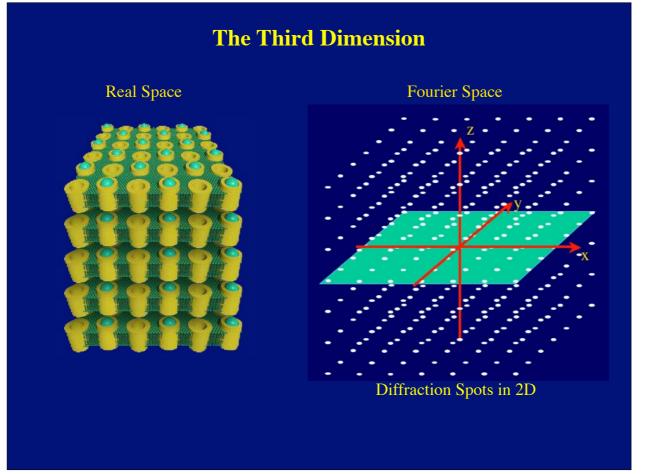
Lattice Determination

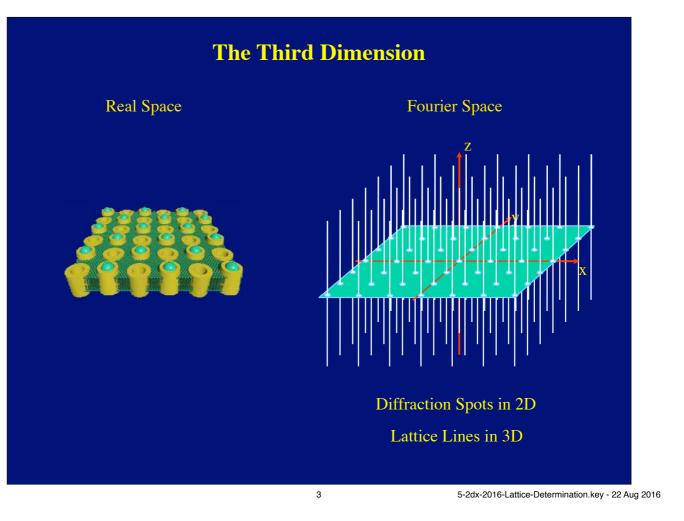
Henning Stahlberg, Biozentrum, Uni Basel, Switzerland c-cina.org

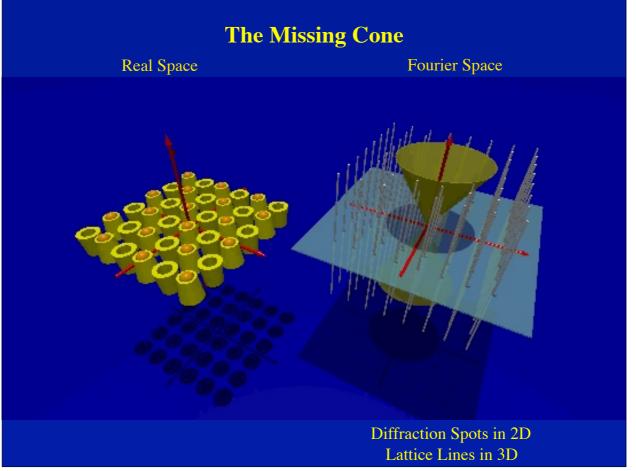
> 2dx Workshop Basel, August 23-26, 2016

> > 1

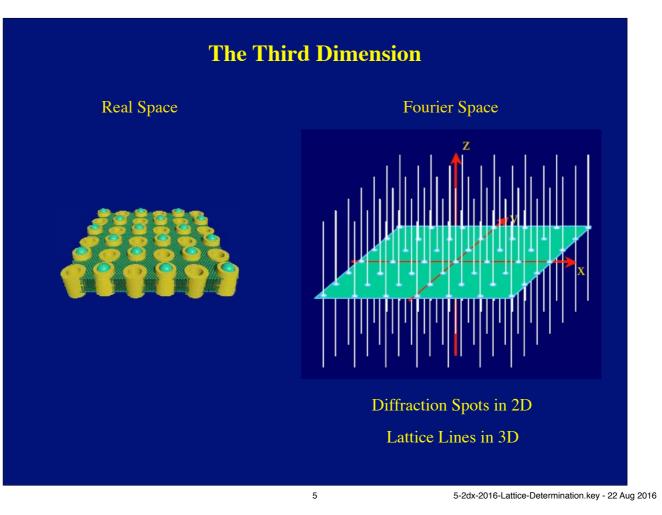
5-2dx-2016-Lattice-Determination.key - 22 Aug 2016



