Coherent diffraction imaging using Crystal Truncation Rods

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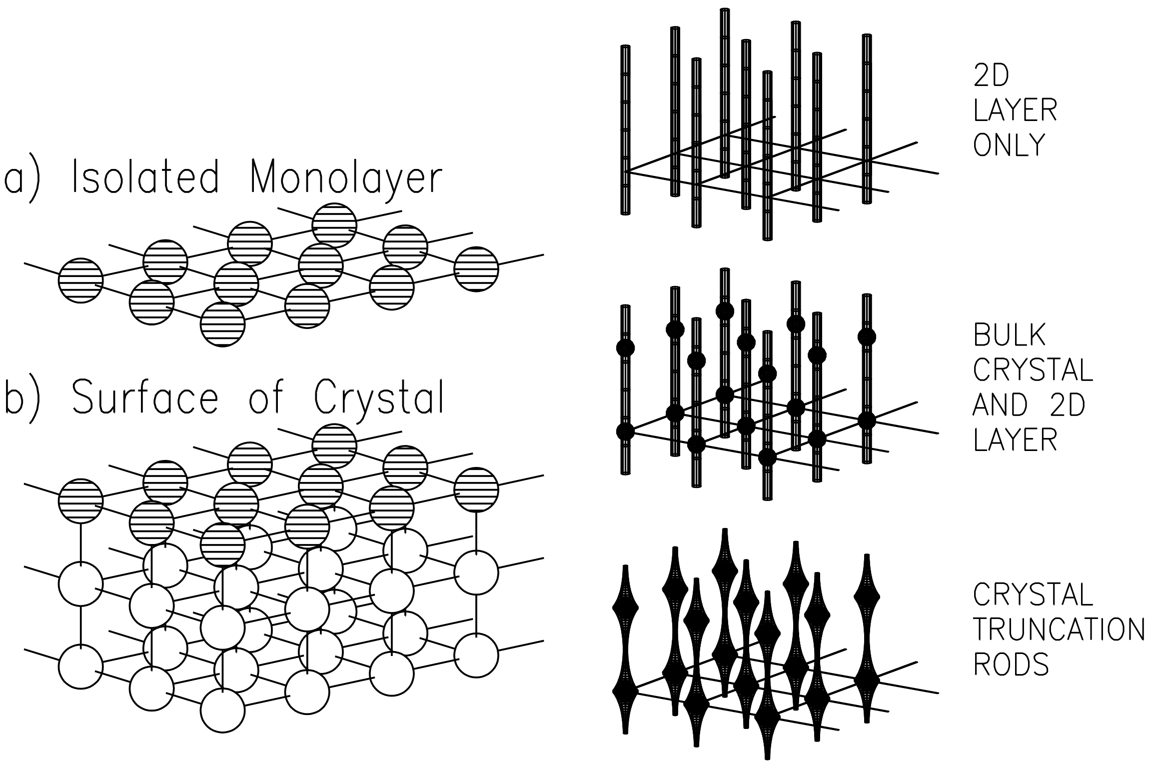
Angel Rodriguez-Fernandez
Diamond Light Source

