Bragg Coherent Diffractive Imaging with Even More Coherence

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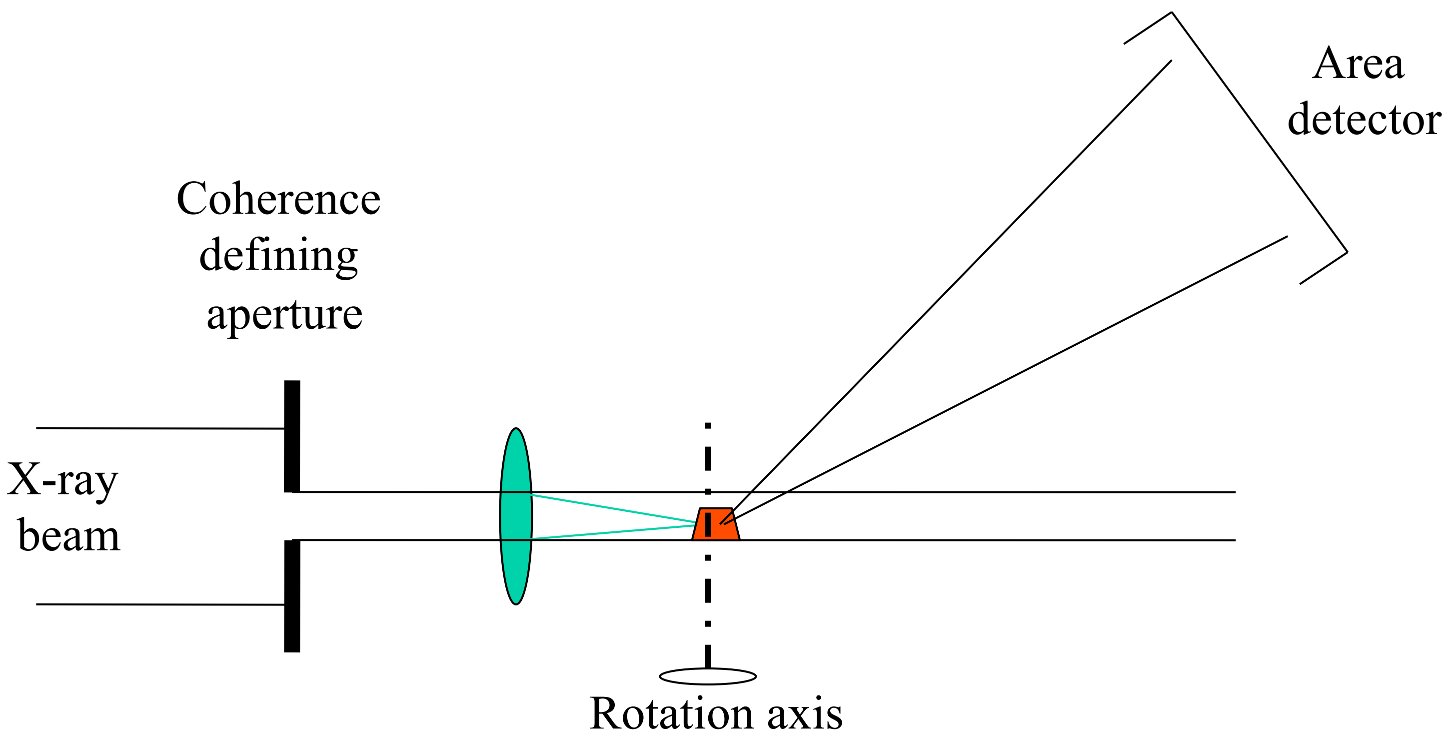
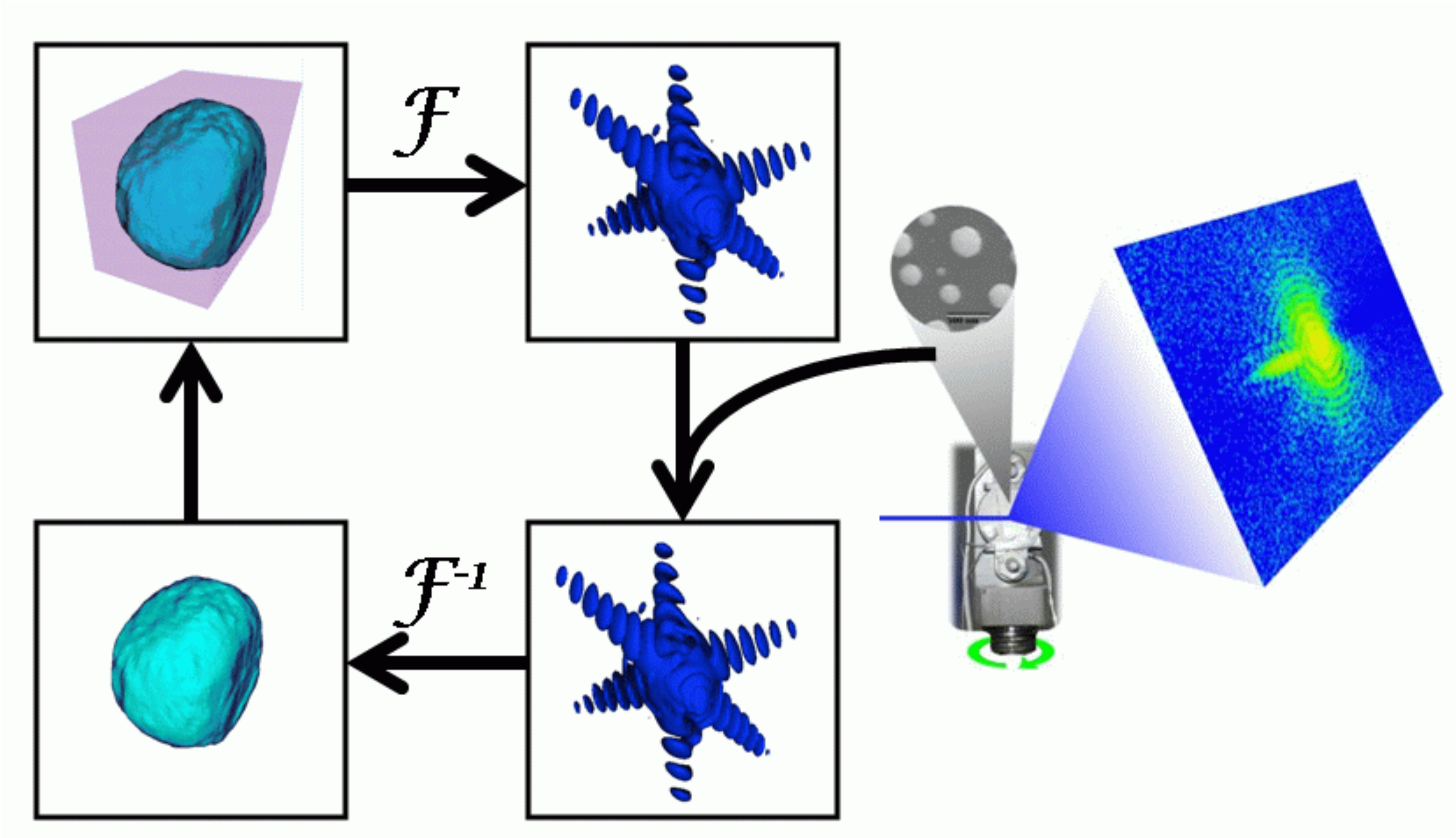
Outline

- Complex density in BCDI images
- Phase domains in $La_{0.5}Ca_{0.5}MnO_3$
- Phase Domain Structures
- Memory effects in $La_{1.875}Ba_{0.125}CuO_4$
- Domain Walls
- Role of Ptychography

