

Bragg Coherent Diffraction Imaging

- Ian Robinson
- Jesse Clark
- Gang Xiong
- Moyu Watari
- Marcus Newton
- Ross Harder
- Steven Leake
- Loren Beitra
- Xiaowen Shi

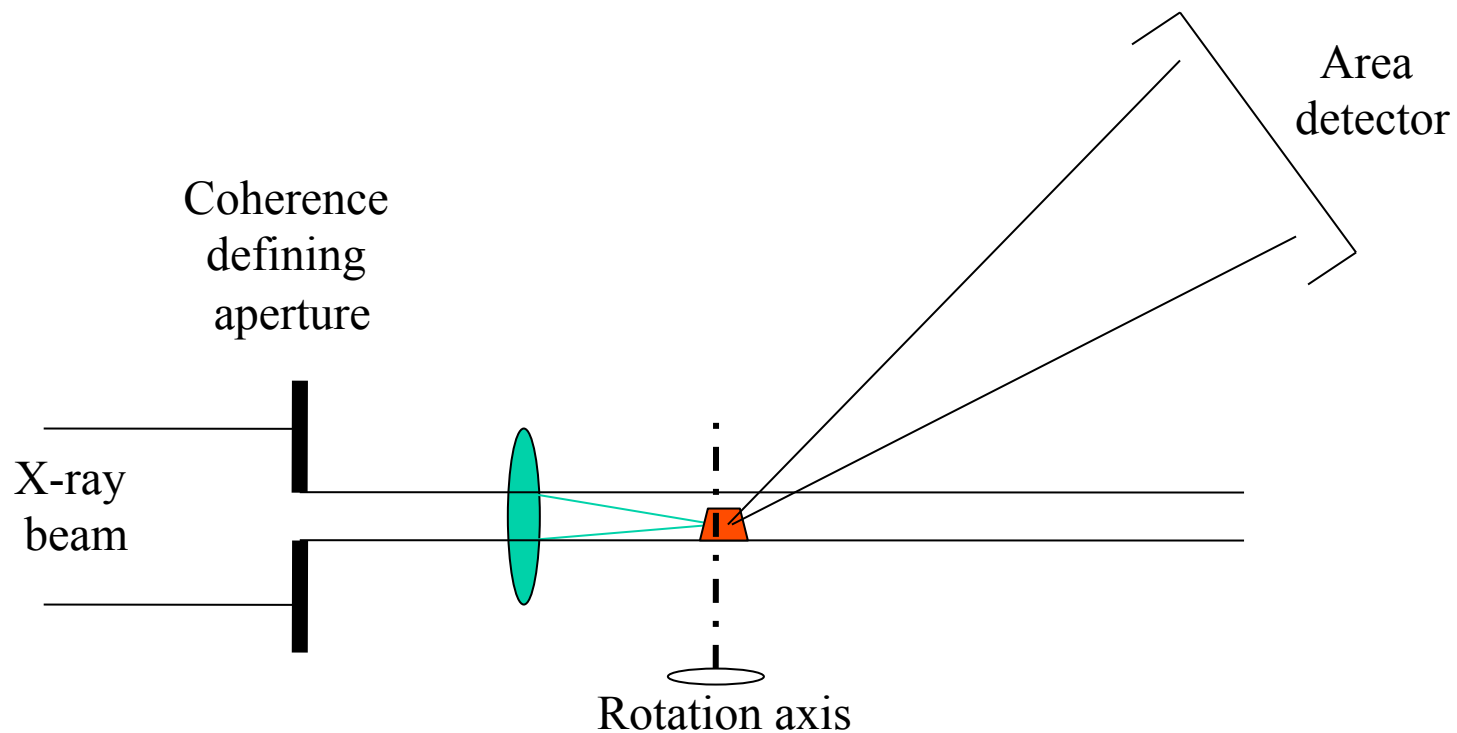
London Centre for Nanotechnology
University College, London
Research Complex at Harwell

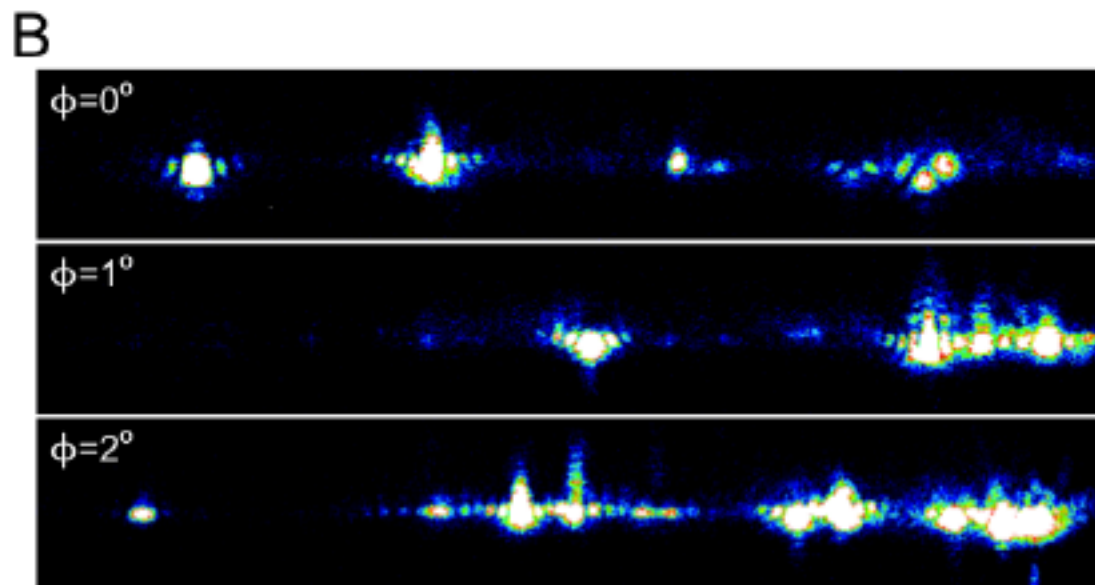
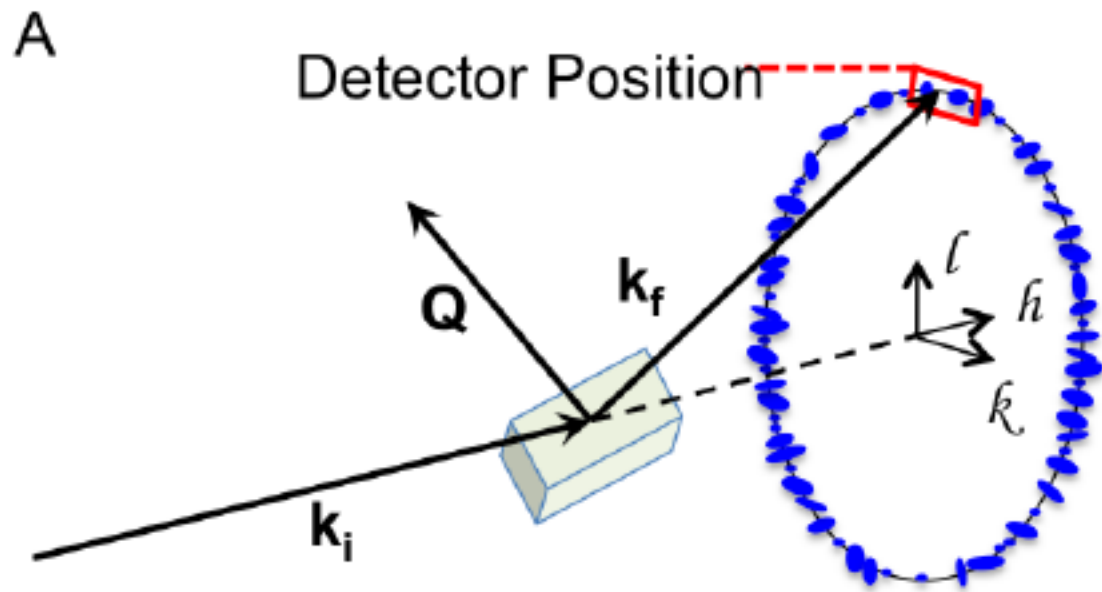
Sao Paulo School
July 2015

Lecture 1 Topics

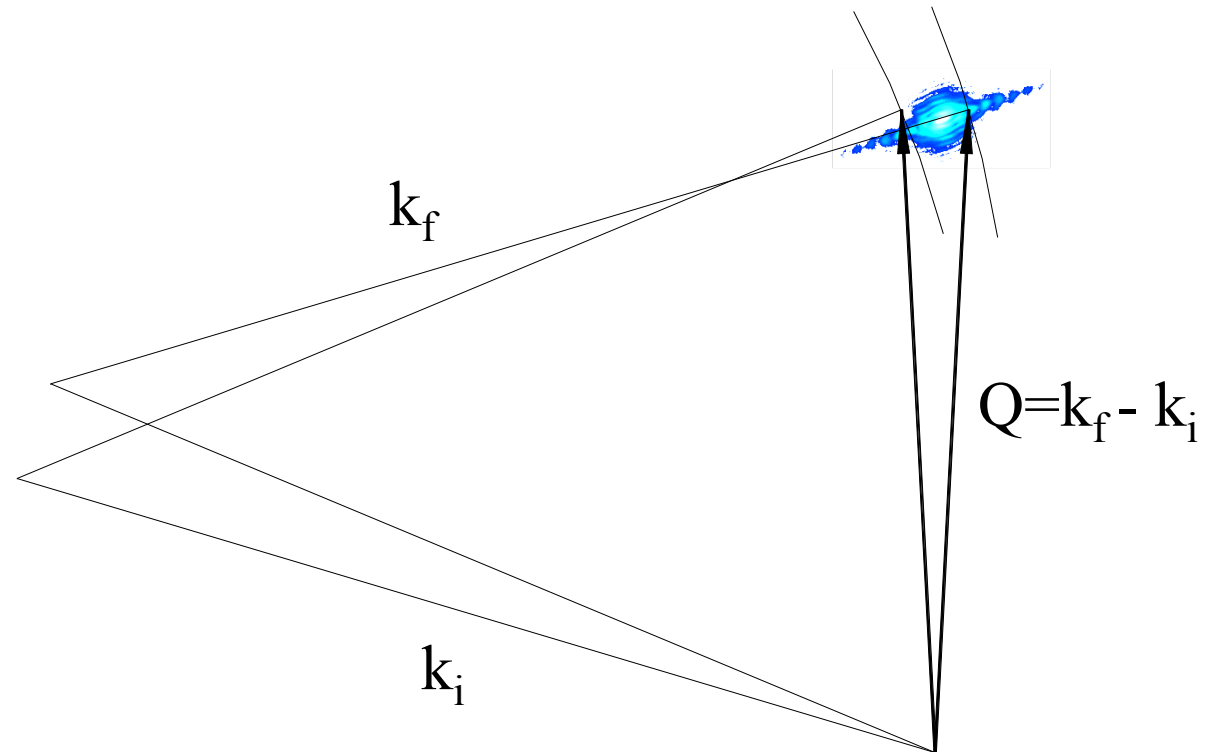
- I. Bragg Diffraction Imaging (BCDI)
- II. Longitudinal Coherence
- III. Transverse Coherence
- IV. Nanocrystal Alloying
- V. Nanocrystal Structures
- VI. Strain Imaging

Lensless X-ray Microscope, 2003

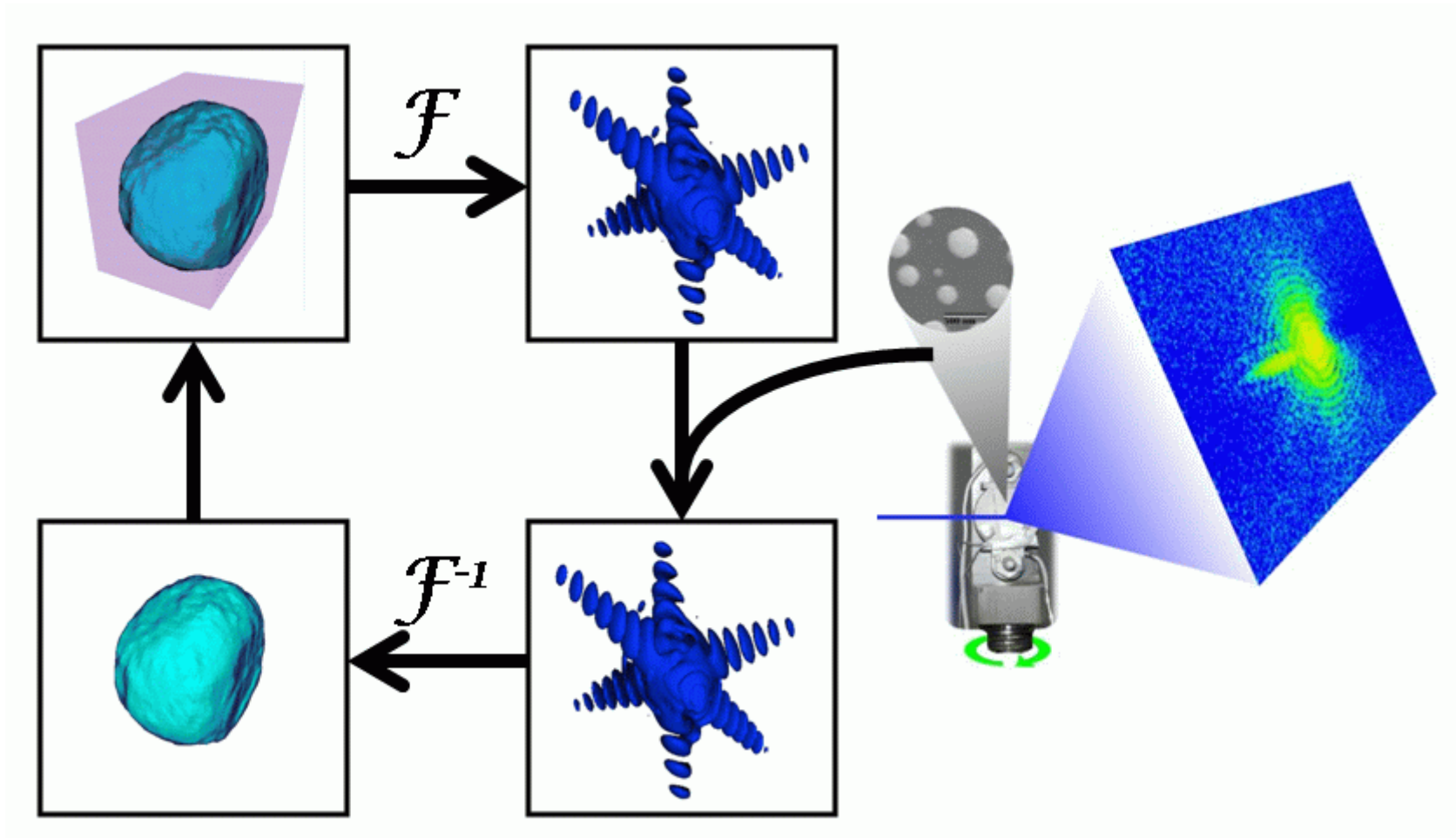




3D Diffraction Method



Generic “Error Reduction” method



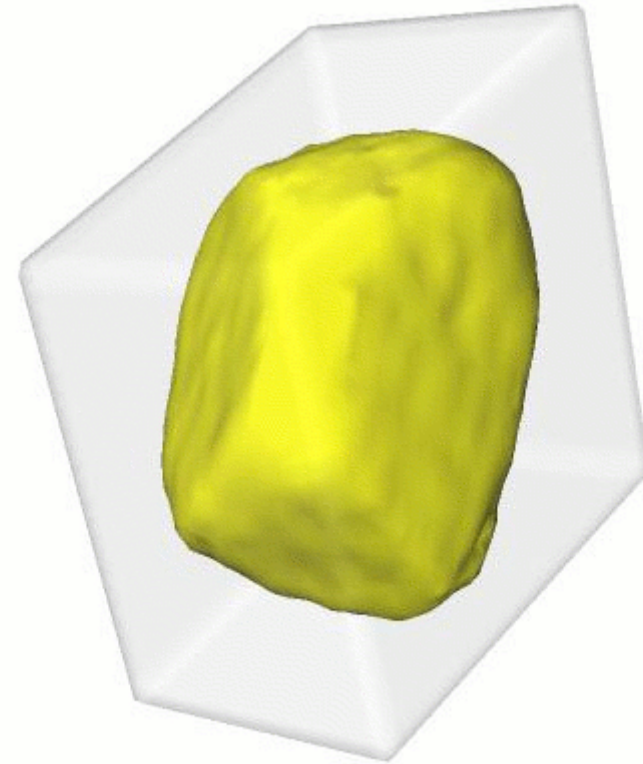
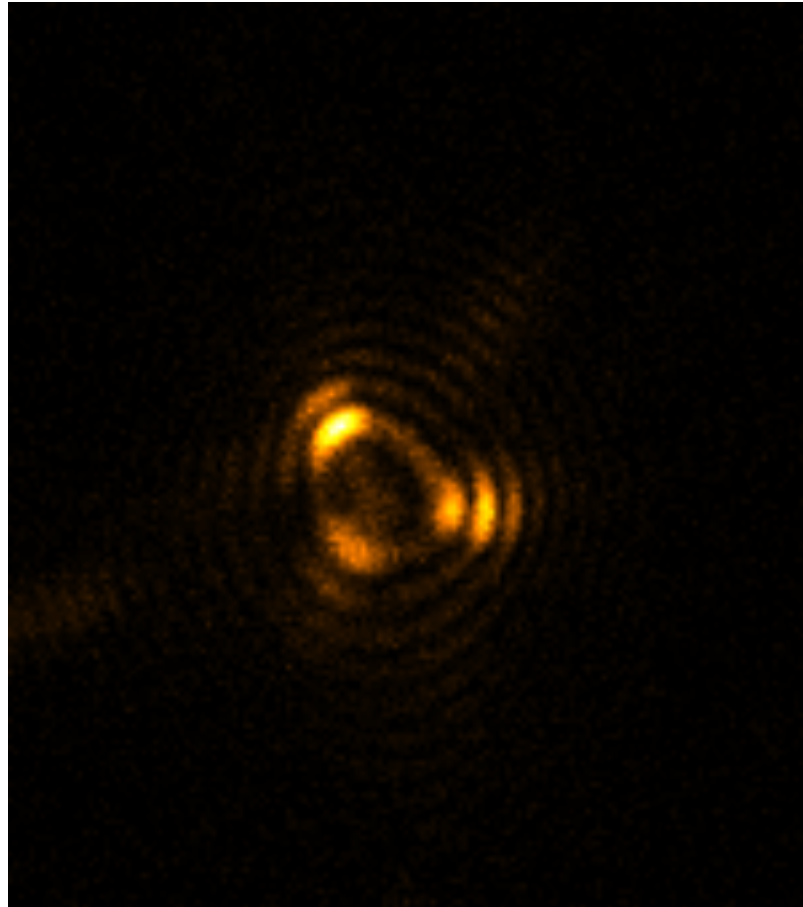
J. R. Fienup *Appl. Opt.* 21 2758 (1982)

R. W. Gerchberg and W. O. Saxton *Optik* 35 237 (1972)

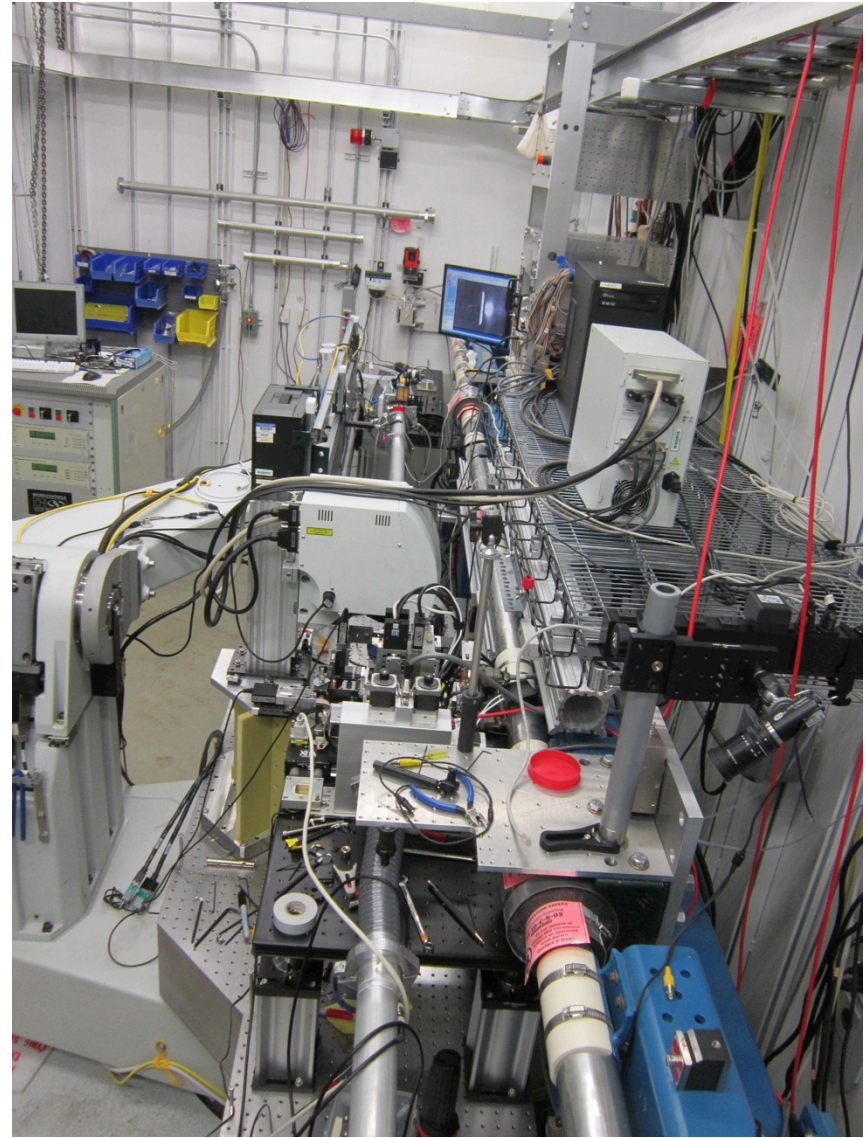
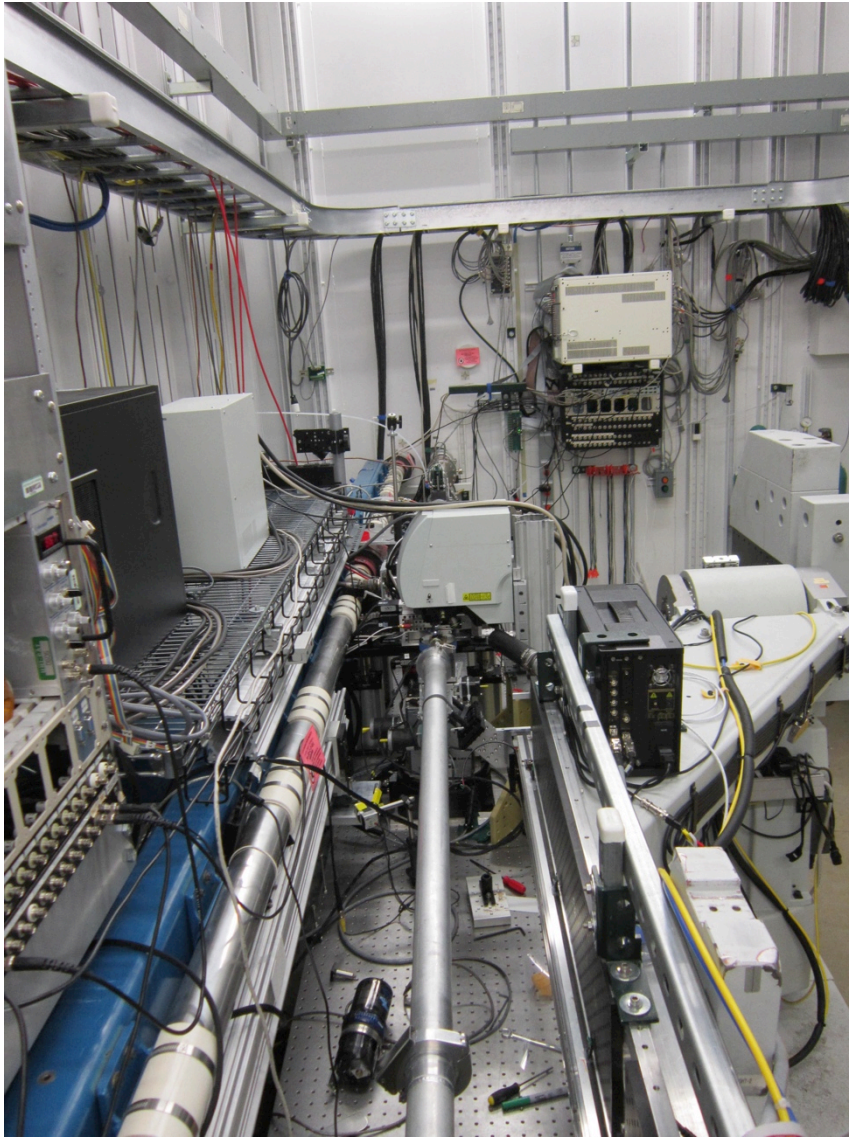
I. K. Robinson Campinas 2015

