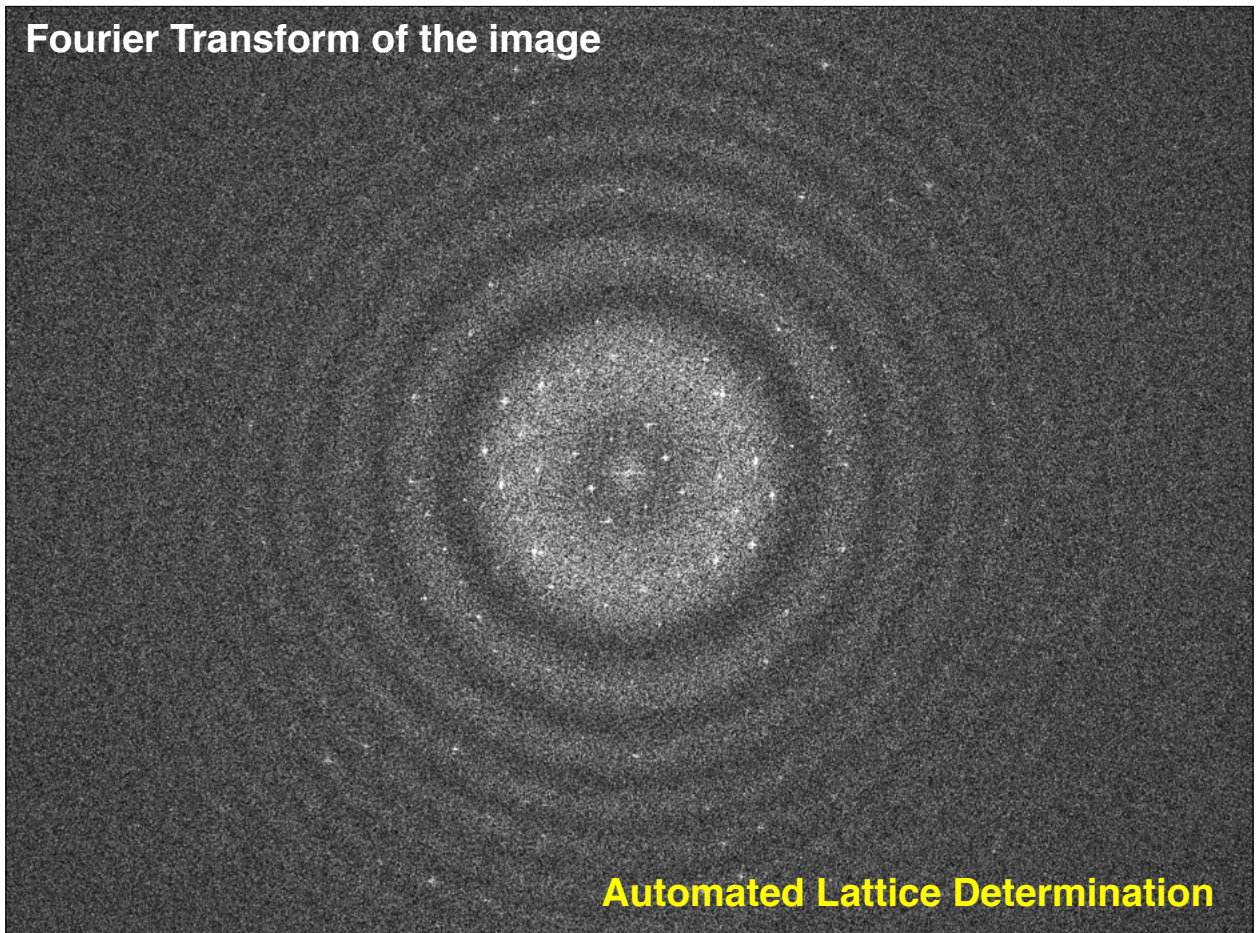
Fourier Transform of the image



7

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Fourier Transform of the image