Bragg Coherent Diffraction Imaging “Lensless” X-ray Microscope, 2003



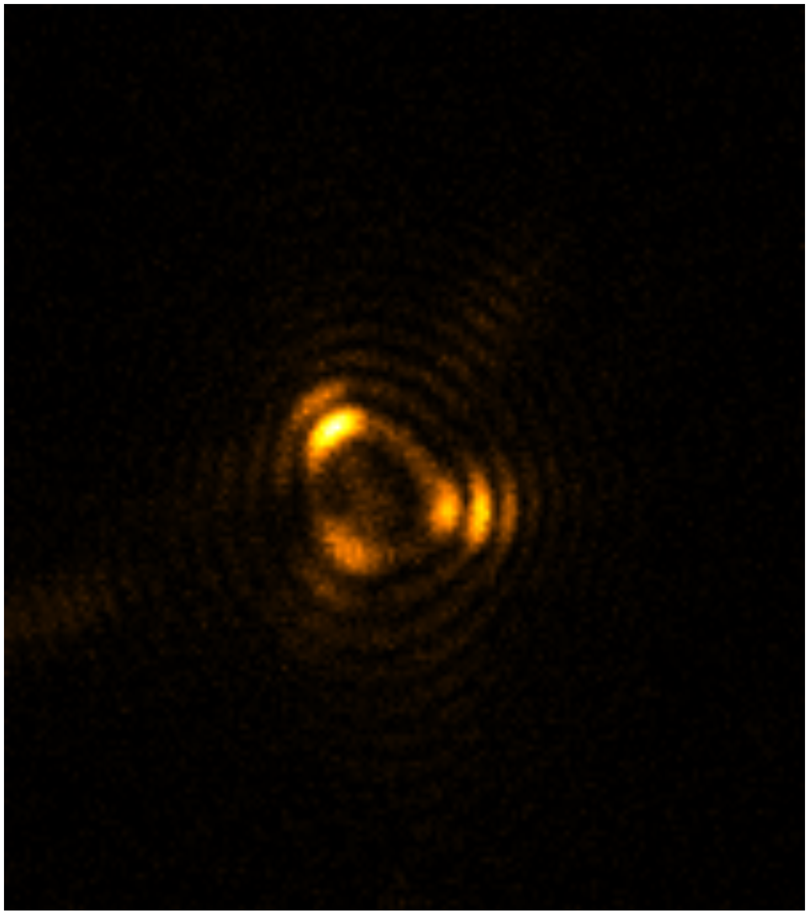
Generic “Error Reduction” method

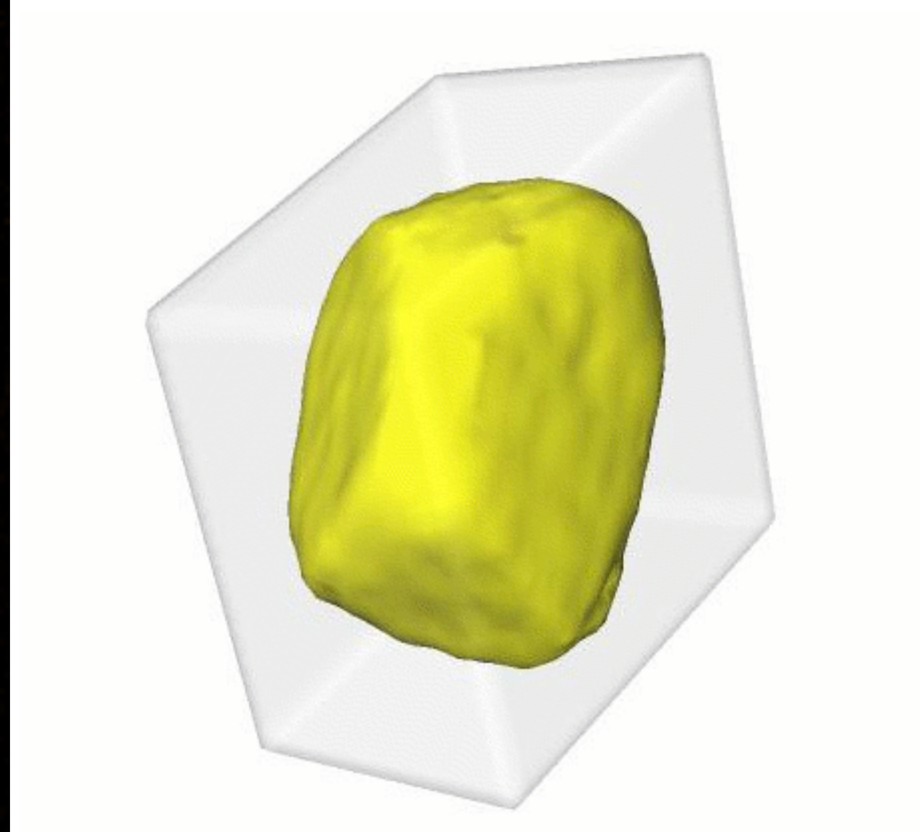


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

Gold nanocrystal reconstruction

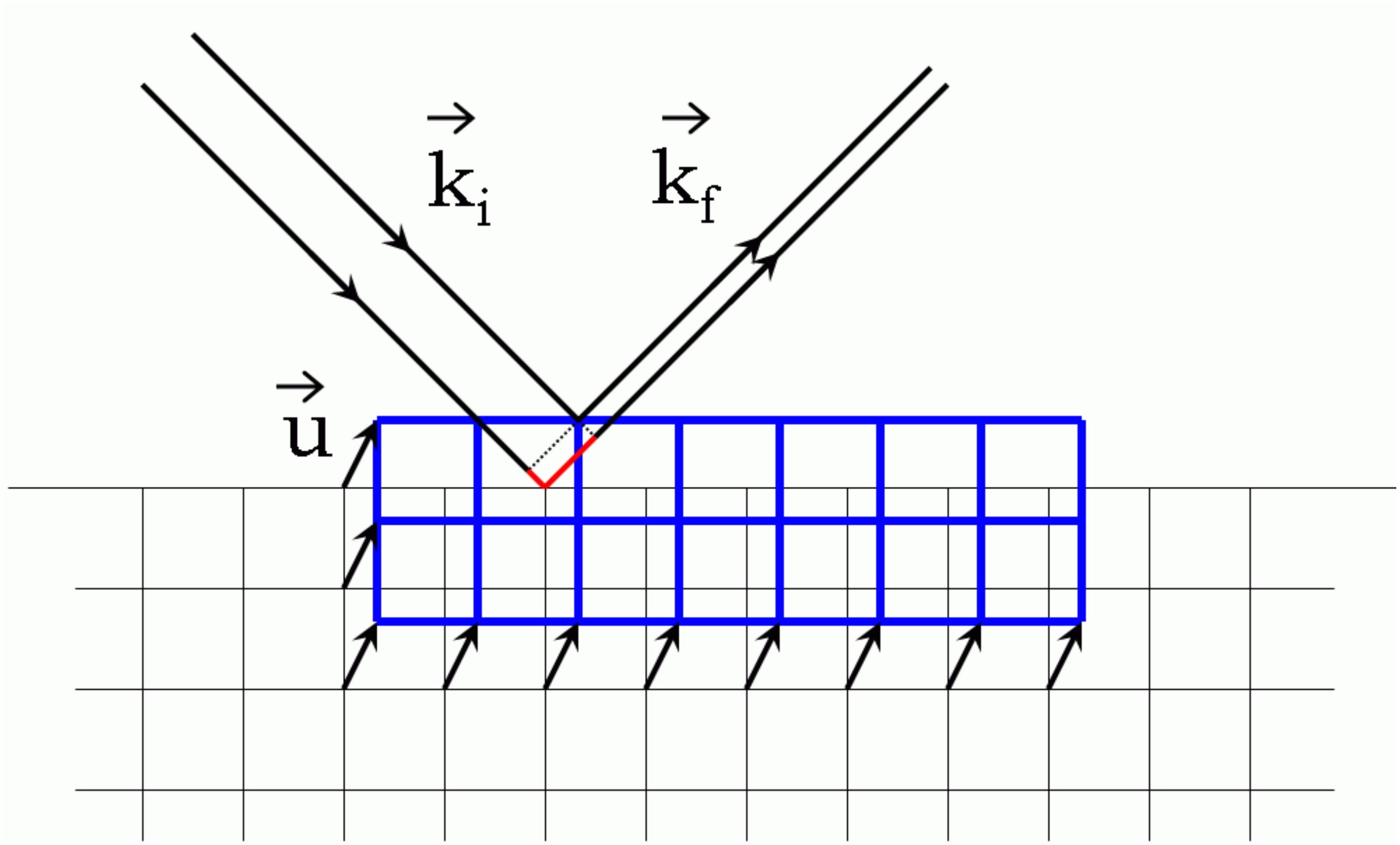
showing support used for 20 HIO followed by 10 ER





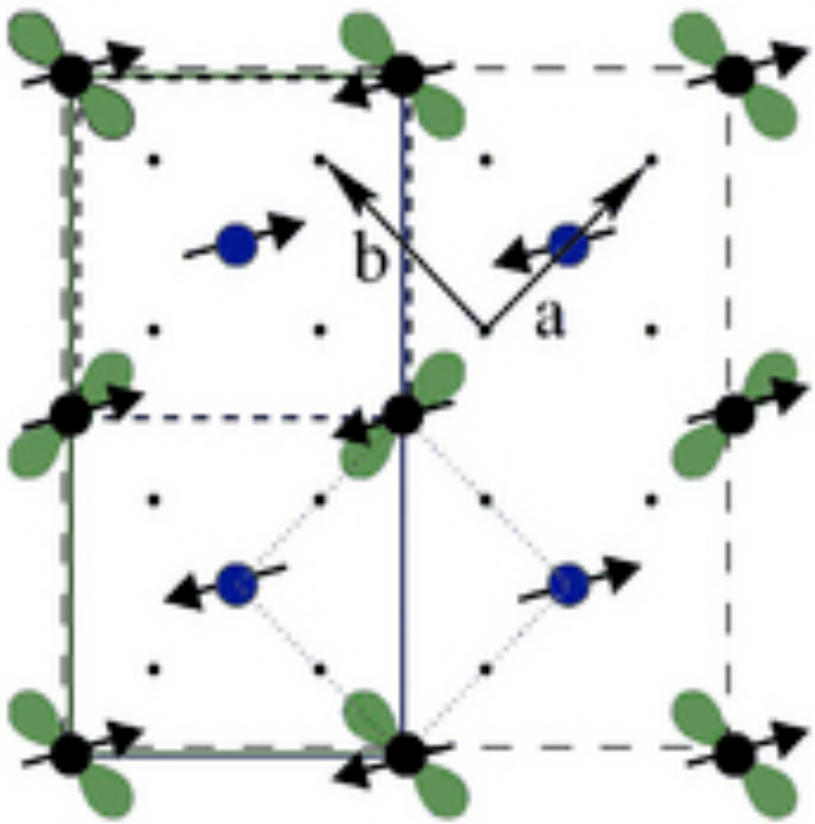
Sensitivity to strain

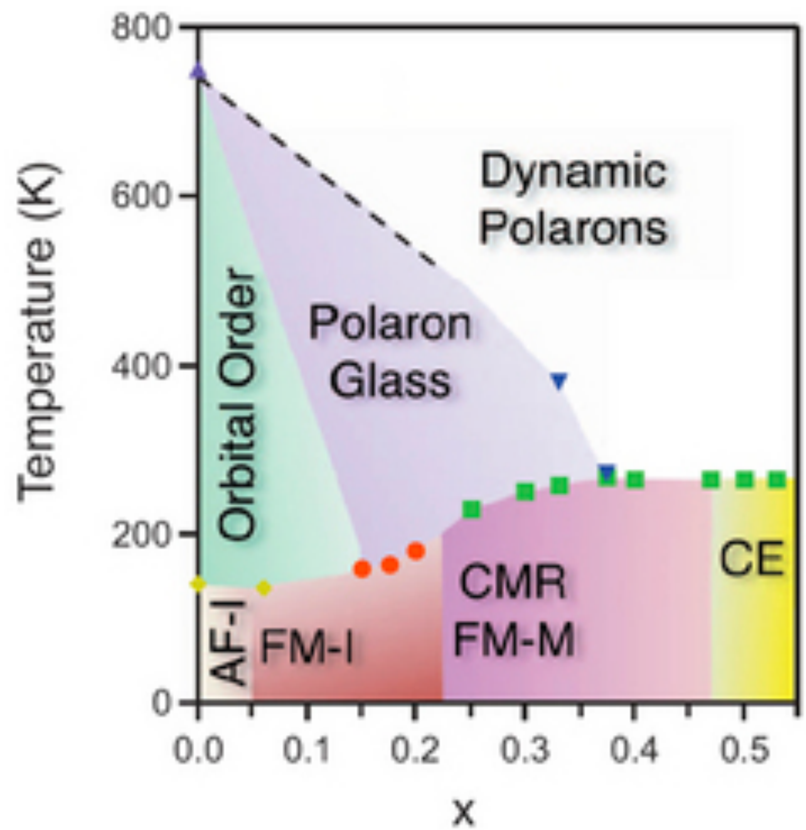
$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$