Gold nanocrystal reconstruction

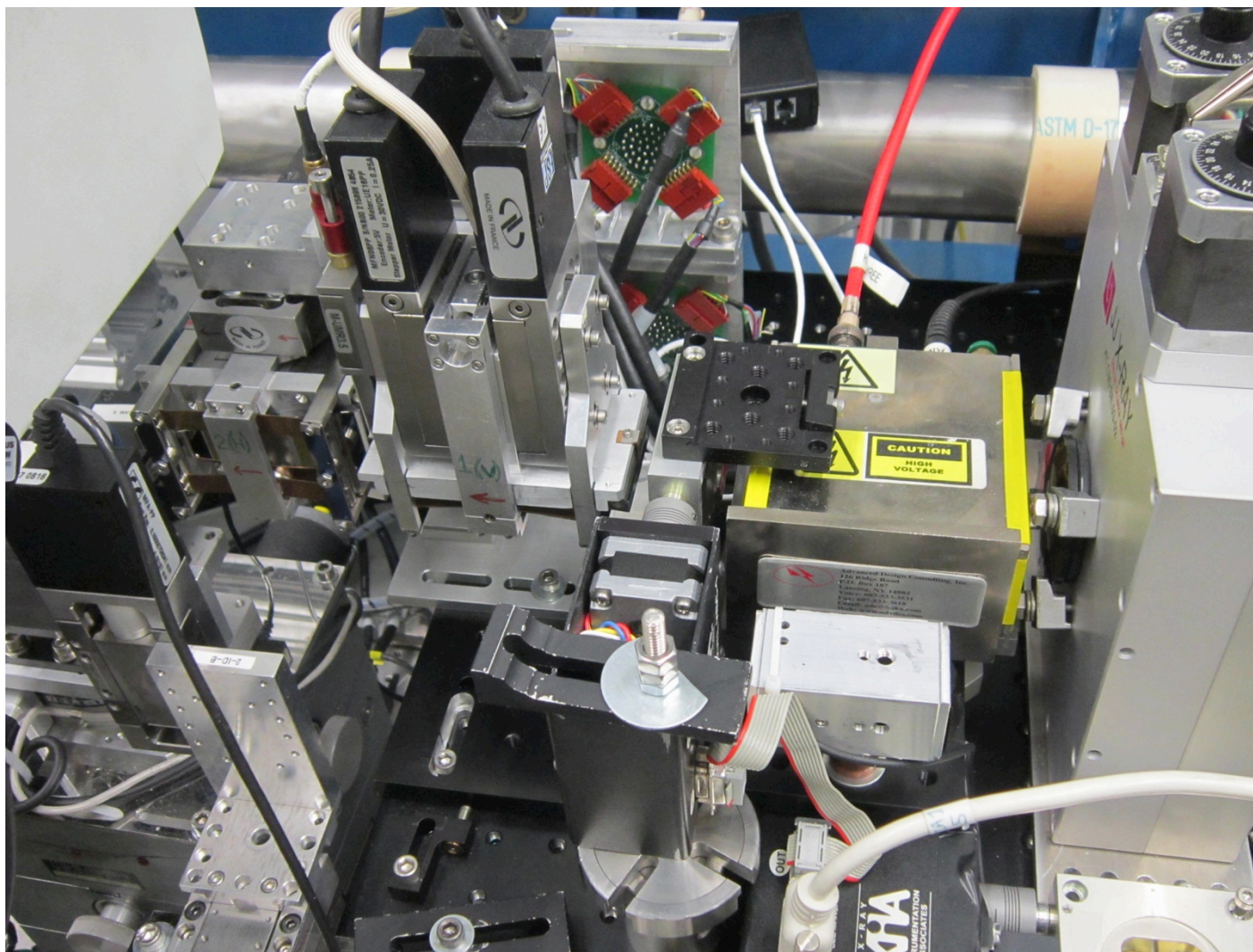
showing support used for 20 HIO followed by 10 ER



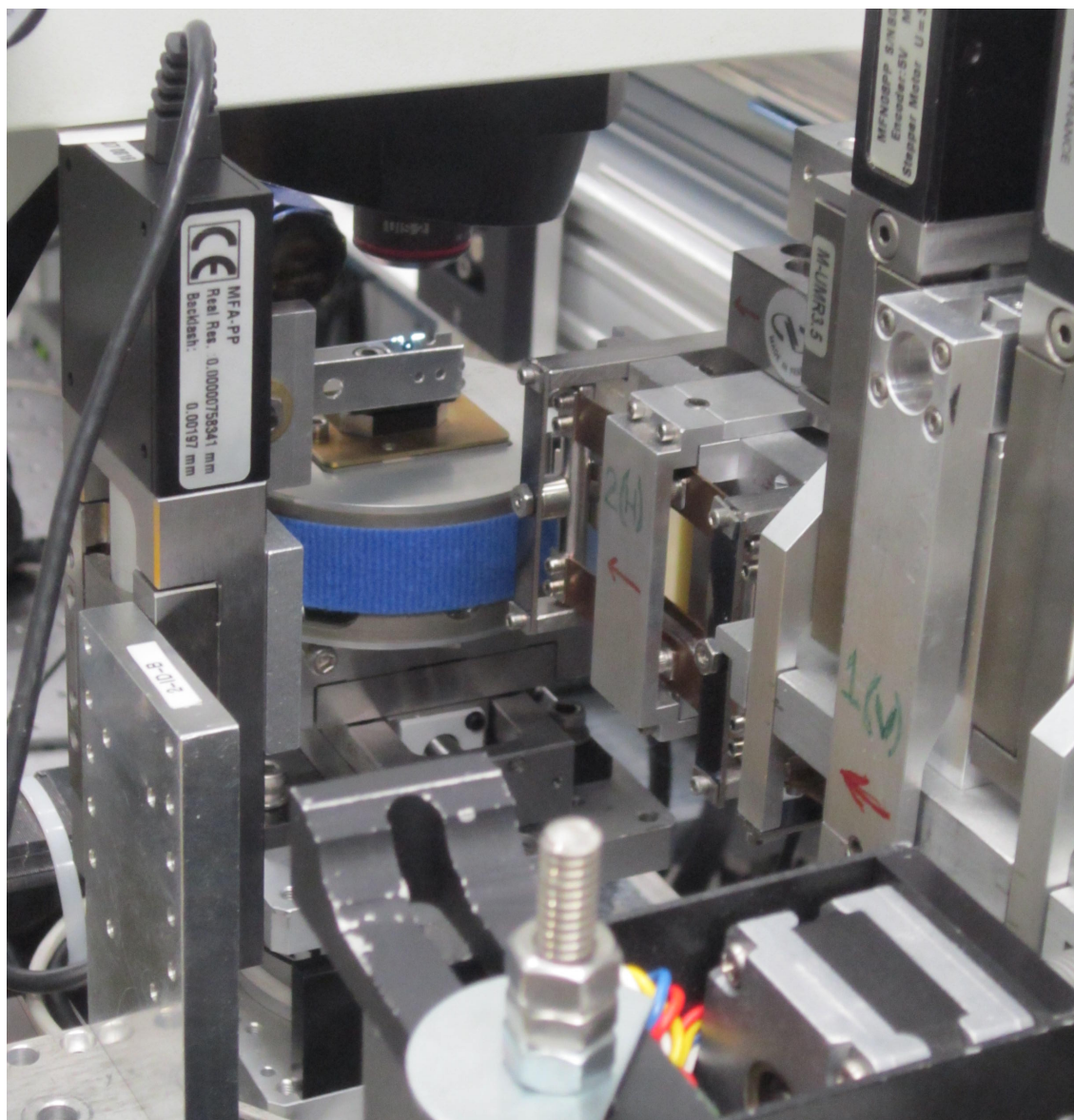




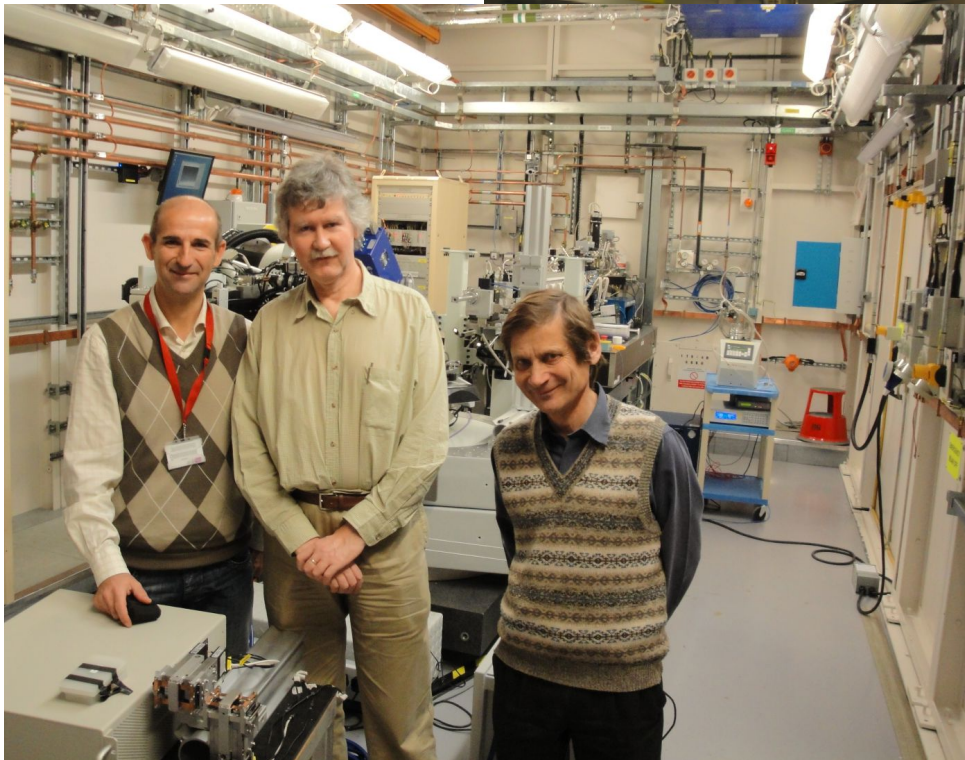
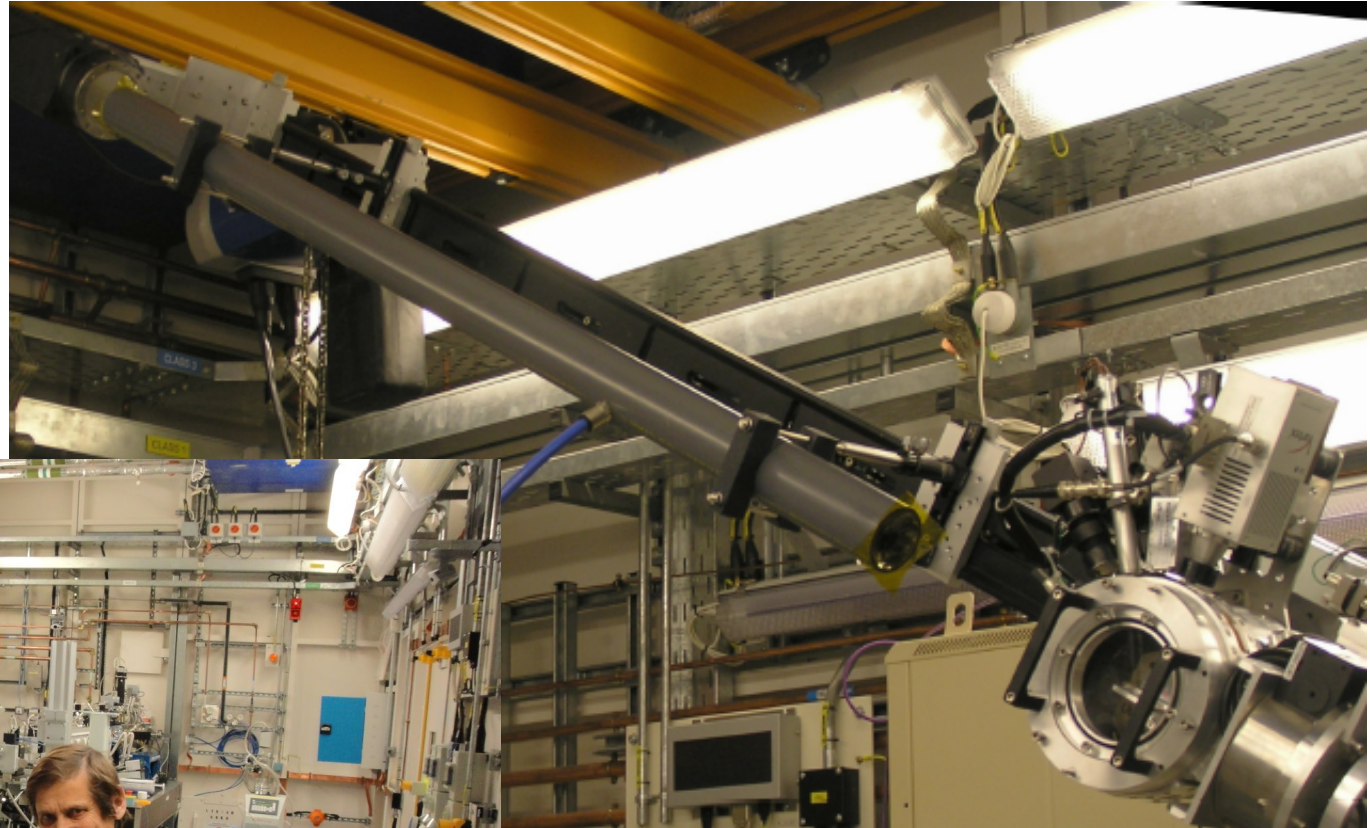
34-ID-C in April 2013



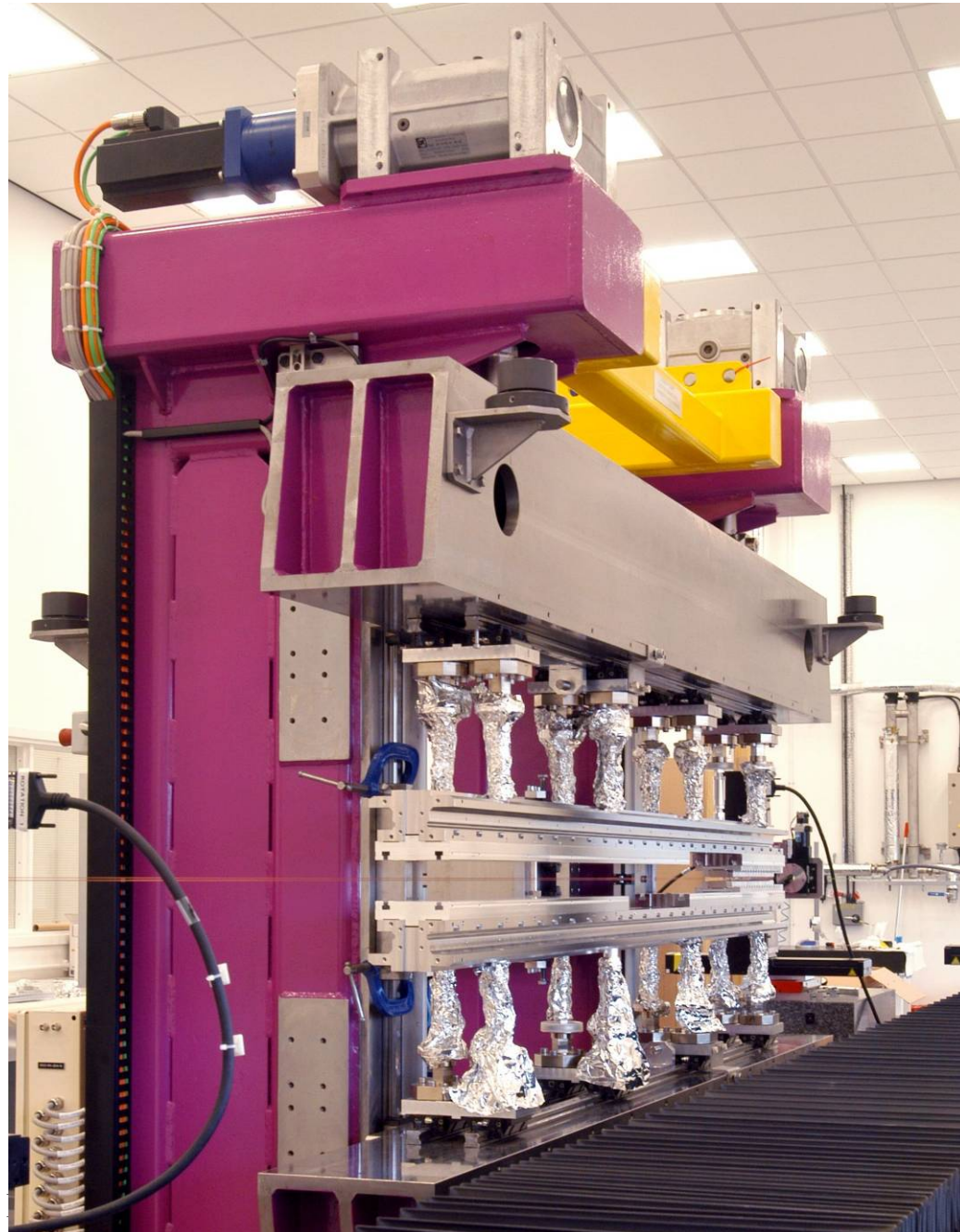
34-ID-C in April 2013



Diamond I-16, Materials and Magnetism



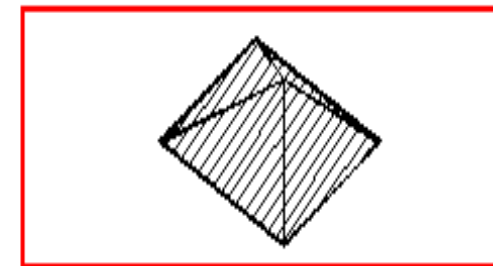
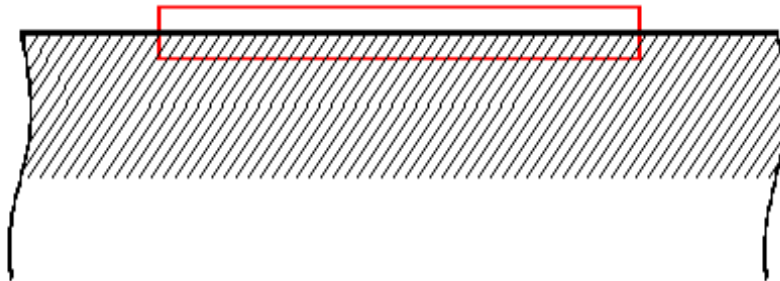
Diamond
in-vacuum
X-ray
Undulator



Coherence at 3rd Generation (undulator) Synchrotron Sources

| Coherence of | ξ_{VER} | ξ_{HORIZ} | ξ_{LONG} | Flux |
|-----------------------|--------------------|----------------------|---------------------|--------------------|
| Raw Undulator | $35\mu\text{m}$ | $9\mu\text{m}$ | $0.004\mu\text{m}$ | 2×10^{12} |
| Si(111) Monochromator | $35\mu\text{m}$ | $9\mu\text{m}$ | $1\mu\text{m}$ | 1×10^{10} |
| C(111) Monochromator | $35\mu\text{m}$ | $9\mu\text{m}$ | $3\mu\text{m}$ | 3×10^9 |