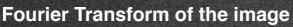


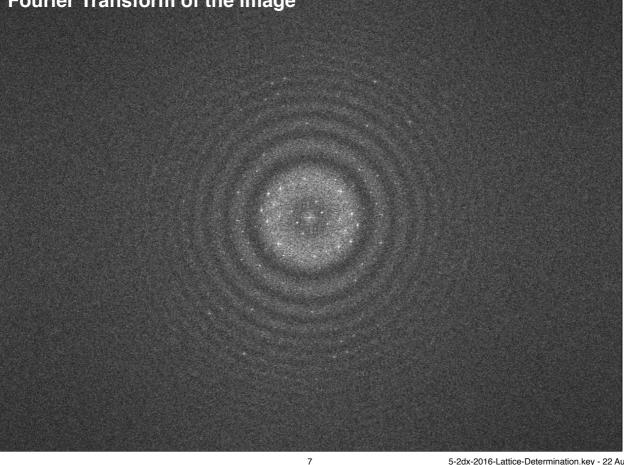


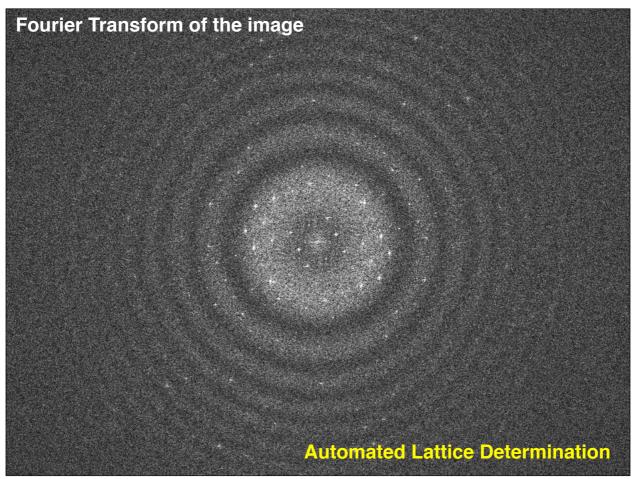
4

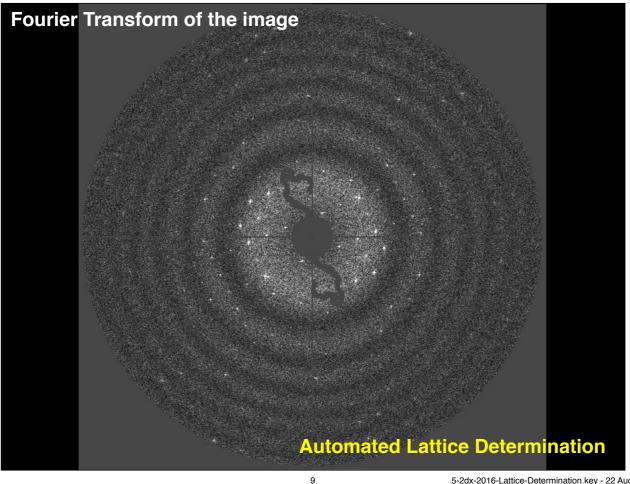


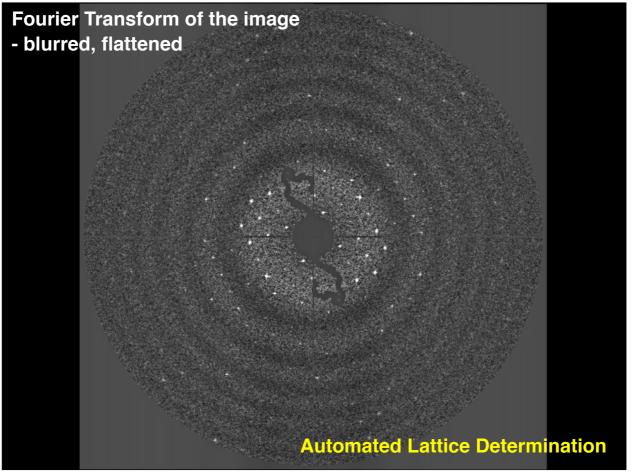
Algorithm Non-tilted mask= 1px Masked СТ Raw nasktran FFT Image FFT Masked 20px FFT Reference 2 V Unbent CC-Map Profile Image maketran Perfect (Apply FFT Defocus) Collection of Amp&Phs Amps Amps Amps & & & origtilt CCP4 apply Phases Phases Phases Amps & Phases