LCMO $La_{1-x}Ca_xMnO_3$

http://www.psi.ch/swissfel/correlated-electron-phases

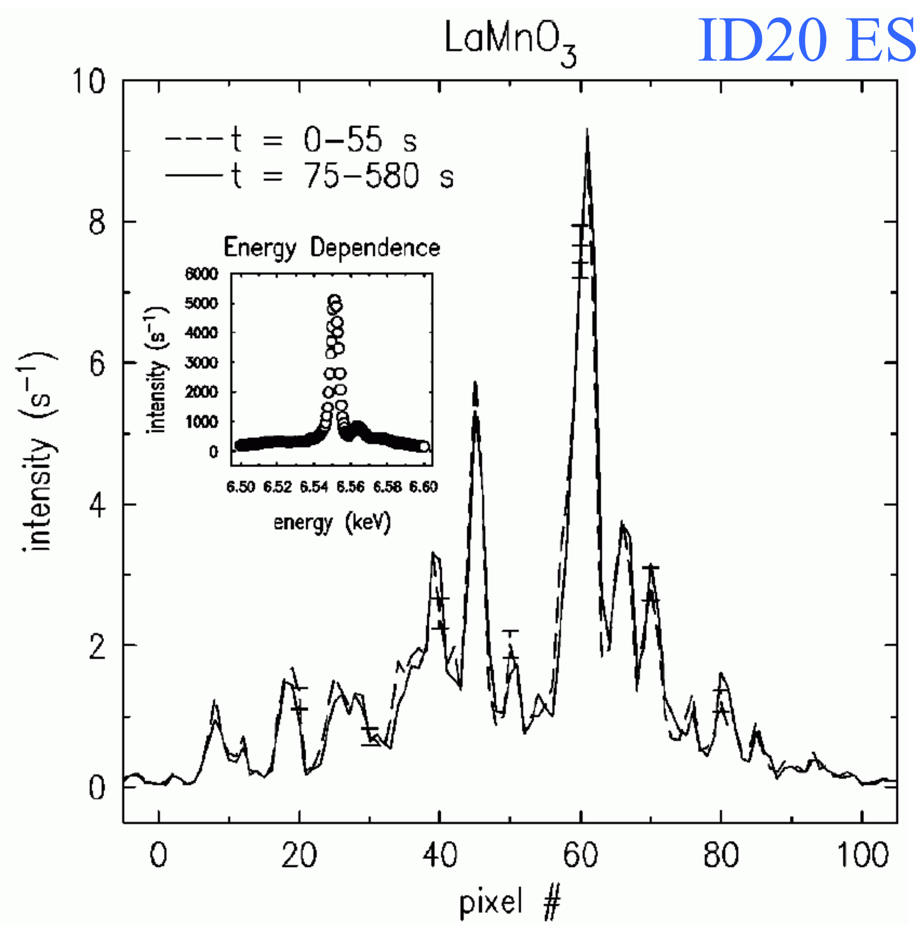


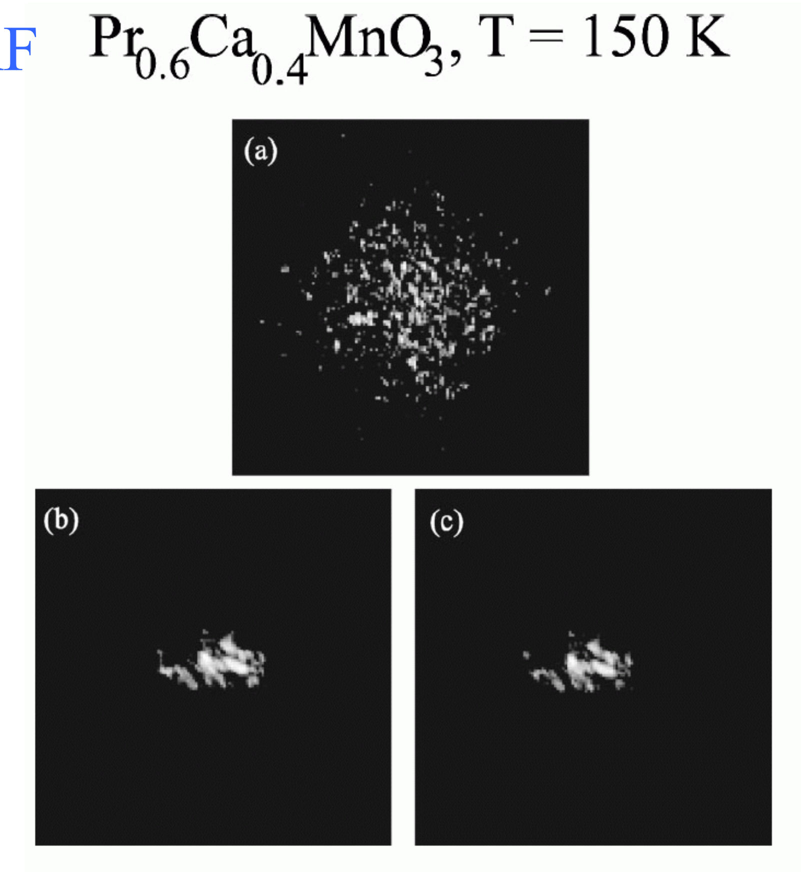


$LaMnO_3$ and $Pr_{0.6}Ca_{0.4}MnO_3$ speckle

C. S. Nelson, J. P. Hill, Doon Gibbs, F. Yakhou, F. Livet, Y. Tomioka, T. Kimura and Y. Tokura, PRB 66 134412 (2002)

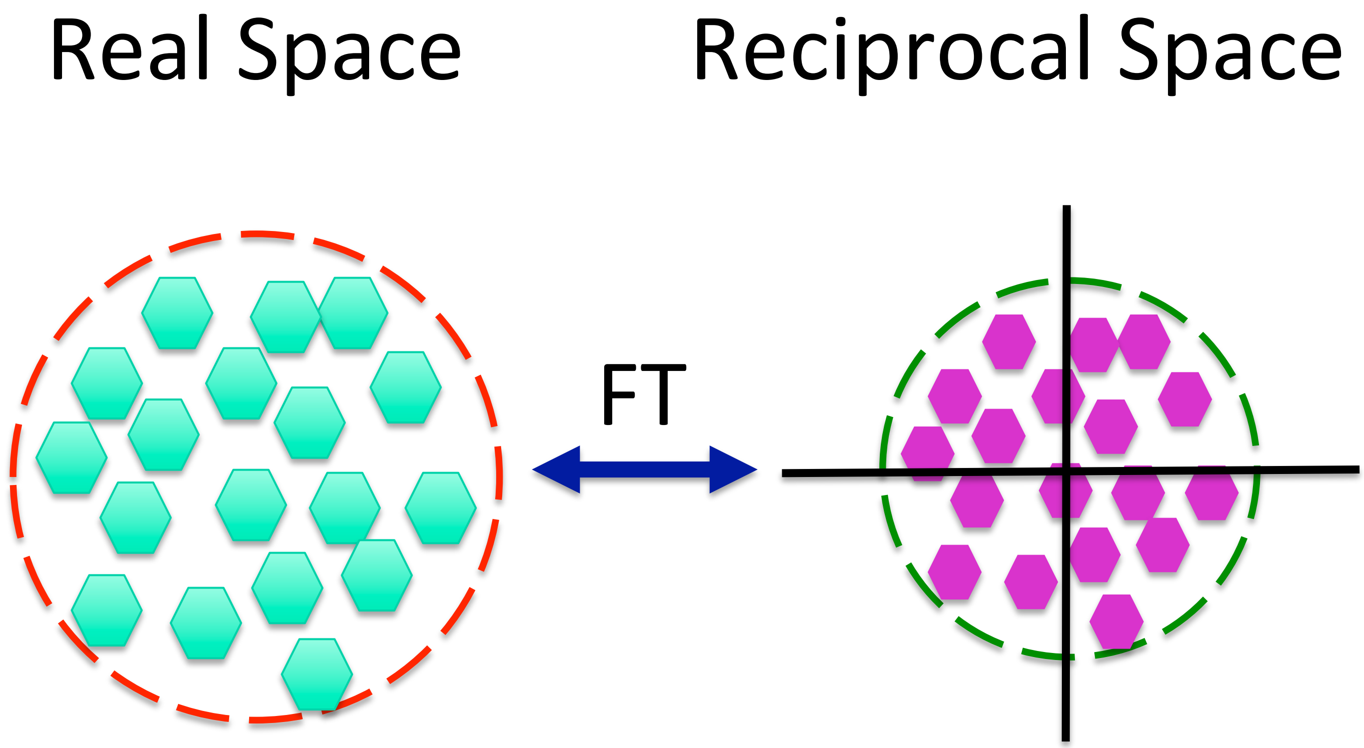
ID20 ESRF





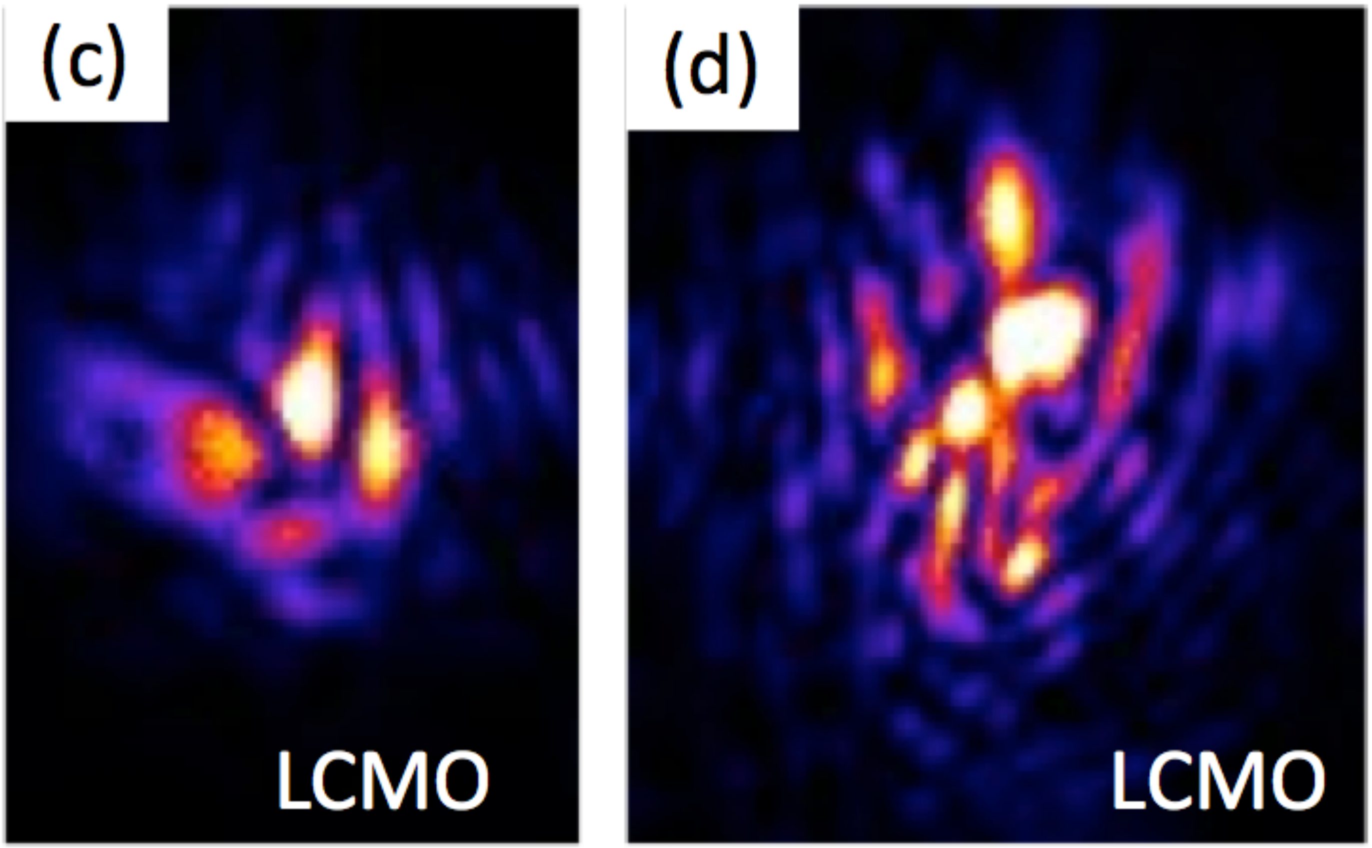
. Images of orbital (a) and charge (b), (c) order