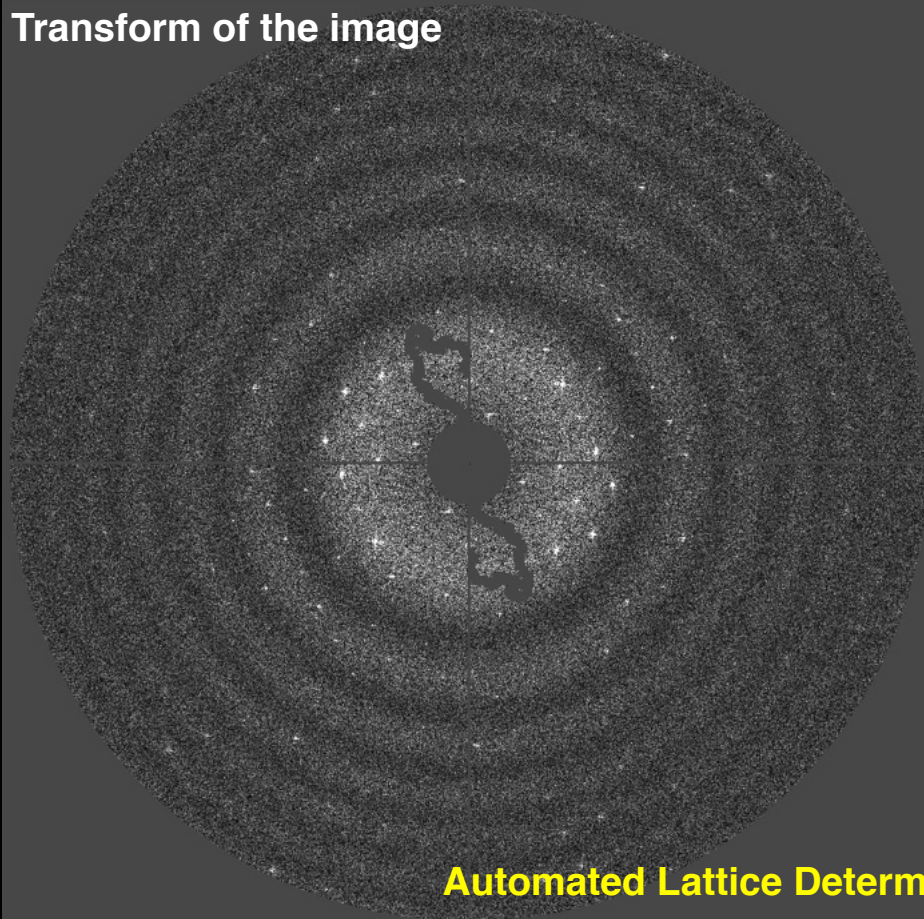


Automated Lattice Determination

8

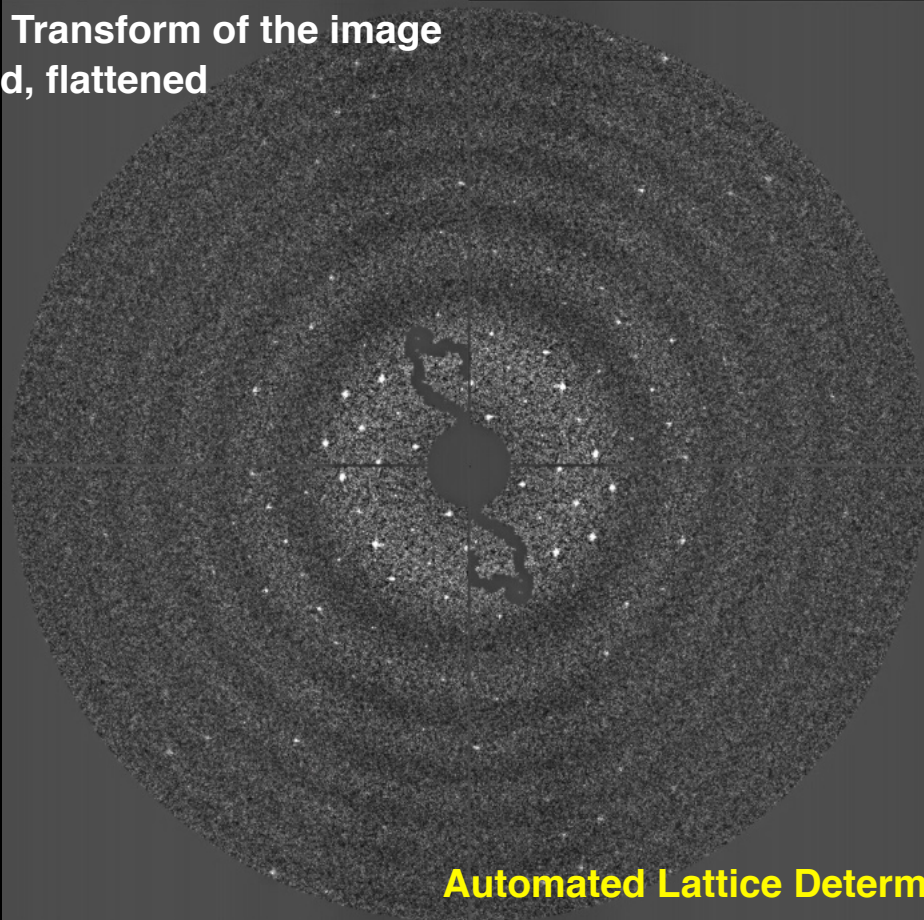
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Fourier Transform of the image