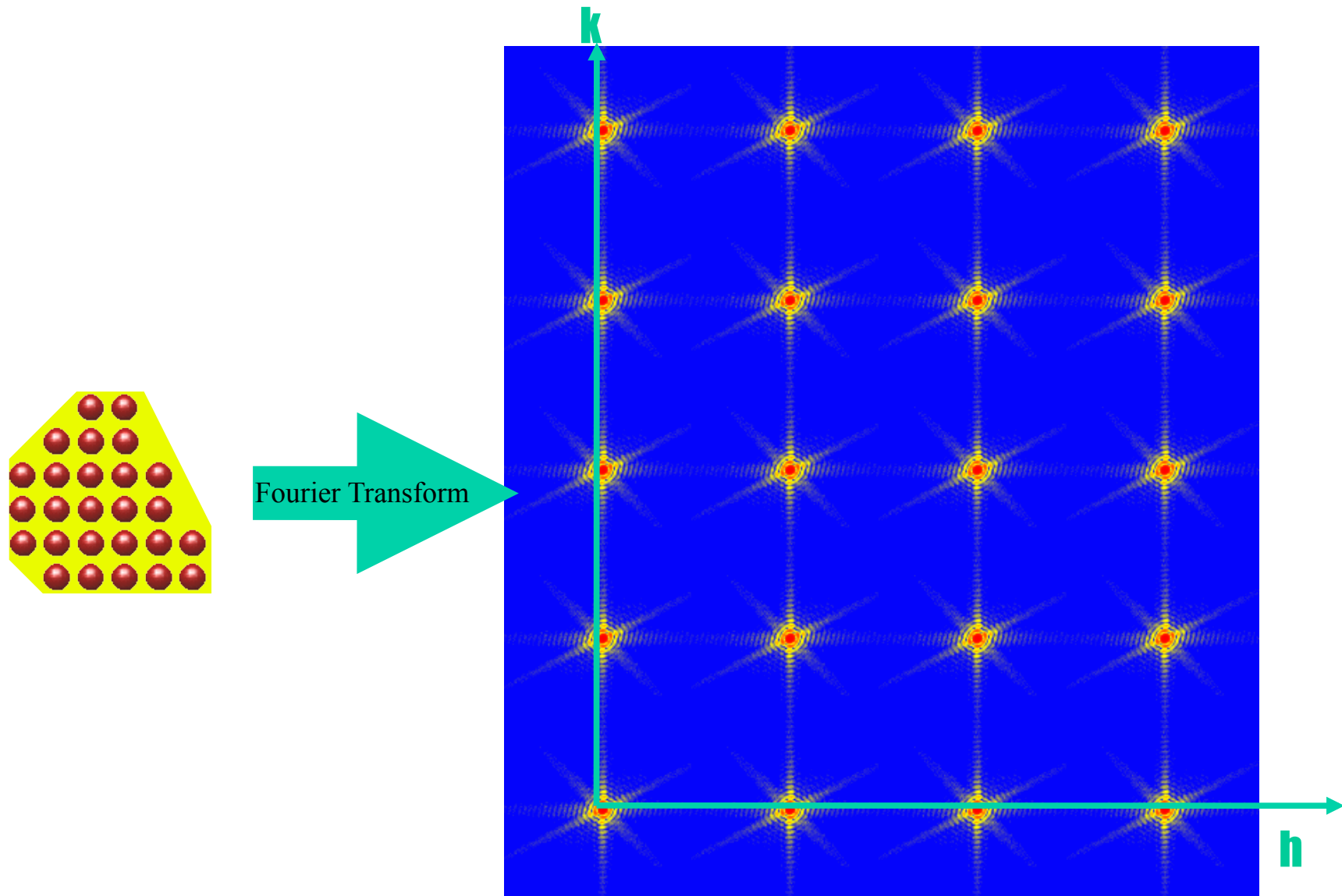
Coherent region defined by slits



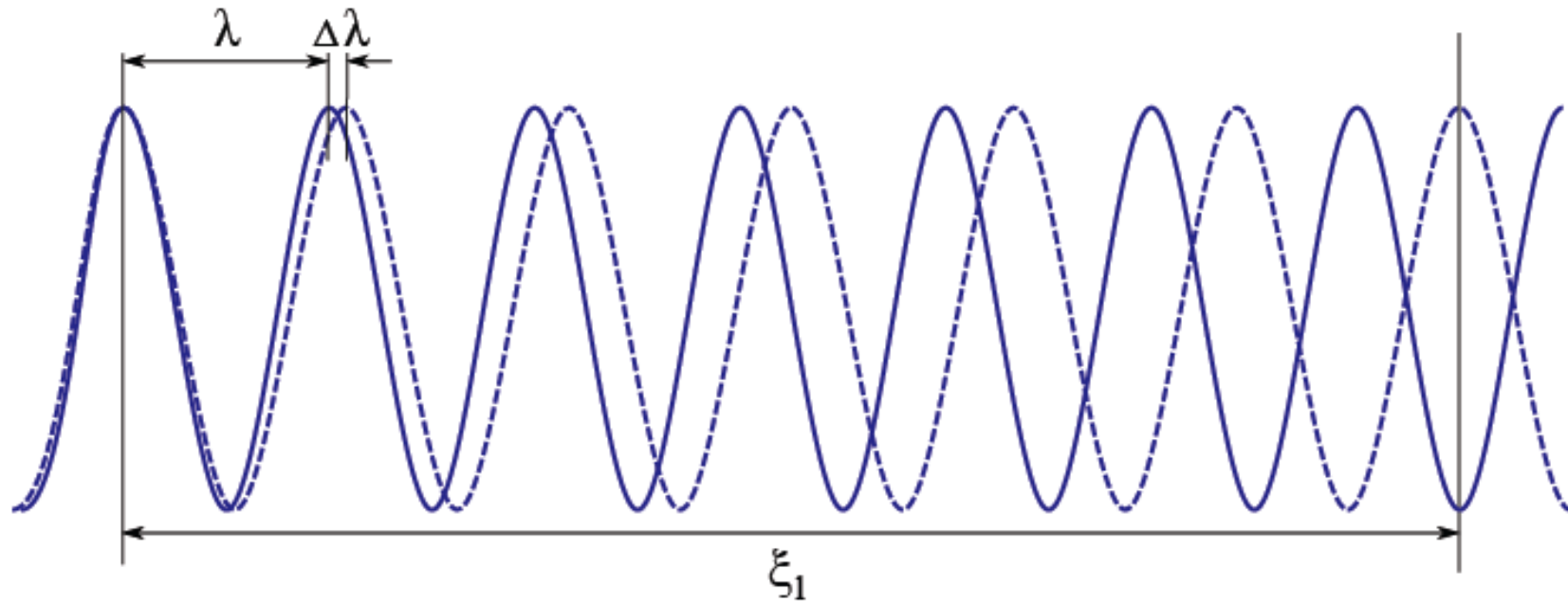
Lecture 1 Topics

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- V. Nanocrystal Structures
- VI. Strain Imaging

Coherent Diffraction from Crystals

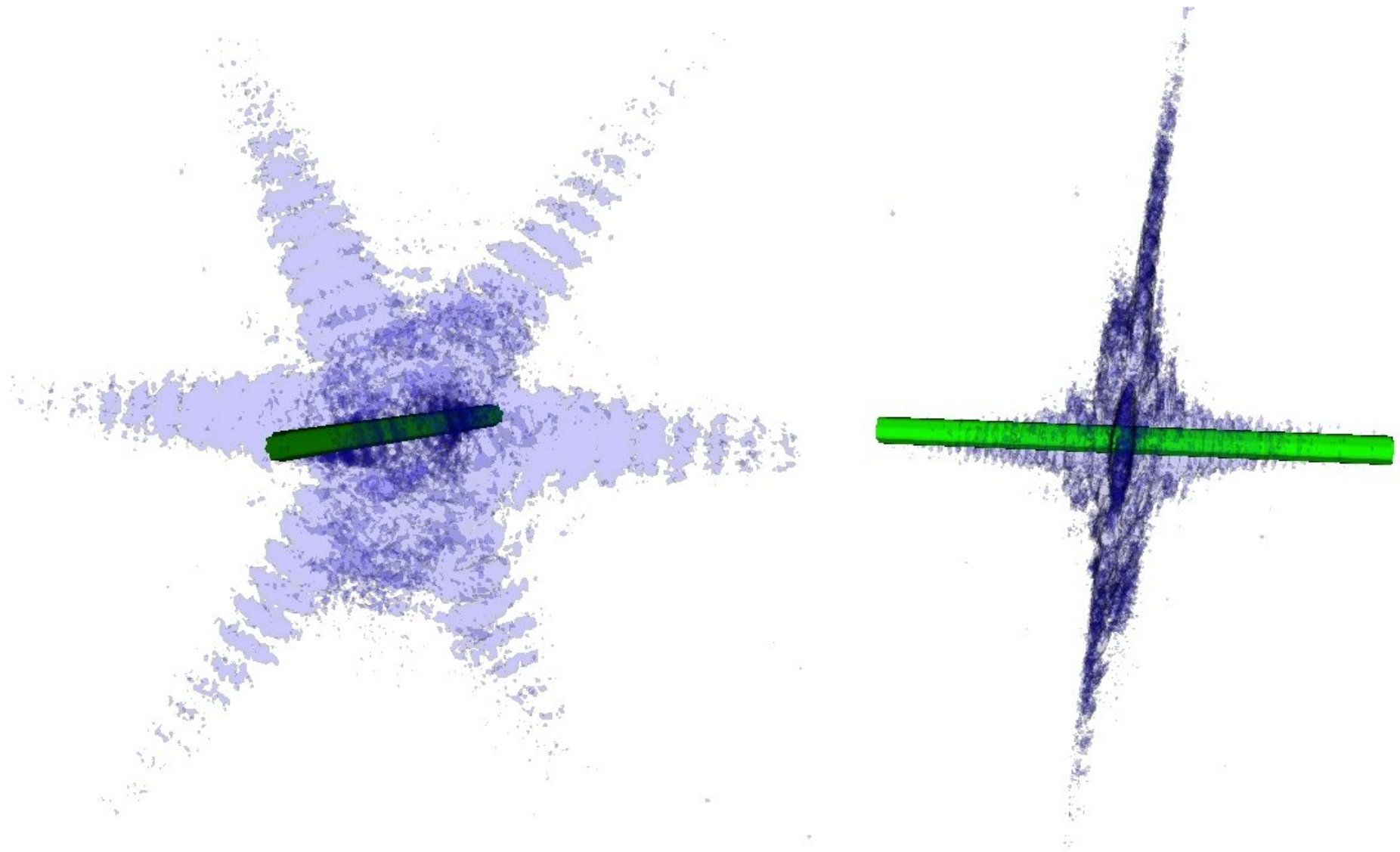


Longitudinal Coherence

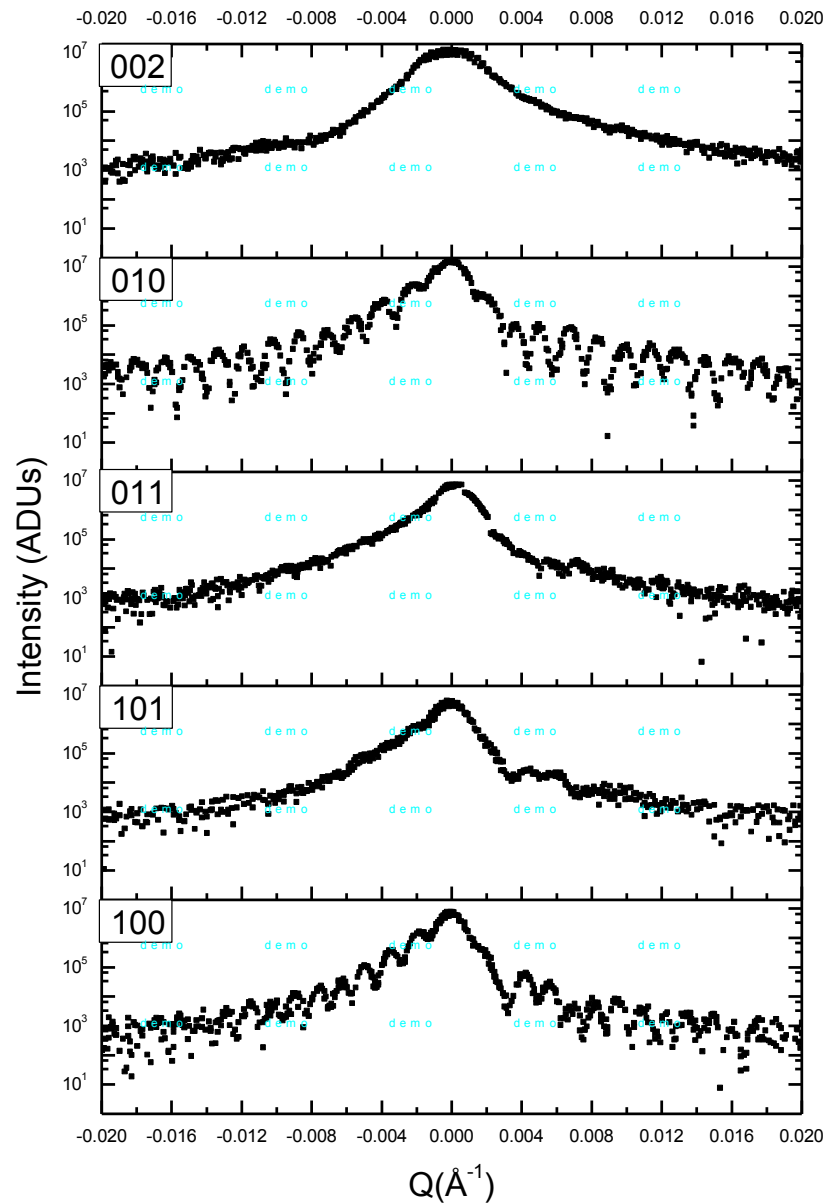


$$\xi_L = \frac{1}{2} \frac{\lambda^2}{\Delta\lambda}$$

How to extract the contrast data



Five Bragg peaks



002 no fringe visibility

010 & 100 good fringe visibility

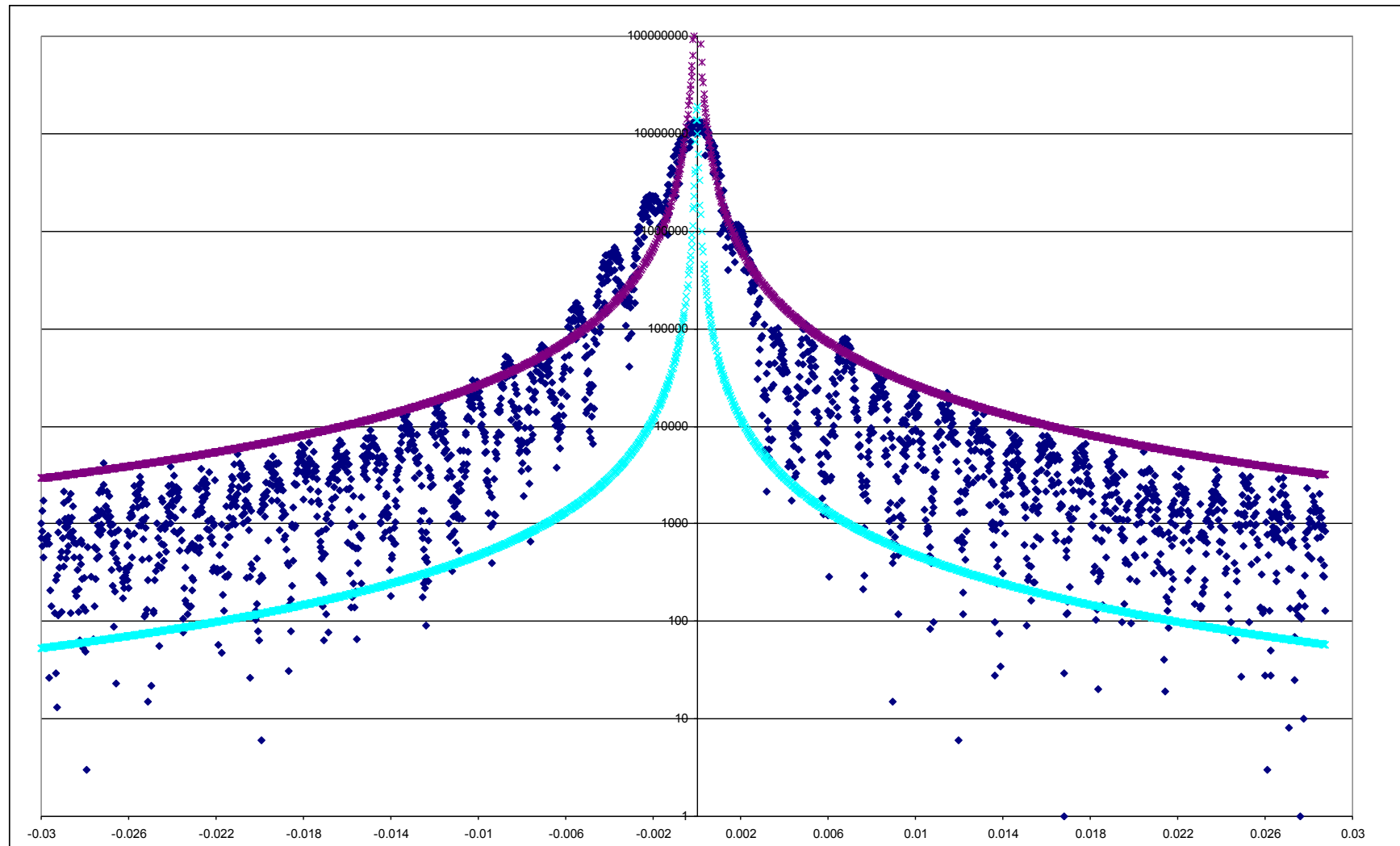
101 & 011 diminished fringe visibility
but fringes still evident

010:011 & 101:100
show complementary fringes
but not between each other

Error in coordinate transform ruled out

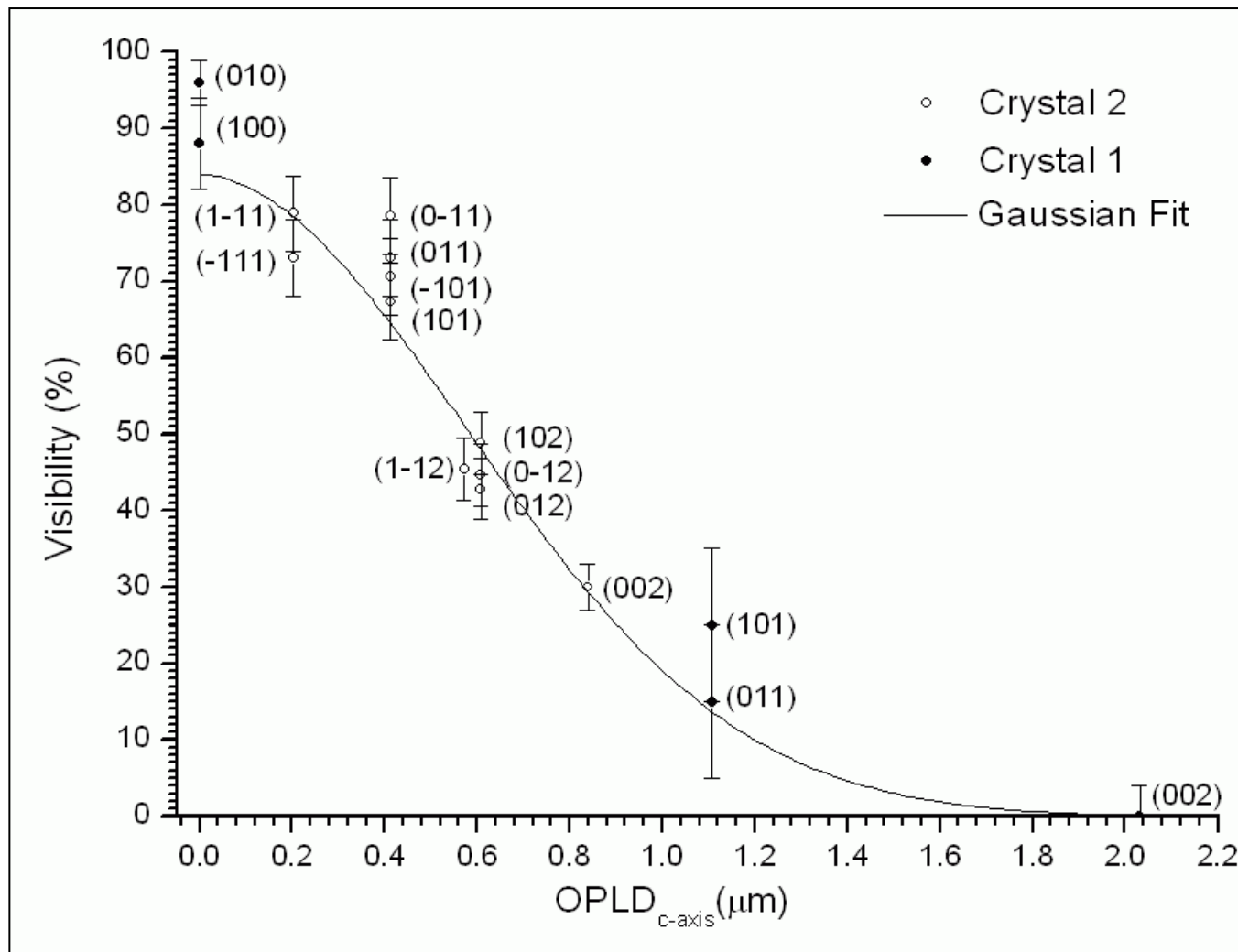
010 and 100 reflections fringe spacing
difference $\sim 20\%$

Fringe Visibility $96 \pm 2\%$ @010



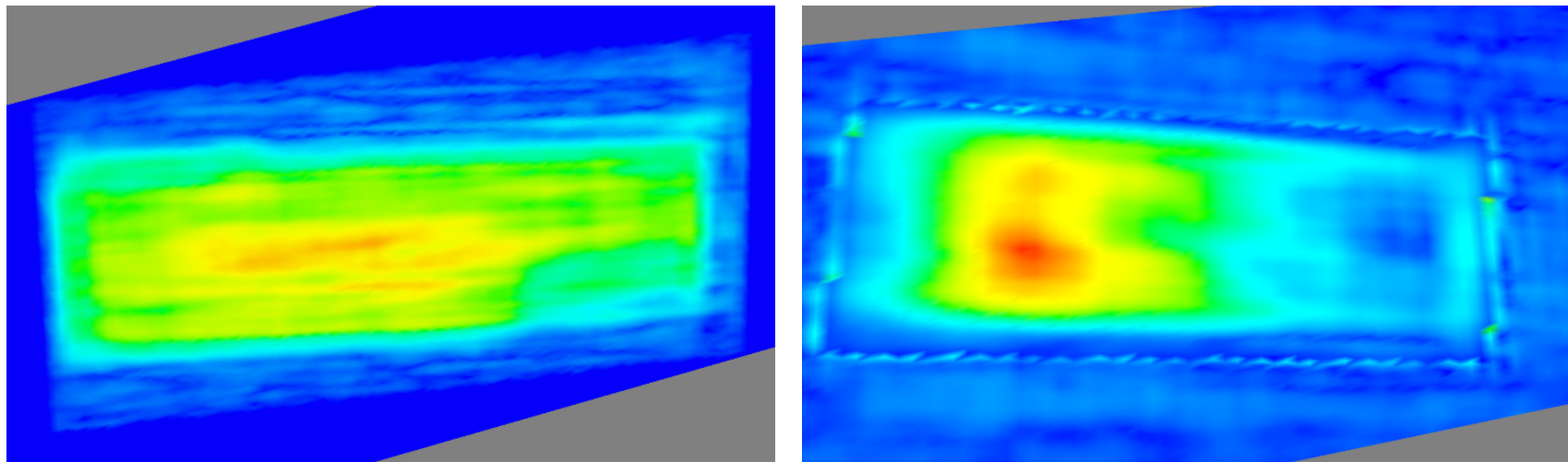
Measured Longitudinal Coherence

Steven Leake et al, Optics Express 17 15853 (2009)