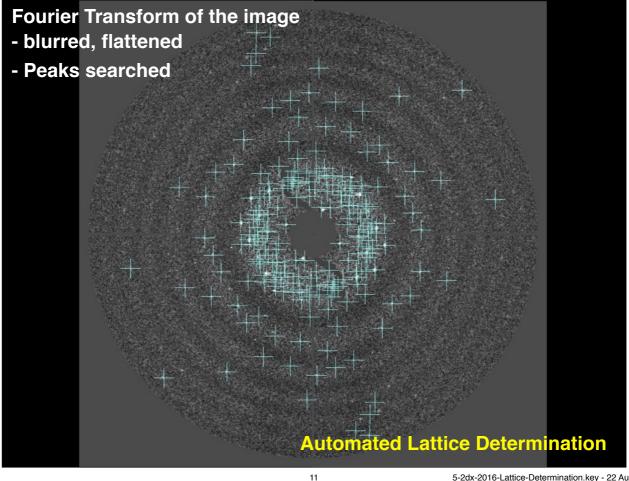


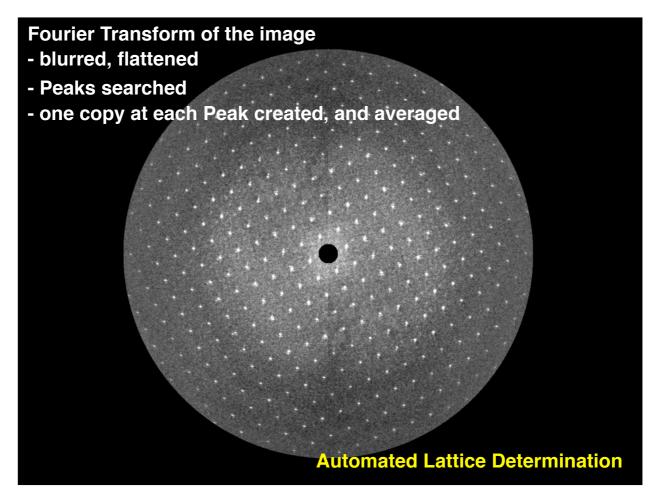






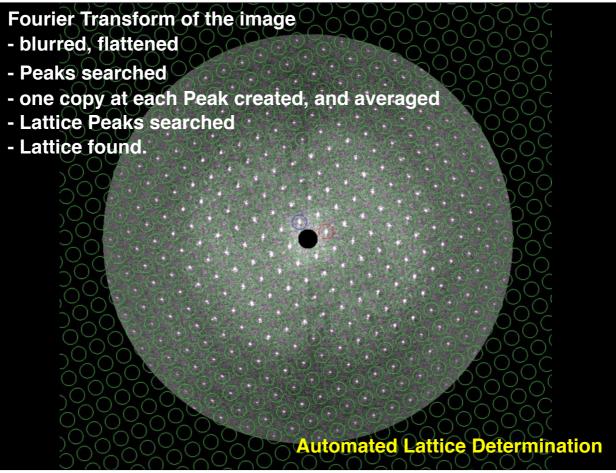


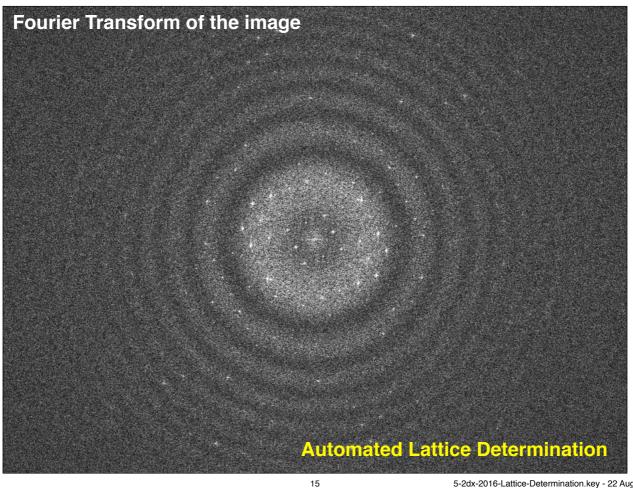


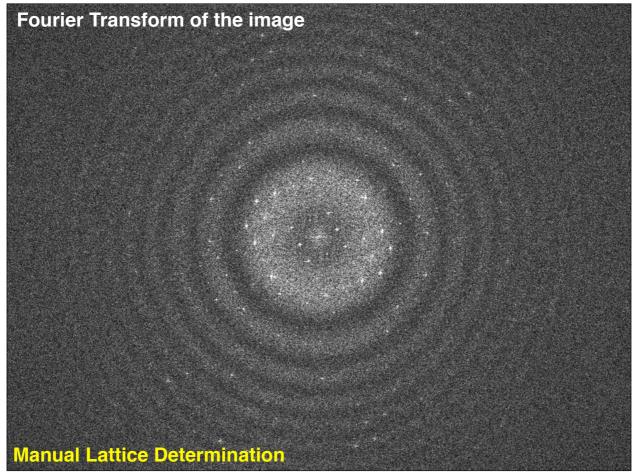


Fourier Transform of the image • blurred, flattened • one copy at each Peak created, and averaged • Lattice Peaks searched

13







Fourier Transform of the image Shift-"R" Two independent spots clicked -Lattice Refinement: <17, -34> <37, 15> i j x v 1 0 1 37 15 0 17 -34 2 1 Current Point: 37 15 Miller Index: Accept First Lattice Add Point Accept Second Lattice **Delete Point** Clear All **Manual Lattice Determination**

17

5-2dx-2016-Lattice-Determination.key - 22 Aug 2016

Fourier Transform of the image

Manual Lattice Determination

- Shift-"R"
- Two independent spots clicked
- Lattice accepted

a	ttice Refinement:	<17, -34>		<37, 15>
	i	j	x	У
1	0	1	37	15
2	1	0	17	-34
Du	rrent Point: 30	4	56	
	rrent Point: 30 ler Index: 2	4	56	
Mi	_	4 Accept First Latti	7	ccept Second Lattice

Fourier Transform of the image

- Shift-"R"

Manual Lattice

- Two independent spots clicked

+

ł

- Lattice accepted
- More spots added, and new lattice accepted

SCOL

50C

$\langle 0 \rangle \sim ($	Lattice Refinement:	<17.1487,	34.4325> <37	.3701, 15.531>
TAUL .	i	j	x	У
	1 -11	2	-115	410
27	2 -8	9	201	415
	3 -5	7	175	281
50	4 -1	-6	-240	-59
56	5 0	1	37	15
	6 1	0	17	-34
	Current Point: -24 Miller Index:	10	-59	
) (Add Point	Accept First Latt	ice Acce	pt Second Lattic
(\cdot)	Delete Point			Clear All

