



Probing Strain and Defects in Single Crystals with CDI

Advanced Photon Source, Argonne National Lab
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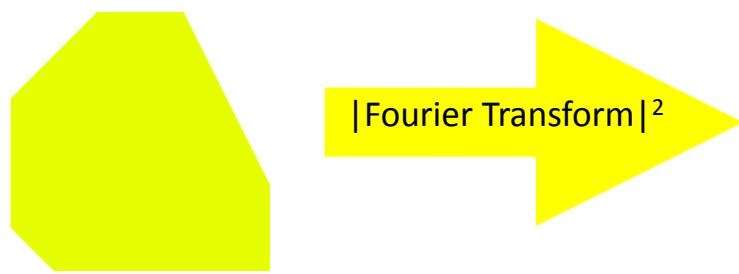
APS Sector 34ID-C

Northwestern University, Materials Science
Karen Chen
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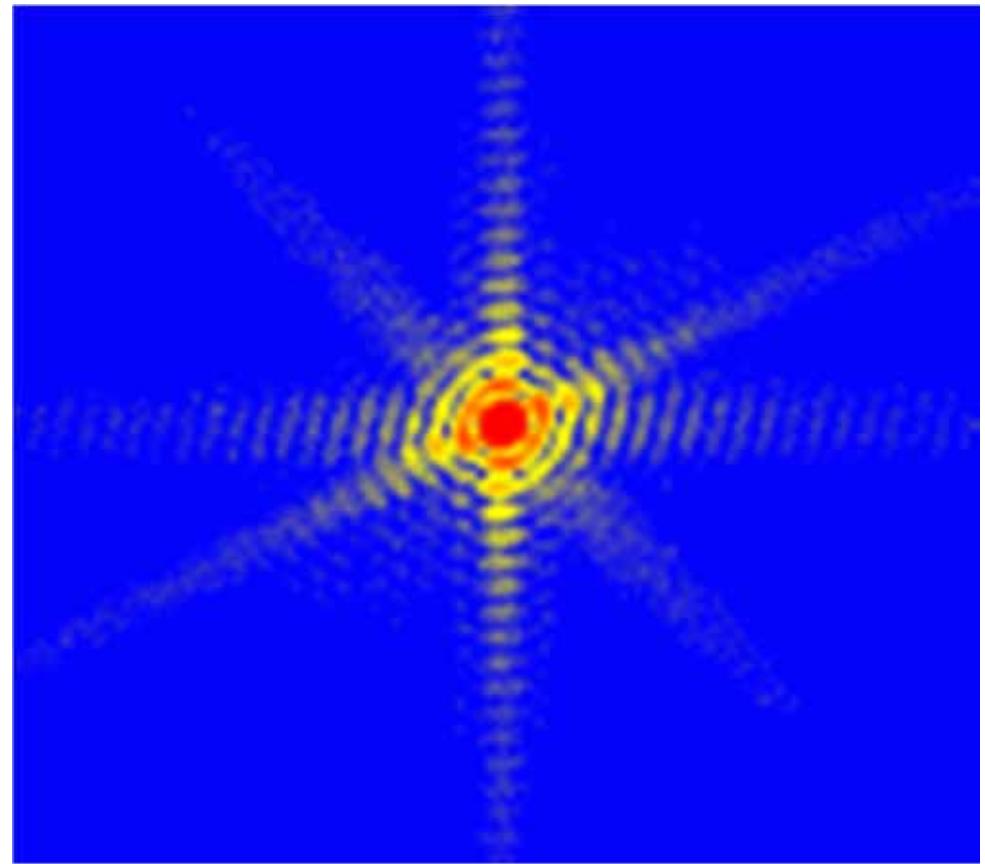
London Centre for Nanotechnology, University College London
Steven Leake
Loren Beitra
Marcus Newton
I.K. Robinson