Density Section of Reconstruction using 100 and 101 reflections

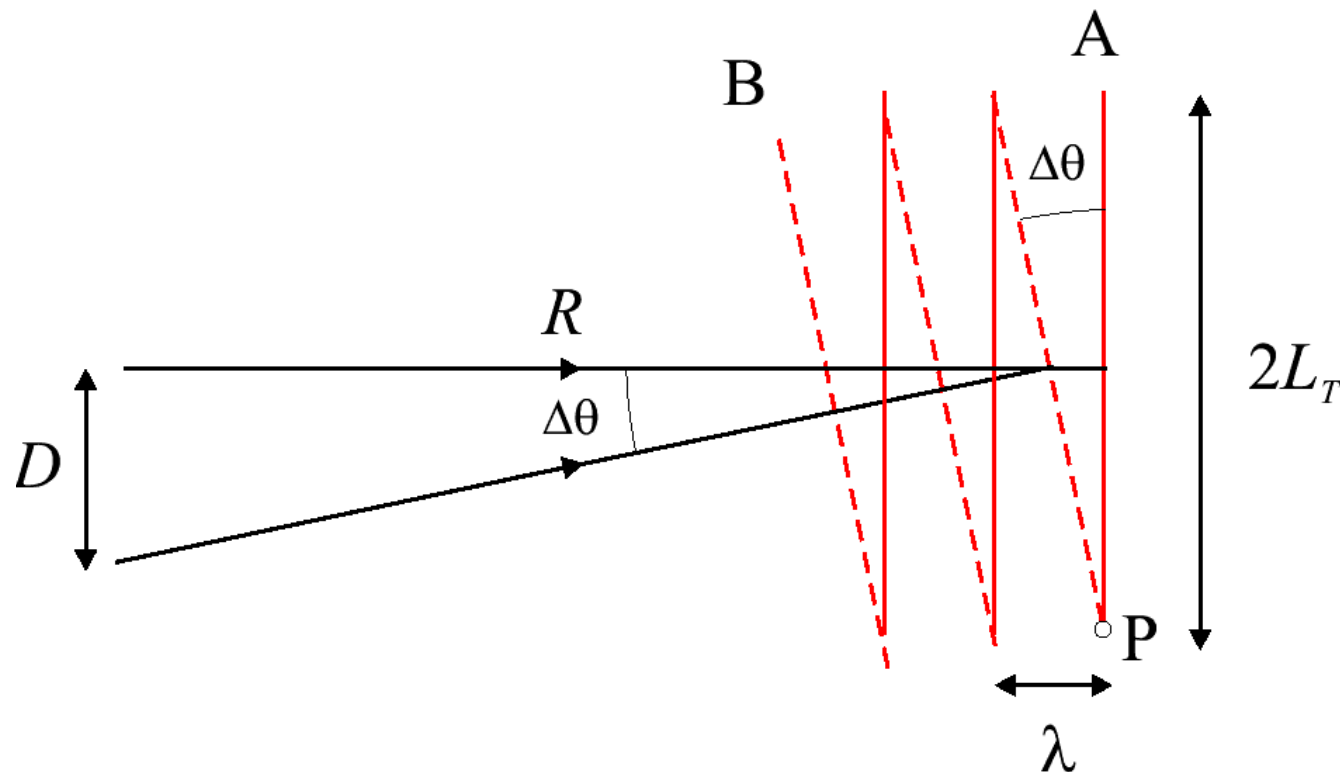
“hot spot” more developed for limited coherence
Steven Leake et al, Optics Express 17 15853 (2009)



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Lateral (Transverse) Coherence



$$L_T = \frac{\lambda R}{2 D}$$

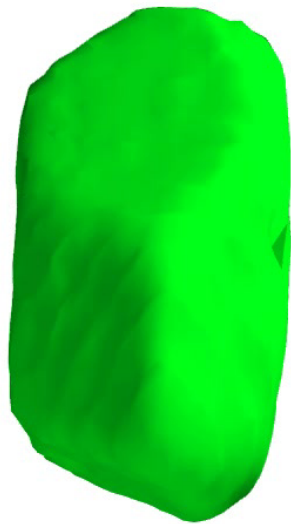
Als-Nielsen and McMorrow (2001)

Vary transverse coherence

using horizontal entrance slit settings

$12\mu m$

High coherence



Assuming perfect coherence

$50\mu m$

Low coherence

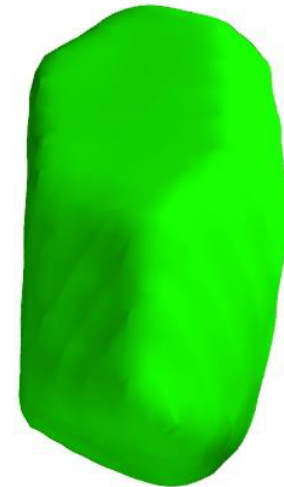


Assuming perfect coherence

I. K. Robinson Campinas 2015

$50\mu m$

Low coherence



Correcting for partial coherence

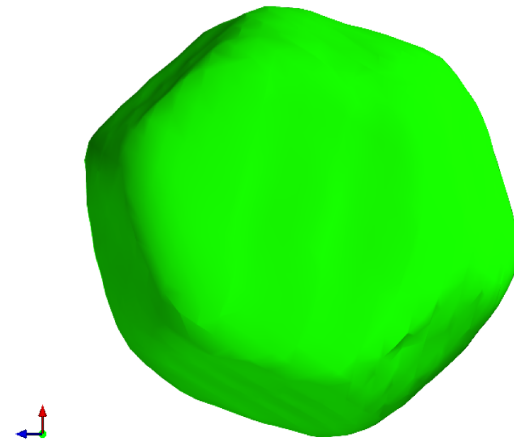
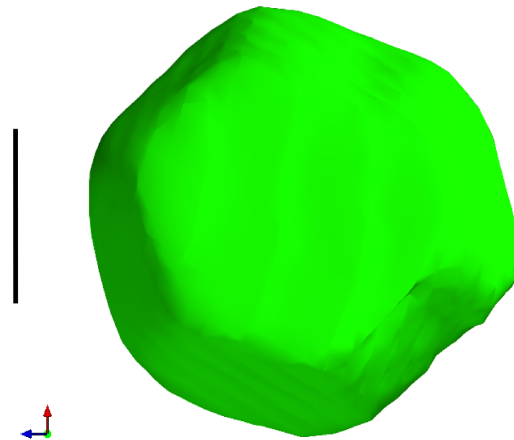
Top view of crystal

Jesse Clark, Nature Comms, 3 993 (2012)

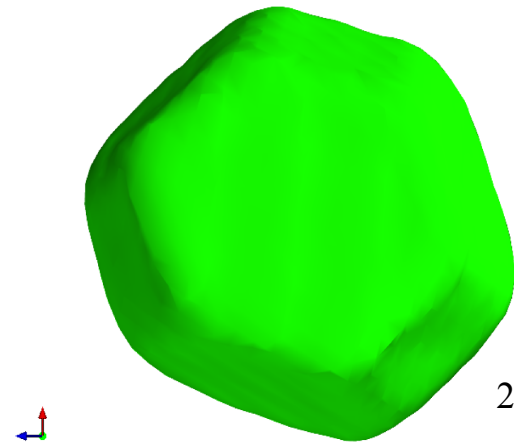
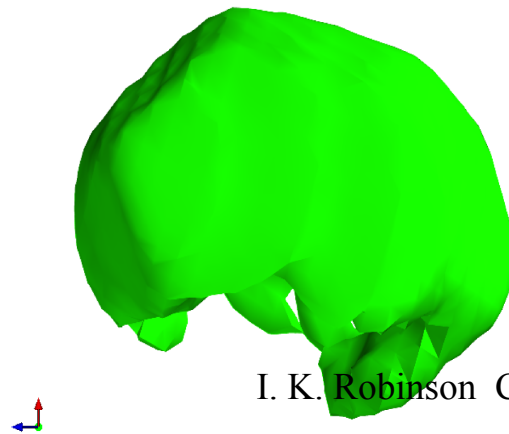
Assuming full
coherence

Correcting for partial
coherence

'High' coherence

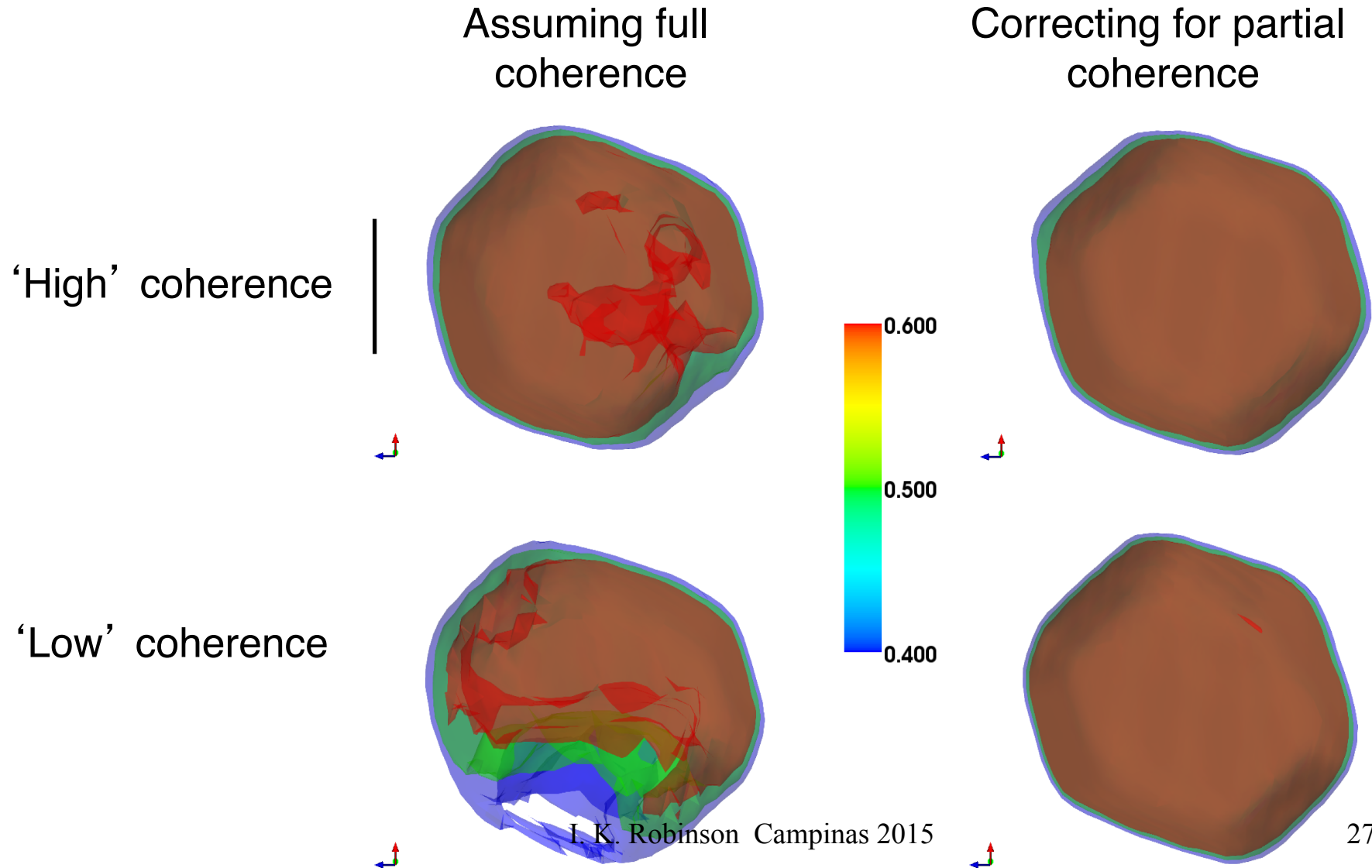


'Low' coherence



Top view of crystal

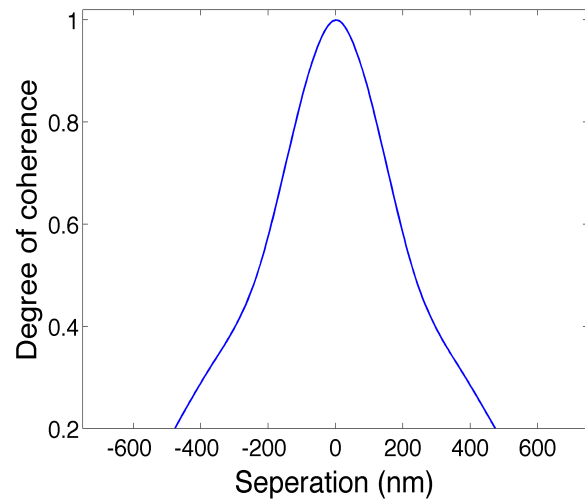
Jesse Clark, Nature Comms, 3 993 (2012)



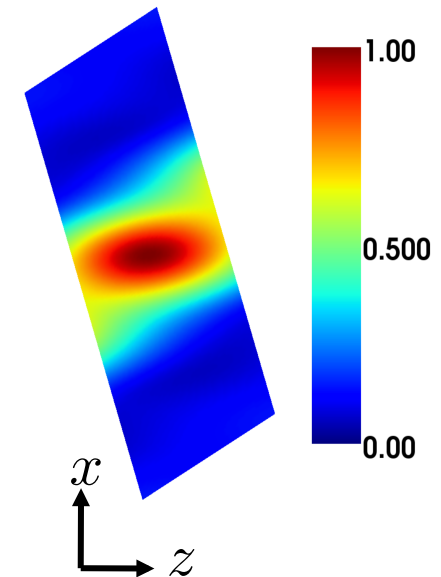
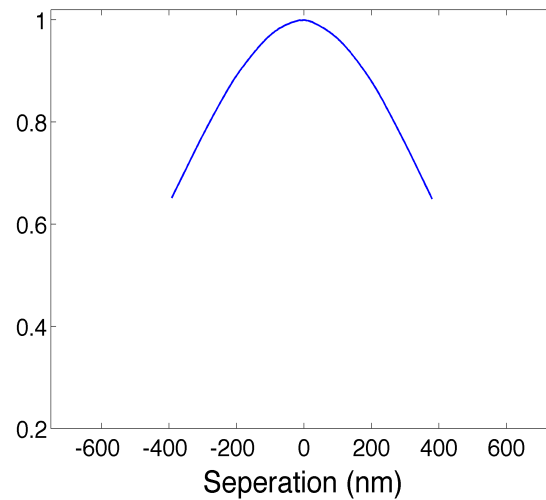
Derived coherence parameters

Jesse Clark, Nature Comms, 3 993 (2012)

x



z



Recovered
(HWHM)

$$l_x = 220 \text{ nm}$$

$$l_z = 485 \text{ nm}$$

Measured/
Estimated

$$l_x = 250 \text{ nm}$$

$$l_z = 660 \text{ nm}$$

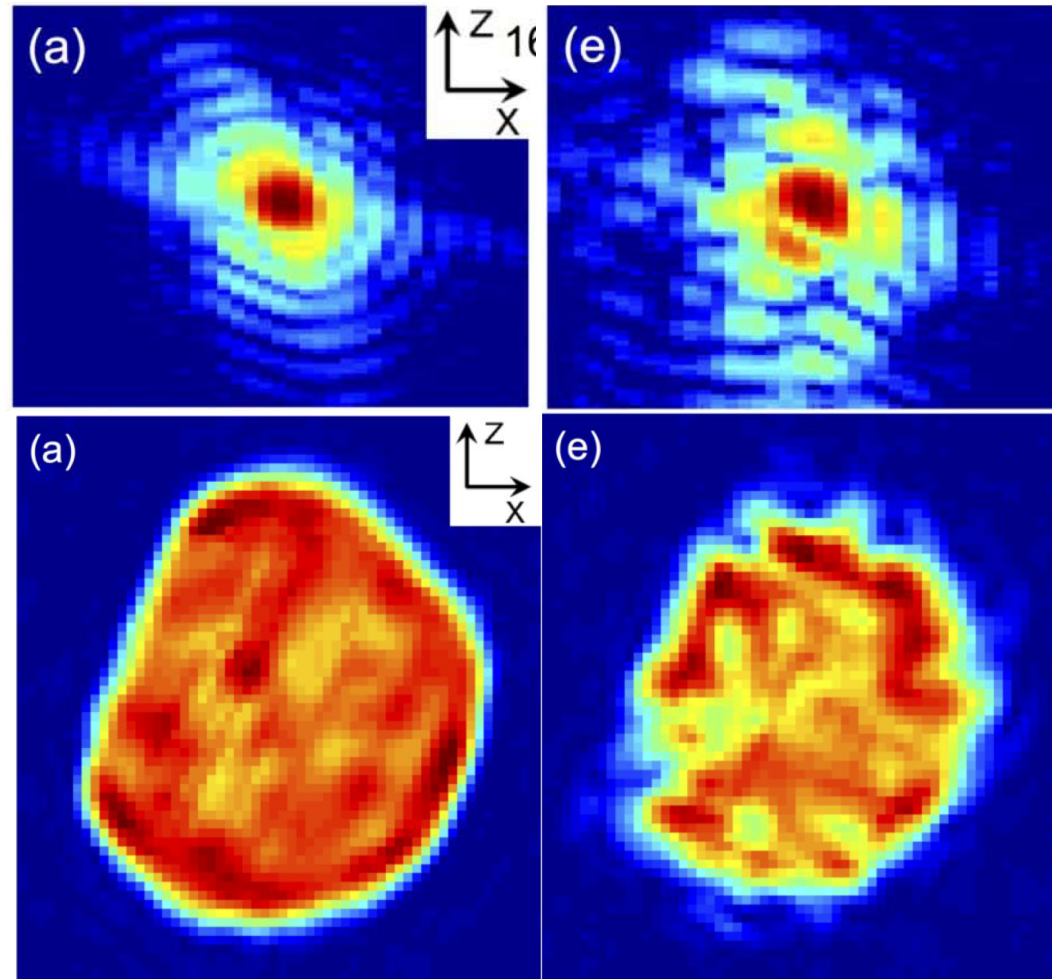
I. K. Robinson Campinas 2015

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Copper Diffusion into Gold Nanocrystal

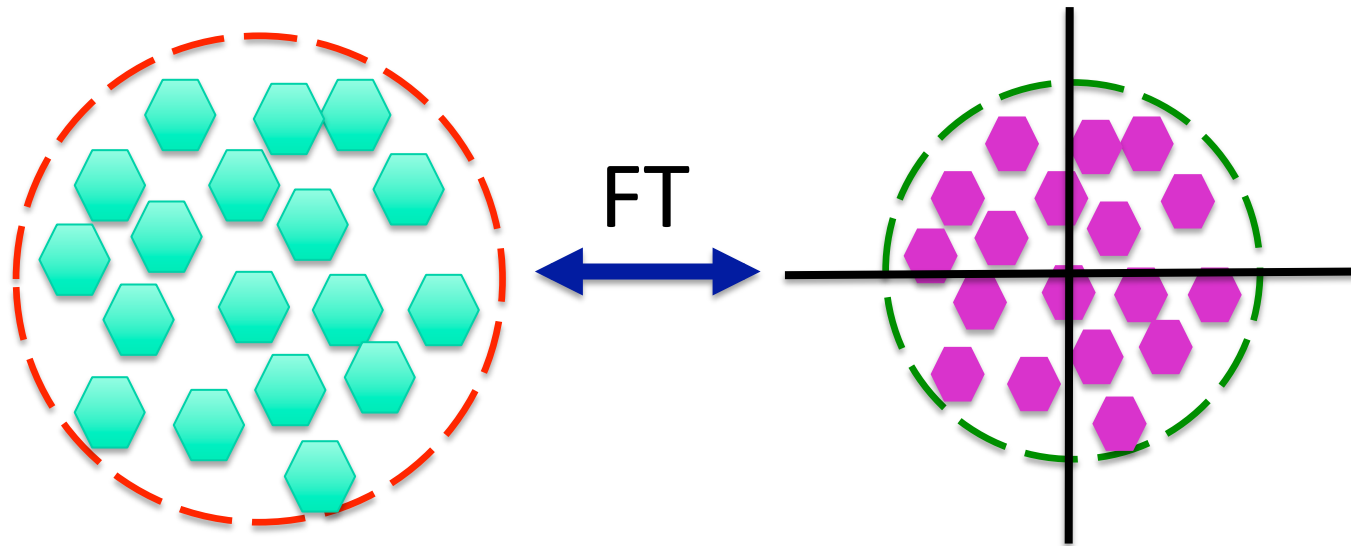
Gang Xiong, et al, Sci Rep 4 6765 (2013)