SXNS18, July 2026

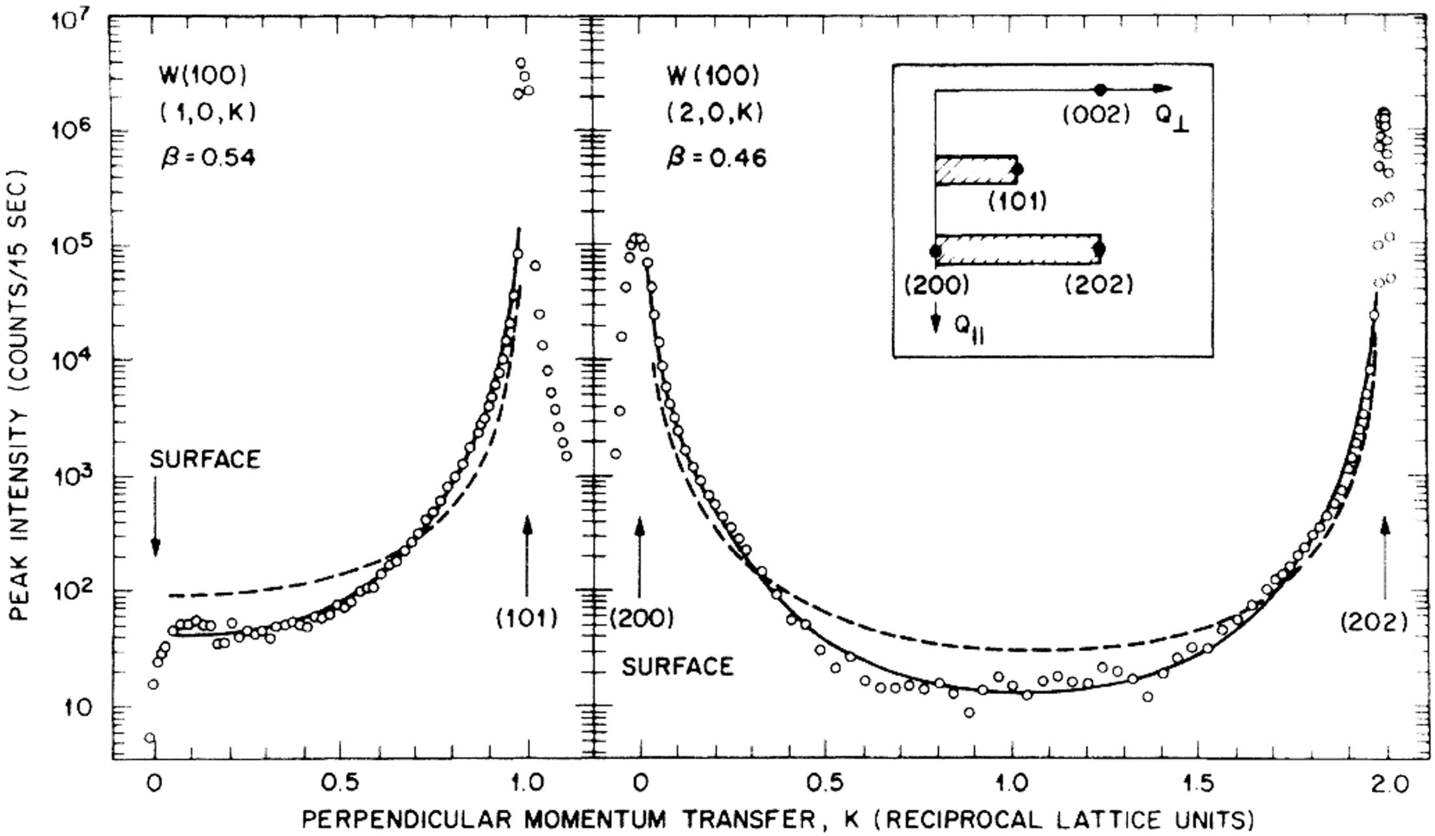
Outline

- Crystal Trucation Rods and SXNS
- Coherent Diffraction Imaging by Ptychography
- Bragg Ptychography
- Imaging of Thin Films and Interfaces
- Future directions

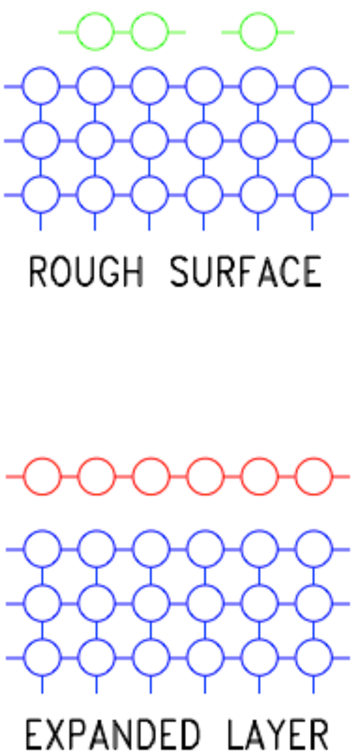
Crystal Truncation Rods (1986)

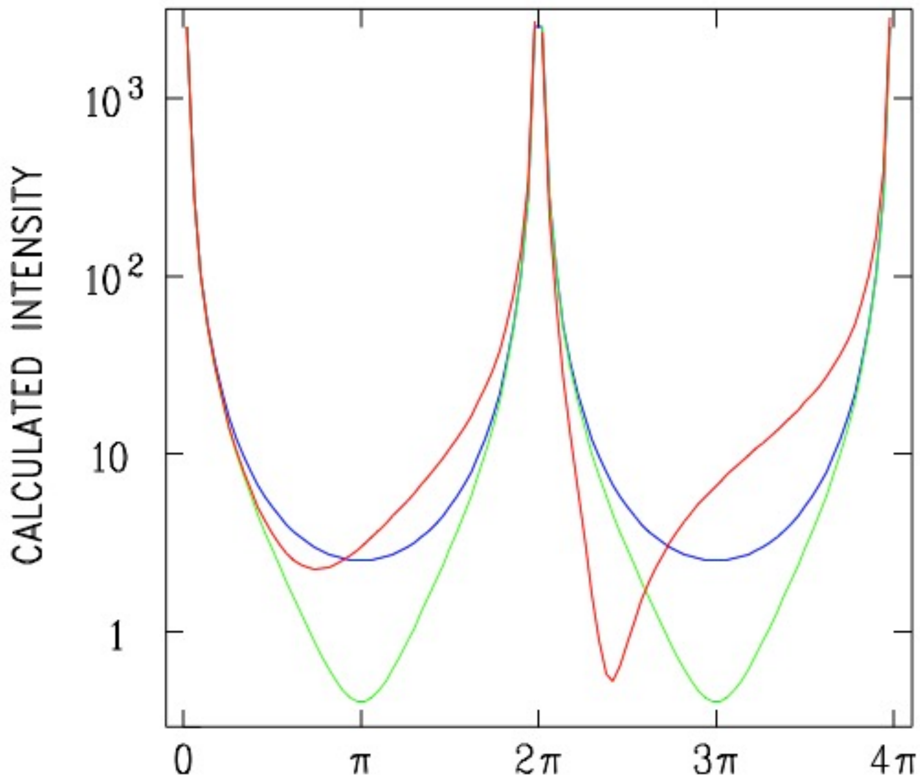


CRYSTAL TRUNCATION RODS AND SURFACE ROUGHNESS



CTR is Sensitive to Surface Structure





Surface Diffraction Overview [SXNS-5]