Automated Lattice Determination

**Fourier Transform of the image
- blurred, flattened**

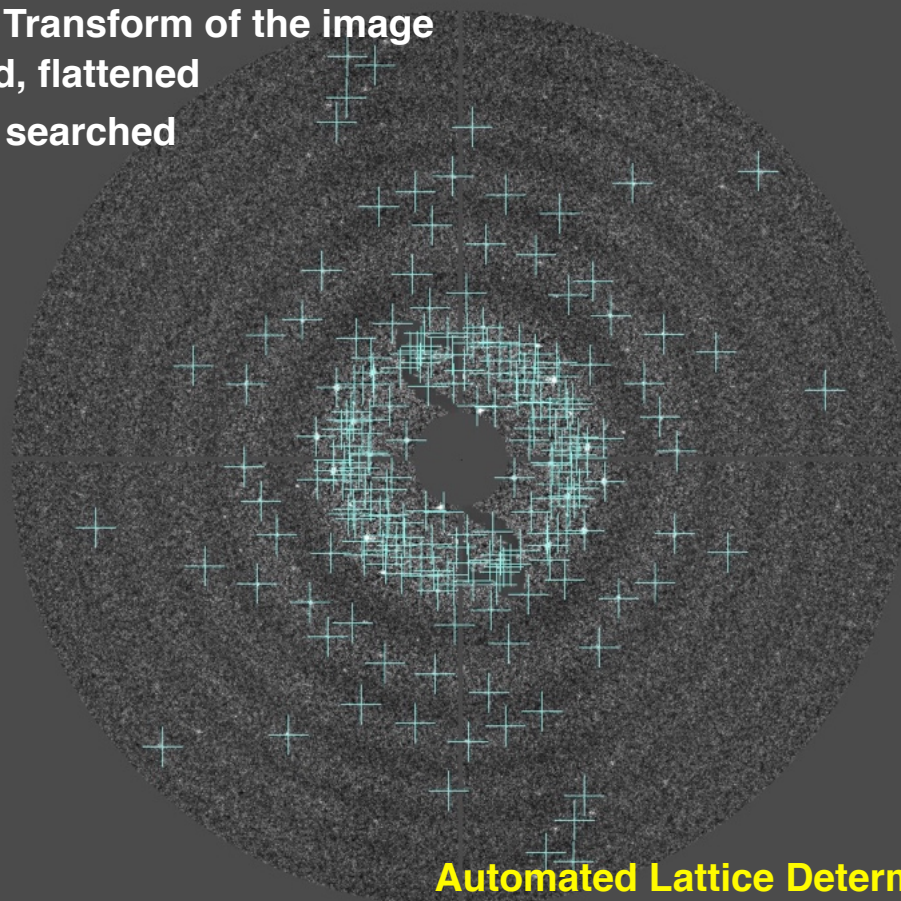


Automated Lattice Determination

Fourier Transform of the image

- blurred, flattened

- Peaks searched