19

					N 🔁									
oK1-P	K2-2014-11-17_MloK1_cAMP/2014-11	-17_12-05-02 🛛 🛋 Mio	K100/MloK1009900	1200										
R	Init Program	Get Lattice & Tilt												
	Init Files and Parameters	Setup Level: Advanced									Results			
R	Calculate FFTs	-				<u></u>	Level.	Auvanceu	0 25	lattic	-			
	Get Defocus & Tilt	Determine Lattice Lattice Determination A	loorithm to nue	1	Yes (No					e E TLTAXIS	"37.3		
Ľ.	Get Derocus & Tilt	Cattice Determination A		vpected is	ttice/e) based		-				E TLTANG	"-23.		
	Get Lattice & Tilt		ss new lattice based			on real celly					E TLTAXA	-23.		
-	Refine Lattice	Lattice Determination:			1.3364		-				-			
	Refine Lattice	Lattice Determination:			140 of 140					LATTIC	-	"-61.		
	Calculate Crystal Tilt from Carb	Lattice Determination:			1.6507						E_TANGL	"-23.3		
	CTE Competies (Bat 1)	Real Unit Cell Length (131.0		131.0				ATEDMAG	2201		
	CTF Correction (Part 1)	Real Cell Angle (for en			90.0					laterr	or_abserror	54	. 01	
	Get SpotList	Regenerate Peak List			Yes	No				laterr	or_rmsderror	1	. 3	
		Initial number of Peaks			200					laterr	or_peaksused	140 0	of 1	
	Unbend I	Number of Peaks			140					laterr	or_nodepeakdensity	, 1	. 65	
	Get SpotList (or refine)	Inner exclusion radius			0.05					LATTIC	E_done			
17		Delta tolerance for latti		1	3.0					SPOTS	done			
8	Unbend II	Test other handedness	also?	1	Yes	No					0			
	Unbend MovieA1	Reciprocal Lattice	-34,4325		37.3701		15.531			Images	-			
12		Second (bad) Lattice	-34.4325		37.3701		10.031			FFT of	Image Downsampled Image			
8	Unbend MovieA2	€ 0/8///////////////////////////////////										•		
	Unbend MovieB	Second lattice exists												
17		Output (Double click for I	ogbrowser)			Verbosity Le	erbosity Level: Low				pectrum			
8	CTF correction (Part 2)	New 2nd lattice would	New 2nd lattice would have been 0.0,0.0,0.0,0.0 (Score = 0.0),							Pre Ba	nd-Pass Powerspect	rum		
	Generate Map	Due to the bad score it will not be used.								Post Band-Pass Powerspectrum				
<u>۰</u>	Contrate map	==== 2dx_getspot - To generate a first spotlist. ====================================								Masked and Band-Passed Powerspect				
		<pre>=== emtil: To calculate the tilt geometry from lattice distortions. ====================================</pre>							Origin-Shifted Average Powerspect					
		2. TILTAXIS =	86.22306 = A	LPHA - P LPHA + P										
		Taking second option.												
	0	==== NOT saving tilt (geometry from la	ttice, b	ecause of lo	w tilt. ====								
	DEPENDENT SCRIPTS 2dx makedirs	==== 2dx calcmag - to	calculate the t	heoretic	al magnifica	tion ======								
	initialize	Theoretical magnification is 22011.695, given magnification is 22500 =================================												
L.		Status	cal lattice is 9	4.065							Preview		-	
		Calc. Mag=	22011	2				Last QVAL=			Preview			
-		Unbend	101	102	103	104	105	IQ6					904	
		Unb.I	35	74	66	96	168	219			, 3 Mode:		-94	
		Unb.II	39	83	65	113	161	228			.4 Origin x,y,z:	0	0	
		MovieA	-	-	-	-	-	-		-			904	
		MovieB	-	-	-	-	-	-		-			808	
		PowerBins			[A]	15	12	9	7	5 3		90 X	90	
		(noise=7)			#	818	77	59	15	7 7	Min Max Means	0.0 3919	9.3	
		Tilt Info Grid TAxis			Defoc. 89.7	Latt. 86.2		SpSplit 89.7		Mer	ge Space Group:			
		Grid TAngle			-16.4	-23.3		-16.4			Symmetry bytes:			
											Phase Origins	0.0 0	0.0	
		Xst. TAxis			25.9	-61.8		25.9	9	25	8.8 RMS:	0.0 0	0.0	