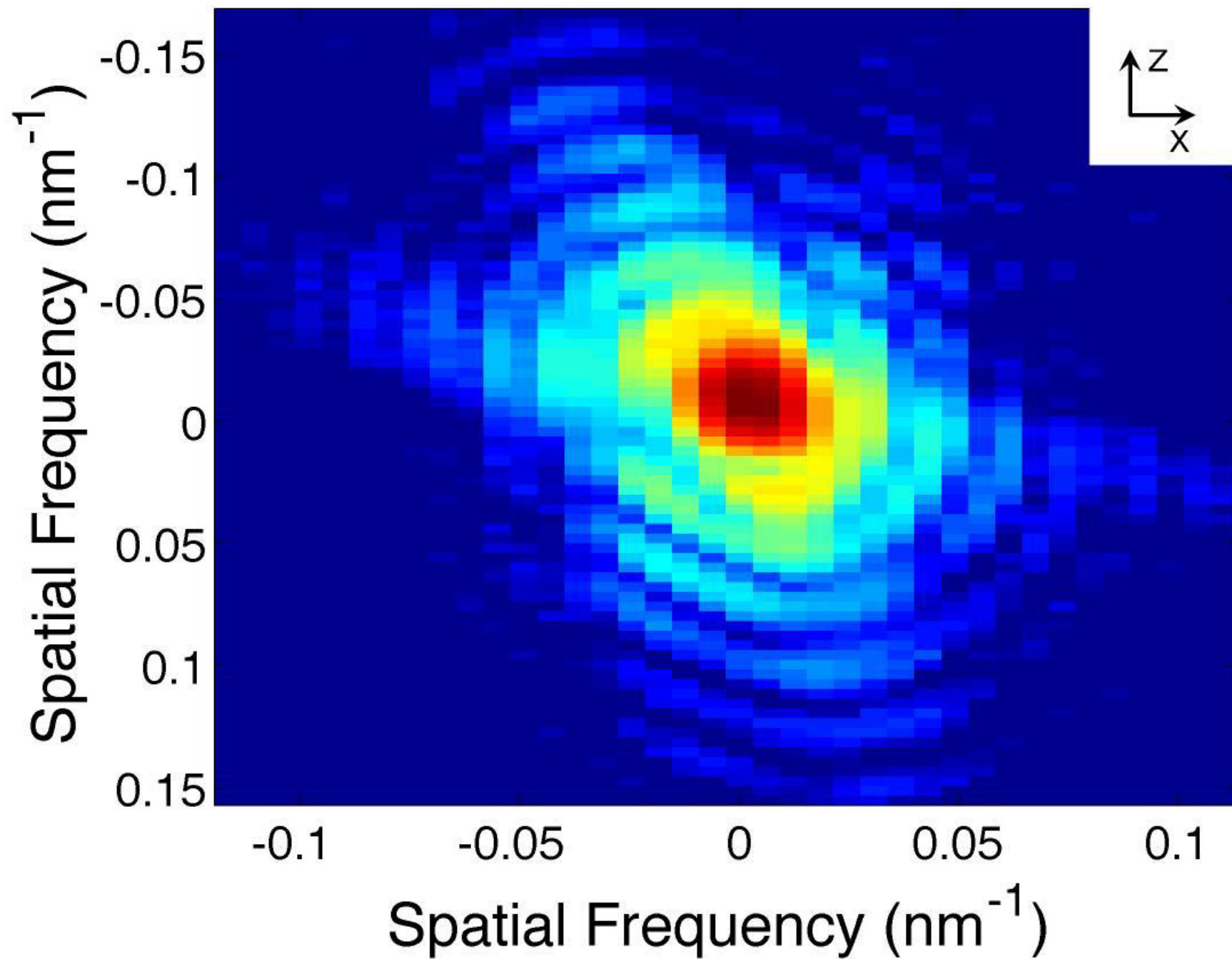


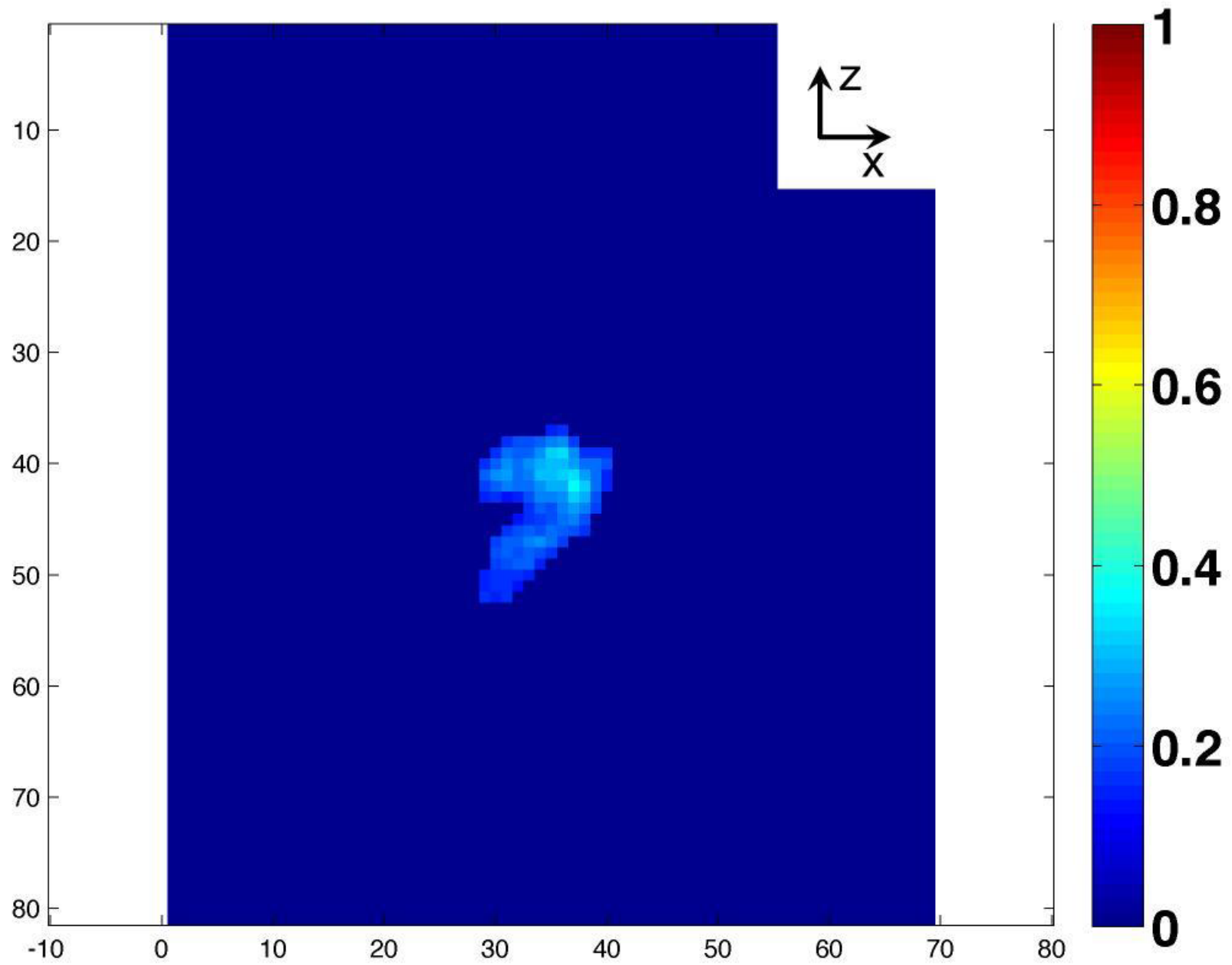
Domain structures give speckled diffraction

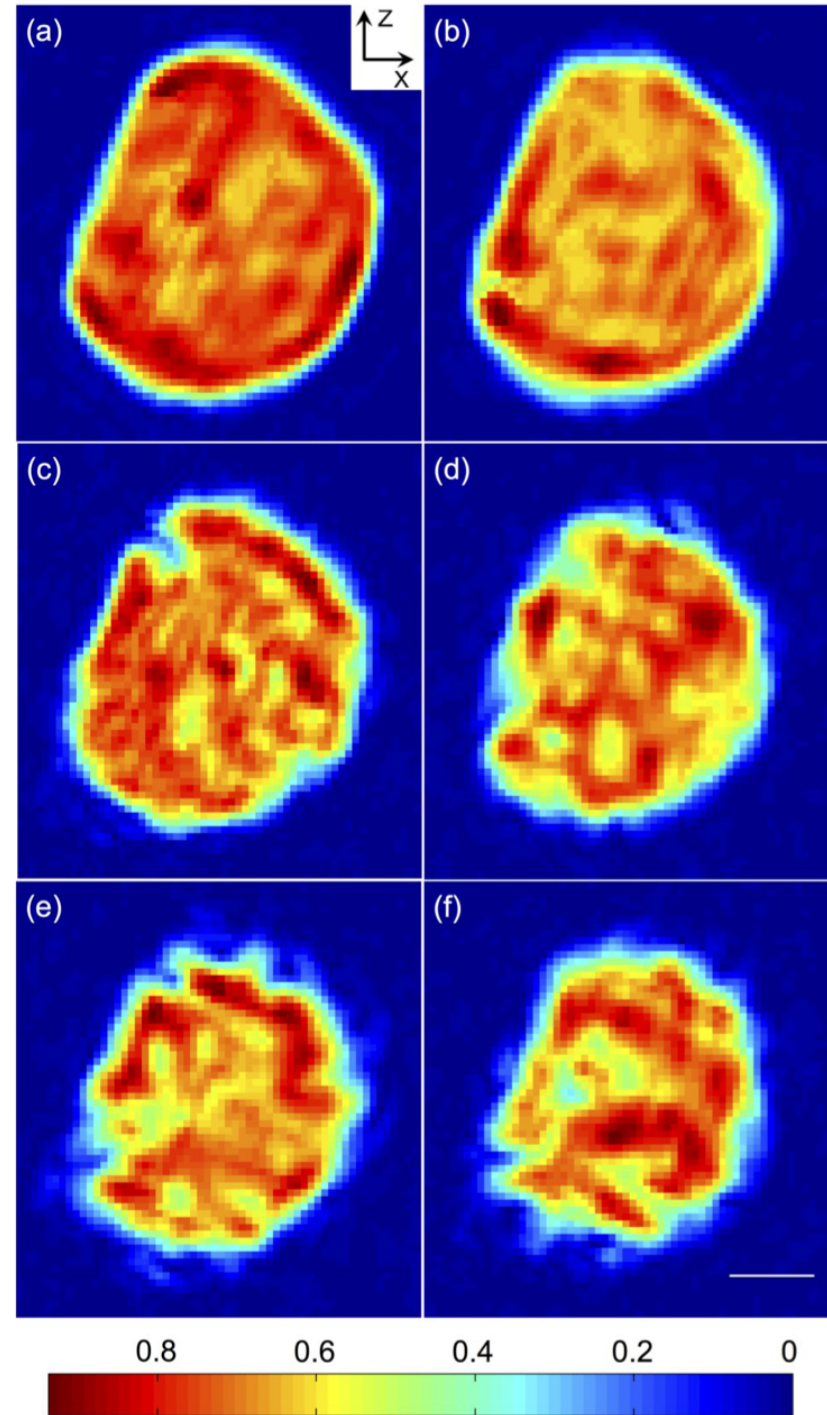
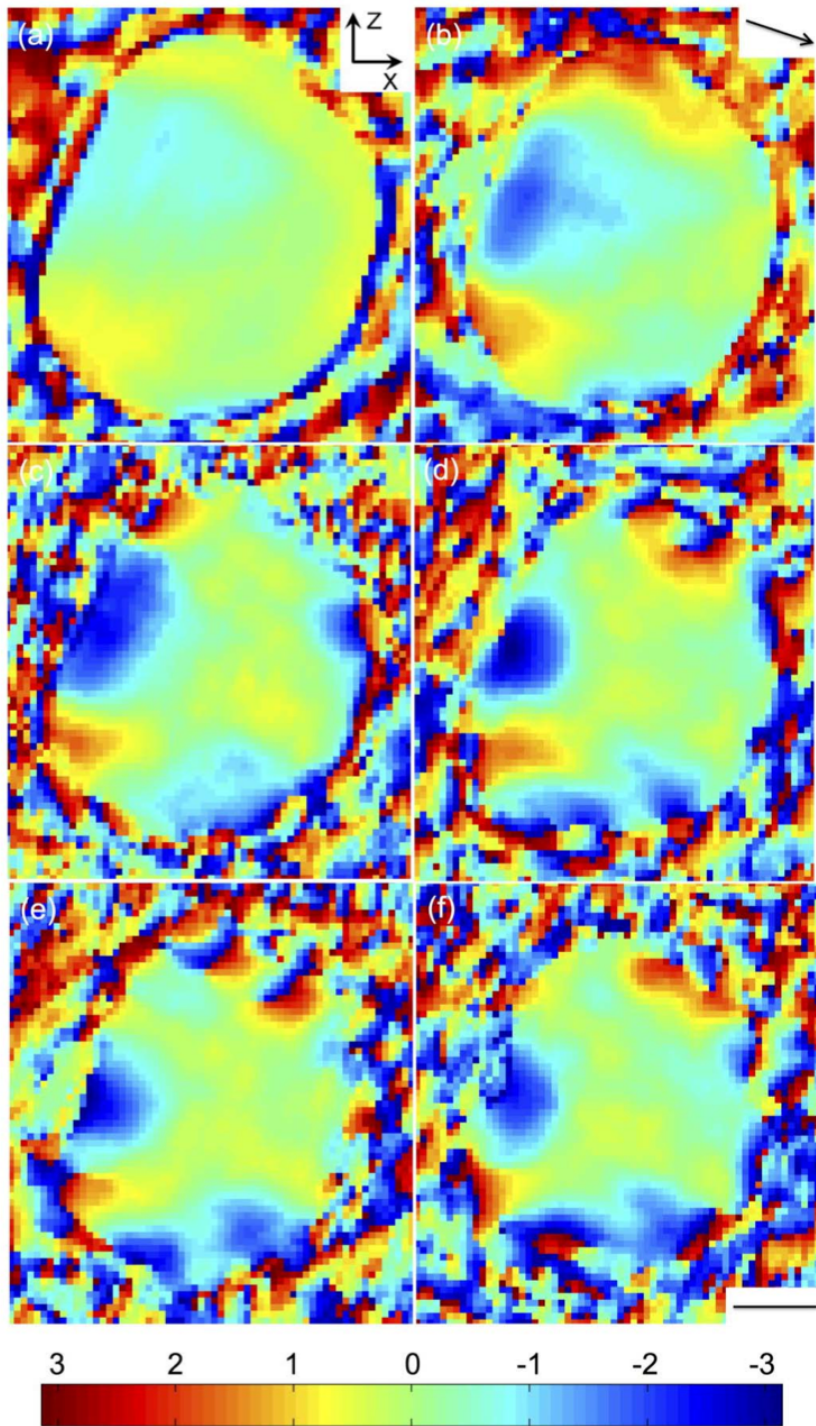
Real Space

Reciprocal Space







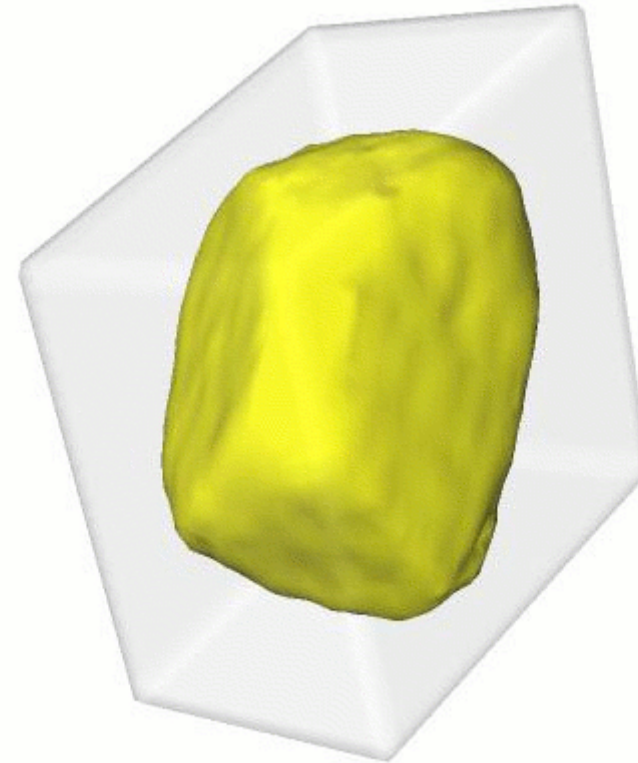
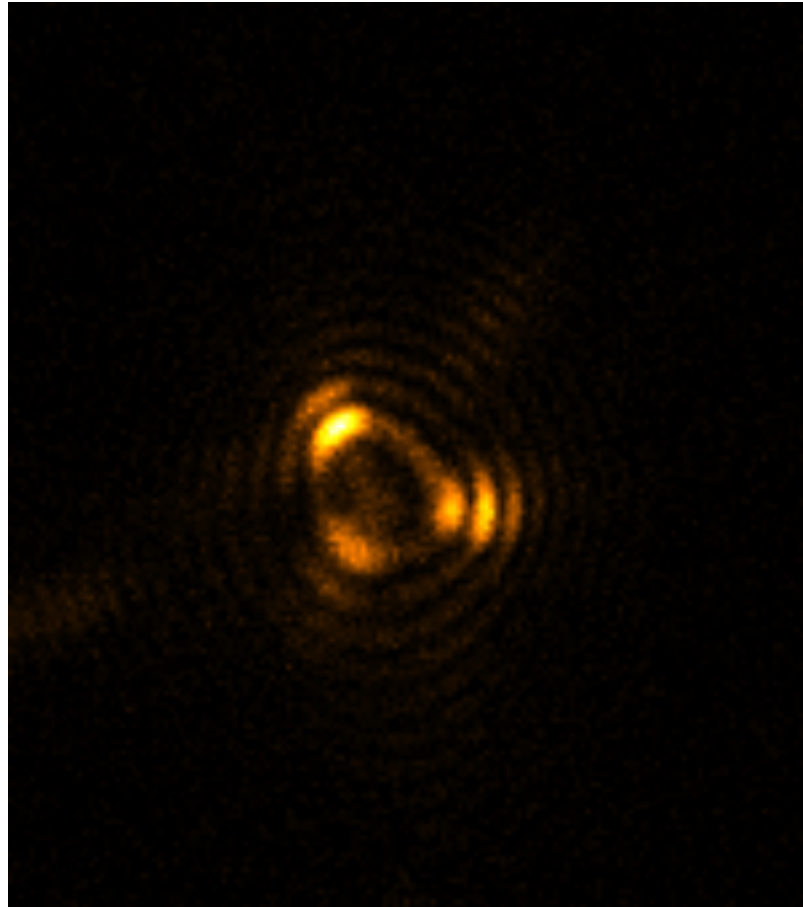


Lecture 1 Topics

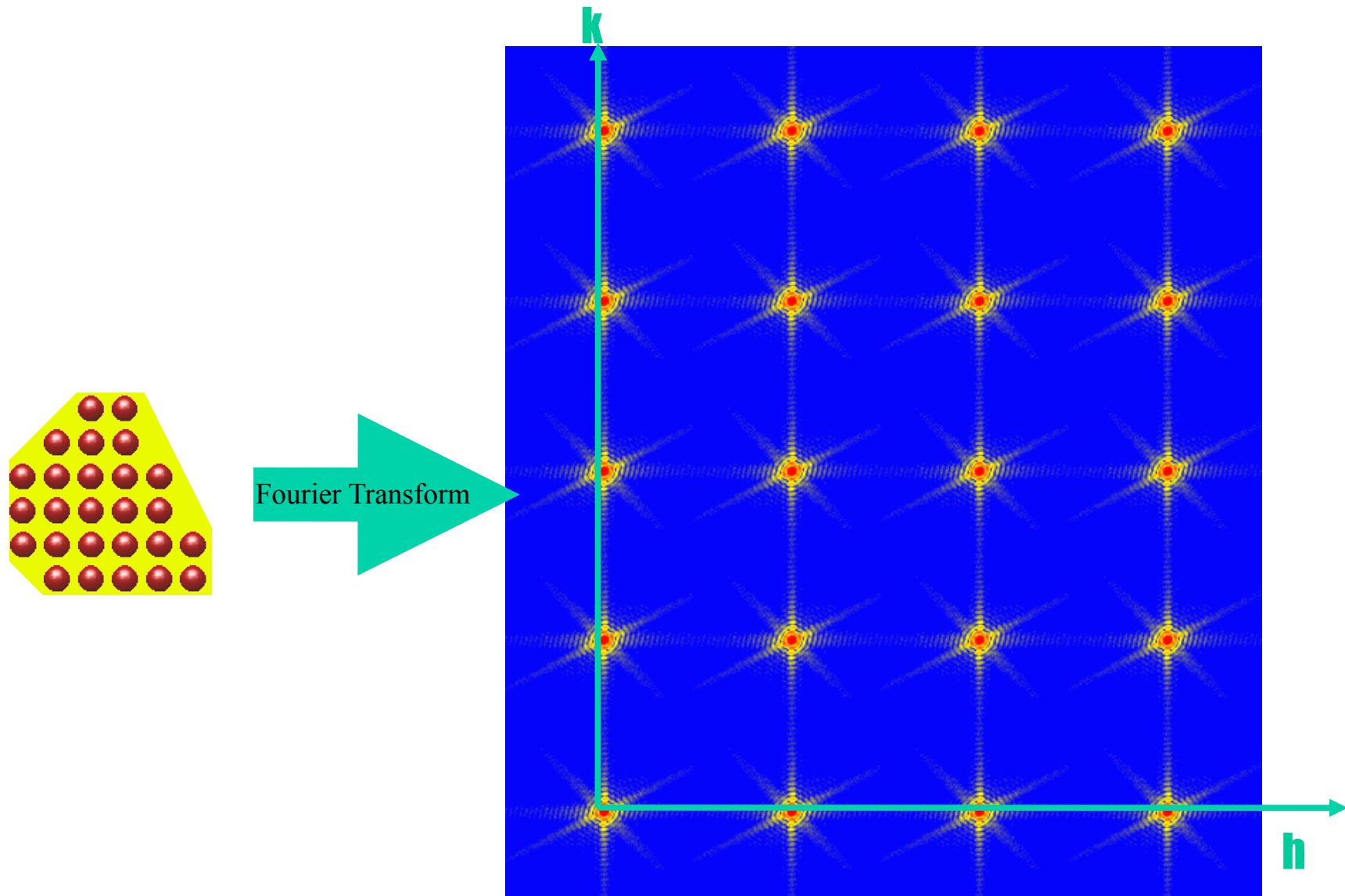
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Gold nanocrystal reconstruction

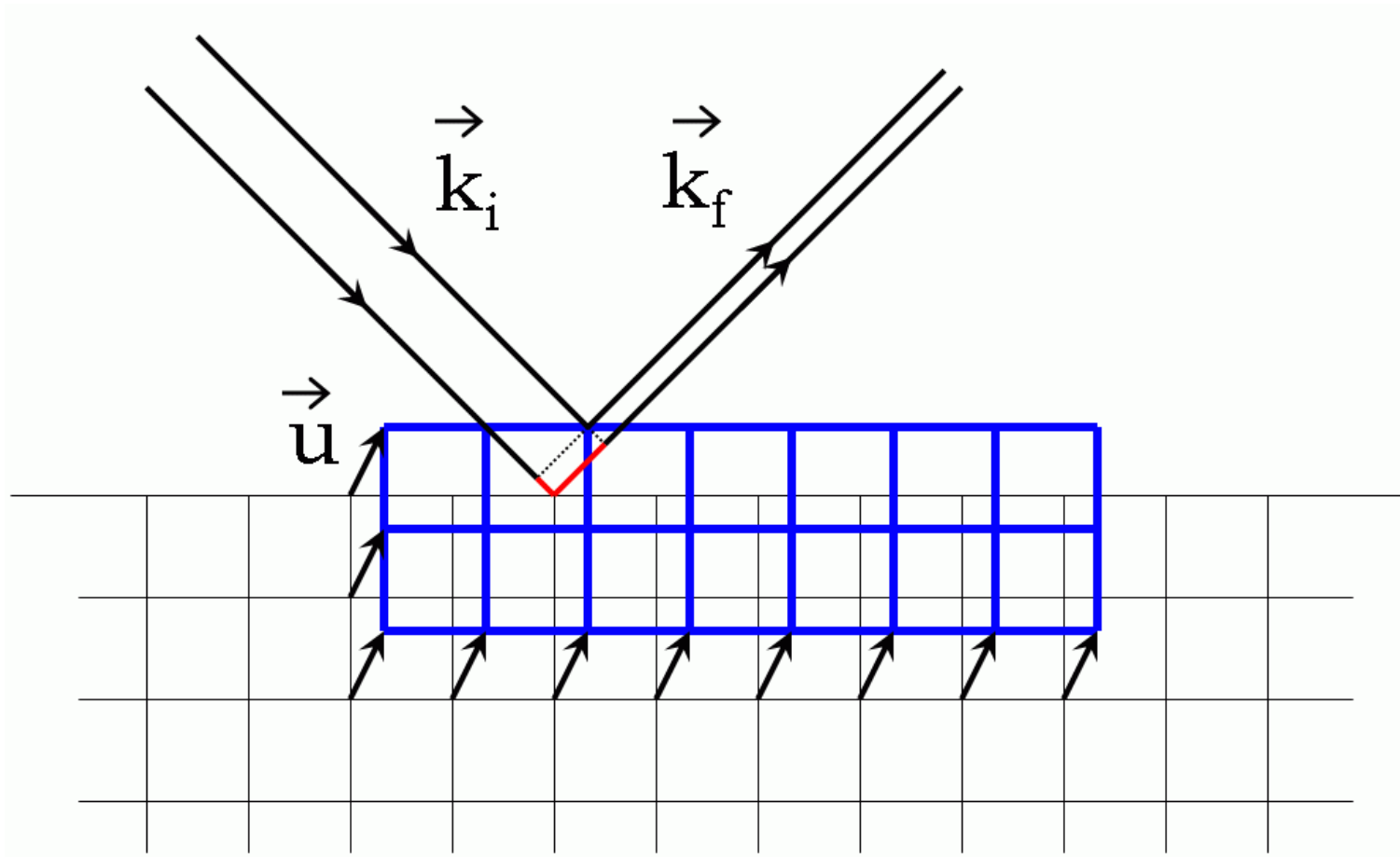
showing support used for 20 HIO followed by 10 ER