Coherent Diffraction from Crystals



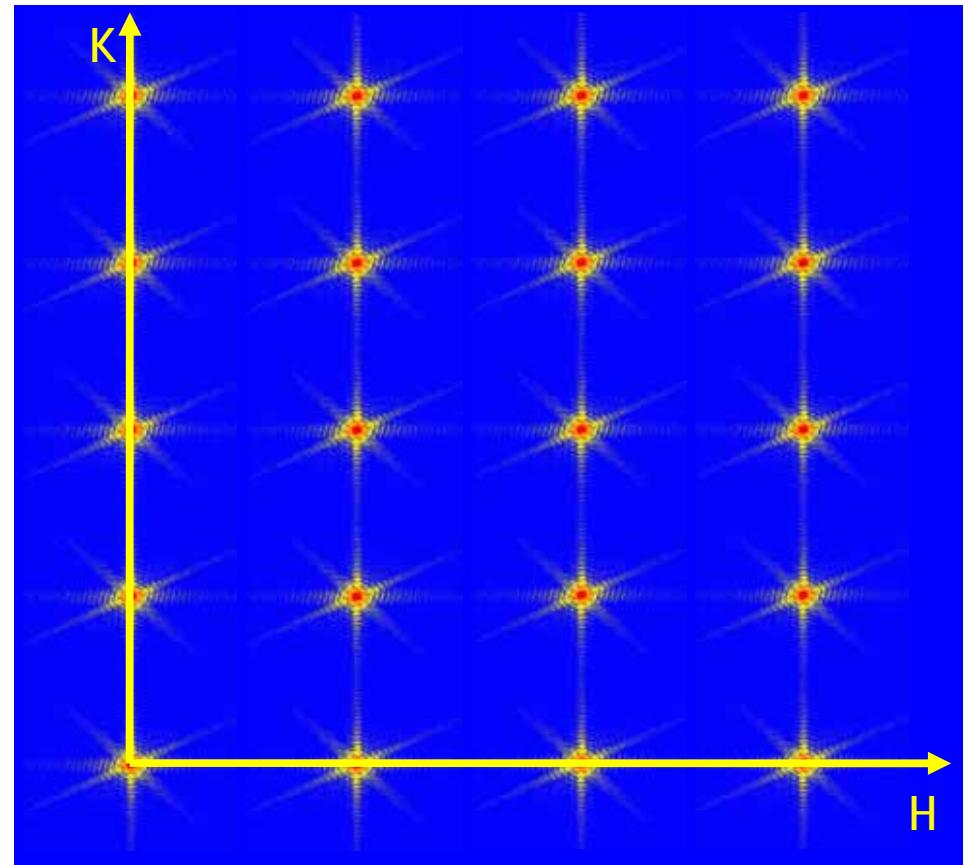
|Fourier Transform|²



Coherent Diffraction from Crystals

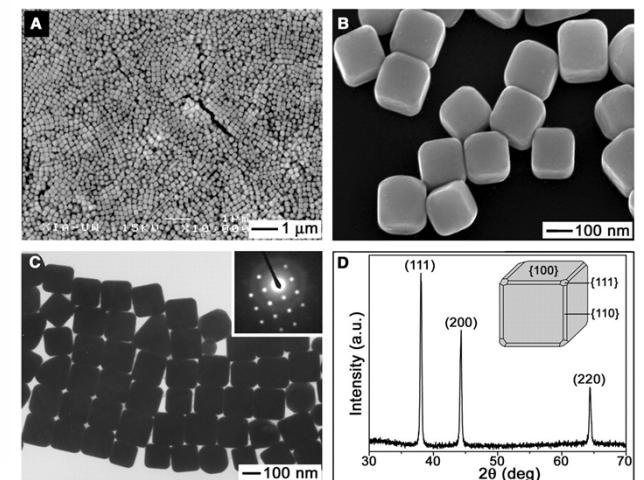
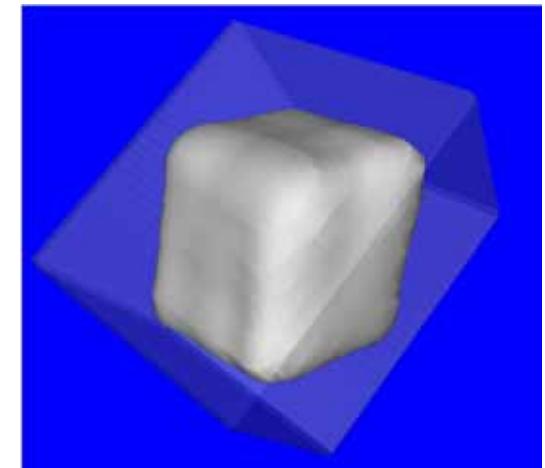
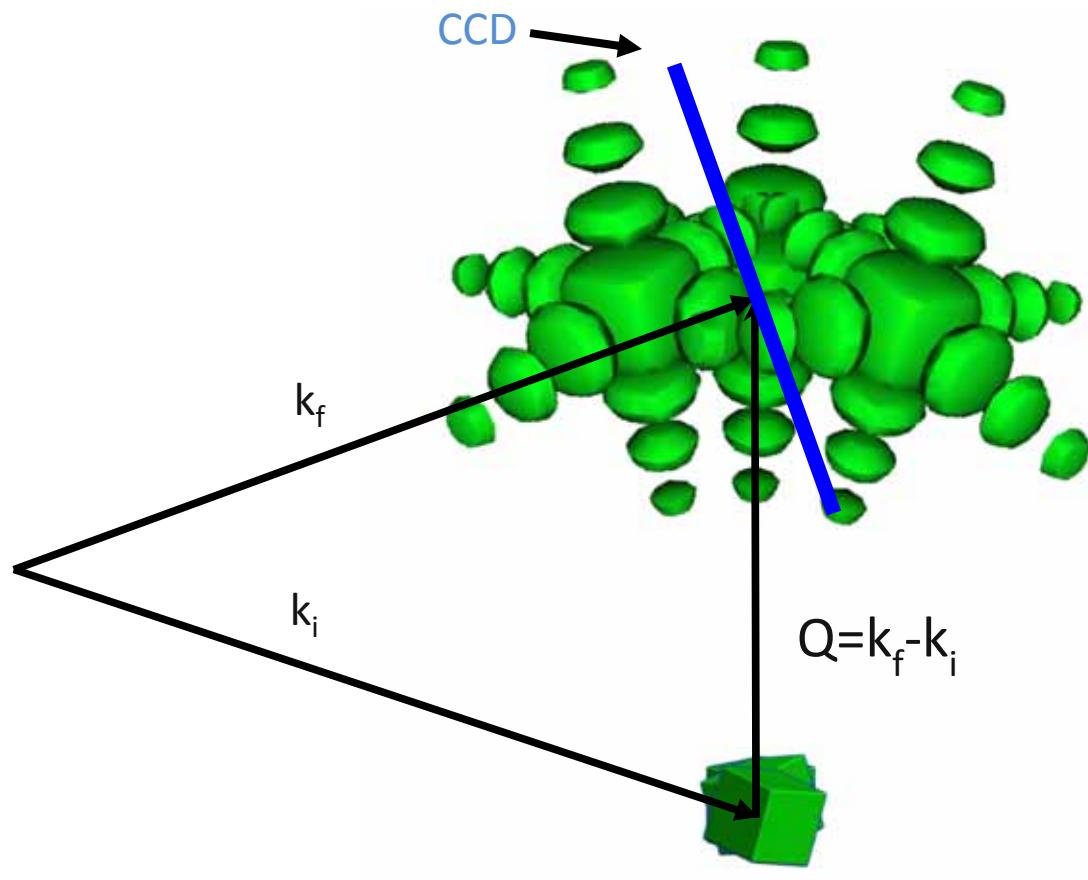


|Fourier Transform|²



Measuring 3D CXD

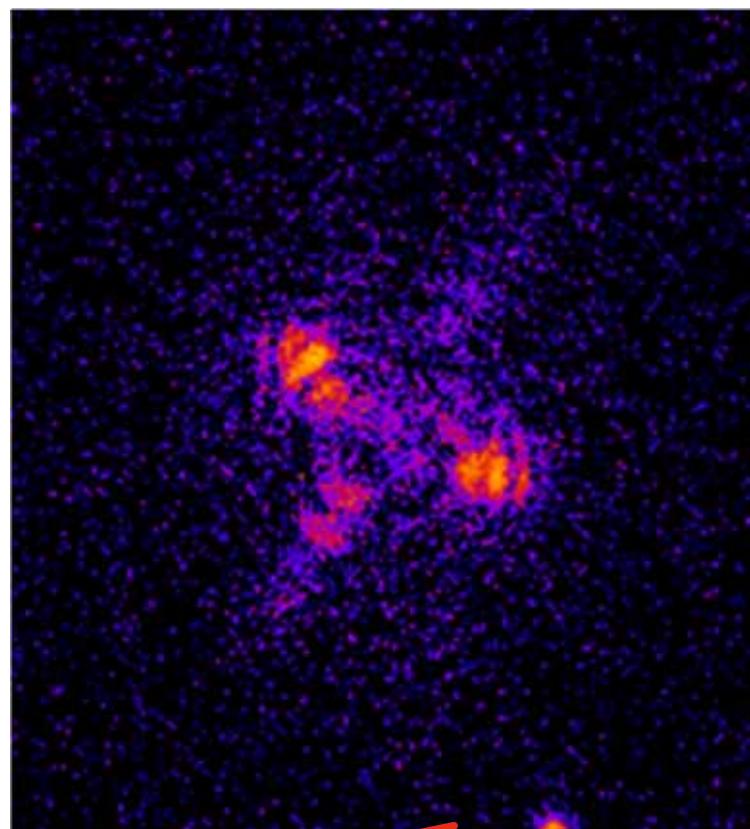
Silver Nano Cube (111)



Yugang Sun and Younan Xia,
Science 298 2177 (2003)



Hi Resolution Imaging?



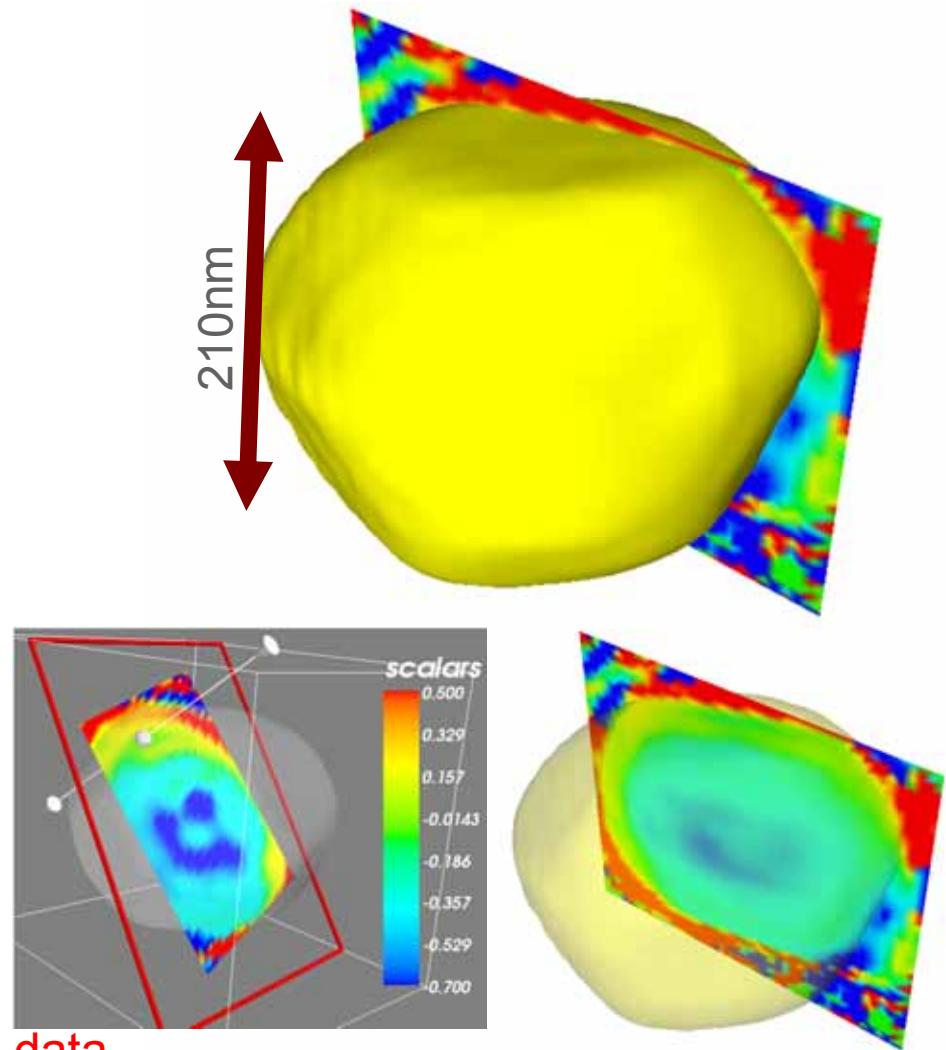
At APS 34-ID-C:

9.25 hours of scanning

0.64 hours of x-ray exposure

~7nm data

210nm



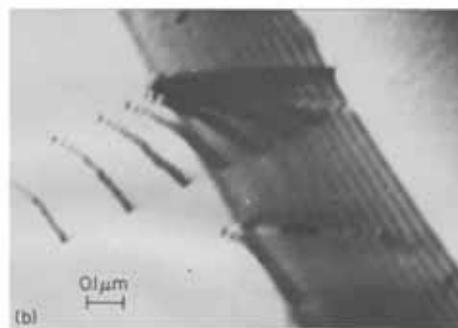
ERL (500x) → 10sec?

http://www.jwave.vt.edu/~rkriz/Projects/create_color_table/color_07.pdf



Slow Dynamics?