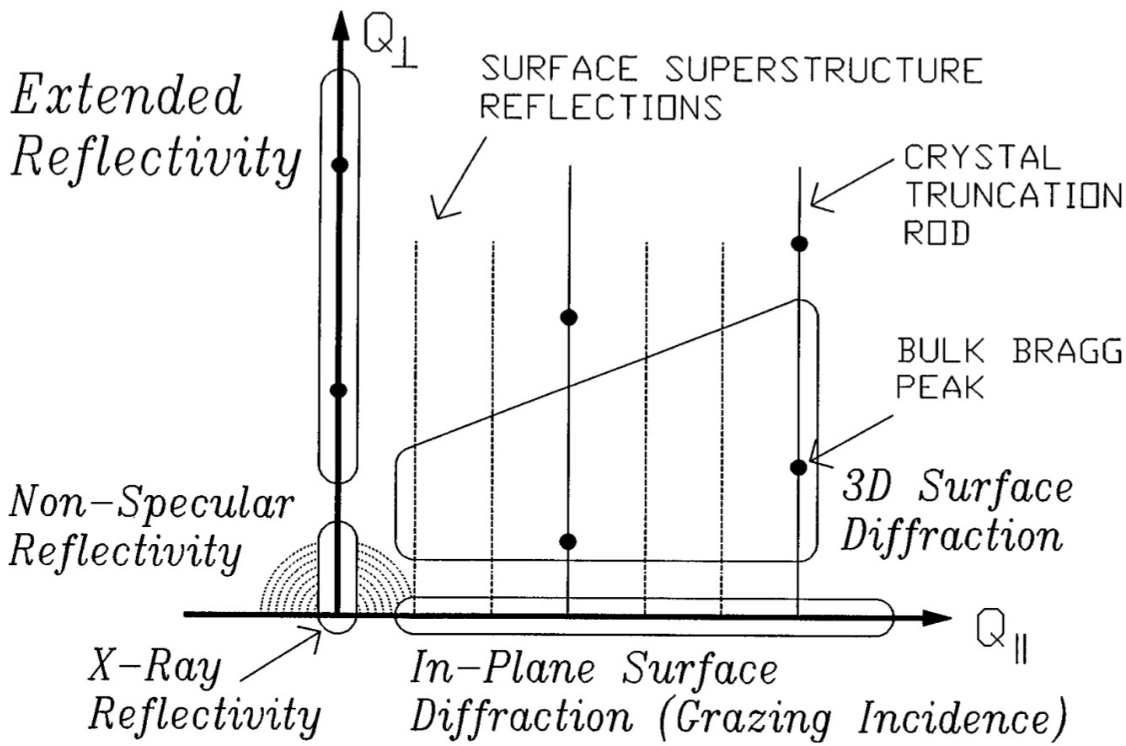


Fig. 1. Schematic map of reciprocal space indicating the names customarily given to different techniques that are sensitive to the surface. From Ref. [20].

Sutton et al, Nature (1991)
X25 (NSLS)

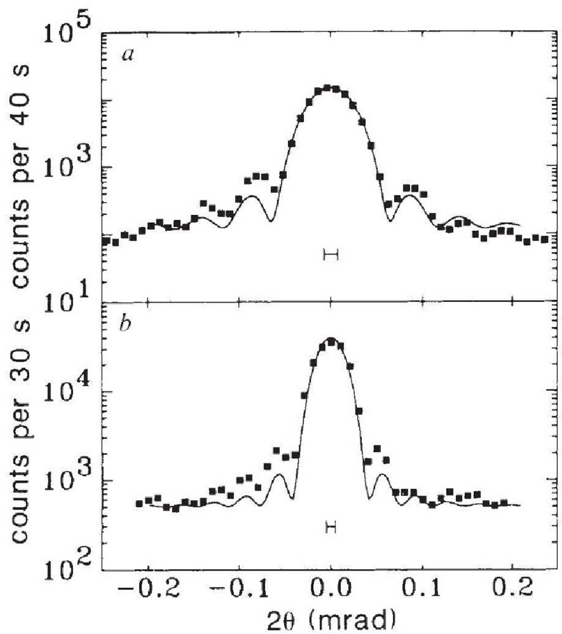


FIG. 2 Fraunhofer diffraction from *a*, 2.5-μm and *b*, 5-μm nominal diameter pinholes. Error bars due to counting statistics are smaller than the symbol size. The solid line represents the calculated diffraction pattern of a circular aperture convolved with the analyser resolution shown by the horizontal bar. A constant background is included in the fit.