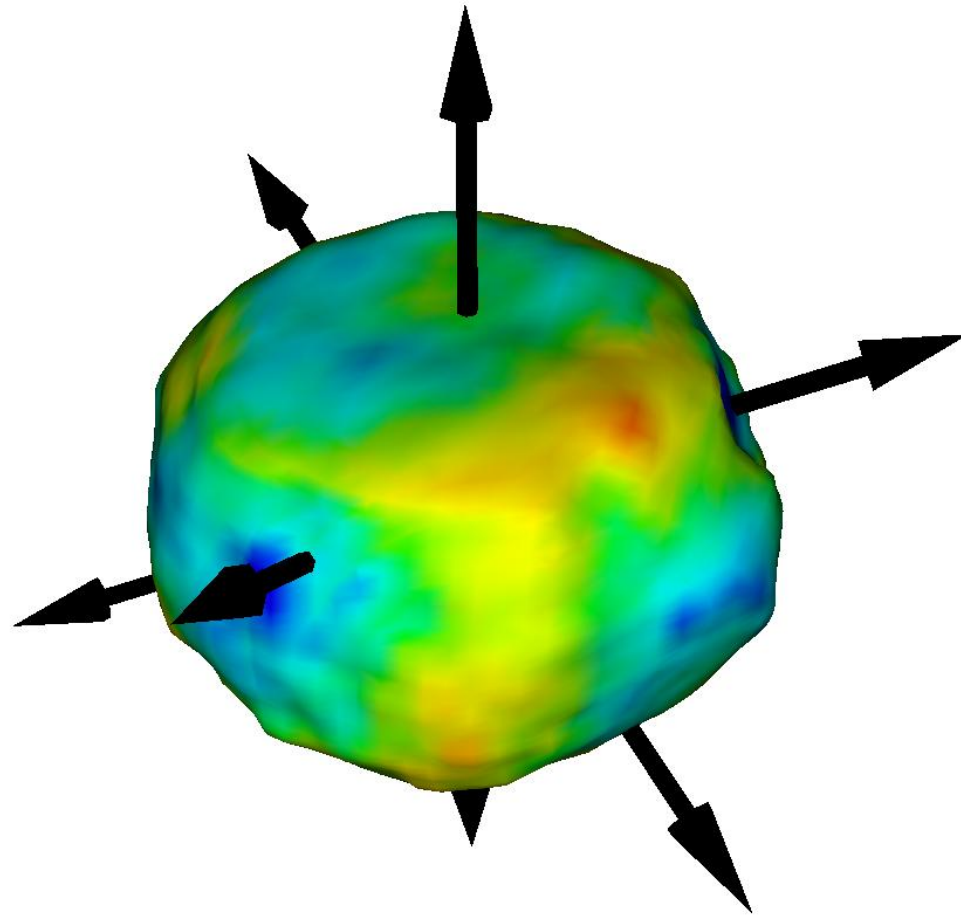
Coherent Diffraction from Crystals



Sensitivity to strain

$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$


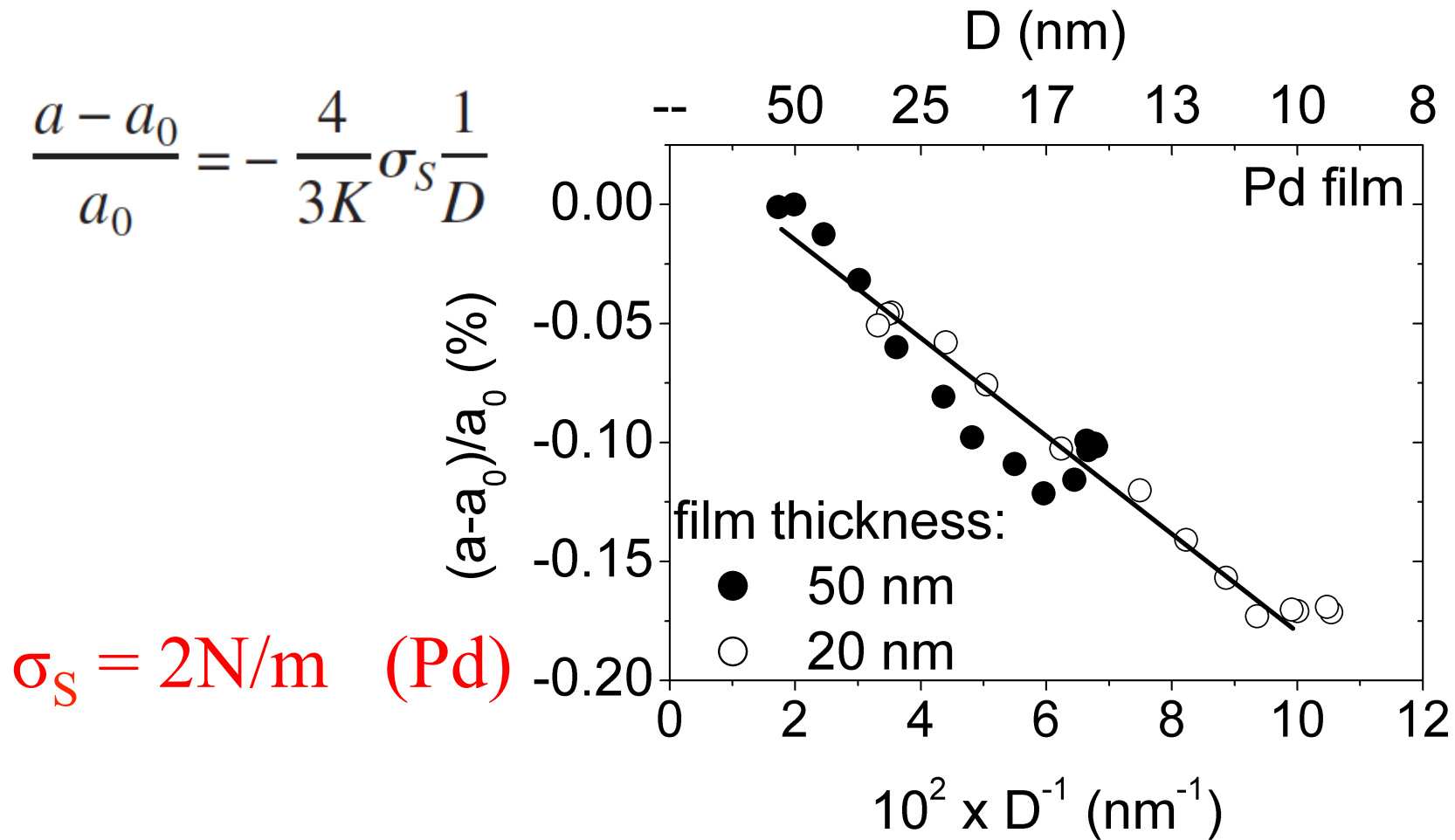
Phase isosurface of residual strain



Contraction of Small Particles

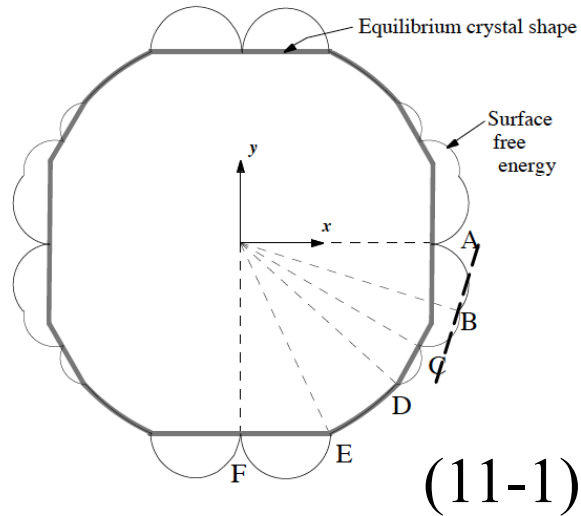
Gibbs Thomson pressure + Bulk modulus

Sheng, Welzel & Mittemeijer, APL 97 153109 (2010)

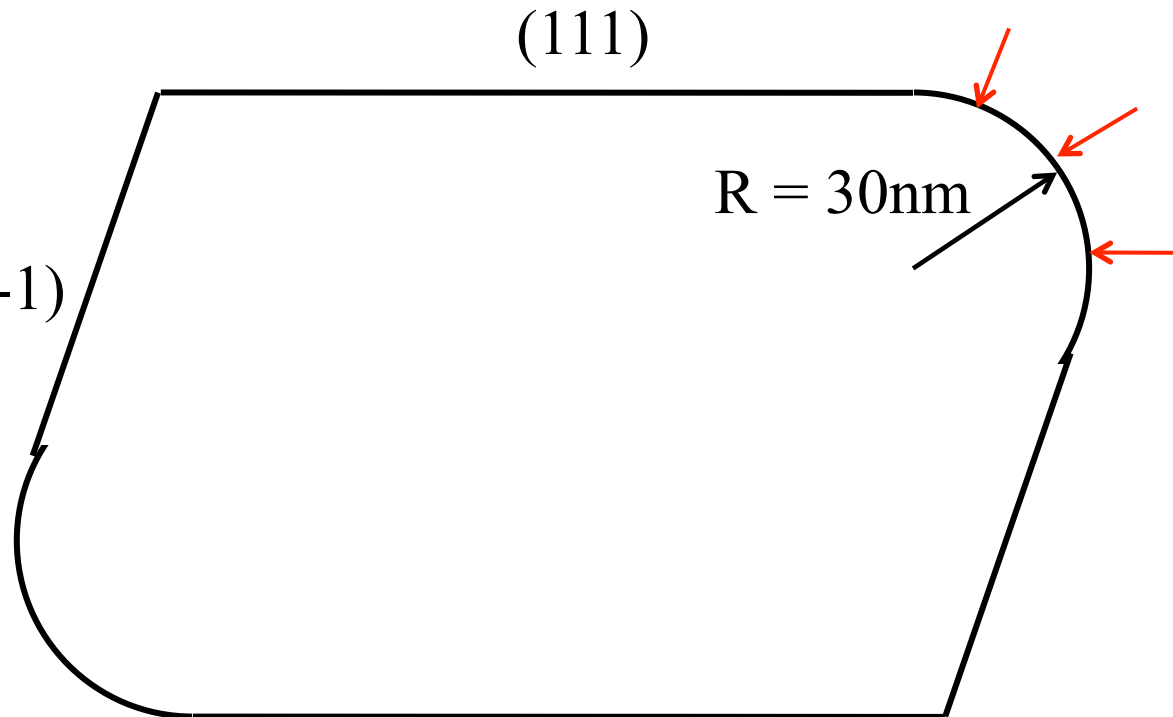


Equilibrium crystal shape

Wulff construction + Gibbs Thomson (Young-Laplace) pressure

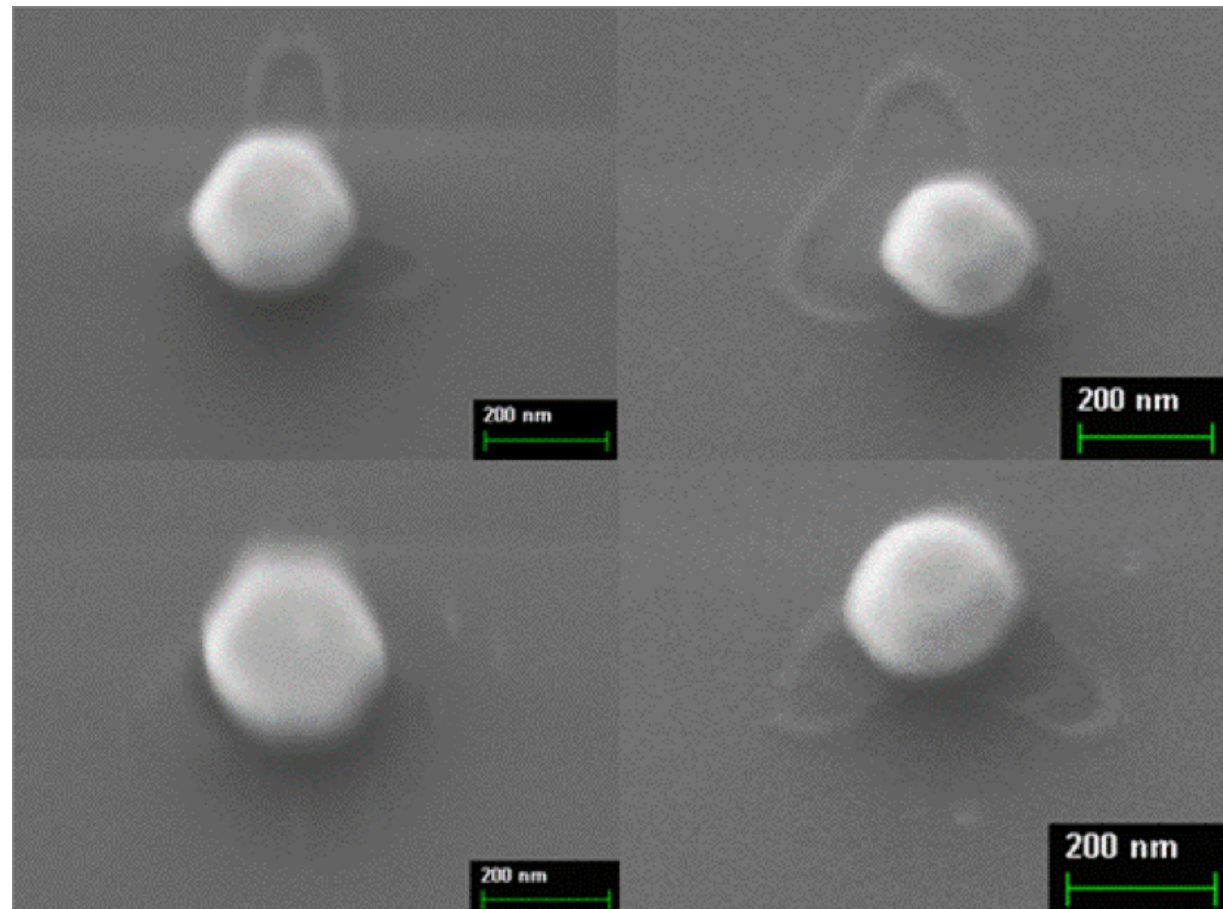
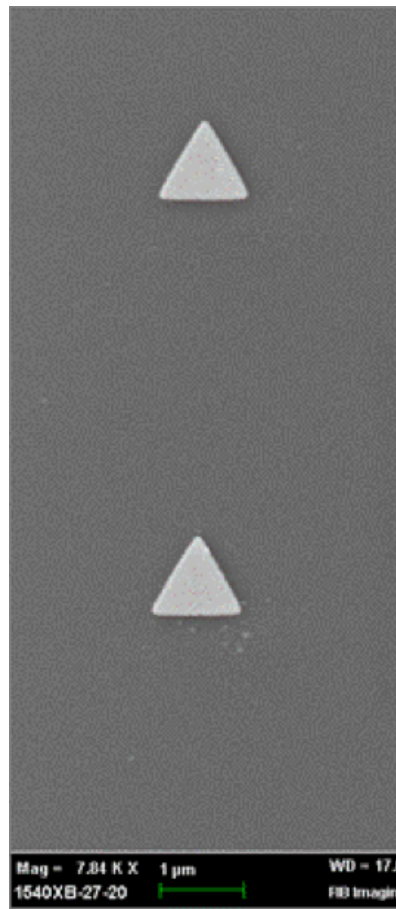


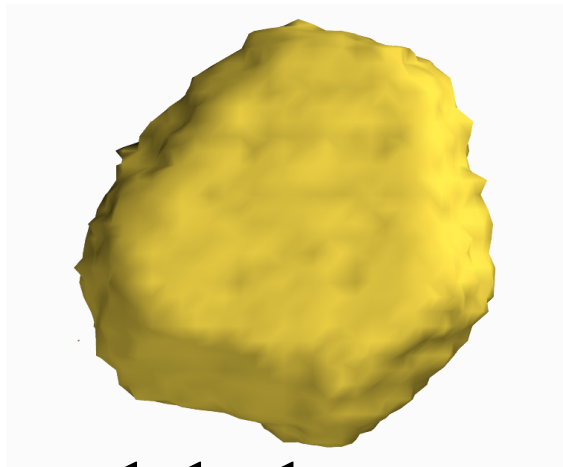
$$\gamma = 2\text{N/m}$$
$$P = 2\gamma/R = 70\text{MPa}$$
$$\varepsilon = 0.1\%, \quad \Phi = 0.6 \text{ rad}$$



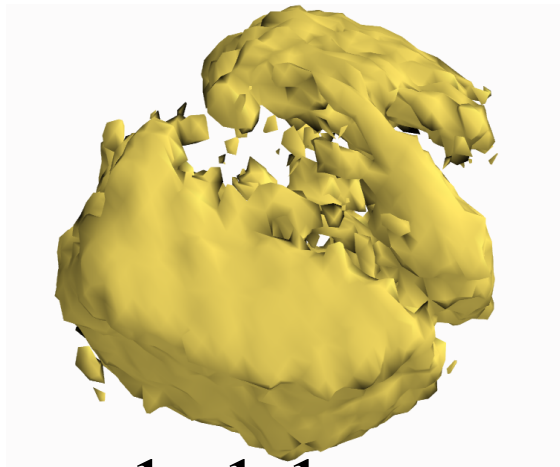
Single Au nanocrystal synthesis

Loren Beitra, Takashi Matsuura

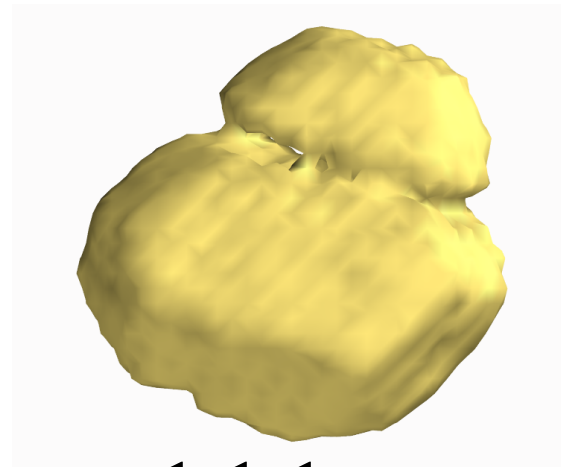




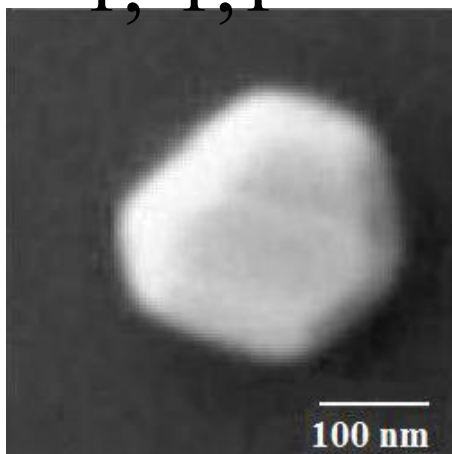
1,1,-1



1,-1,1

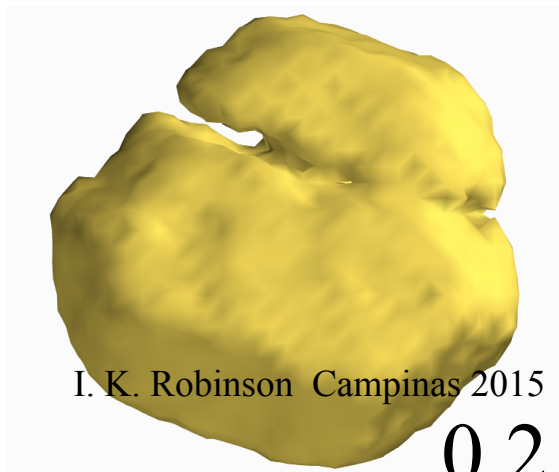
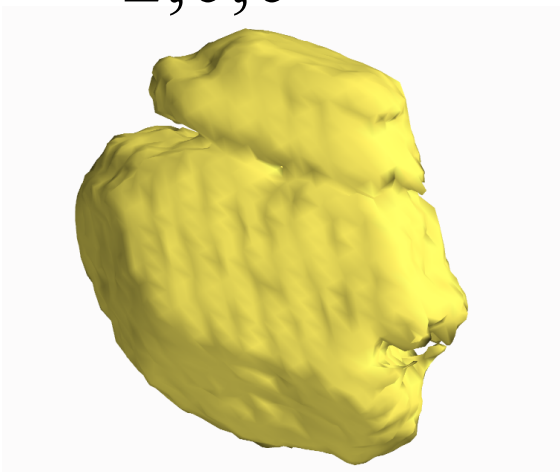