- 10 seconds is “almost” static on the scale of hours.
 - Grain Growth (annealing twins in fcc metals)
 - Defect annealing
 - Domain evolution
 - Surface Melting
 - Equilibrium Crystal Shapes

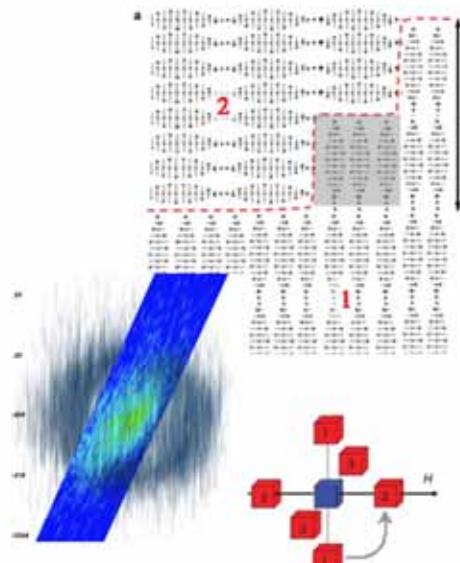
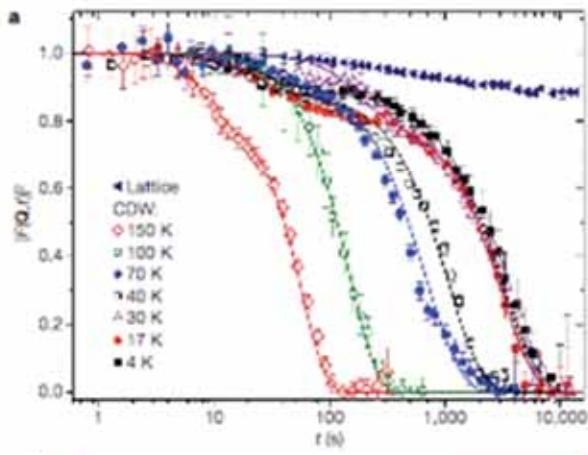


Meyers & Murr,
Acta Metallurgica (1977)

Grain boundary precipitates
in Ni superalloy

Courtesy of Jim Stubbins UIUC

Charge Density wave in Cr



J. C. HEYRAUD and J. J. METOIS
Acta Metallurgica (1980)

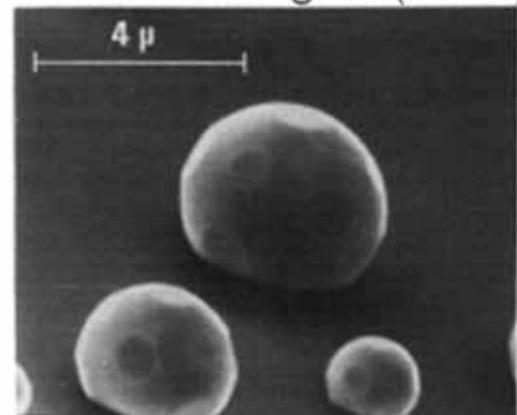
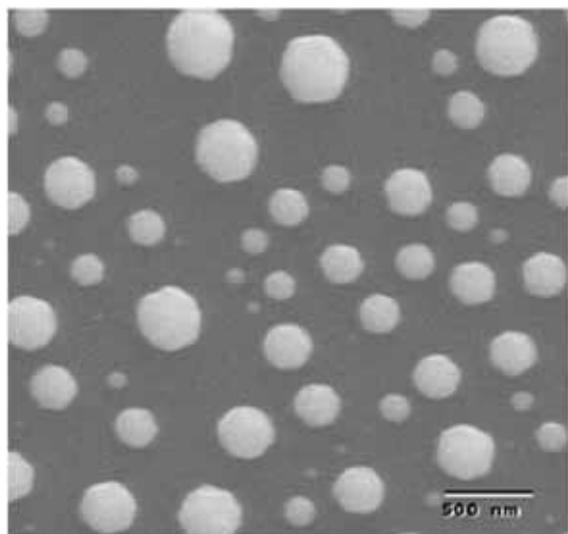
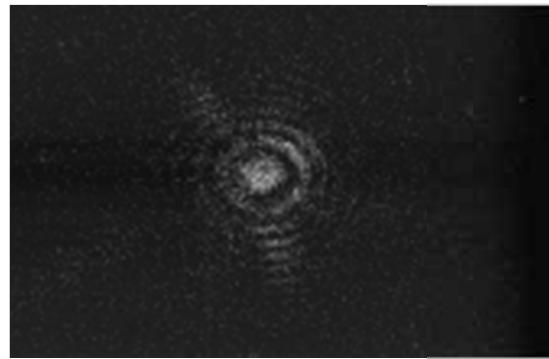


Fig. 2. Equilibrium shape of gold crystallites on graphite obtained after 70 h at 1273 K. Pressure $\sim 10^{-9}$ torr.

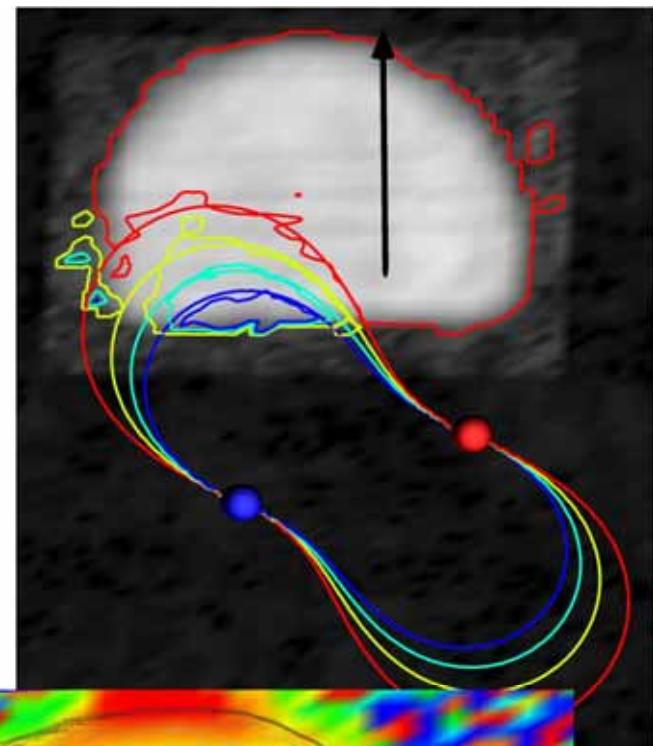
3D Reconstruction of Lead



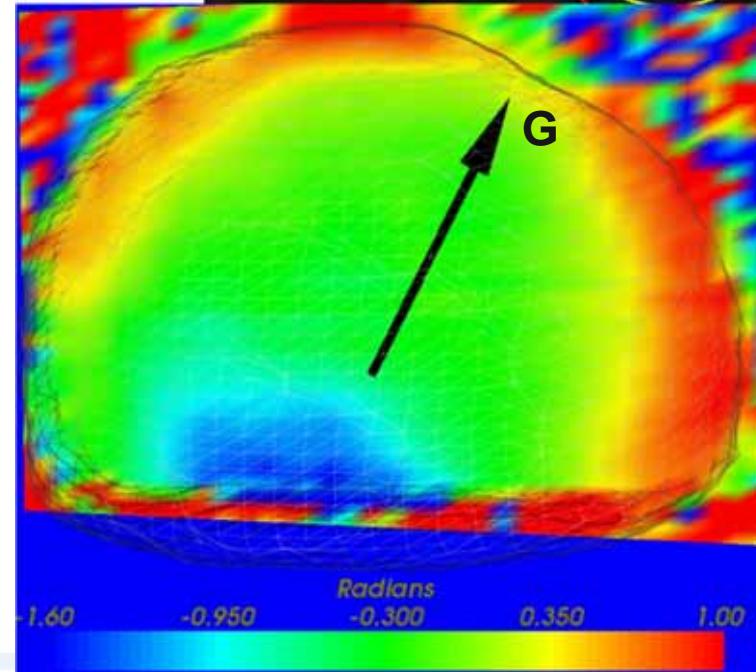
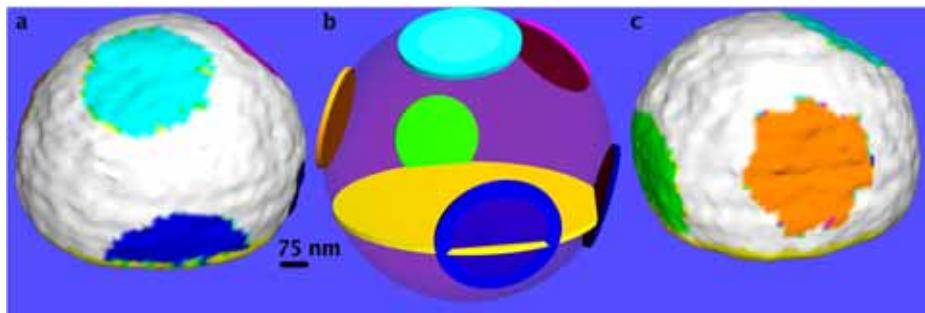
(111) Bragg spot