Domain structures give speckled diffraction



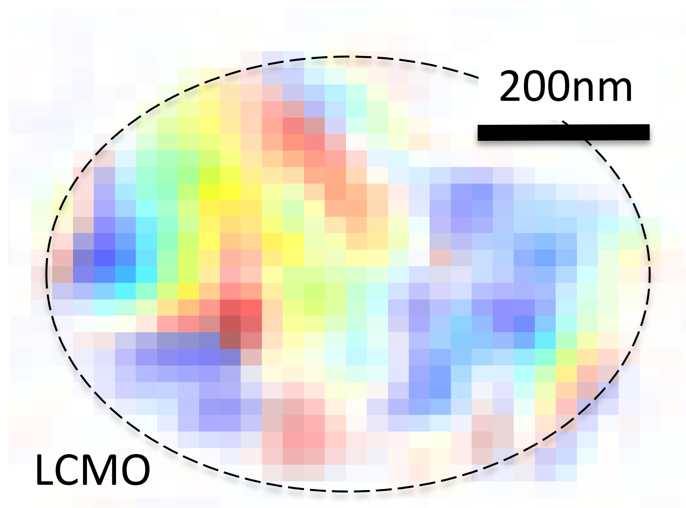
BCDI from $La_{0.5}Ca_{0.5}MnO_3$

LCMO-500, Ian McNulty and Jon Logan, 34-ID-C Argonne



BCDI from $La_{0.5}Ca_{0.5}MnO_3$

Ian McNulty and Jon Logan, 34-ID-C Argonne



LCMO_500_test31.png

TEM of twins in $La_{0.67}Ca_{0.33}MnO_3$

Q. Chen, J. Tao, J.M. Zuo, J.C.H. Spence, JMR **16** 2959 (2001)

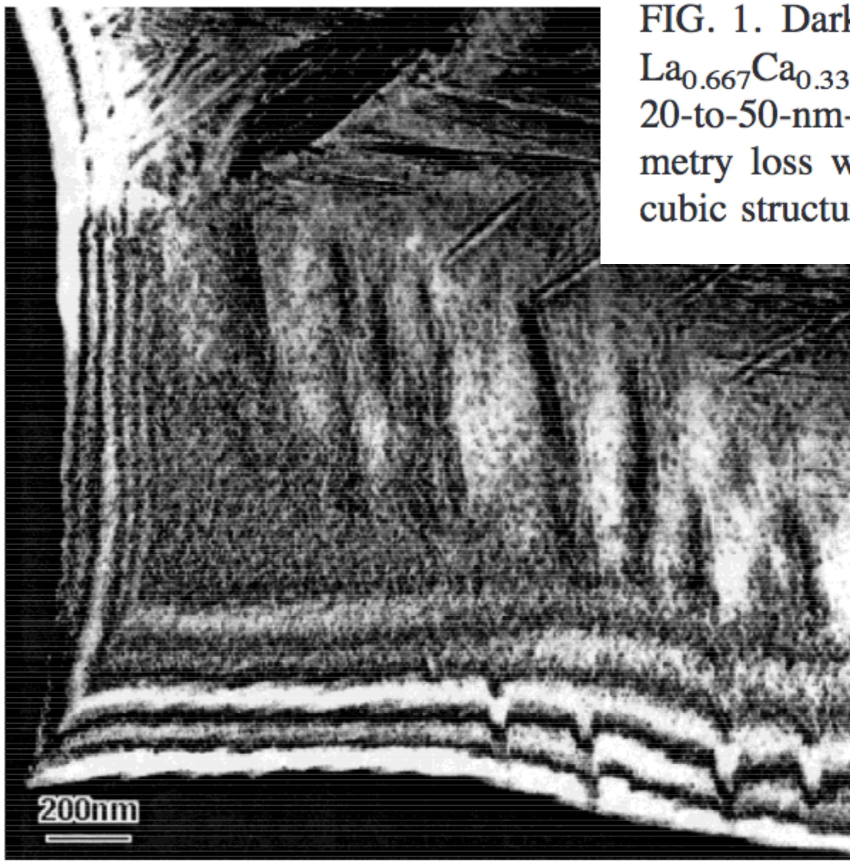
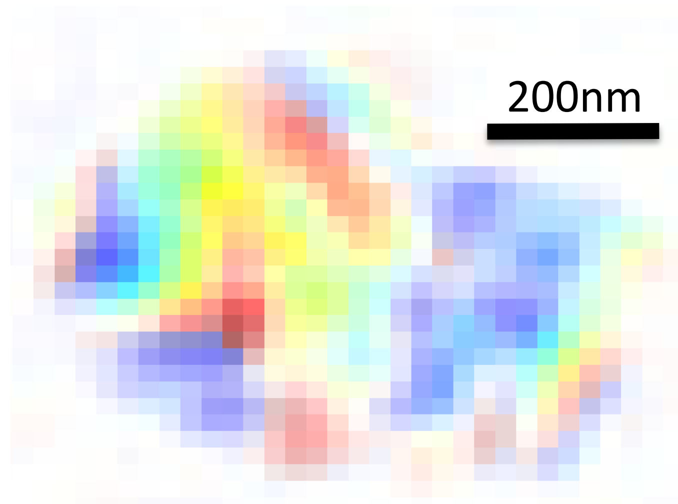


FIG. 1. Dark field image using $(\bar{1}2\bar{1})$ diffraction spot taken from a $La_{0.667}Ca_{0.333}MnO_3$ sample prepared without intermediate grinding; 20-to-50-nm-thick twins are shown. These twins are formed by symmetry loss when the material transforms from the high-temperature cubic structure to the room-temperature *Pnma* structure.



TEM of PLD films of $LaCaMnO_3$

O. I. Lebedev, G. Van Tendeloo, S. Amelinckx, B. Leibold and H.-U. Habermeier, PRB **58** 8065 (1998)

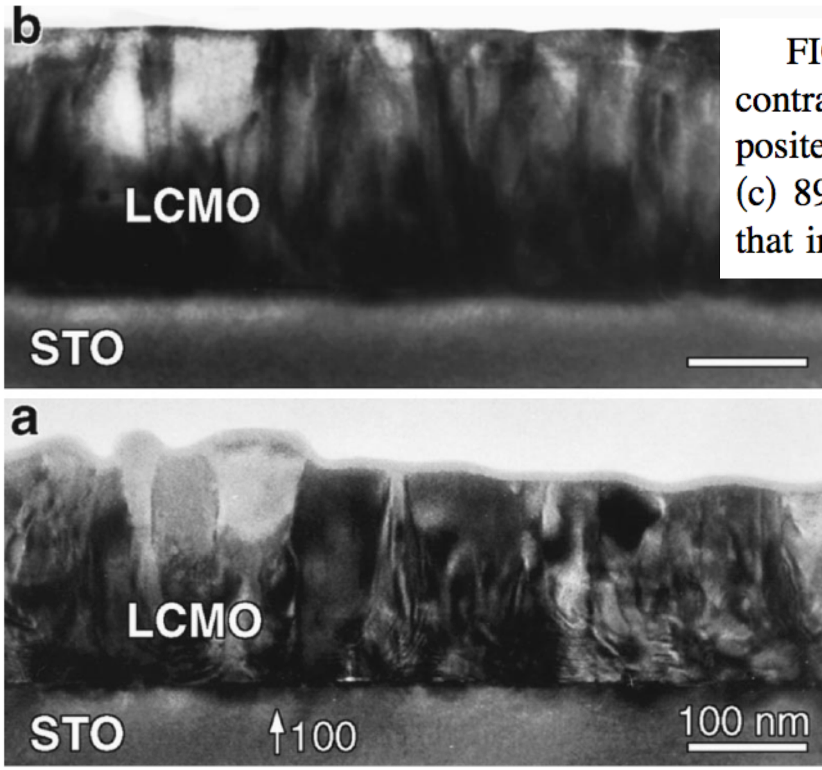
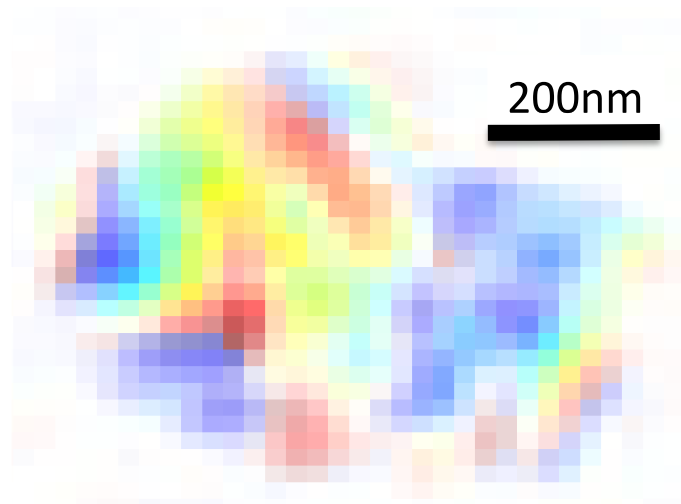
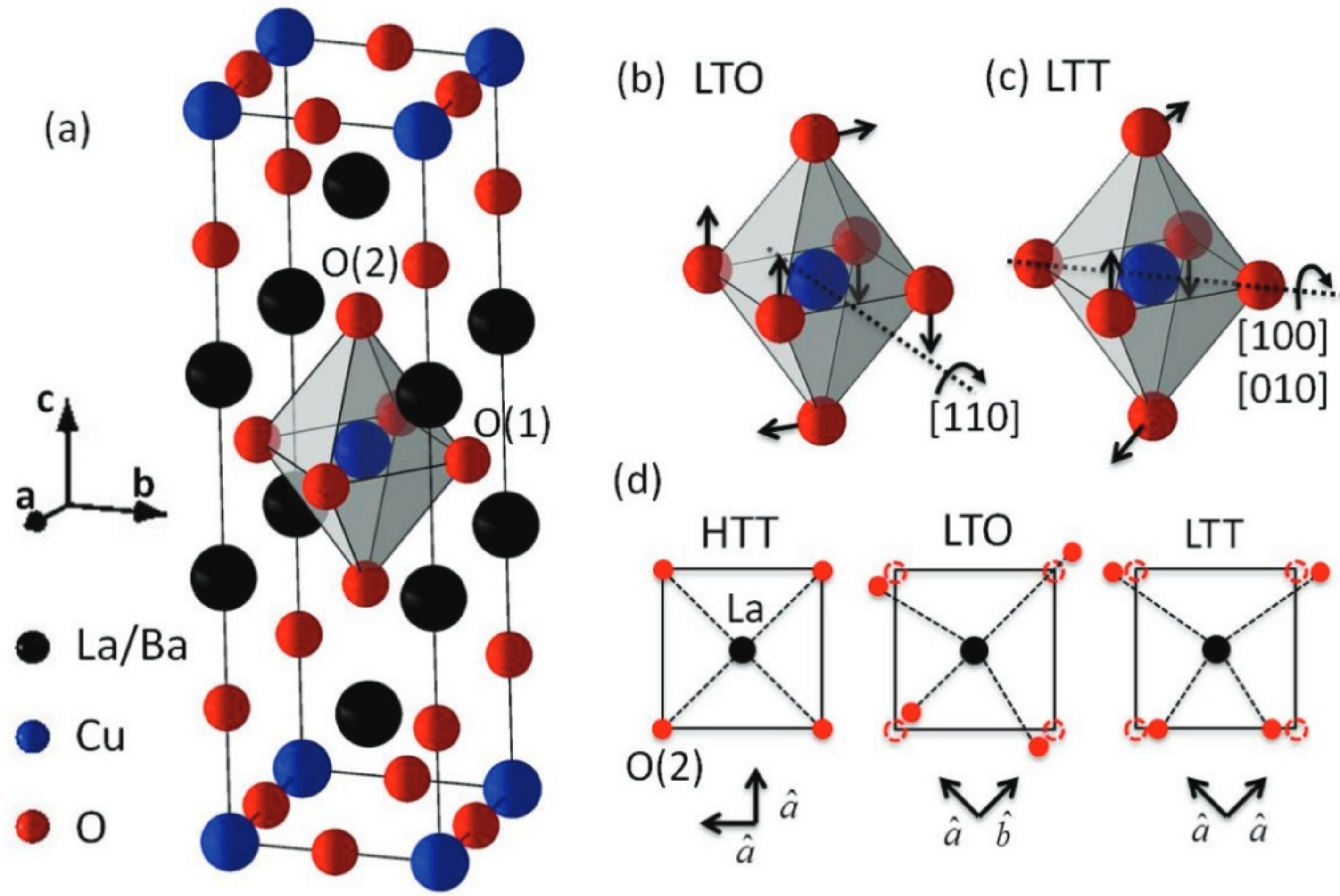


FIG. 1. Low magnification multibeam bright field diffraction contrast image of the columnar texture of (La, Ca)MnO_3 film deposited at different substrate temperatures: (a) 530 °C, (b) 720 °C, (c) 890 °C. The substrate is STO limited by a cube plane. Note that in (c) a perfectly epitaxial transition layer has been formed.