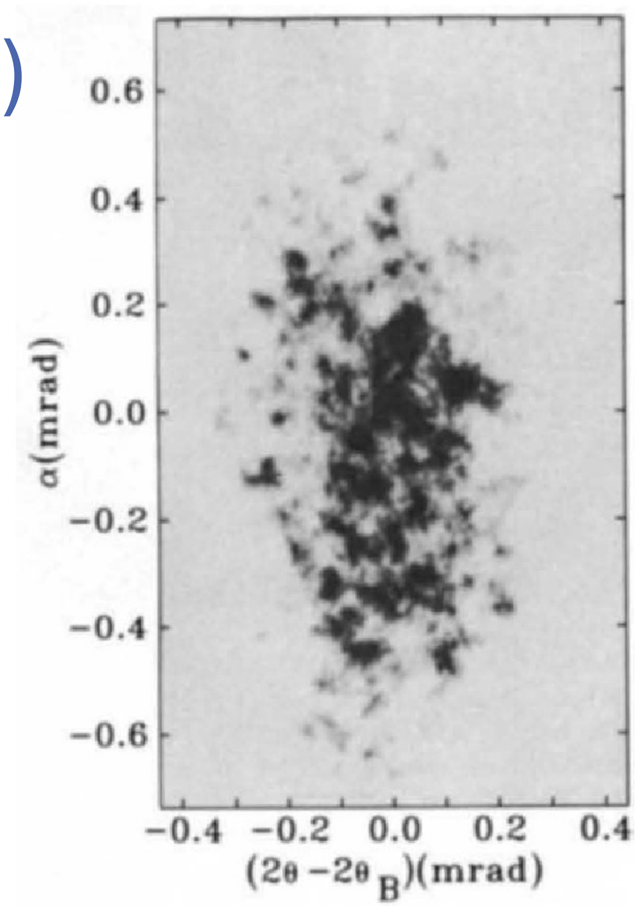
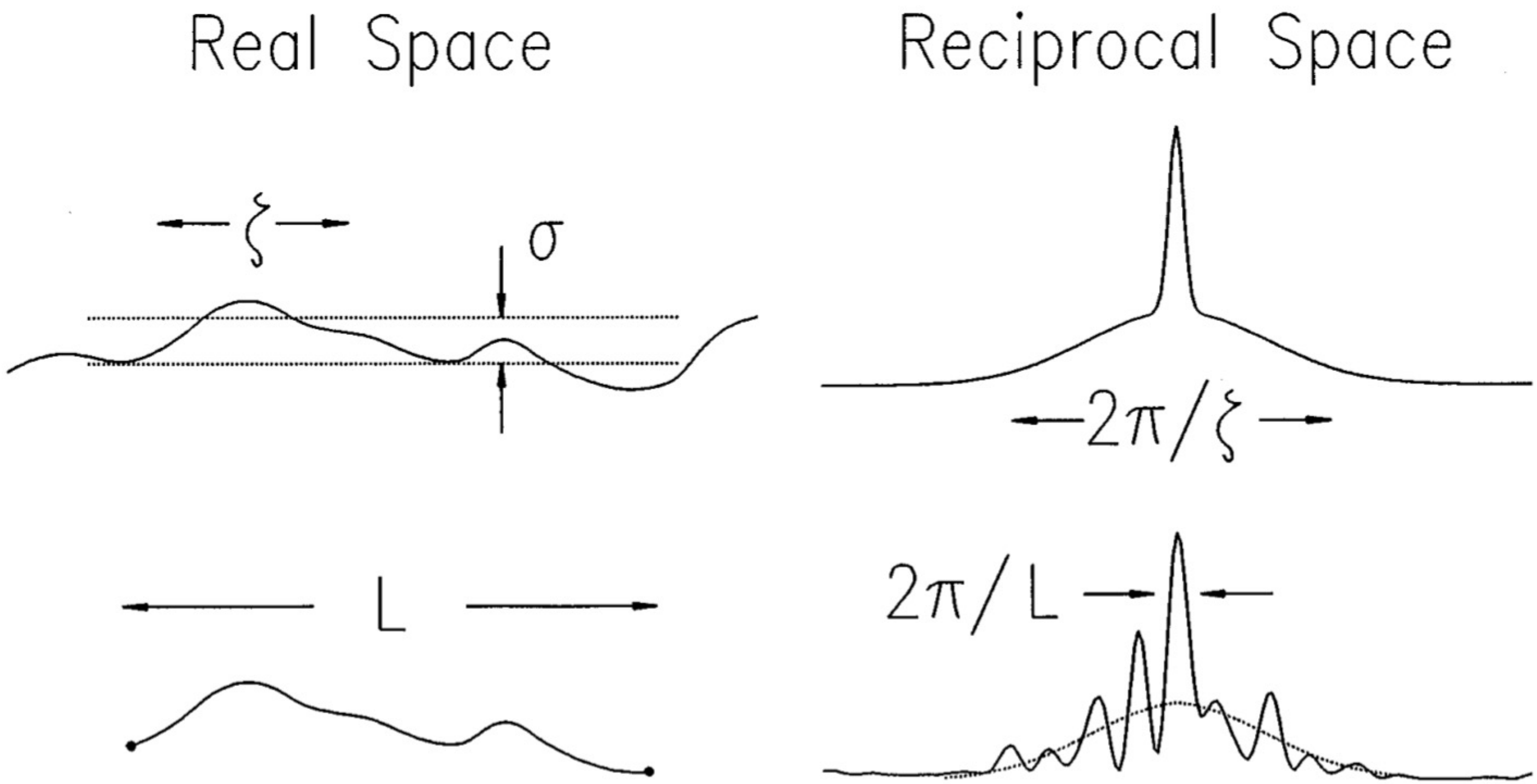


FIG. 3 Photograph of the speckle pattern in the diffuse (001) peak of Cu_3Au. The collimating pinhole is 2.5 μm.