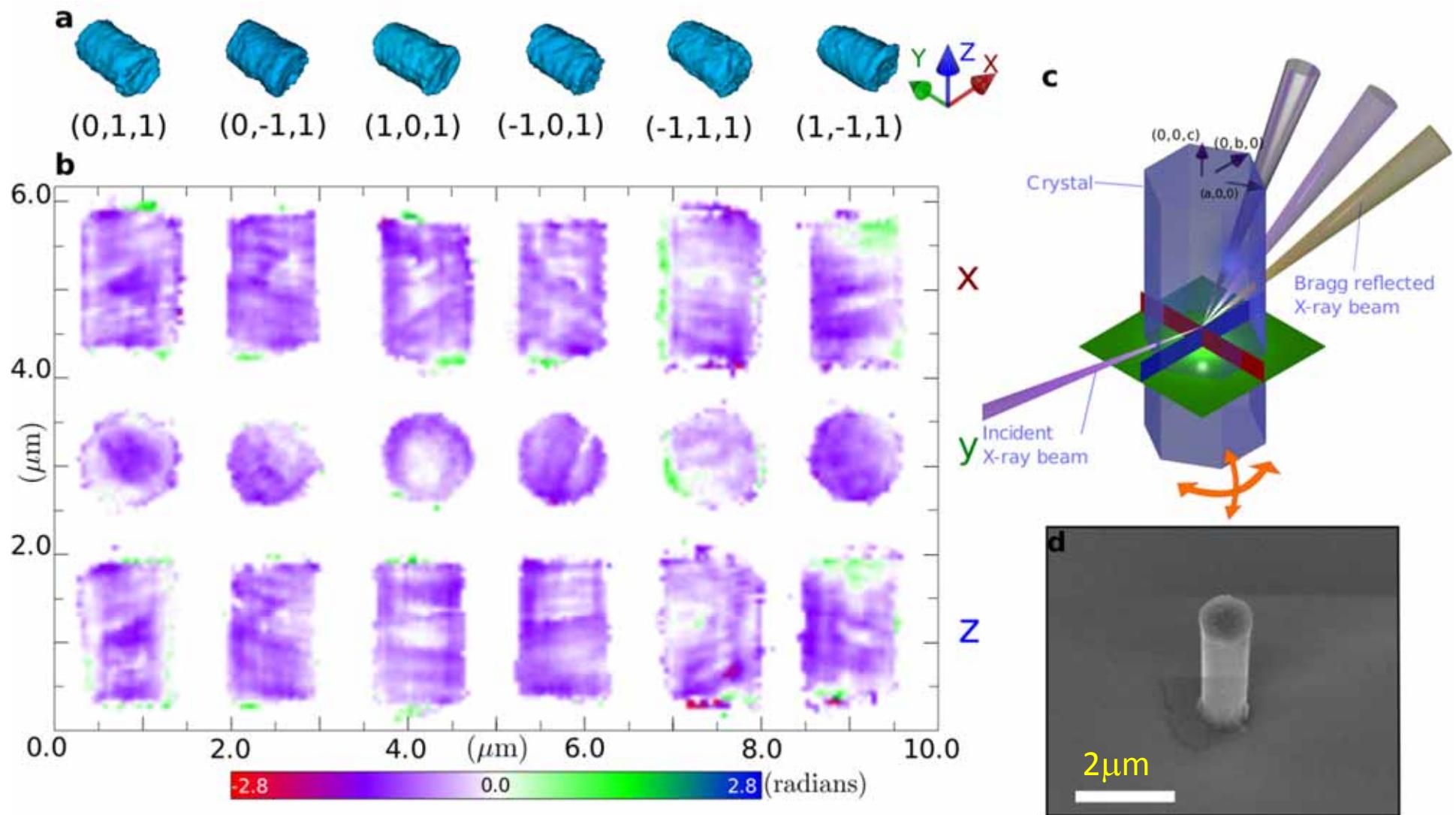
7.9 hour scan
2.1 hour x-ray exposure



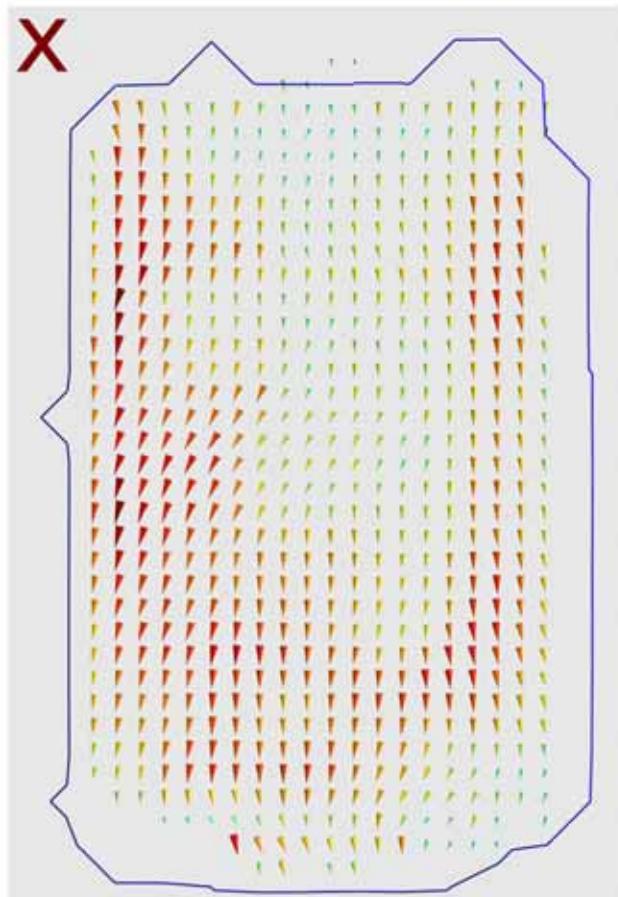
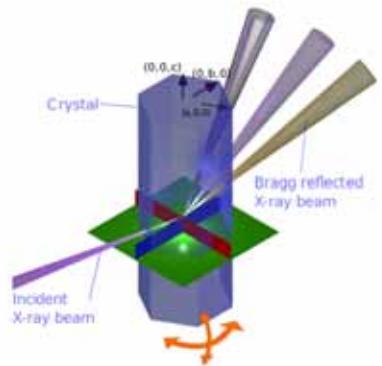
Nature, Vol. 442 p. 63 (July 6 2006)
PhysRevB.76.115425 (2007)



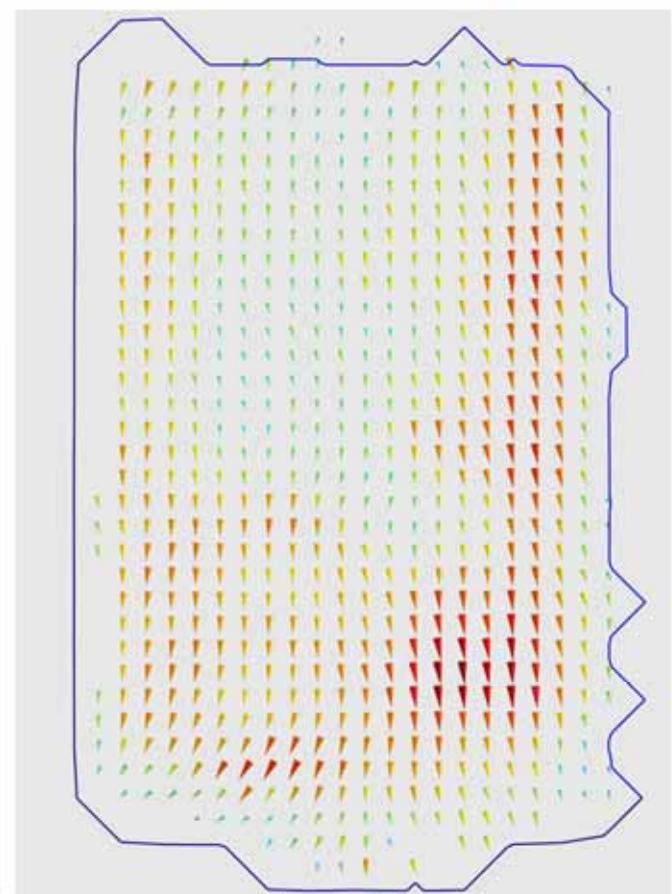
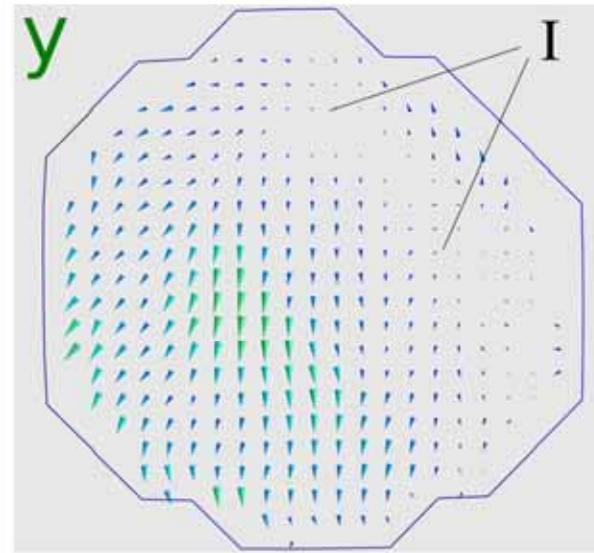
3D Strain Map in ZnO