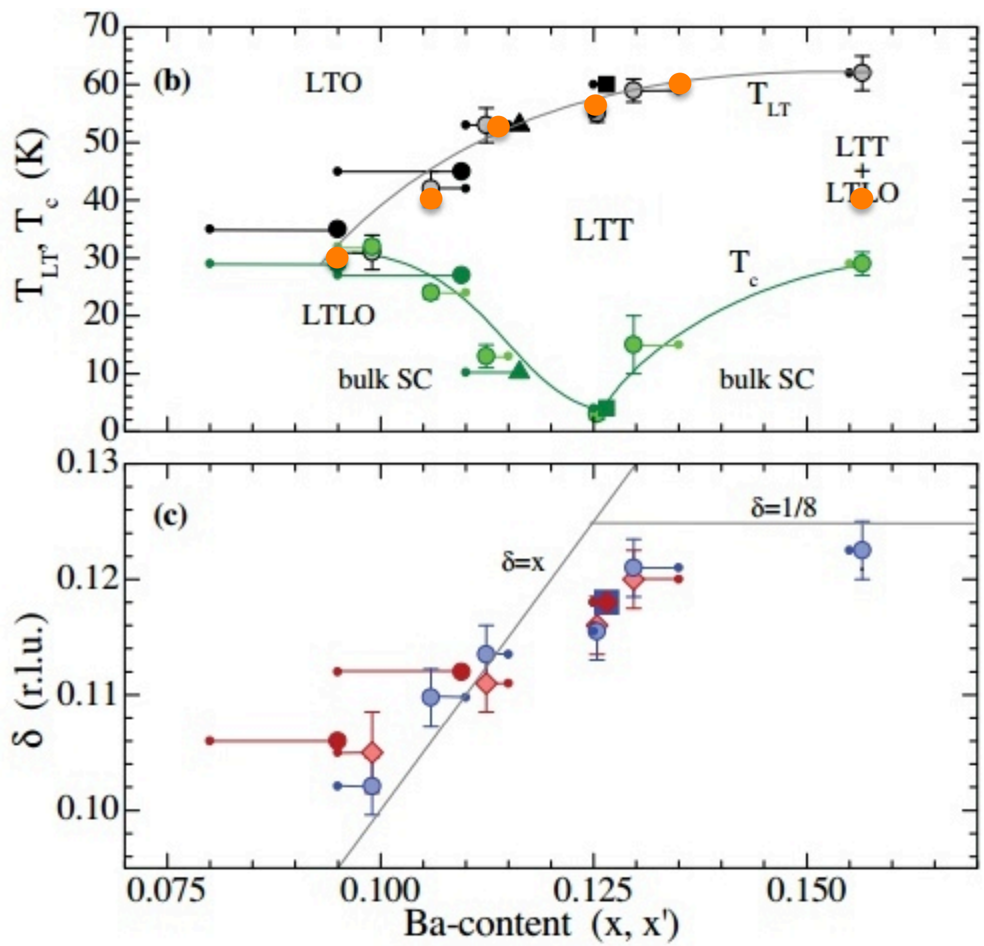
HTT-LTO-LTT phases of $La_{2-x}Ba_xCuO_4$

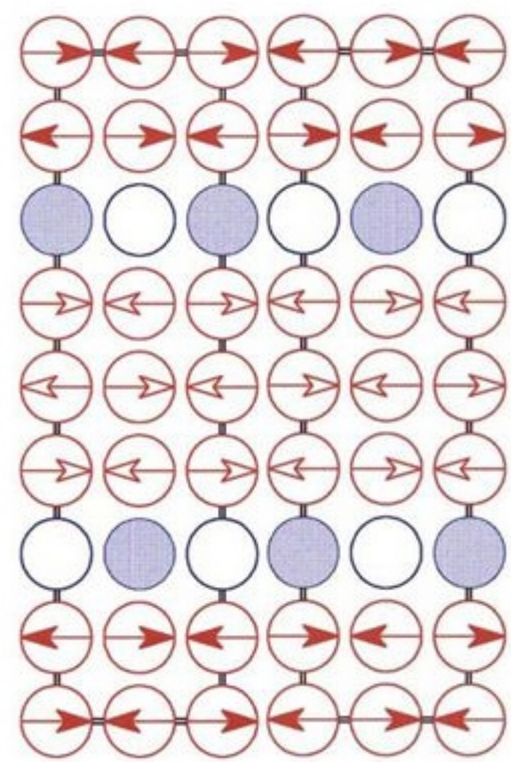
G. Fabbris et al, Phys. Rev B 88 060507 (2013)



Stripes with Doping $La_{2-x}Ba_xCuO_4$

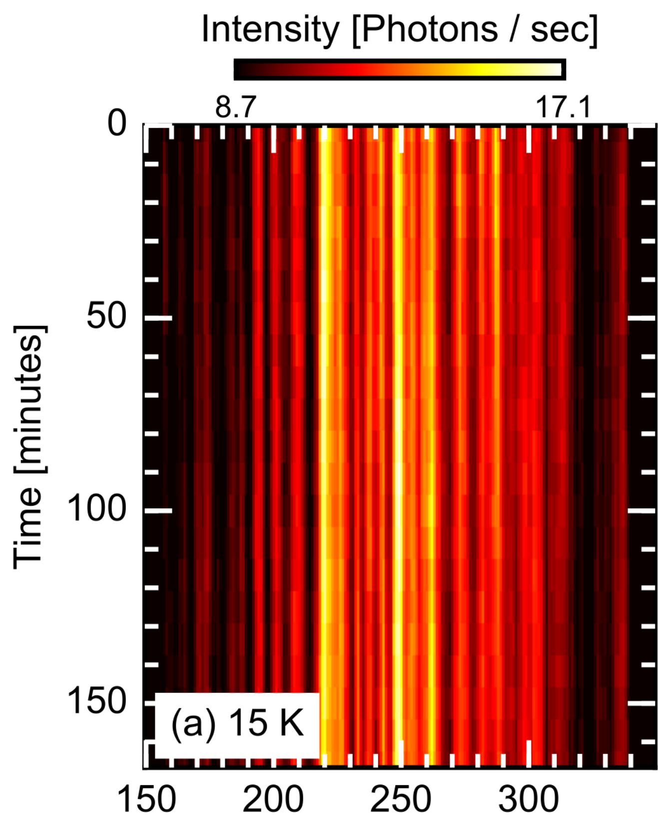
M. Hucker et. al., Phys. Rev. B **83** 104506 (2011)

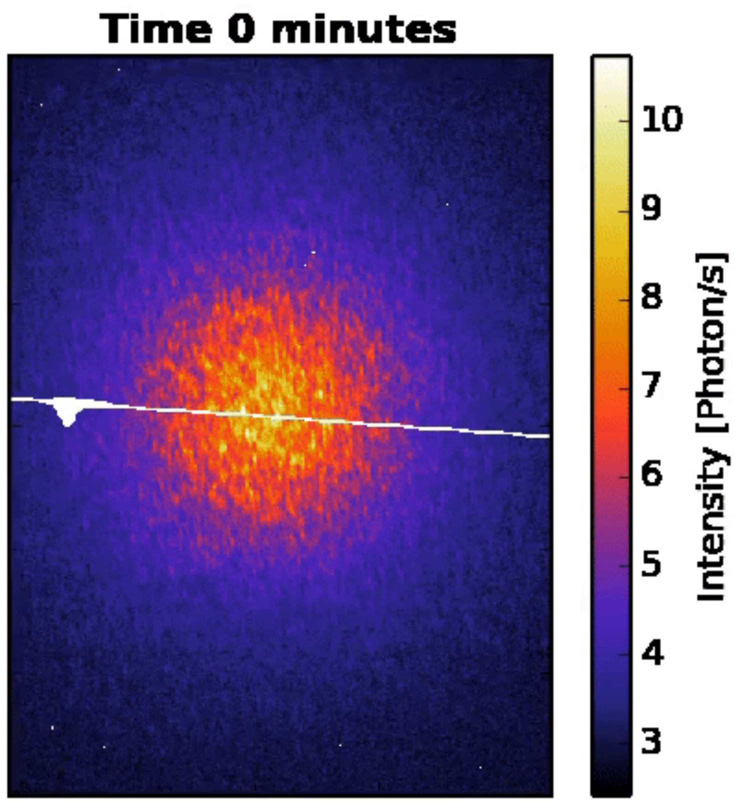




$La_{1.875}Ba_{0.125}CuO_4$ "stripe" fluctuations

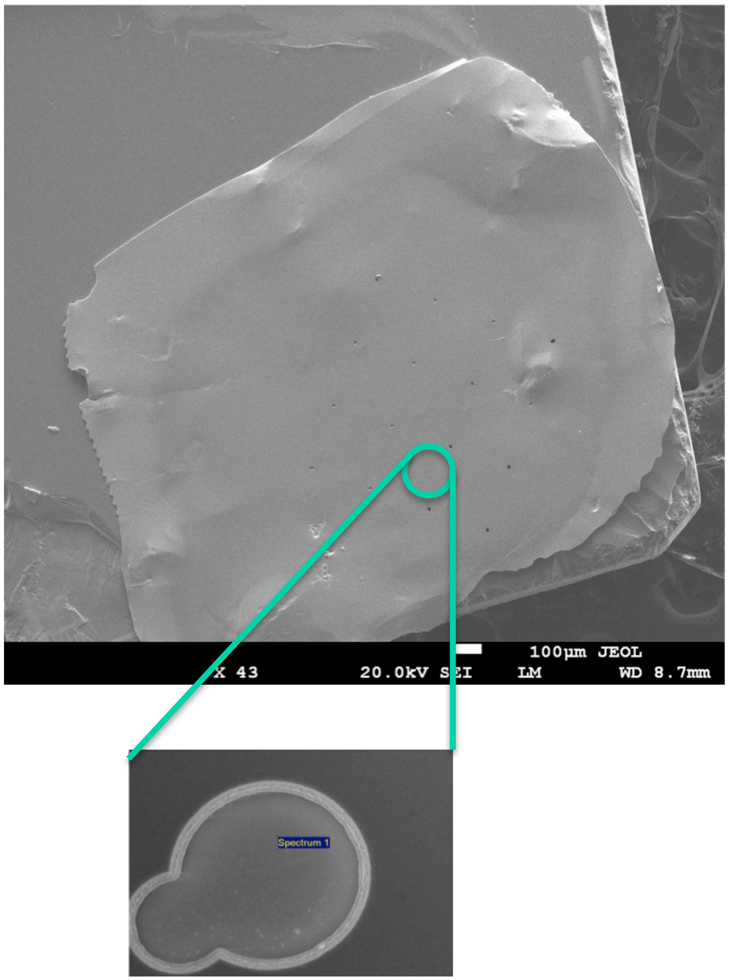
X.M. Chen, V. Thampy, C. Mazzoli, A. M. Barbour, H. Miao, G.D. Gu, Y. Cao, J. M. Tranquada, M. P. M. Dean and S. B. Wilkins, Phys. Rev. Letts. **117** 167001 (2016)