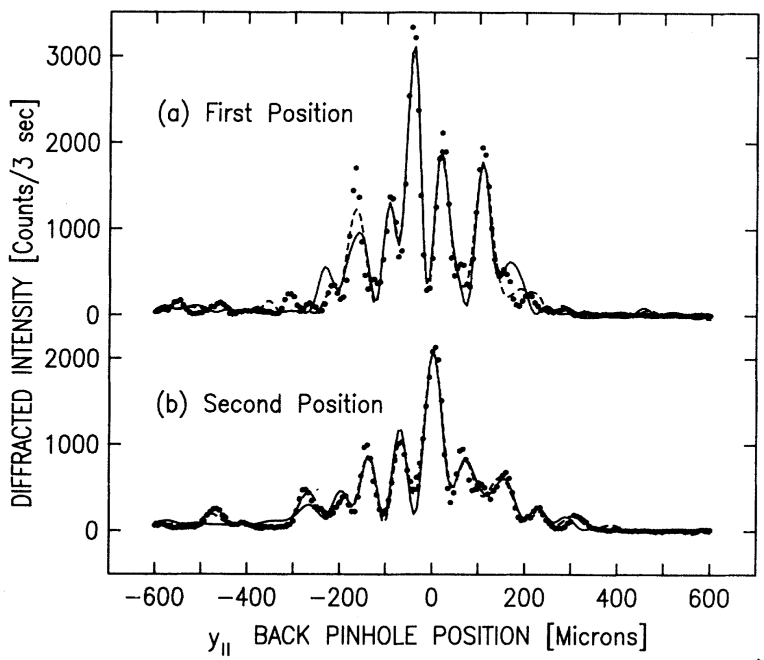
NATURE · VOL 352 · 15 AUGUST 1991

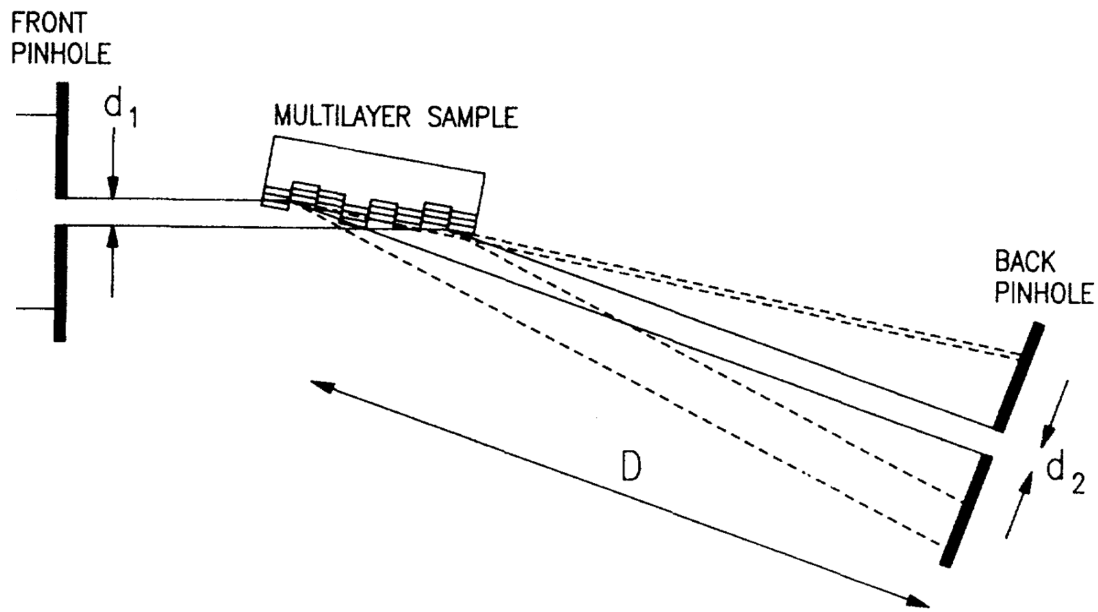
Surface Morphology as Speckle [SXNS-5]



Multilayer speckle at ESRF ID-10 “Troika” (1995)