3D Strain Map in ZnO



$$u_j = \xi_{ji} q_{ki} \phi_k; \quad \xi_{ji} = (q_{kj} q_{ki})^{-1}$$

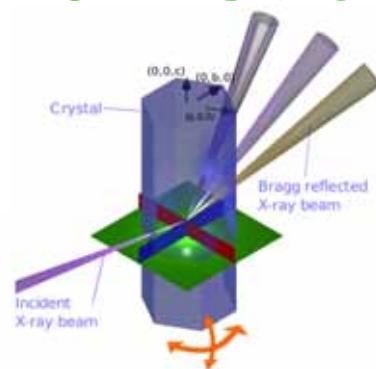


0.0 0.09 nm

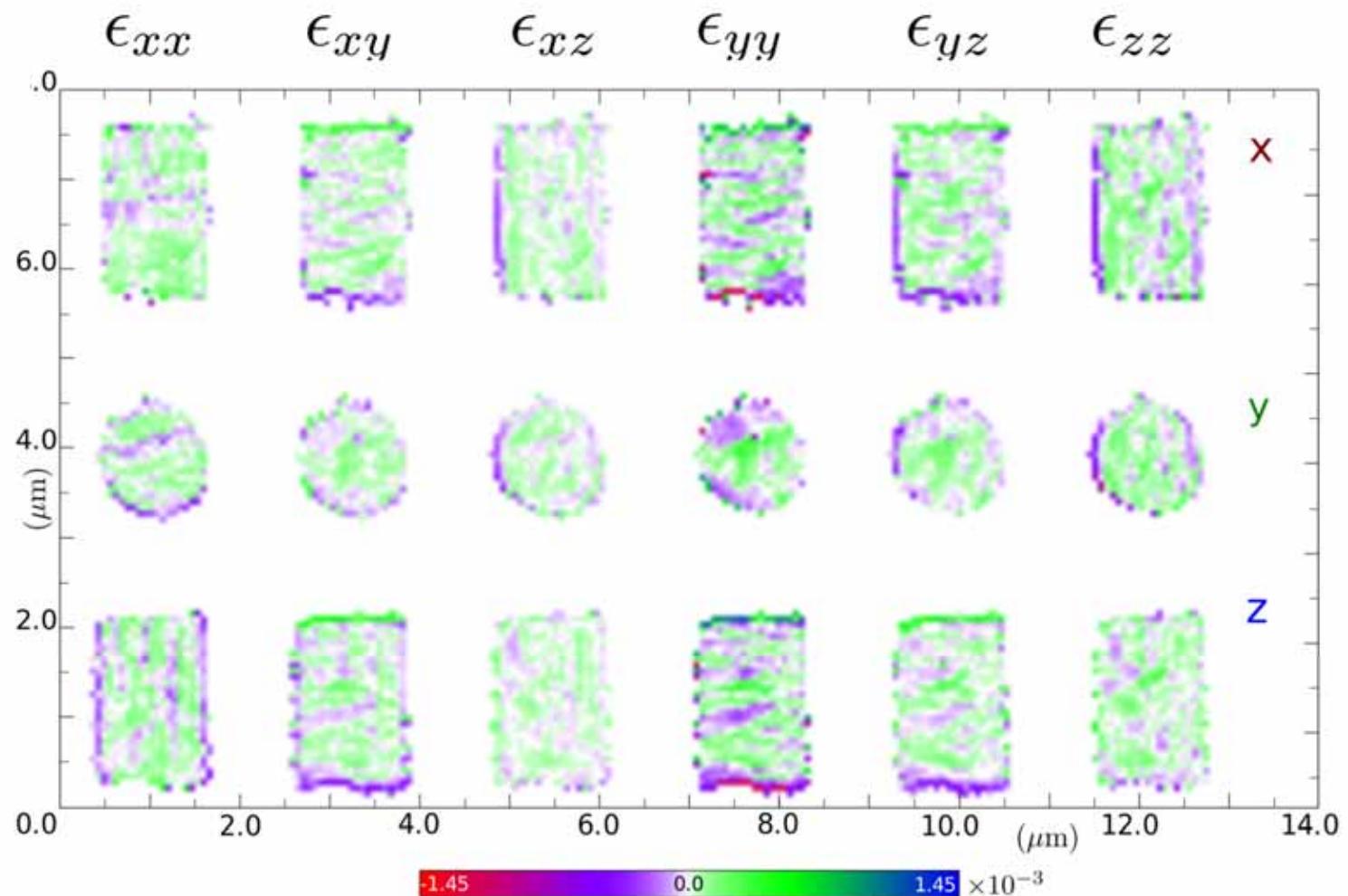
Nature Materials 9, 120 - 124 (2010)



3D Strain Map in ZnO

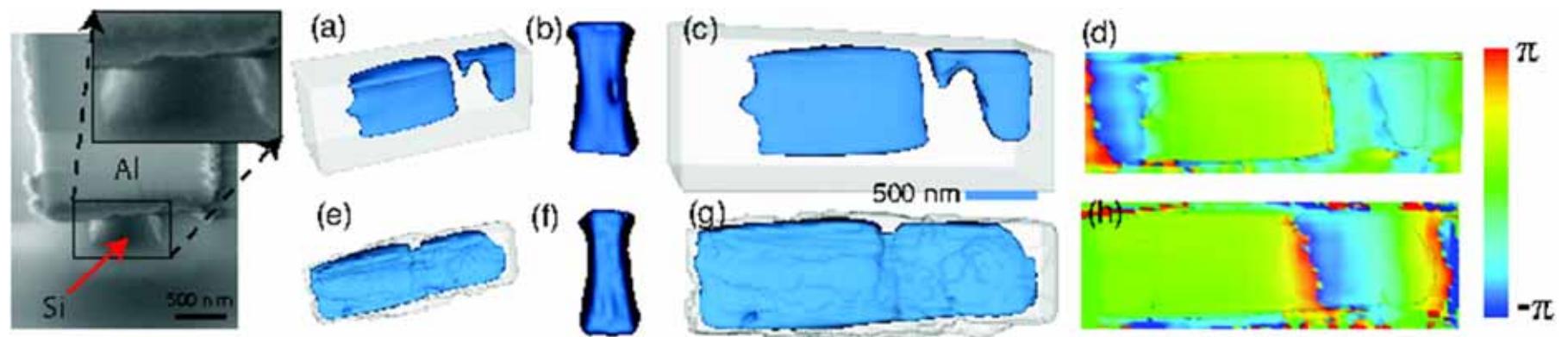
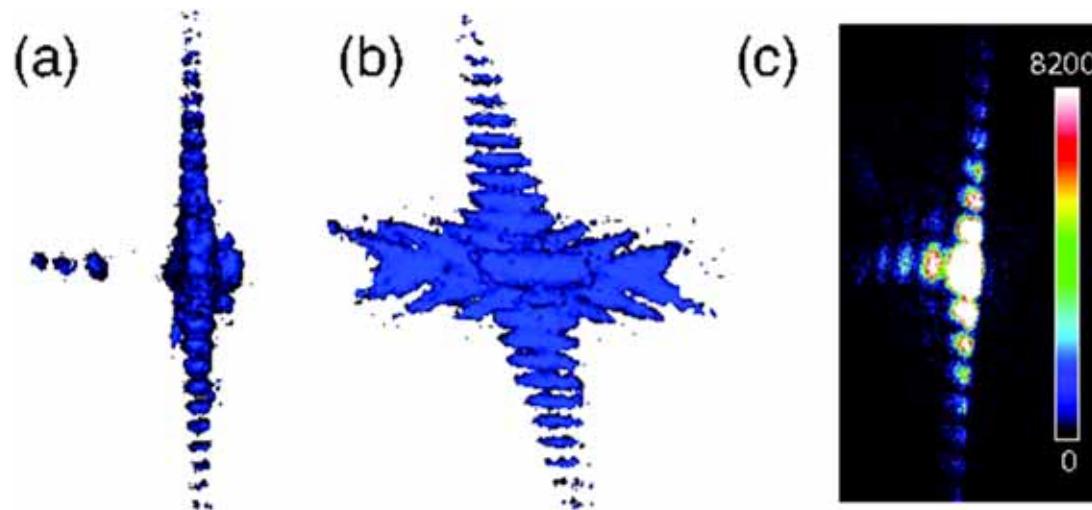


$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right), \quad \tau_{ij} = \left(\frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j} \right)$$



Highly Strained crystals?