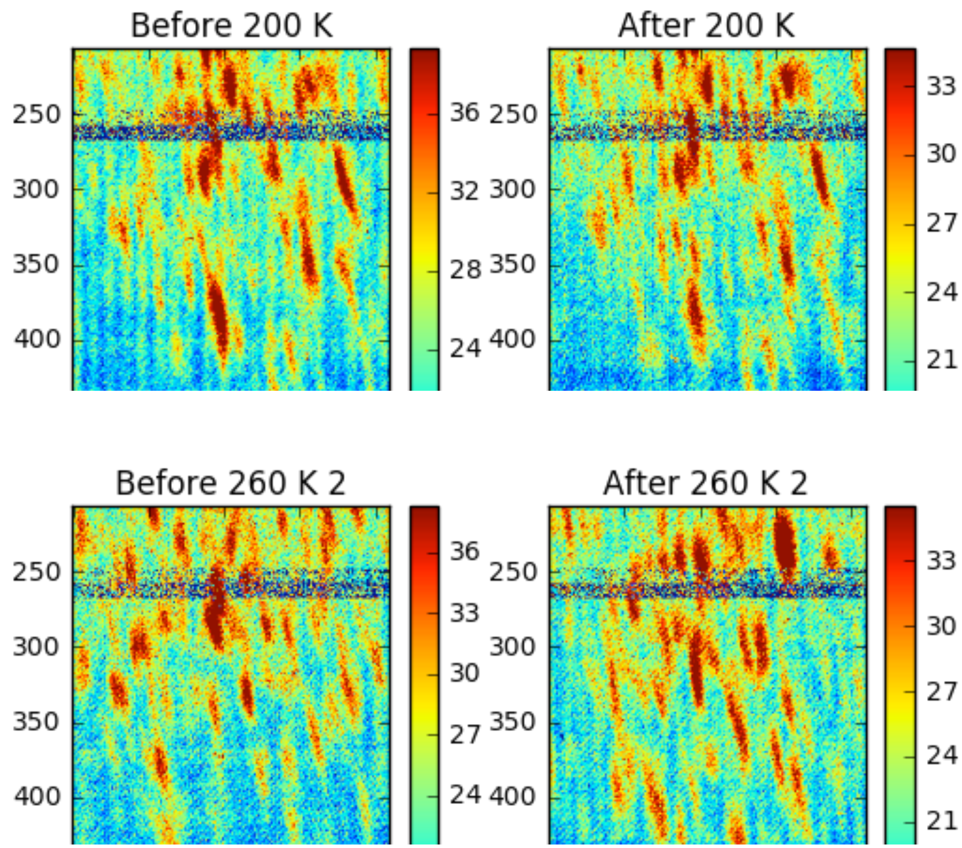




$La_{1.875}Ba_{0.125}CuO_4$ pinning persistence

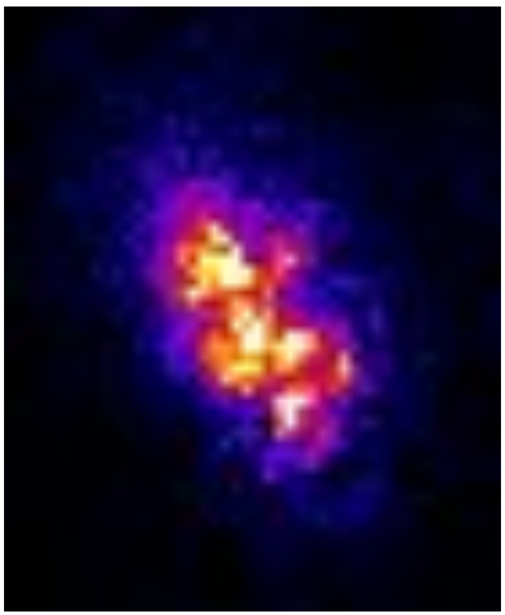
NSLS-II CSX beamline
931eV Cu-L_3 resonance

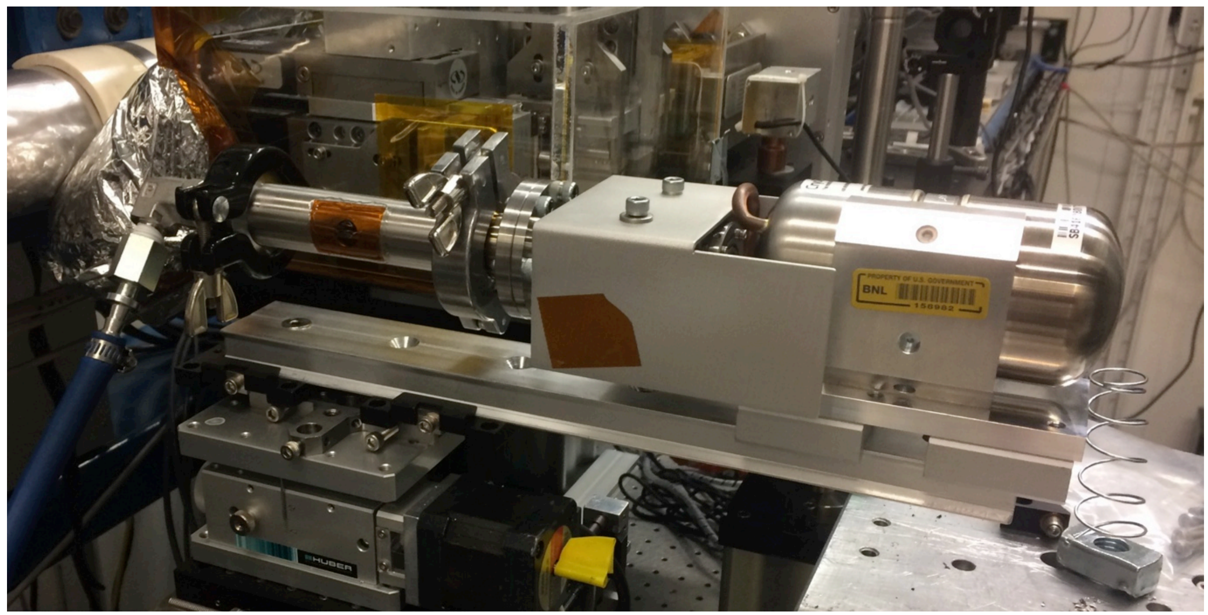




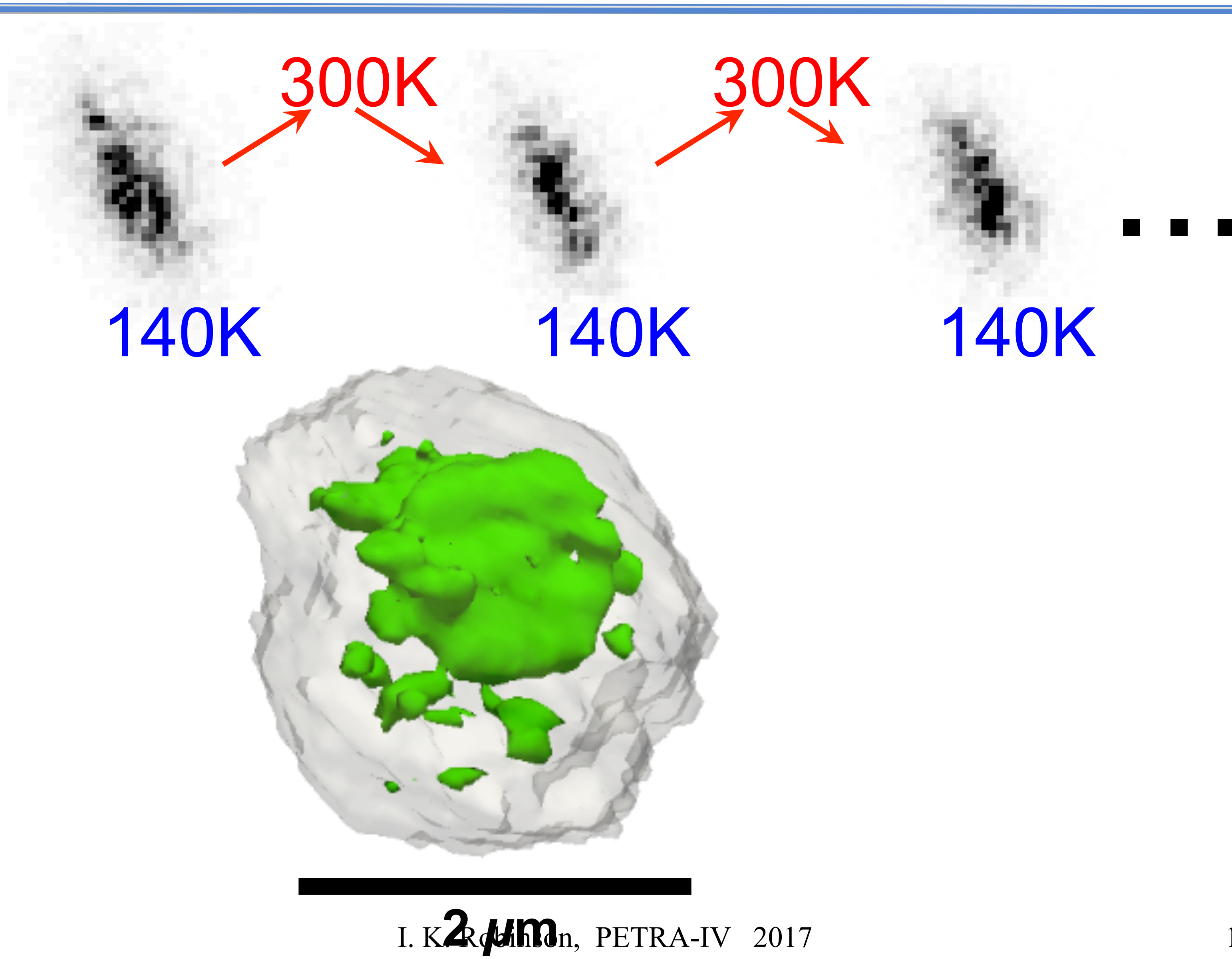
Tools to Image LBCO Domain Walls

- 012 peak forbidden in HTT, allowed in LTO phase
- Need well-formed micron-sized crystals for BCDI
- Need ultra-stable cryostat on a BCDI beamline
- Preliminary tests by grinding large crystals