-1,1,1



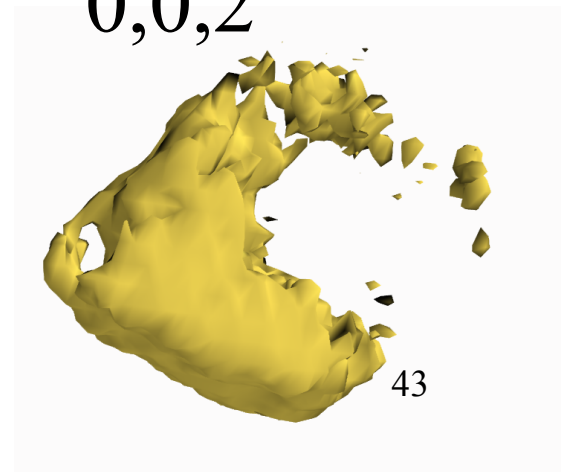
100 nm

2,0,0



I. K. Robinson Campinas 2015

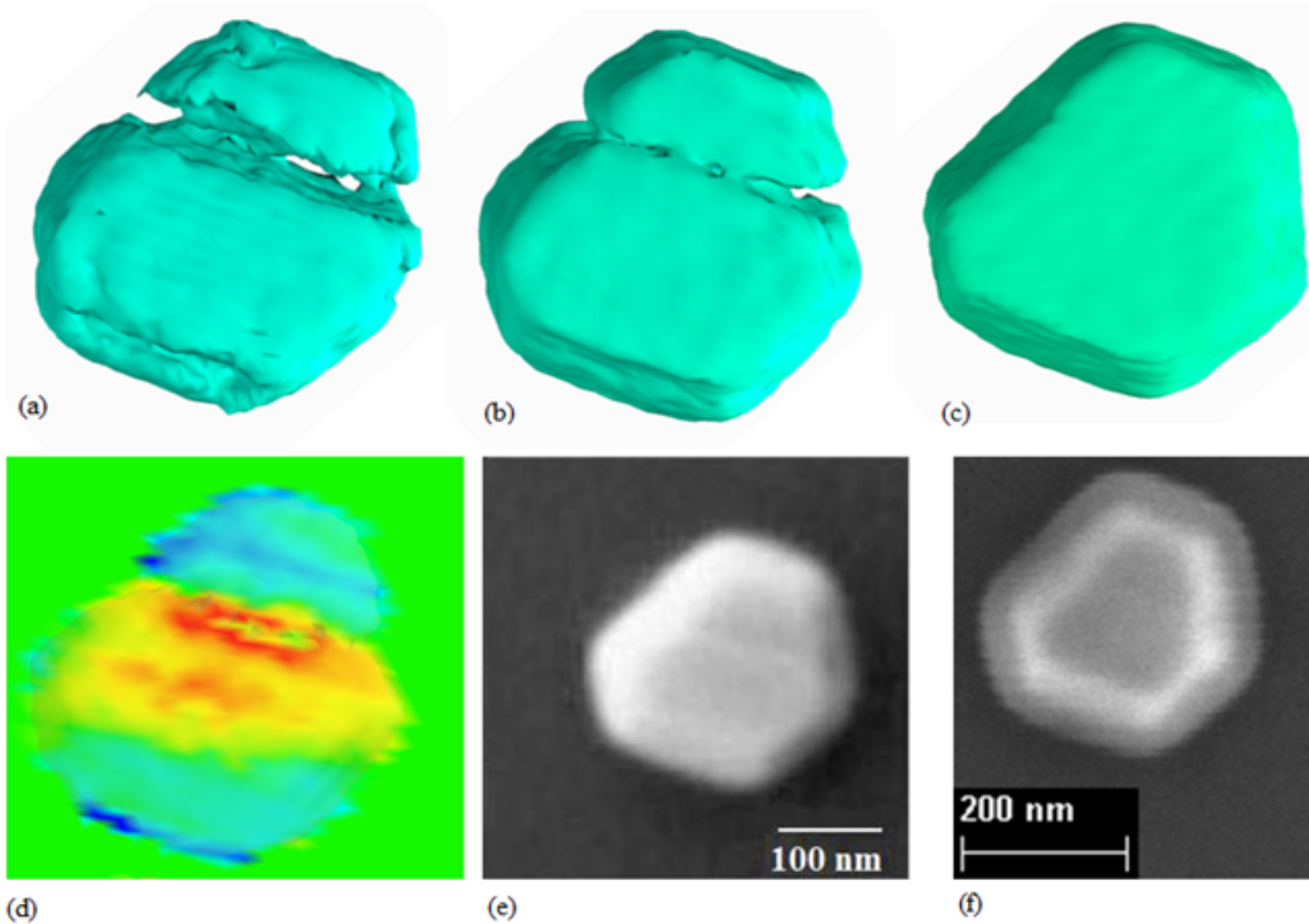
0,2,0



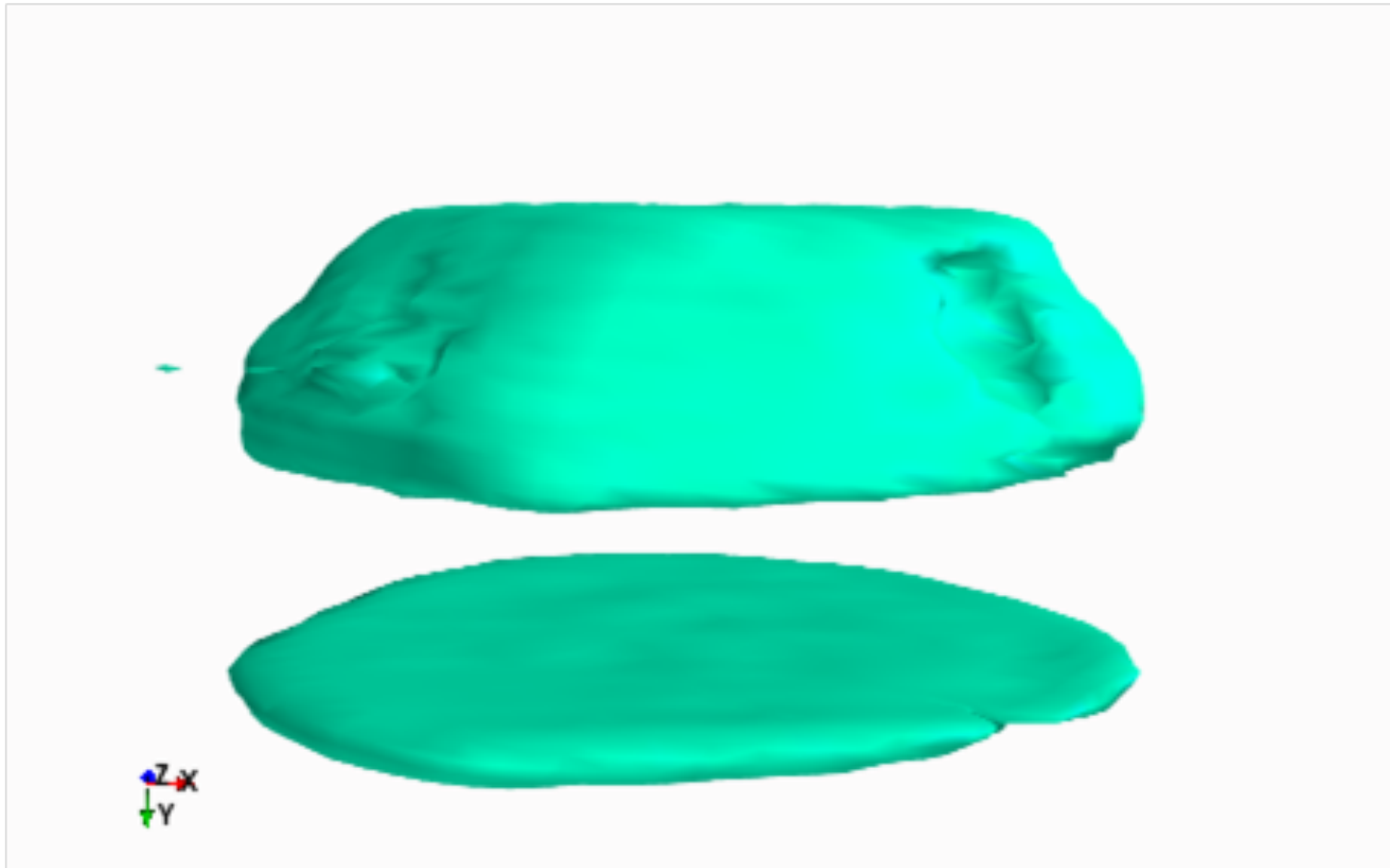
0,0,2

43

Different Bragg Peaks

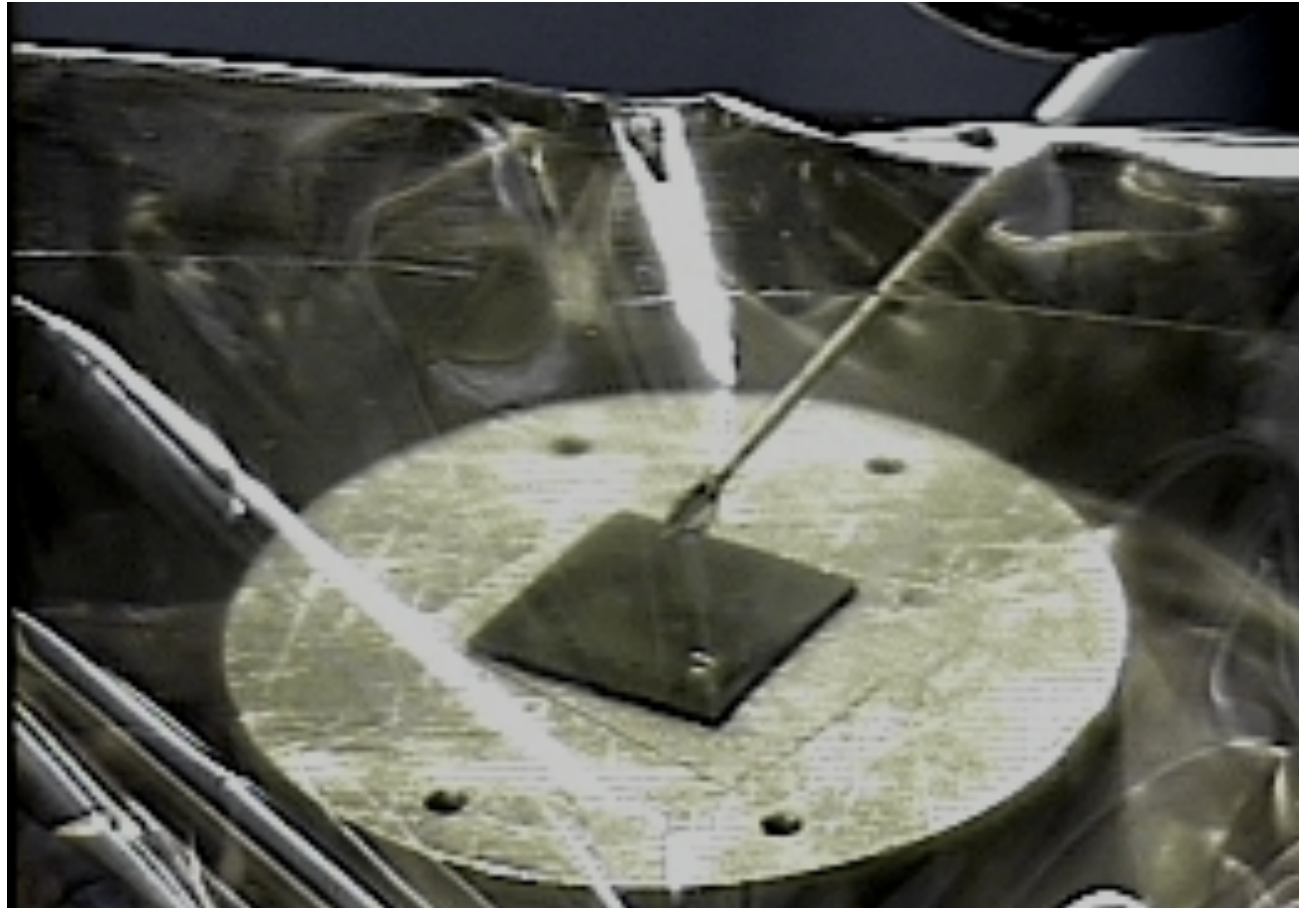


Horizontally Faulted Slab



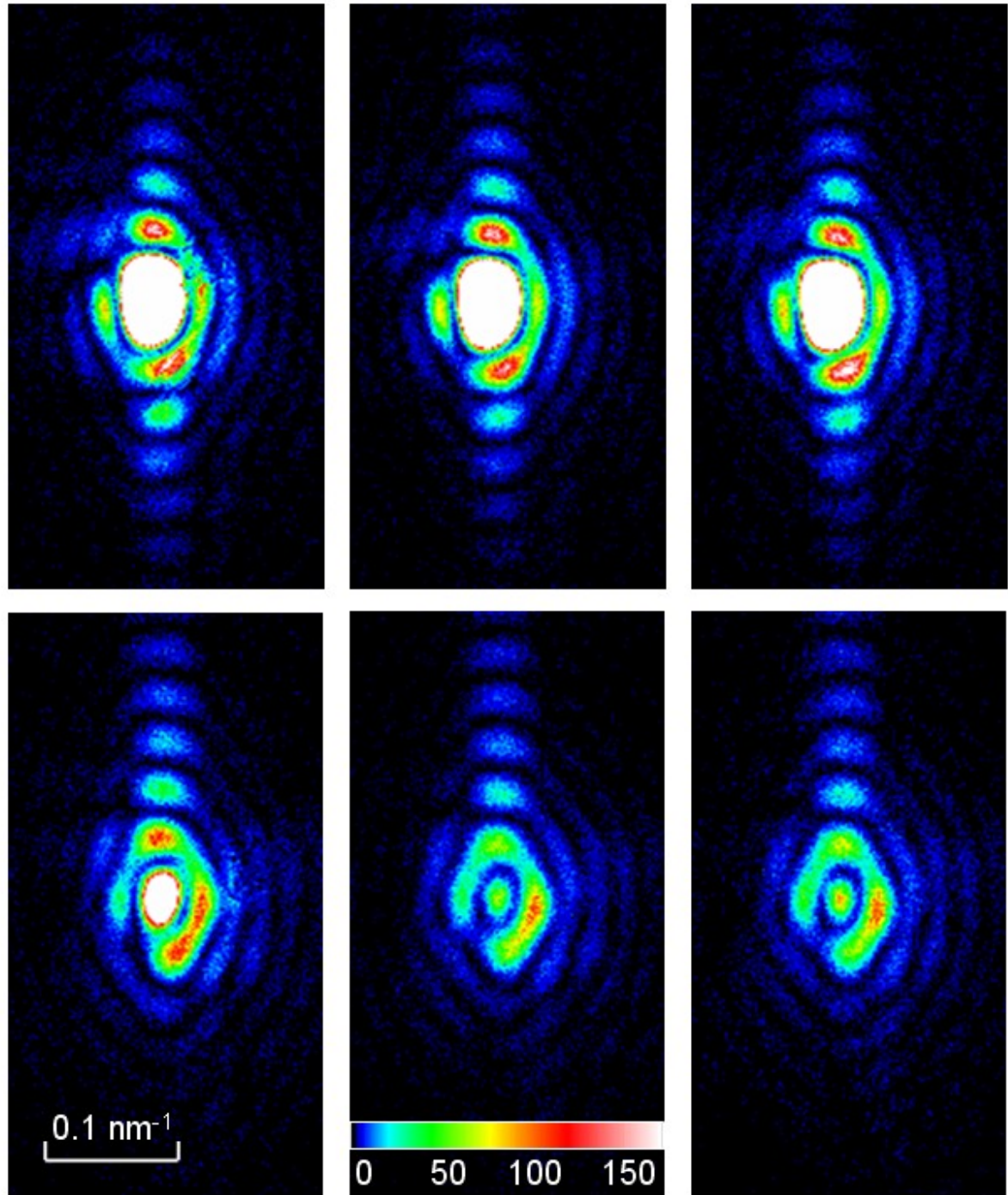
Dosing with C_3H_7SH in ethanol

Moyu Watari, Rachel McKendry, Manuel Voegtli, Gabriel Aeppli,
Yeong- Ah Soh, Xiaowen Shi, Gang Xiong, Xiaojing Huang,
Ross Harder and Ian Robinson, Nature Materials (2011)



Rocking curve of Au crystal

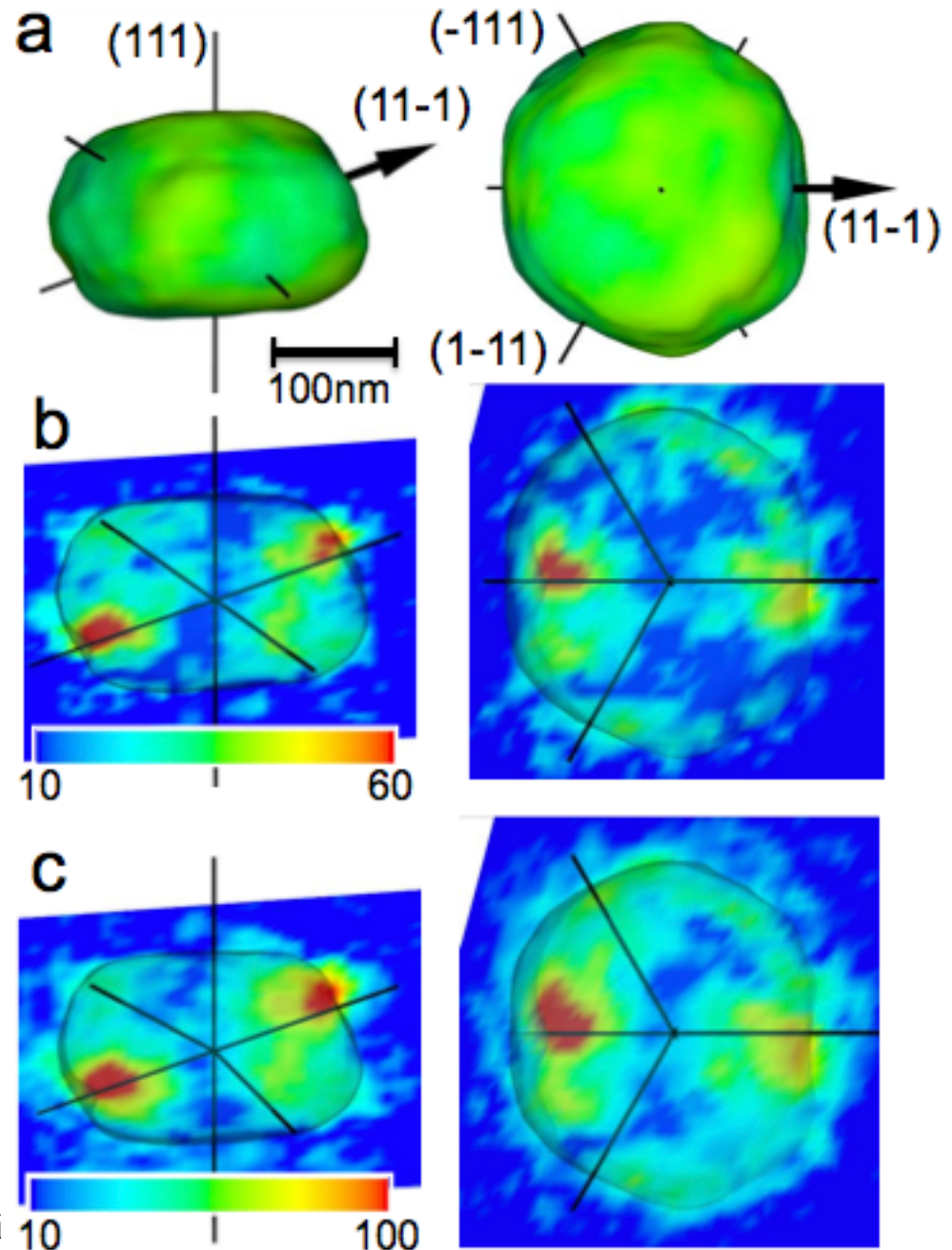
Before dosing /
dose 1 / dose 2



Difference Fourier:

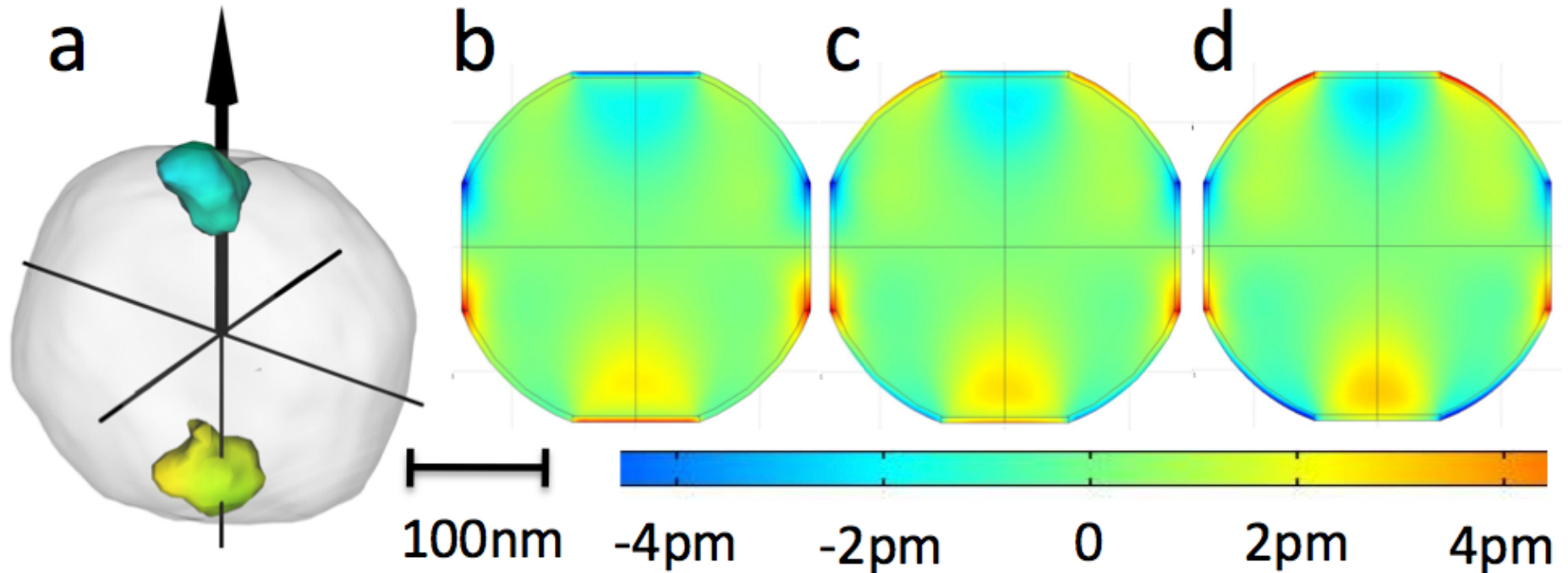
Magnitude of phase
change caused by
dosing