Silicon on Insulator (SOI)
Reactive Ion Etched from a thin film
to form nanostructured “bars” or “wires”



Huang et al. (submitted PRB)



Codes?

<http://code.google.com/p/pythonphasing/>

The screenshot shows the Google Code interface for the 'pythonphasing' project. At the top, there's a navigation bar with links like 'Project Home', 'Downloads', 'Wiki', 'Issues', 'Source', and 'Administer'. Below the navigation bar, there's a 'Summary' section with links for 'Updates' and 'People'. A tip message for project owners is displayed: 'Tip: Project owners, see our [Getting Started](#) guide for steps to configure your project.' On the left, there's a sidebar with sections for 'Project Information' (including 'Star project', 'Activity' marked as 'Medium', and 'Project feeds'), 'Code license' (GPLv2), and 'Recent changes' (empty). The main content area contains a brief description of the project: 'A library of phasing codes, and other supporting codes, for inverting CXD to images. These are particularly developed for phasing CXD measured in the vicinity of Bragg spots at APS 34id-c. The majority of the library is written in C and run from python scripts. The C code is wrapped with swig.' It also notes that documentation is basically API docs.

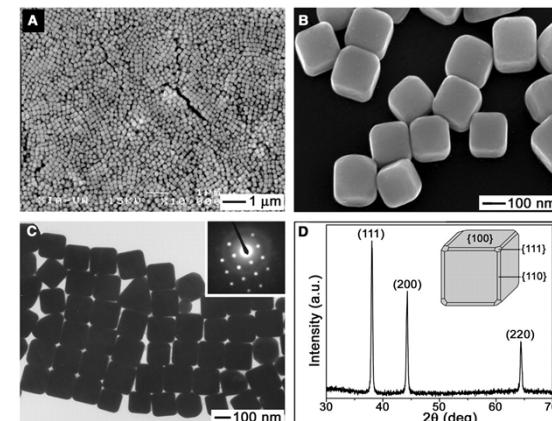
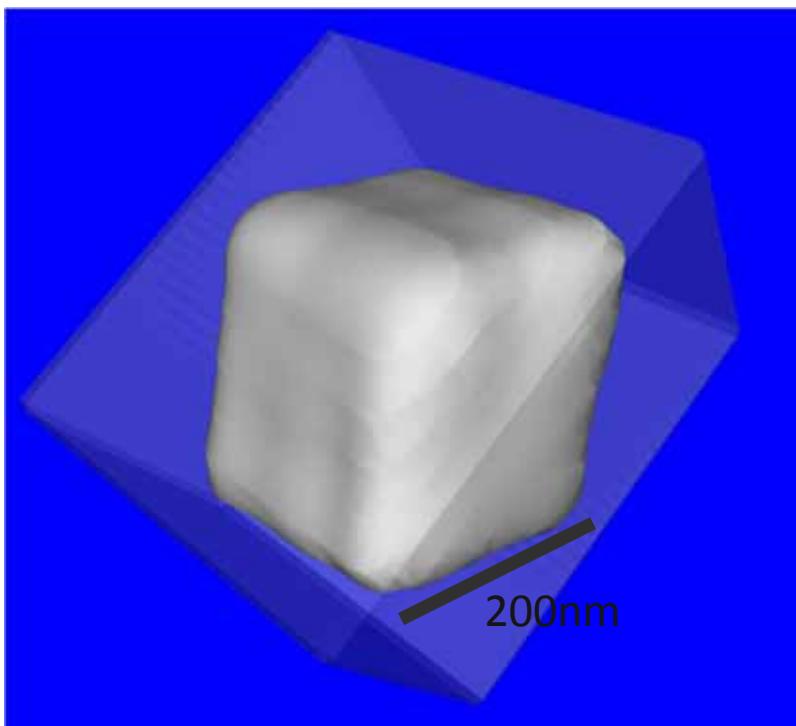
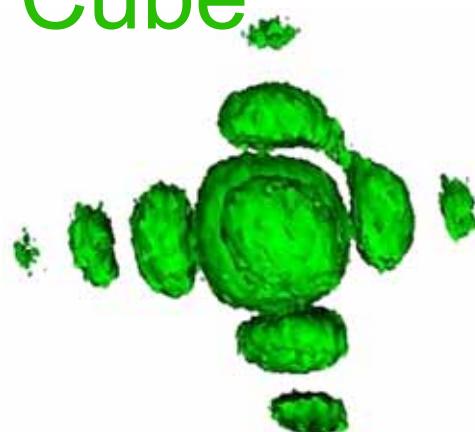
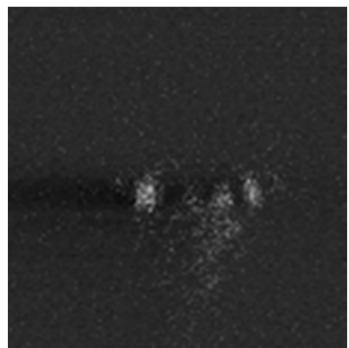
<http://code.google.com/p/mypythonphasing/>

<http://code.google.com/p/pythonphasing-scripts/>

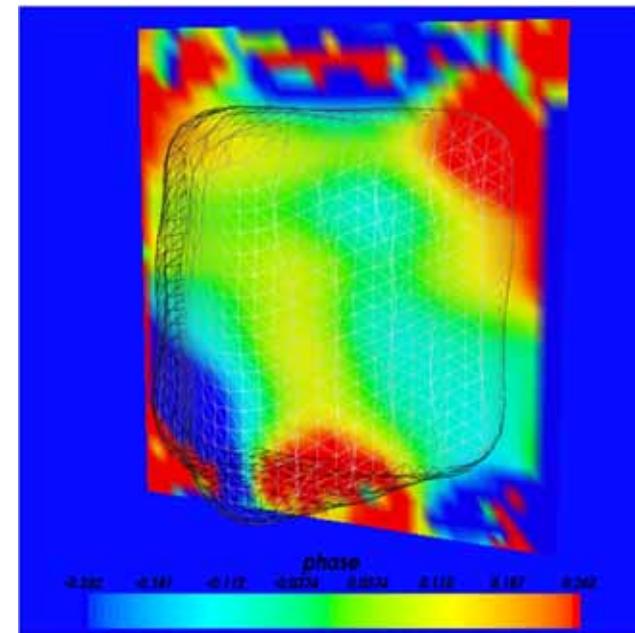
<http://groups.google.com/group/pythonphasing>