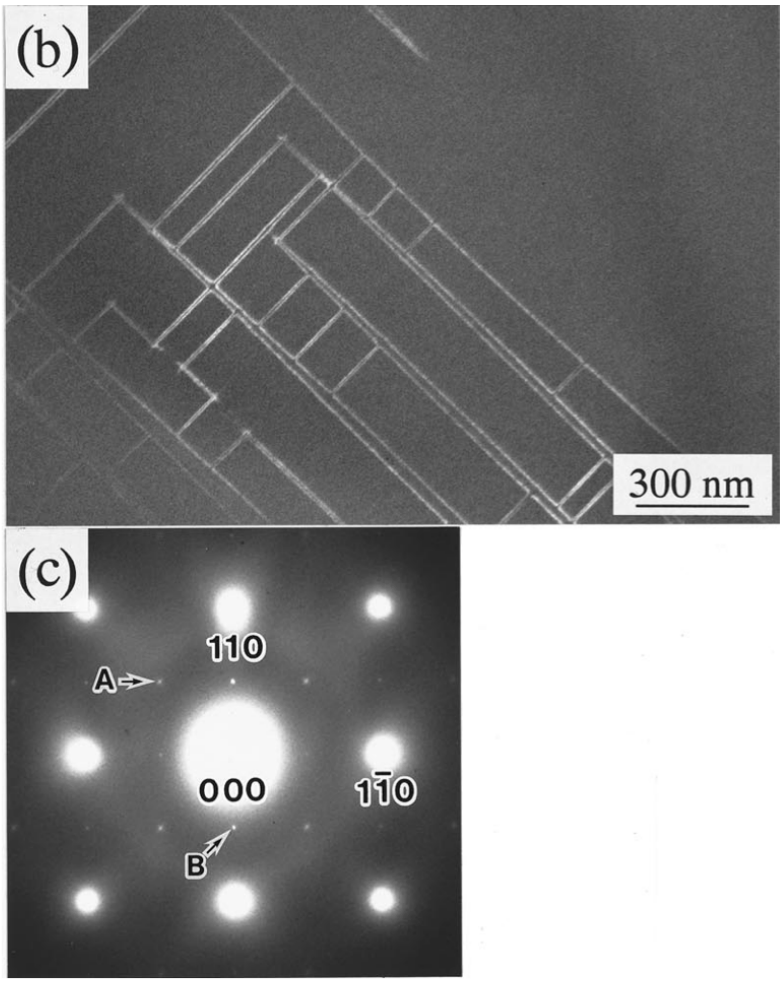


Preliminary Images of LBCO Domain Walls



$La_{1.9}Sr_{0.1}CuO_4$ Domain Walls are LTT

Y. Horibe, Y. Inoue, Y. Koyama, PRB **61** 11922 (2000); Yimei Zhu et al PRL **73** 3026 (1994)

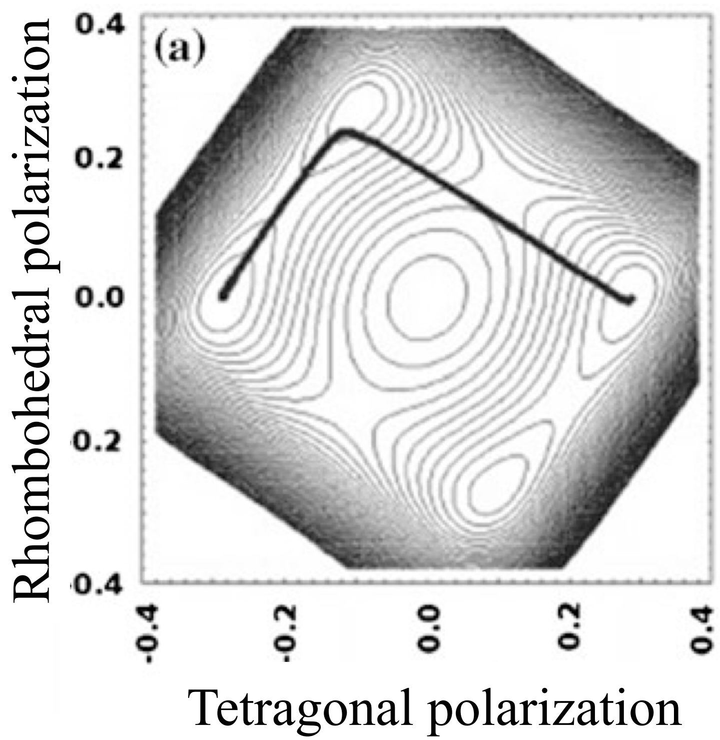


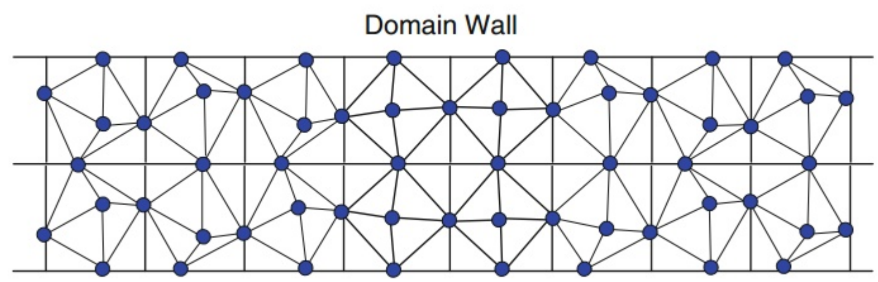
- TEM Image of $La_{1.9}Sr_{0.1}CuO_4$
- 12K in LTO phase
- Using (100) LTT peak
- 10nm of LTT phase in domain walls between LTO twins

Phase space trajectory calculated for orthorhombic 120° domain walls in oxides

P. Marton, I. Rychetsky and J. Hlinka, Phys. Rev. B **84** 139906(E) (2011)

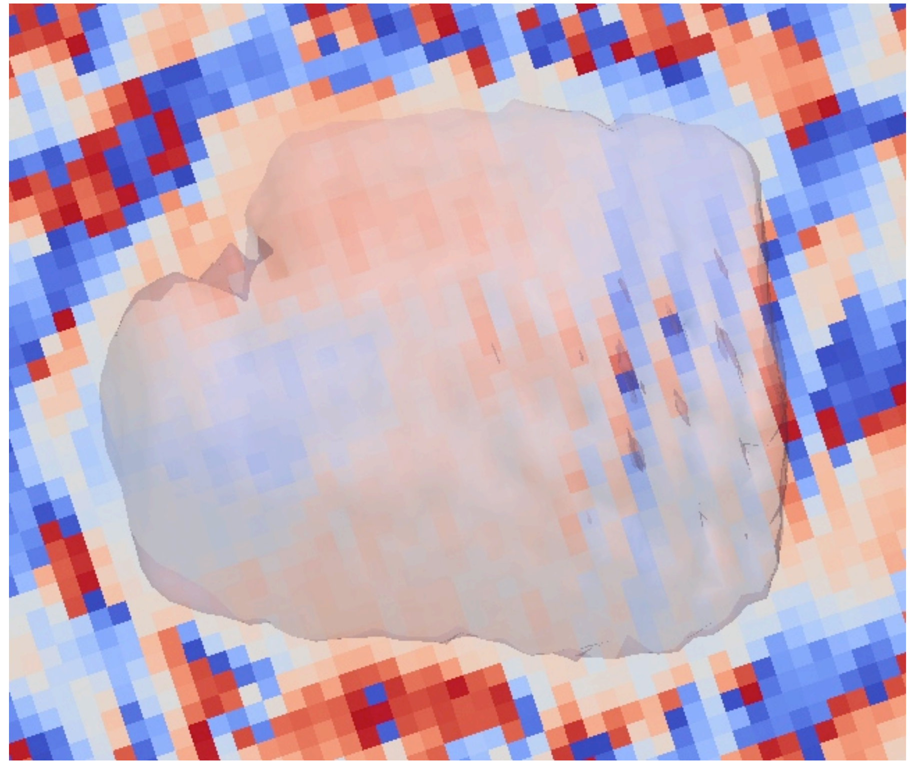
G. Catalan,. Ferroelectrics **433** 65–73 (2012)

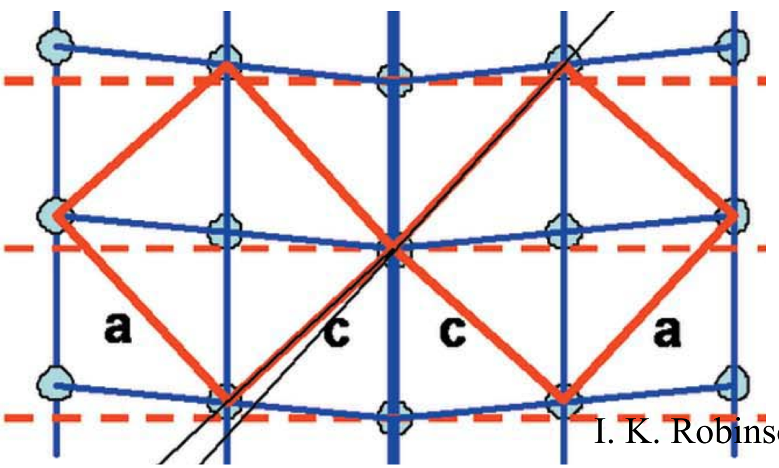




Domain wall can have different crystal structure from the dominans

$BaTiO_3$ bicrystal imaged by BCDI





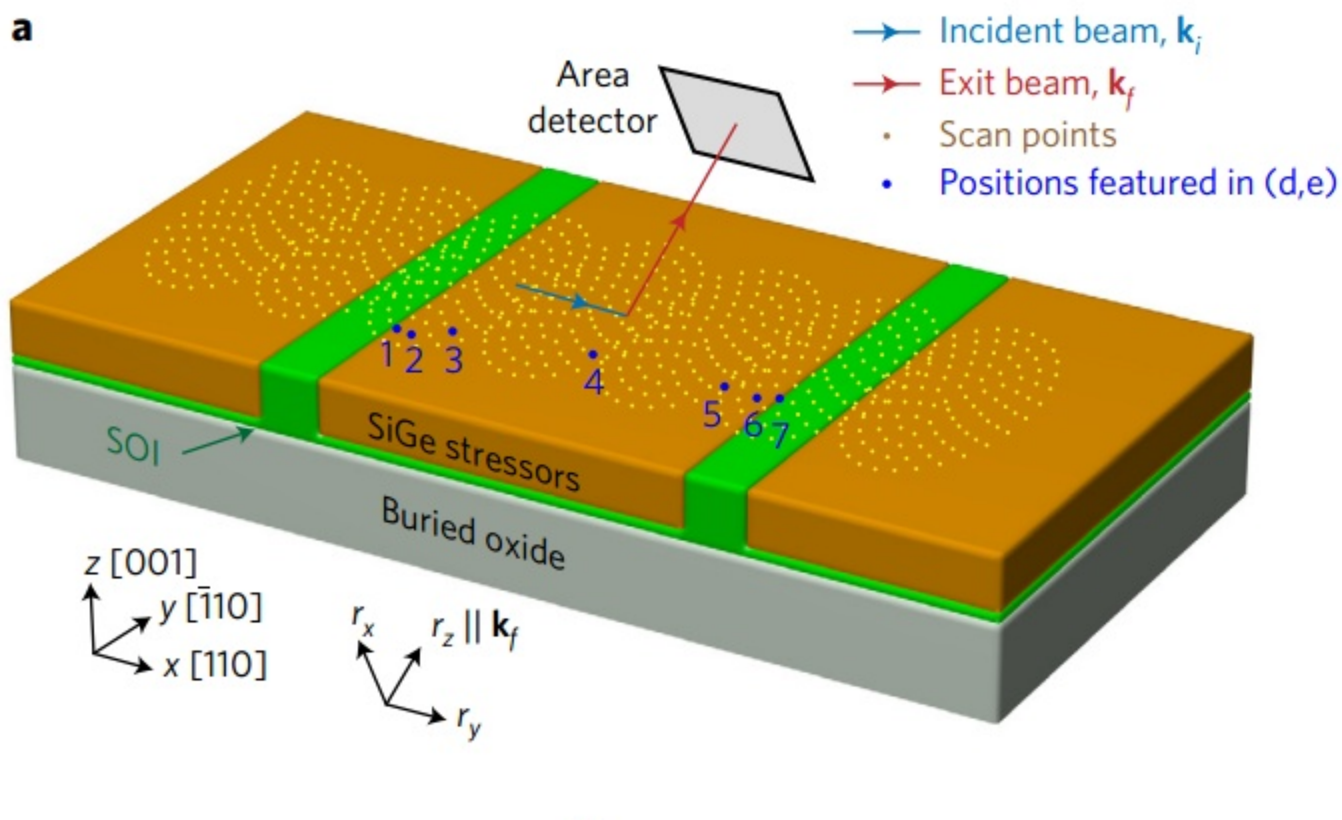
Support *vs* Ptycho constraint for crystals?