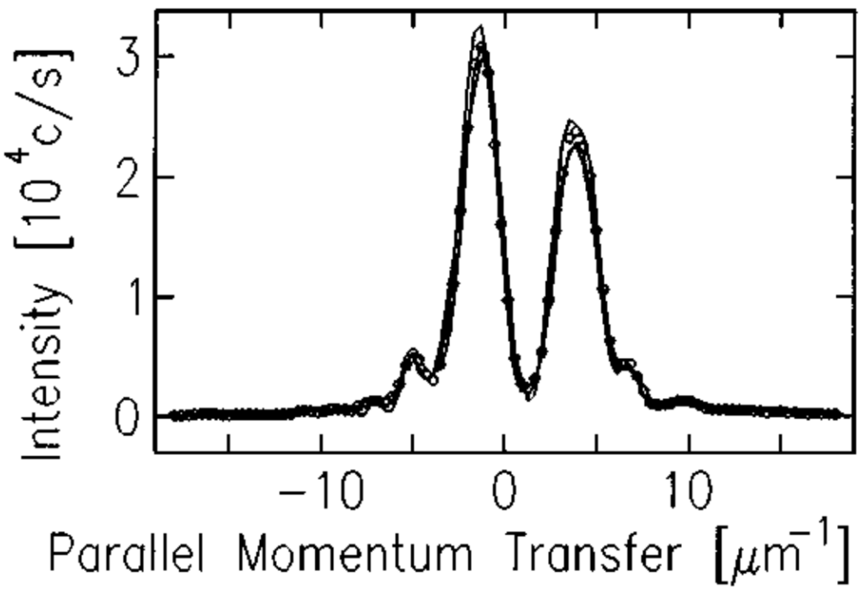
I. K. Robinson, R. Pindak, R. M. Fleming, S. B. Dierker, K. Ploog, G. Grübel, D. L. Abernathy and J. Als-Nielsen, Phys. Rev. B 52 9917 (1995)

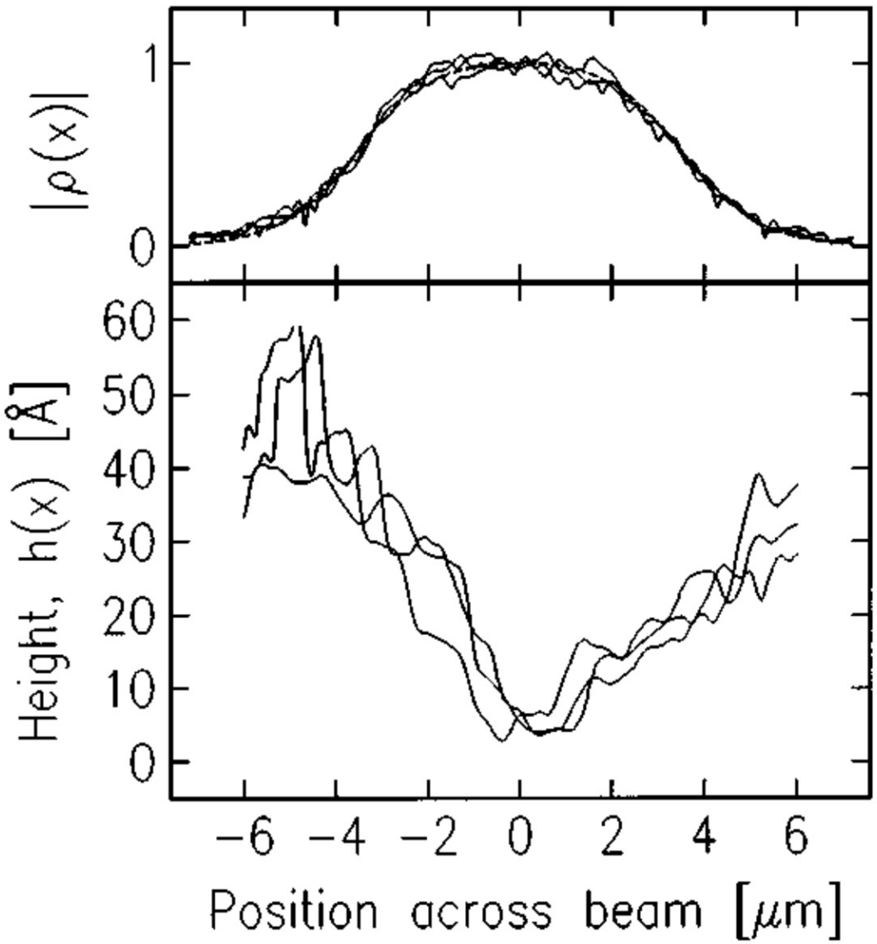




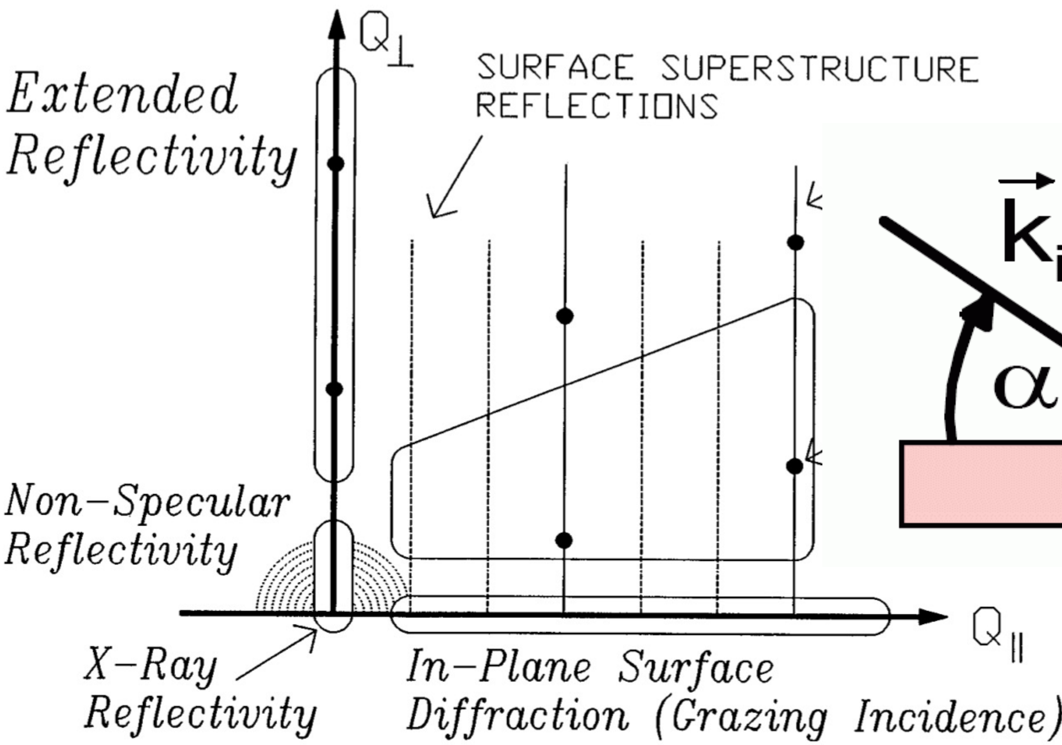
Reconstruction of Surface Morphology of Si wafer