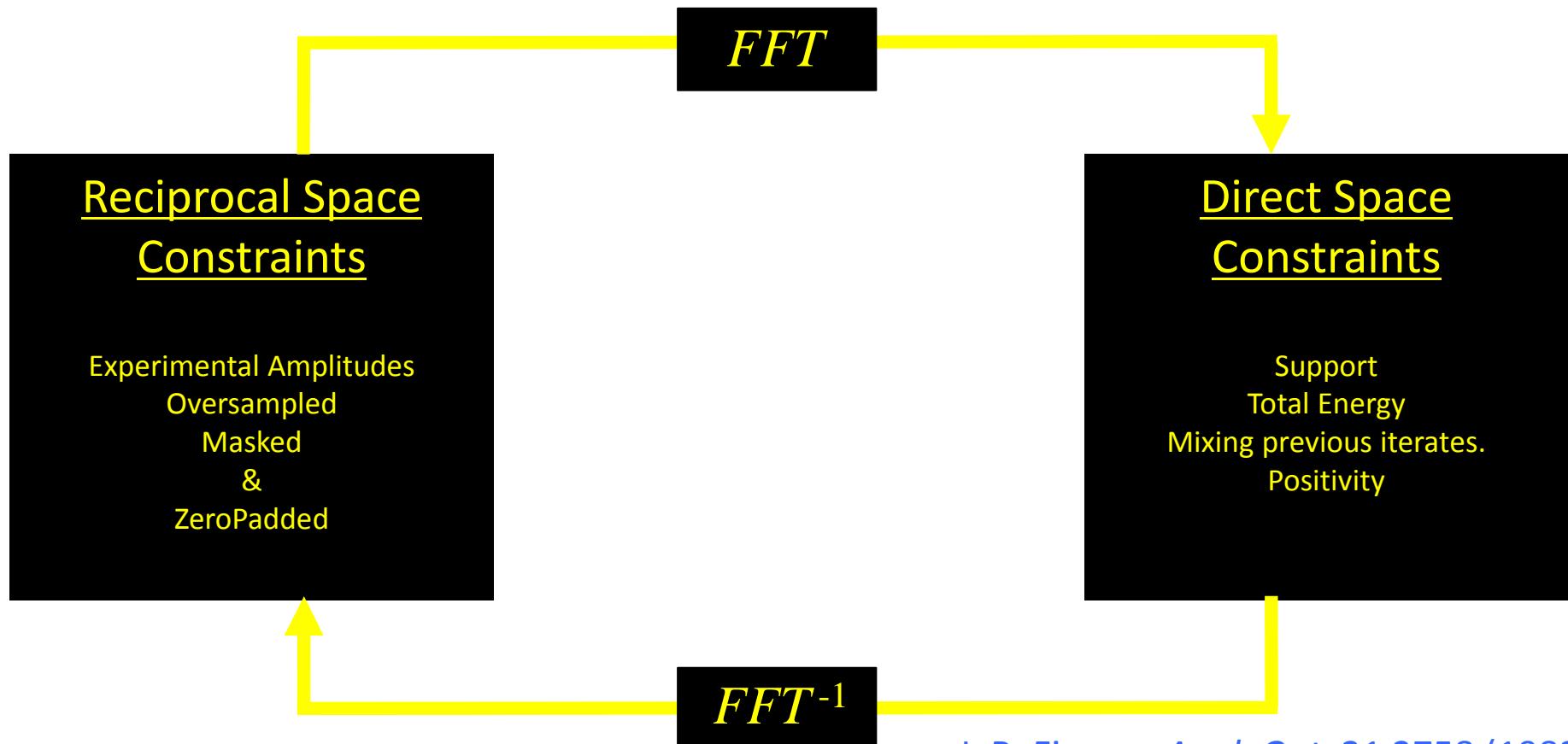
3D Ag Nano Cube



Yugang Sun and Younan Xia,
Science 298 2177 (2003)



Input Output Algorithms



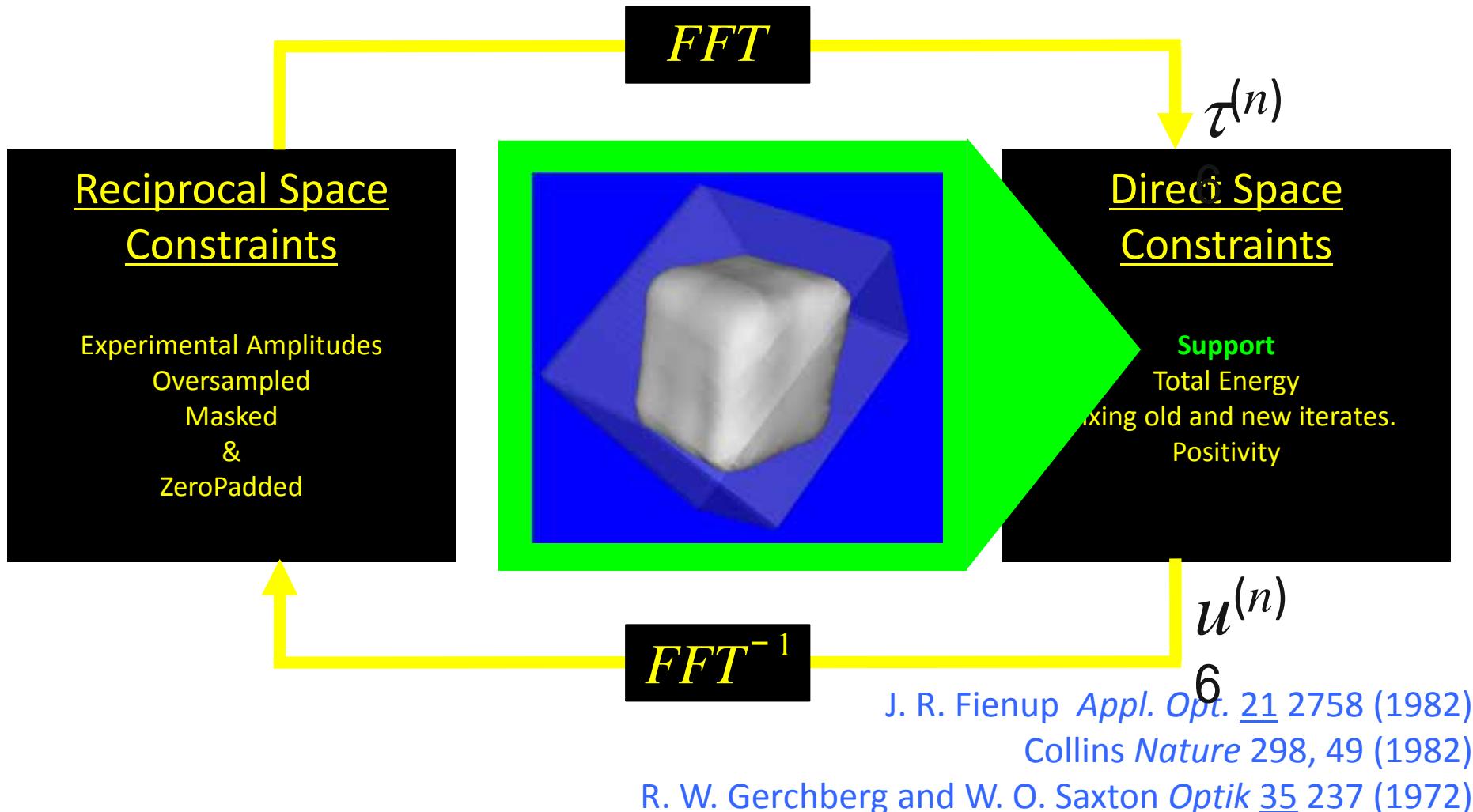
J. R. Fienup *Appl. Opt.* 21 2758 (1982)

Collins *Nature* 298, 49 (1982)

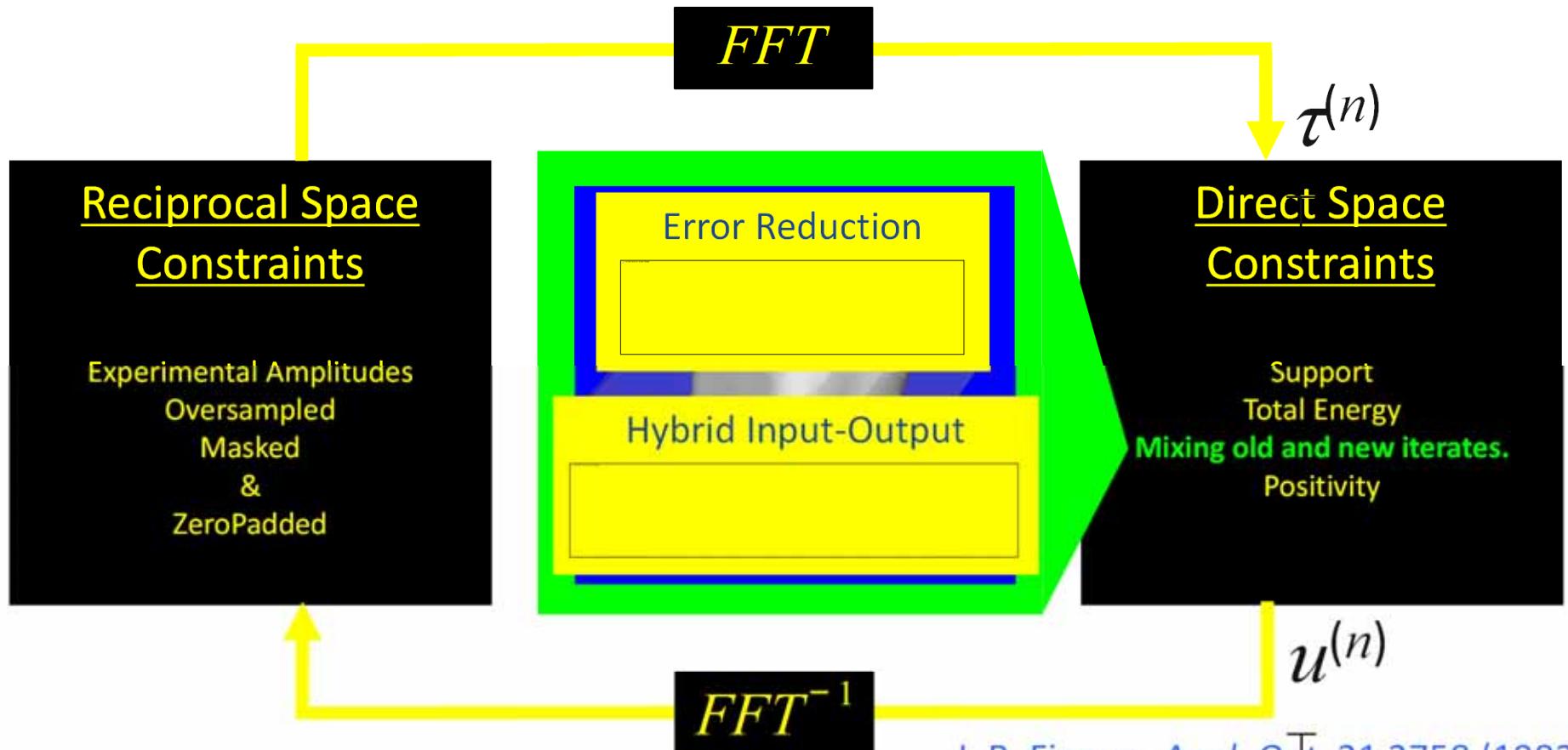
R. W. Gerchberg and W. O. Saxton *Optik* 35 237 (1972)