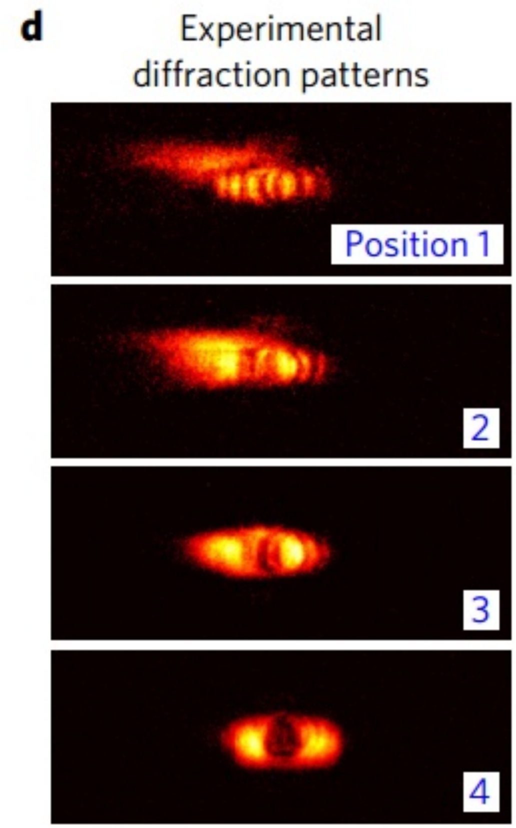
- Support
  - Flares in diffraction
  - Reaches higher Q?
  - Shrink-wrap search
  - Oversampling well-determined
  - Naturally 3D

- Ptychography
  - Increase overlap arbitrarily
  - Better convergence
  - Able to image probe
  - Extended objects
  - Hard to extend to 3D

Bragg Projection Ptychography

Hruszkewycz et al Nat. Mat. **5** 026105 (2017)





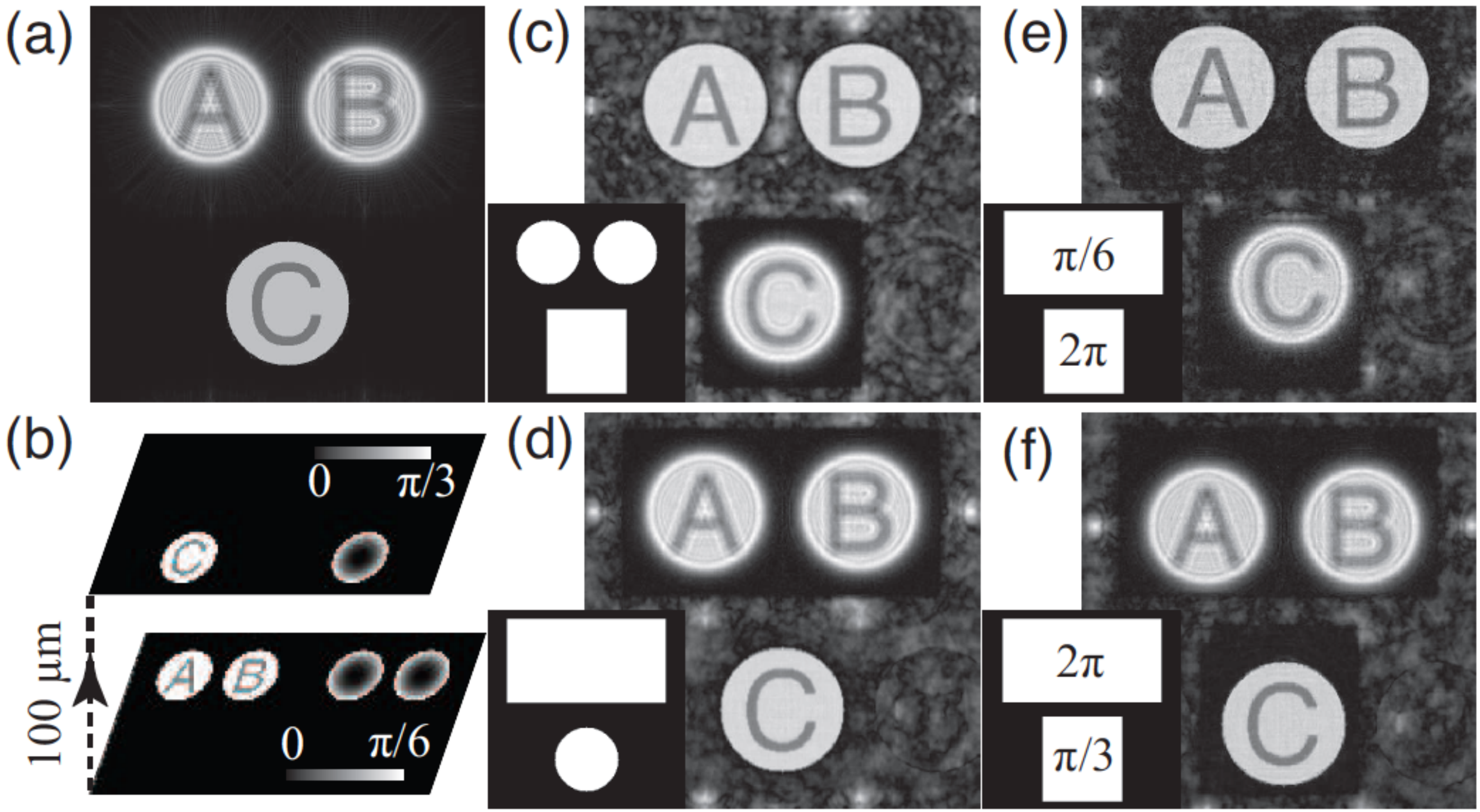
Free-space propagation

$$t'(\mathbf{r}') = \int t(\mathbf{r}) e^{ik(\mathbf{r}-\mathbf{r}')^2/2d} d\mathbf{r},$$

- Box -> box with fringes
- Real Gaussian -> complex *wider* Gaussian
- Real sharp object -> defocused complex object
- Propagated objects all have the same Fourier transform
- Inversion of far-field diffraction is non-unique

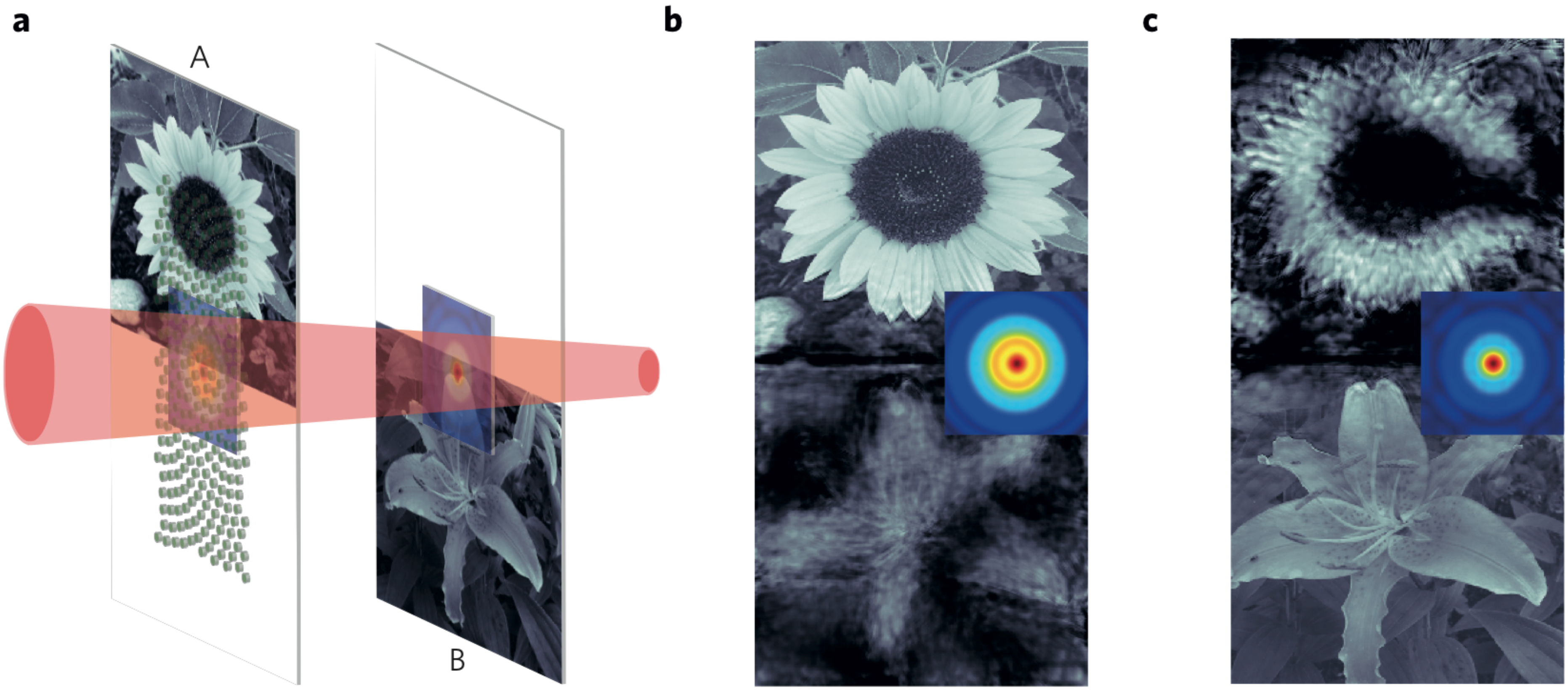
2D reconstruction support tests

J. C. H. Spence, U. Weierstall and M. Howells, Phil. Trans. 360, 875 (2002)
Xiaojing Huang, et al, Physical Review B 83 224109 (2011)



Propagation uniqueness in Ptychography

Ian Robinson and Xiaojing Huang, Nature Mater 16 160 (2017)



Bragg Coherent Diffraction Imaging

- Complex density in BCDI images
- Phase domains in $La_{0.5}Ca_{0.5}MnO_3$
- Mosaic of displacements, not angles
- Memory effects in $La_{1.875}Ba_{0.125}CuO_4$
- Challenge to obtain unique phases
- Role of Ptychography