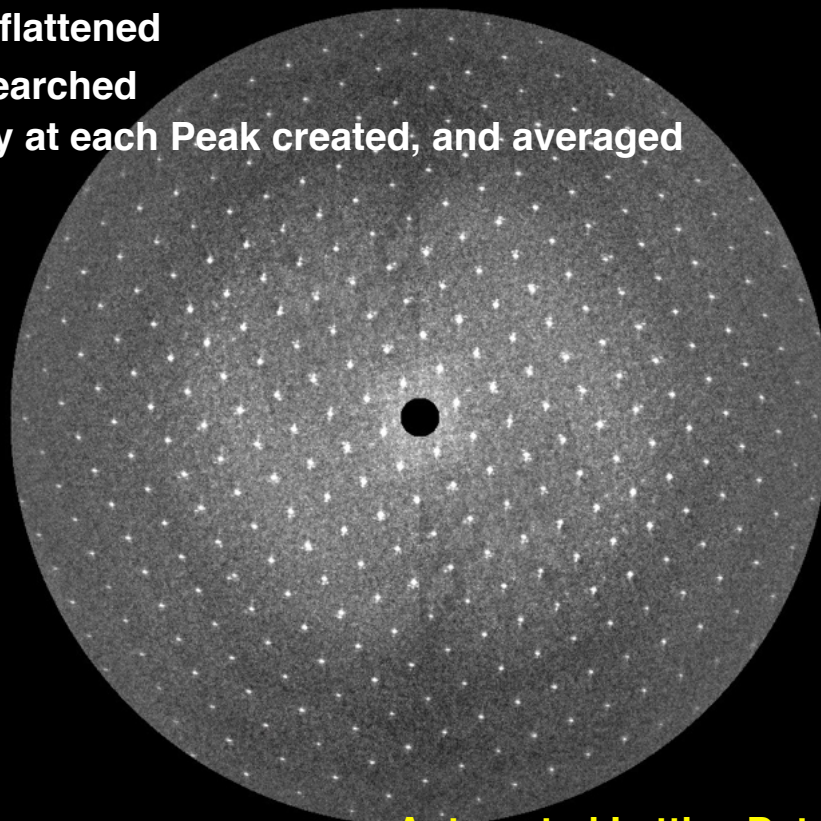
Automated Lattice Determination

Fourier Transform of the image

- blurred, flattened

- Peaks searched

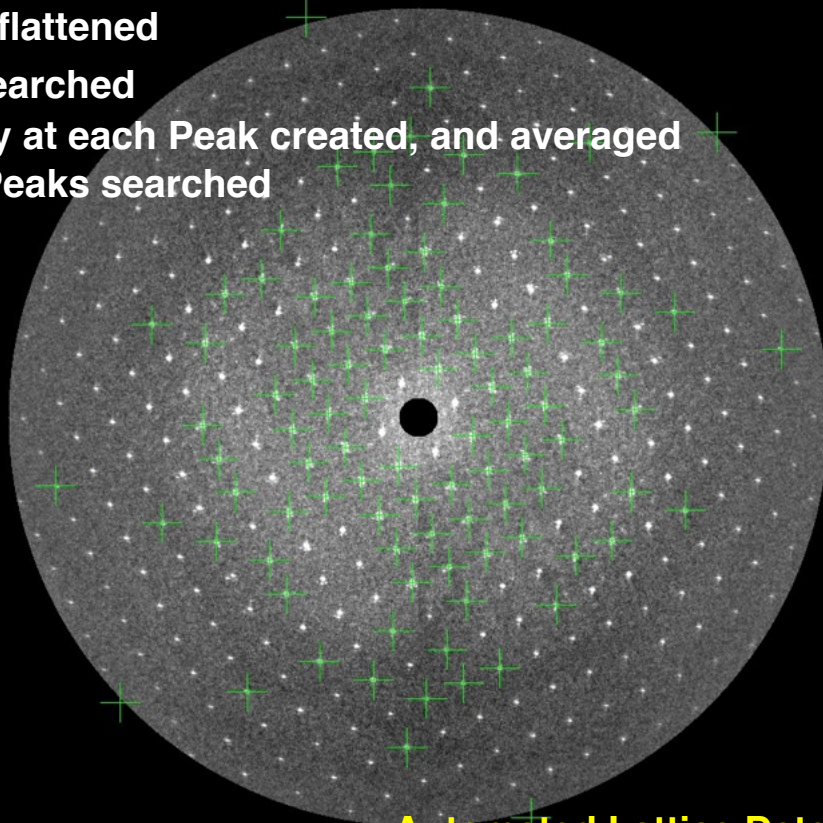
- one copy at each Peak created, and averaged