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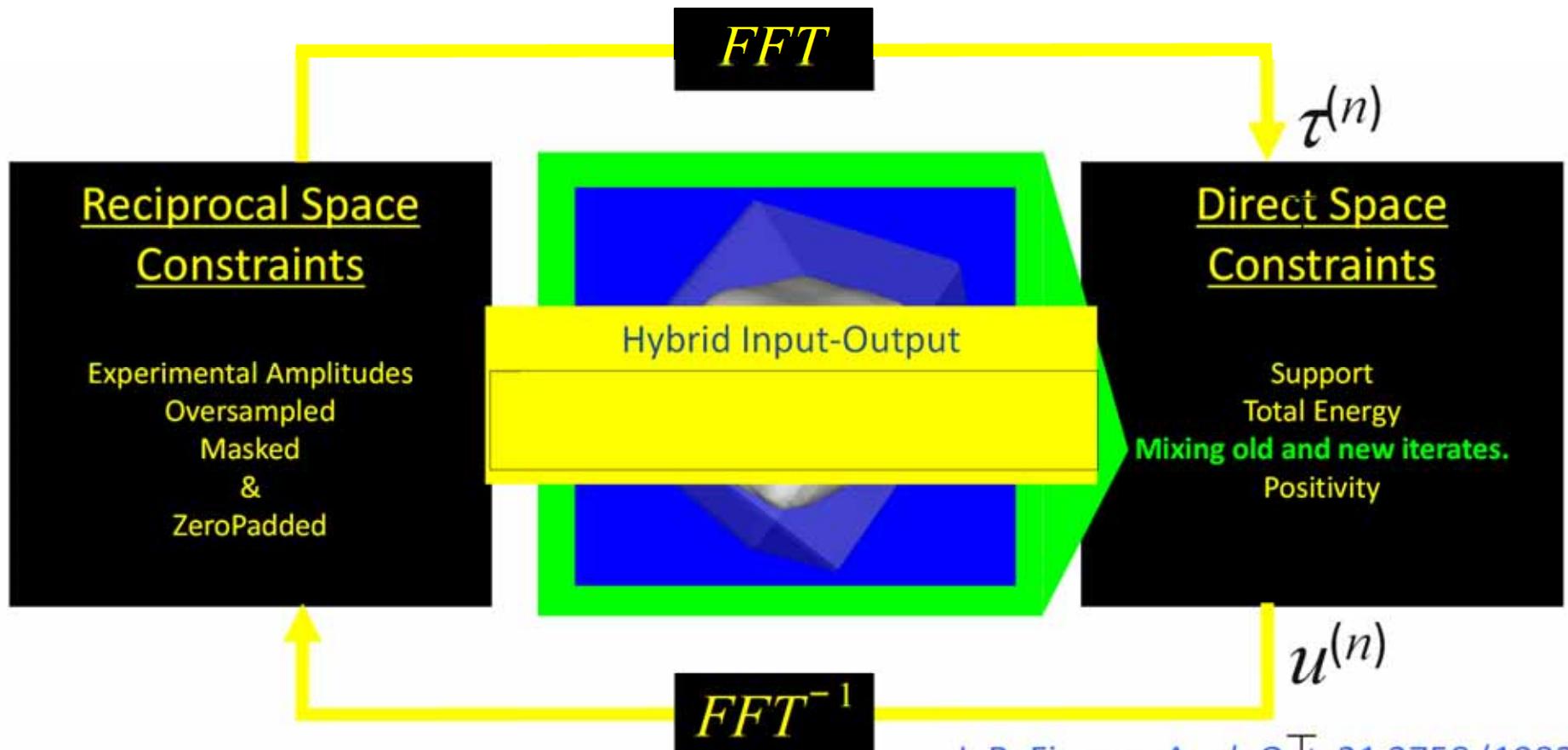
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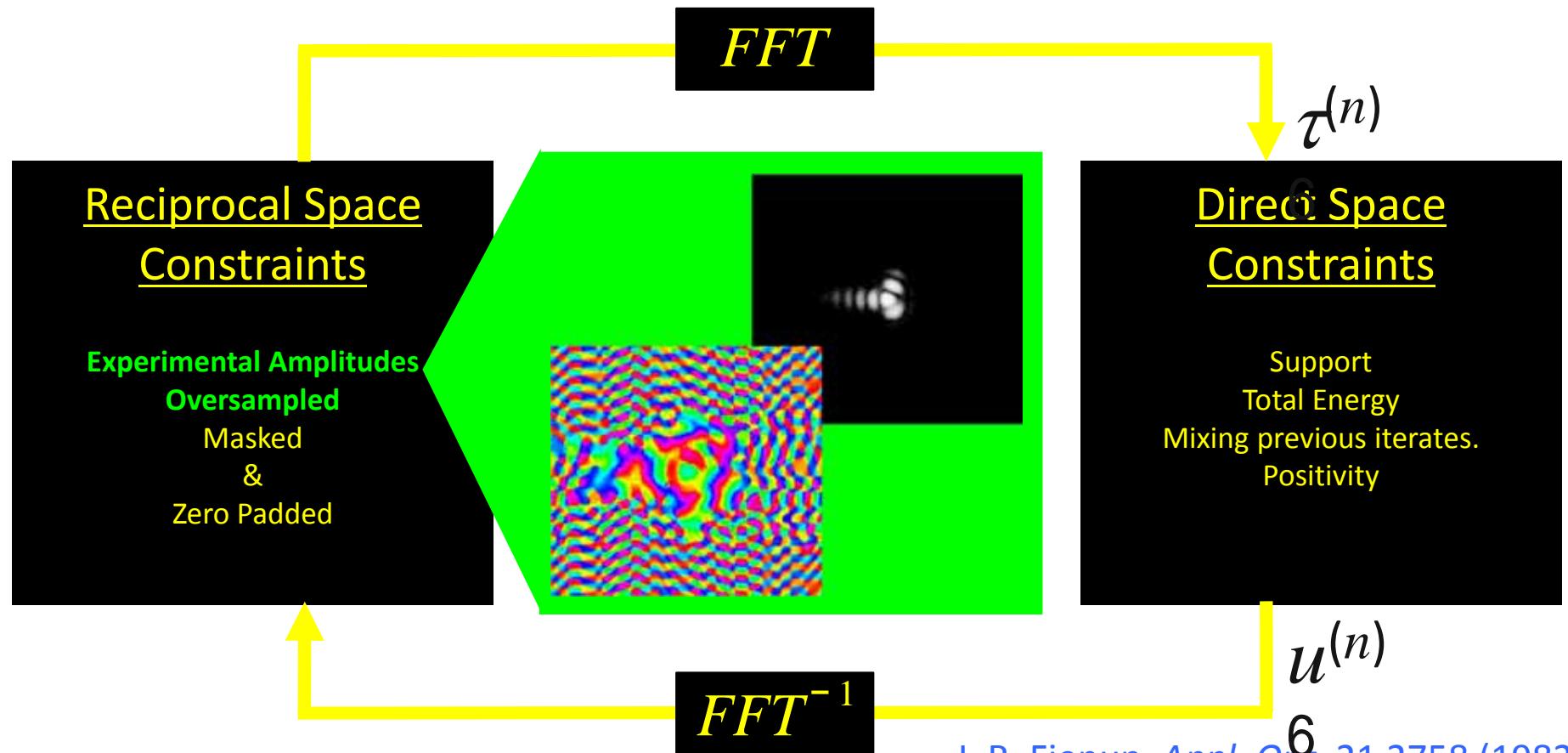
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