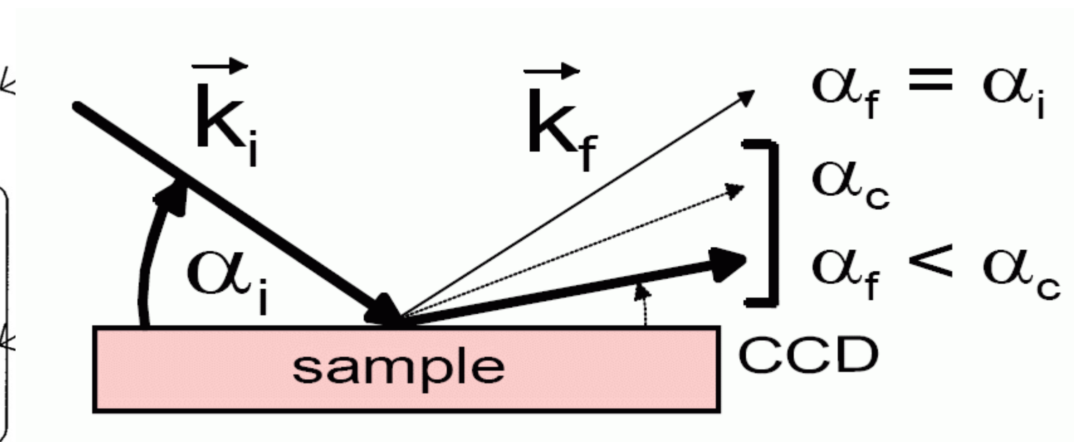
[Vartanyants et al PRB 55 13193 (1997)]