Automated Lattice Determination

Fourier Transform of the image

- blurred, flattened
- Peaks searched
- one copy at each Peak created, and averaged
- Lattice Peaks searched



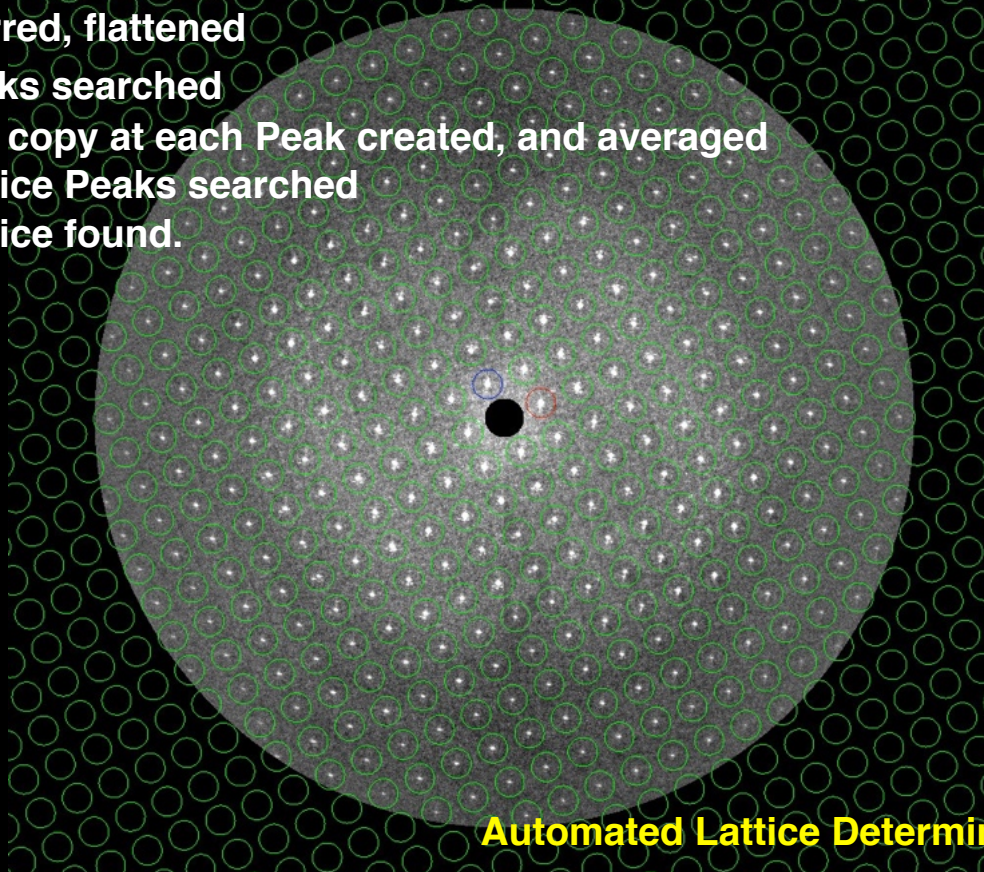
Automated Lattice Determination

13

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Fourier Transform of the image

- blurred, flattened
- Peaks searched
- one copy at each Peak created, and averaged
- Lattice Peaks searched
- Lattice found.