M. Watari et al,
Nature Materials (2011)

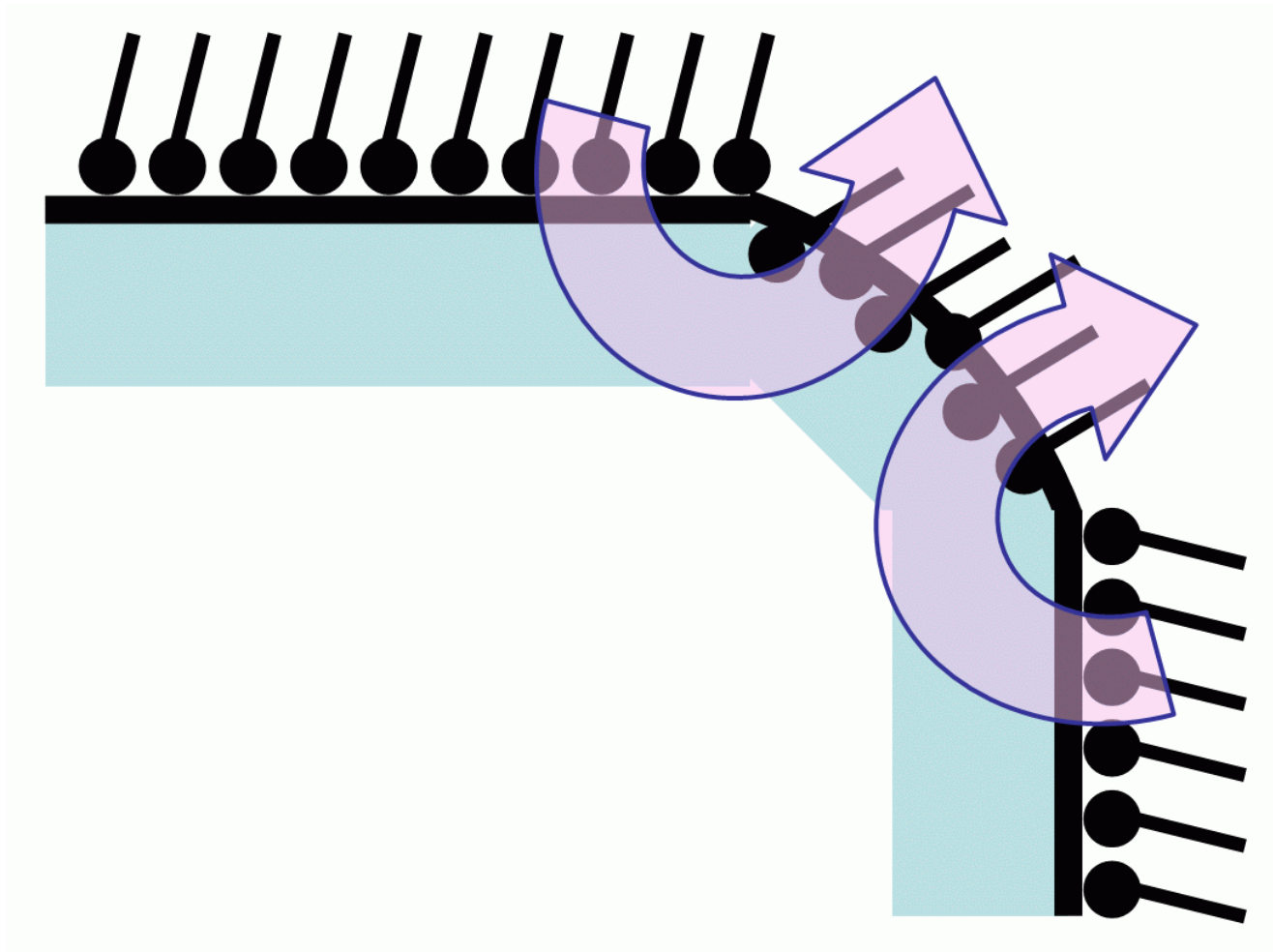


Finite-element Analysis

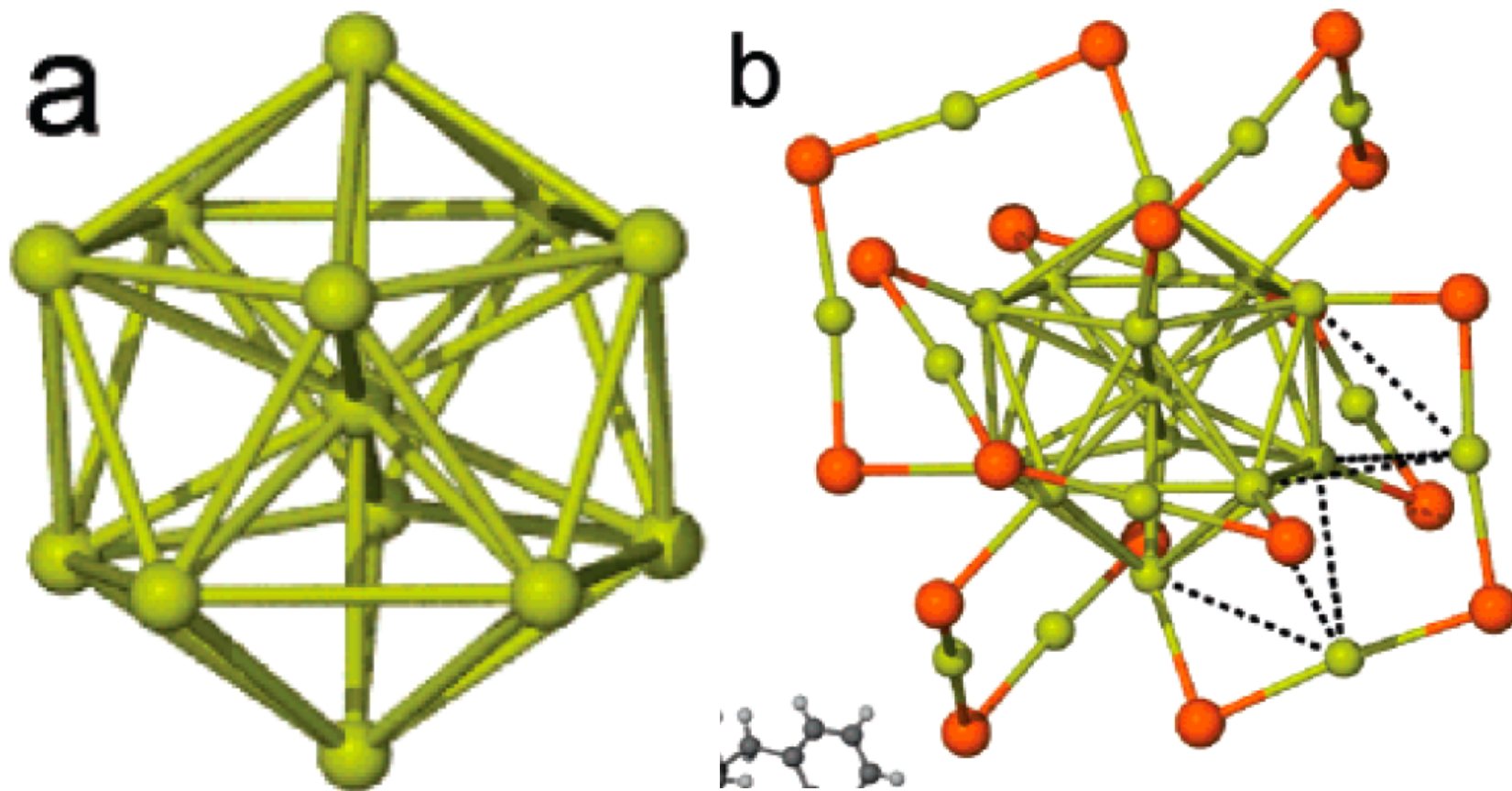
Differential stress introduced in “skin”
 $\pm 3 \times 10^8 \text{ Pa}$ in 5nm thickness = 1.5N/m



Differential adsorption, thiol/Au



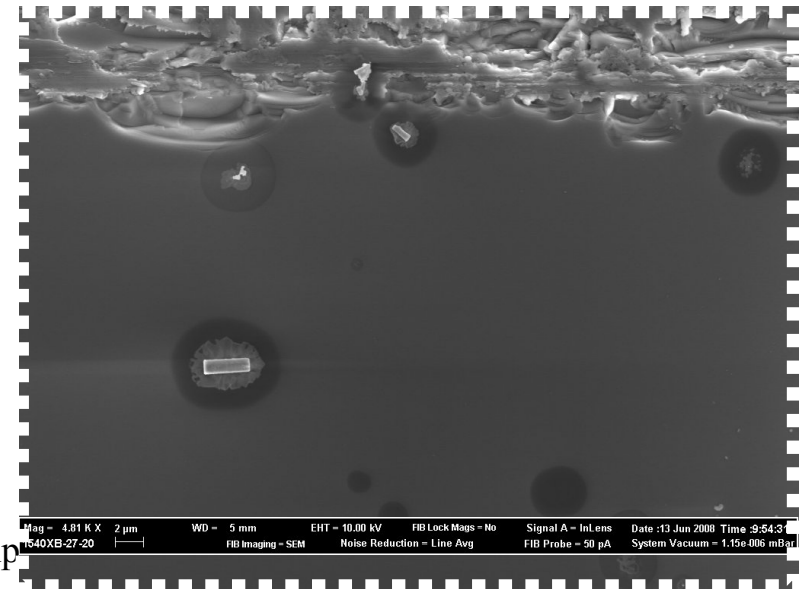
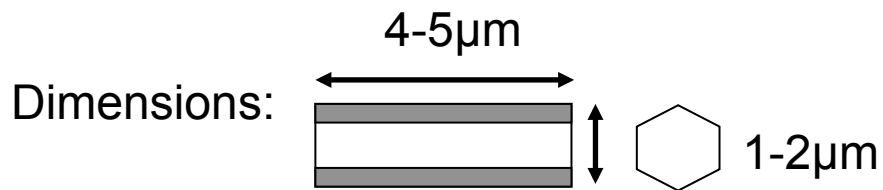
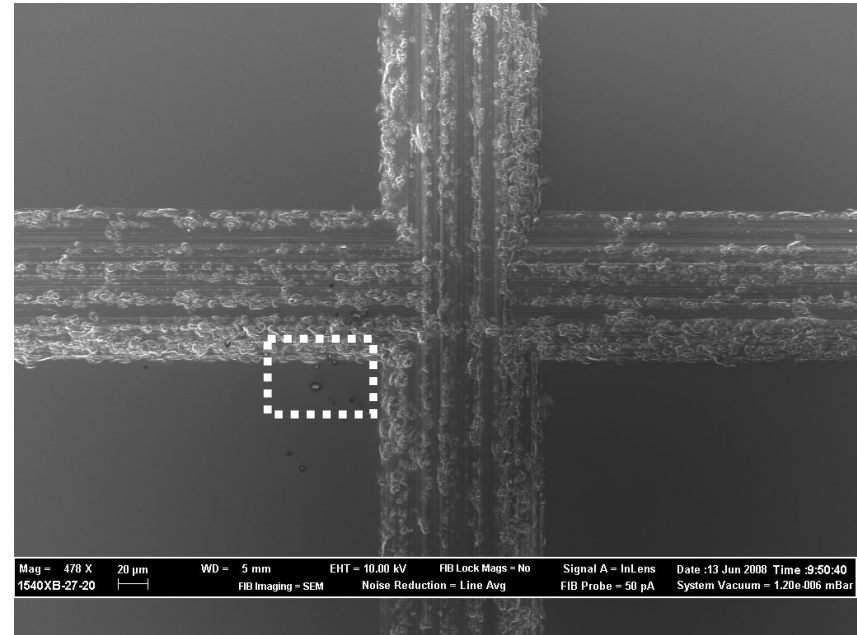
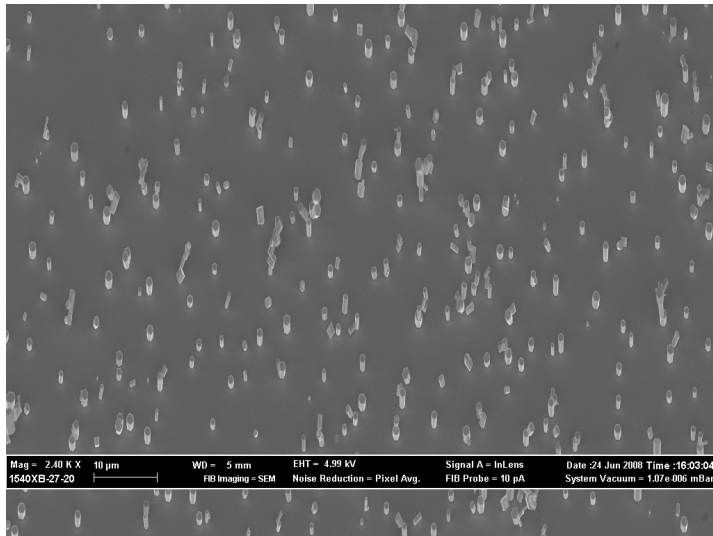
Gold-sulphur structure $\text{Au}_{13}(\text{Au}_2\text{RS}_3)_6$ $=\text{Au}_{25}\text{RS}_{18}$ Heaven et al, JACS 130 3755 (2008)



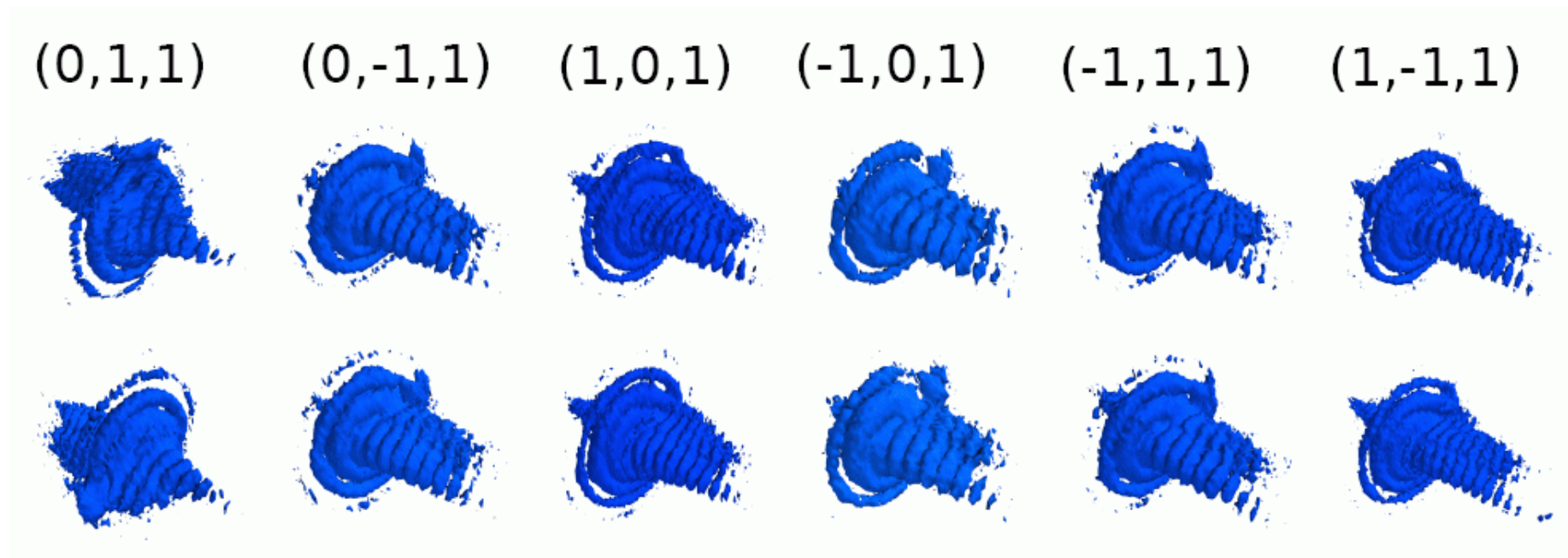
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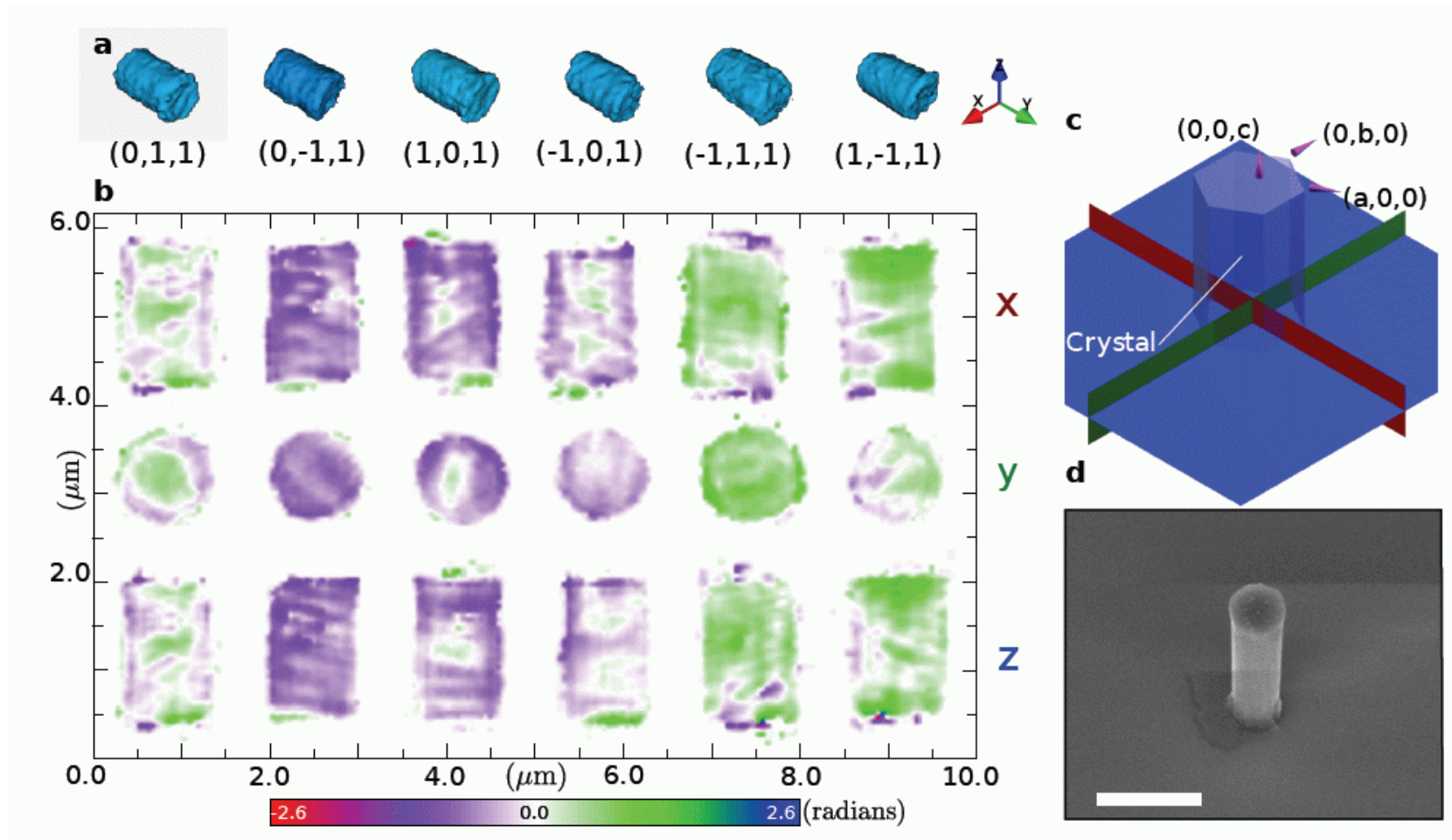
ZnO Sample Preparation



Extension to 6 Bragg Peaks

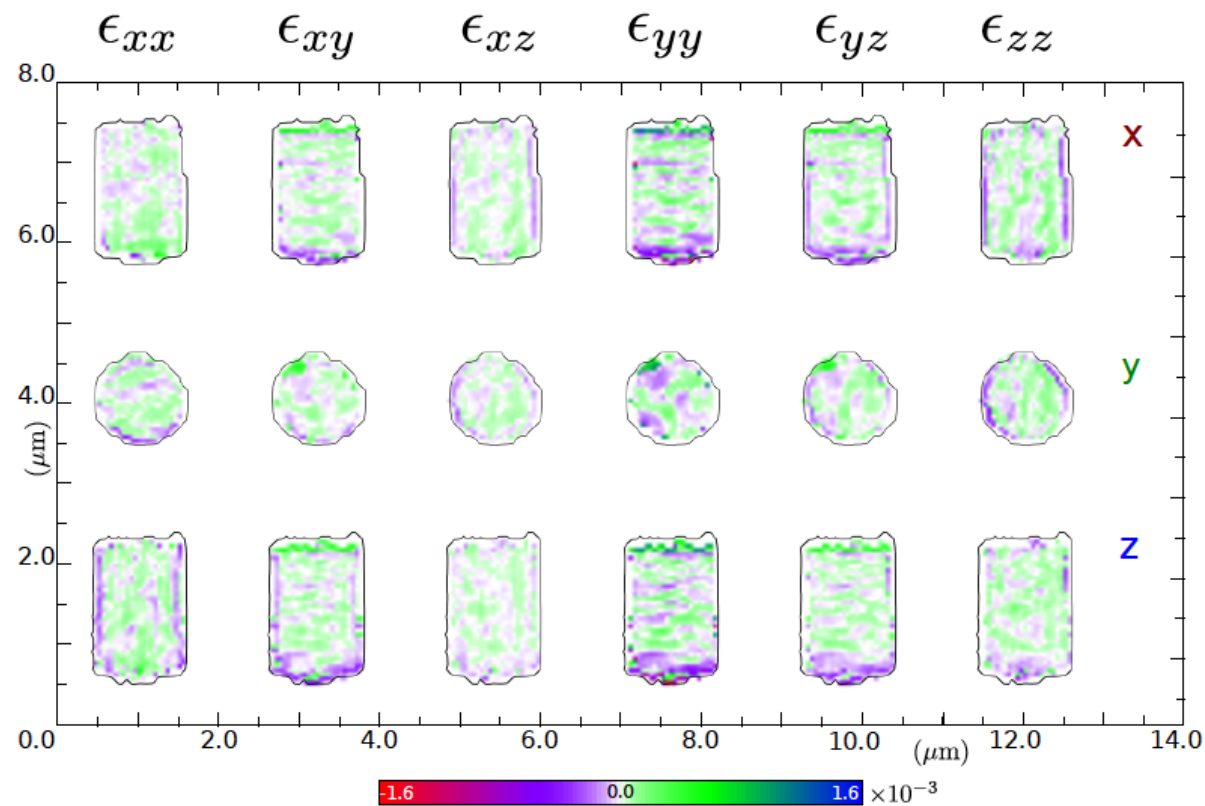


Extension to 6 Bragg Peaks

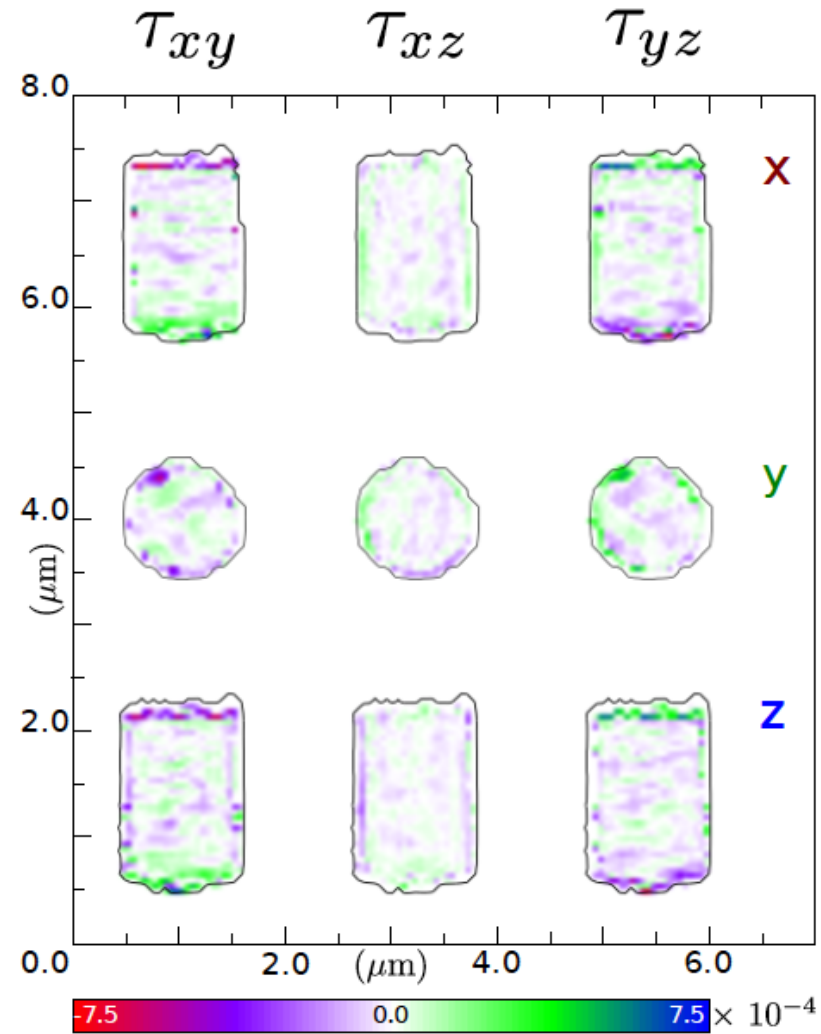


Full Strain Tensor

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right), \quad \tau_{ij} = \left(\frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j} \right)$$



ZnO Rigid-body Rotations



Phasing packages, databases

Marcus Newton, Filipe Maia



The Interactive Phase Retrieval Suite

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Maximizing data availability

Welcome to the Coherent X-ray Imaging Data Bank (CXIDB), a new database which offers scientists from all over the world a unique opportunity to access data from Coherent X-ray Imaging (CXI) experiments.

What is Bonsu?

Bonsu, the interactive phase retrieval from coherent X-ray diffraction images and routines for data manipulation and analysis.

Bonsu is open-source, is designed and implemented in Python, and handles data in formats such as:

- SPE
- HDF5 (indirectly through [h5py](#))
- VTK
- NumPy

To discover new features planned for future releases, please see the [roadmap](#).

A General Tool for Phase Retrieval...

Bonsu aims to be an encompassing tool to enable scientists to perform phase retrieval in a reproducible manner across the board.

Lecture 1 Topics

- I. Bragg Diffraction Imaging (BCDI)
- II. Longitudinal Coherence
- III. Transverse Coherence
- IV. Nanocrystal Alloying
- V. Nanocrystal Structures
- VI. Strain Imaging