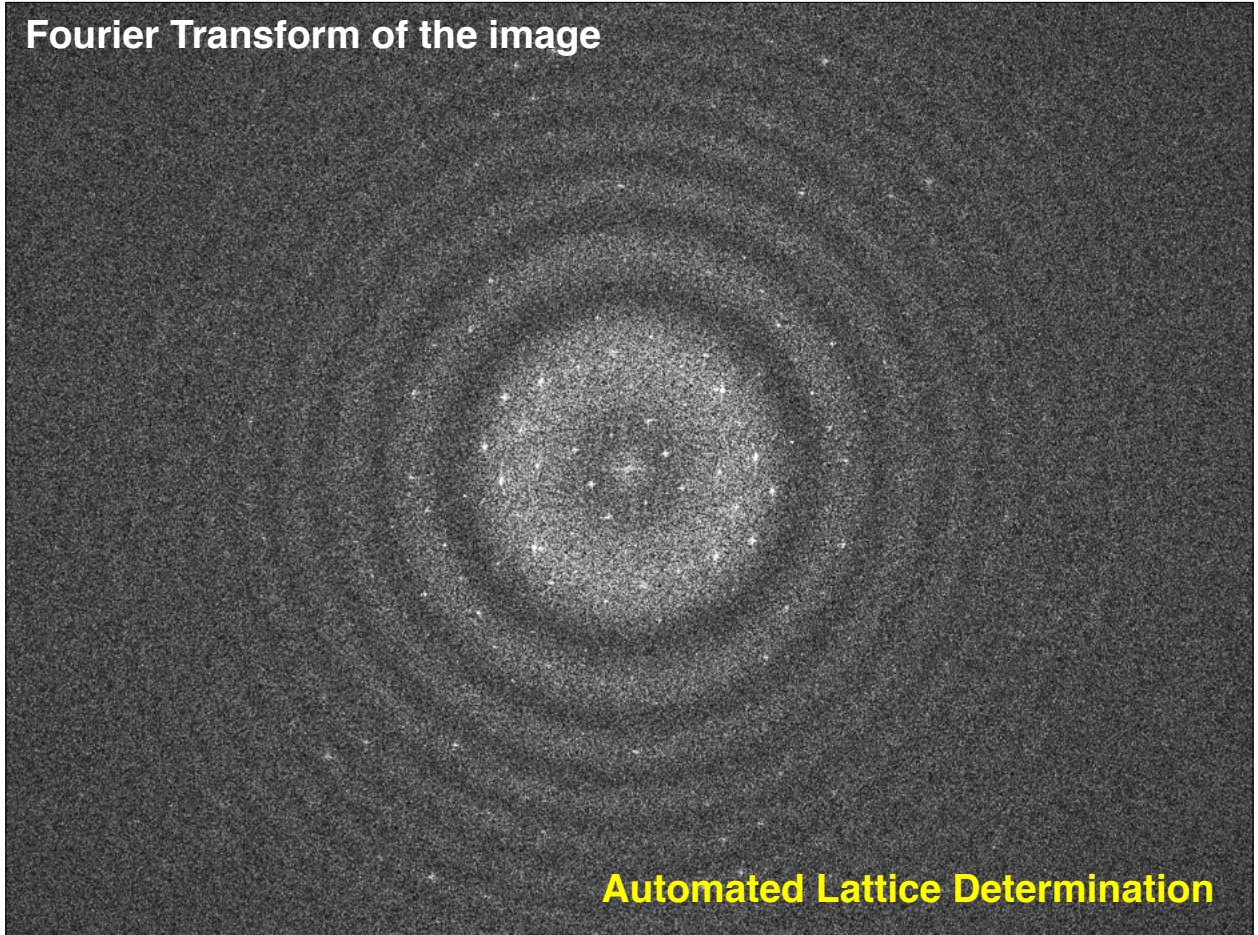


Automated Lattice Determination

14

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Fourier Transform of the image

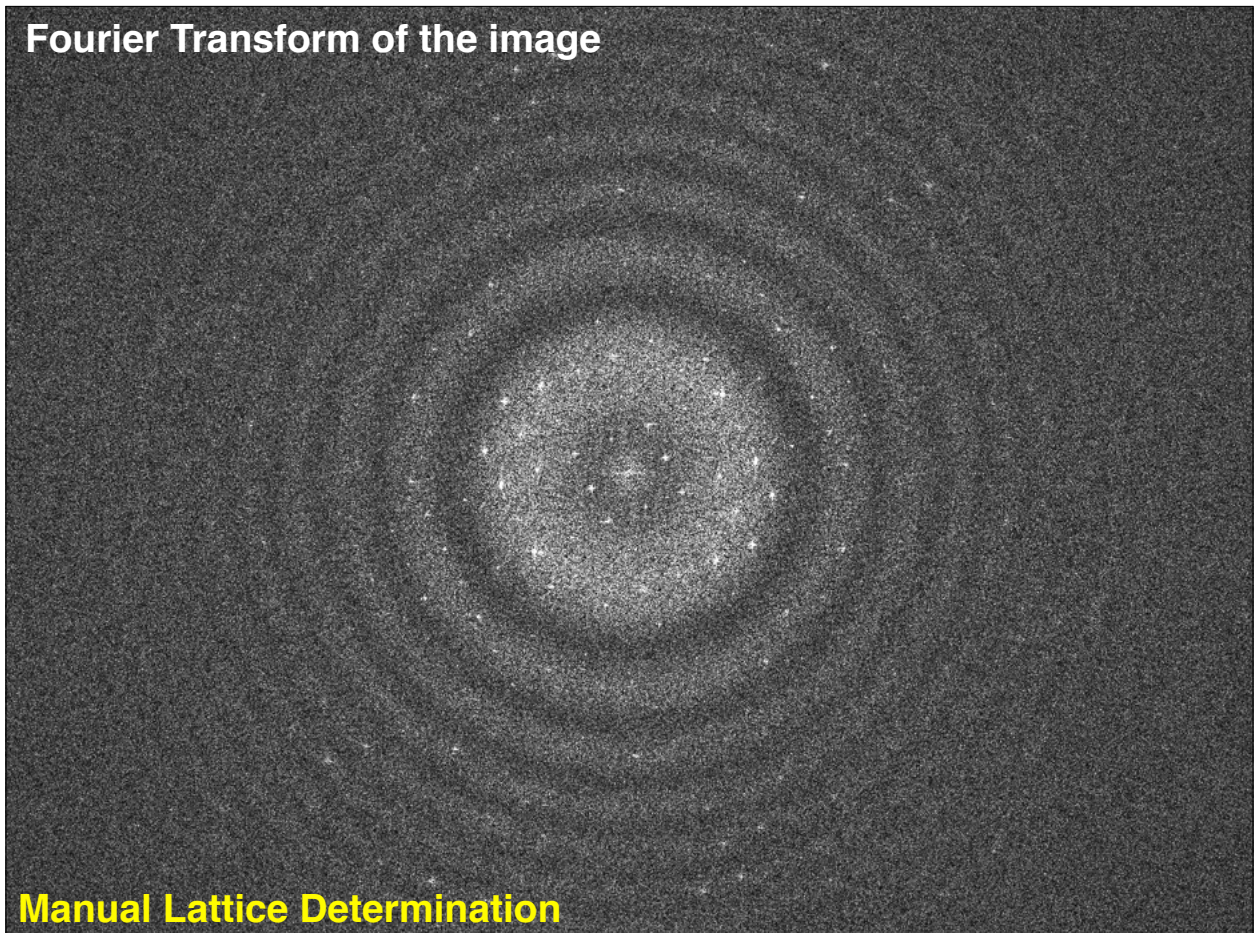


Automated Lattice Determination

15

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Fourier Transform of the image



Manual Lattice Determination

16

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Fourier Transform of the image

- Shift-“R”
- Two independent spots clicked

Manual Lattice Determination

Lattice Refinement:		<17, -34>	<37, 15>
i	j	x	y
1	0	37	15
2	1	17	-34

Current Point: 37 15

Miller Index:

17

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Fourier Transform of the image

- Shift-“R”
- Two independent spots clicked
- Lattice accepted

Manual Lattice Determination

Lattice Refinement:		<17, -34>	<37, 15>
i	j	x	y
1	0	37	15
2	1	17	-34

Current Point: 304 56

Miller Index: 2 7

18

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Fourier Transform of the image

- Shift-“R”
- Two independent spots clicked
- Lattice accepted
- More spots added, and new lattice accepted

Manual Lattice Determination

Lattice Refinement: <17.1487, -34.4325> <37.3701, 15.531>

	i	j	x	y
1	-11	2	-115	410
2	-8	9	201	415
3	-5	7	175	281
4	-1	-6	-240	-59
5	0	1	37	15
6	1	0	17	-34

Current Point: -240 -59
Miller Index:

Add Point Accept First Lattice Accept Second Lattice

Delete Point Clear All

19

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Get Lattice & Tilt (Level: Advanced)

Setup

Determine Lattice: Yes No

Lattice Determination Algorithm to run: **0=FindLattice (search for one or two expected lattice(s) based on real coil)**

1=GetLattice (guess new lattice based on peaks in FFT)

Lattice Determination: RMSD Error: 1.3364

Lattice Determination: Peaks used: 140 of 140

Lattice Determination: Node/Peak Density: 1.6507

Real Unit Cell Length (for entire project): 131.0 131.0

Real Cell Angle (for entire project): 90.0 90.0

Regenerate Peak List: Yes No

Initial number of Peaks: 200

Number of Peaks: 140

Inner exclusion radius for first peak list generation: 0.05

Delta tolerance for lattice refinement: 3.0

Test other handedness also?: Yes No

Reciprocal Lattice: 17.1487 -34.4325 37.3701 15.531

Second (bad) Lattice: 0.0 0.0 0.0 0.0

Second Lattice exists: Yes No

Output (Double click for logbrowser) Verbose Level: Low

```

==== 2dx_getspot - To generate a first spotlist.
==== 2dx_lencalc: to calculate some values for the tilt geometry determination.
==== emtil: to calculate the tilt geometry from lattice distortions.
1. TILTAXIS = -41.33106 = ALPHA - PHITLT
2. TILTAXIS = 86.22306 = ALPHA + PHITLT
Taking second option.

==== NOT saving tilt geometry from lattice, because of low tilt.
==== 2dx_calcmag - to calculate the theoretical magnification
==== Theoretical magnification is 22011.695, given magnification is 22500
==== Angle in reciprocal lattice is 94.065.
    
```

Status

Calc. Mag=	22011.7						Last QVAL=	460.4
Unbend	IQ1	IQ2	IQ3	IQ4	IQ5	IQ6	QVAL	
Unb. I	35	74	66	96	168	219	415.3	
Unb. II	39	83	65	113	161	228	460.4	
MovieA	-	-	-	-	-	-	-	
MovieB	-	-	-	-	-	-	-	

Preview

FFTR/MioK10099001200_red_fft.mrc	1904	1904	1904
Mode:	0	0	0
Origin x,y,z:	1904	1904	1
Sample x,y,z:	3808	3808	1
Cell Axes:	90	90	90
Cell Angles:	x	y	z
Basis Vectors:	0.0	0.0	3919.3
Min, Max, Mean:	0	0	57.1
Space Group:			
Symmetry Bytes:			
Phase Origin:	0.0	0.0	0.0
RMS:			
Labels:			

20

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