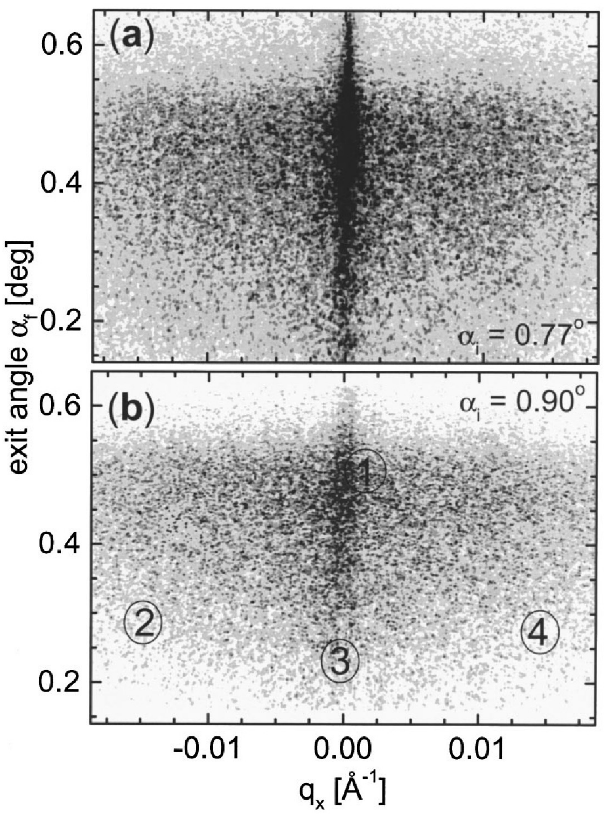
Coherent GISAXS and GESAXS

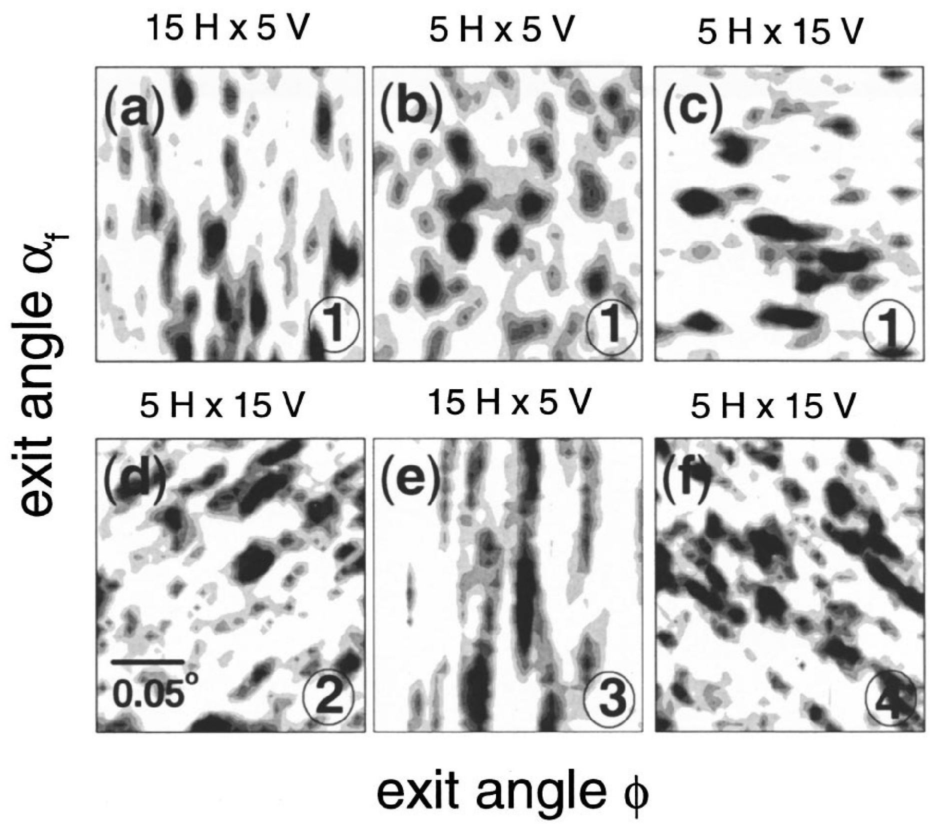




GESAXS Geometry sees film nanostructure

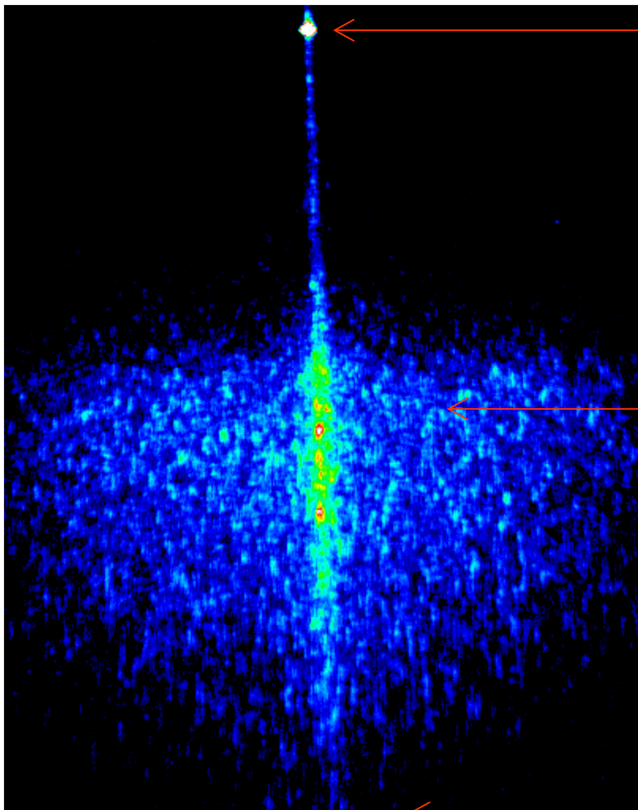
F. Pfeiffer, W. Zhang and I. K. Robinson, Appl. Phys. Letters 84 1847-9 (2004)





Coherent Structure in “Yoneda” Peak 34-IC-C

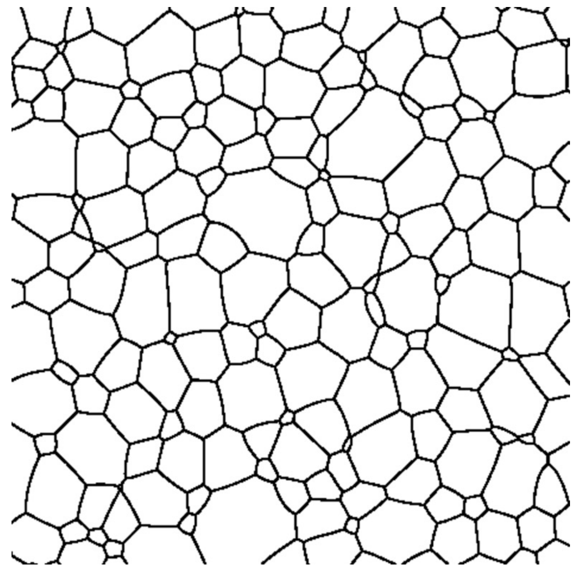
Grazing-exit diffraction from a 100 nm Au polycrystalline film



Specular ($\alpha_f \sim \alpha_i$)

$\alpha_f \sim \alpha_c$

$\alpha_f \sim 0$

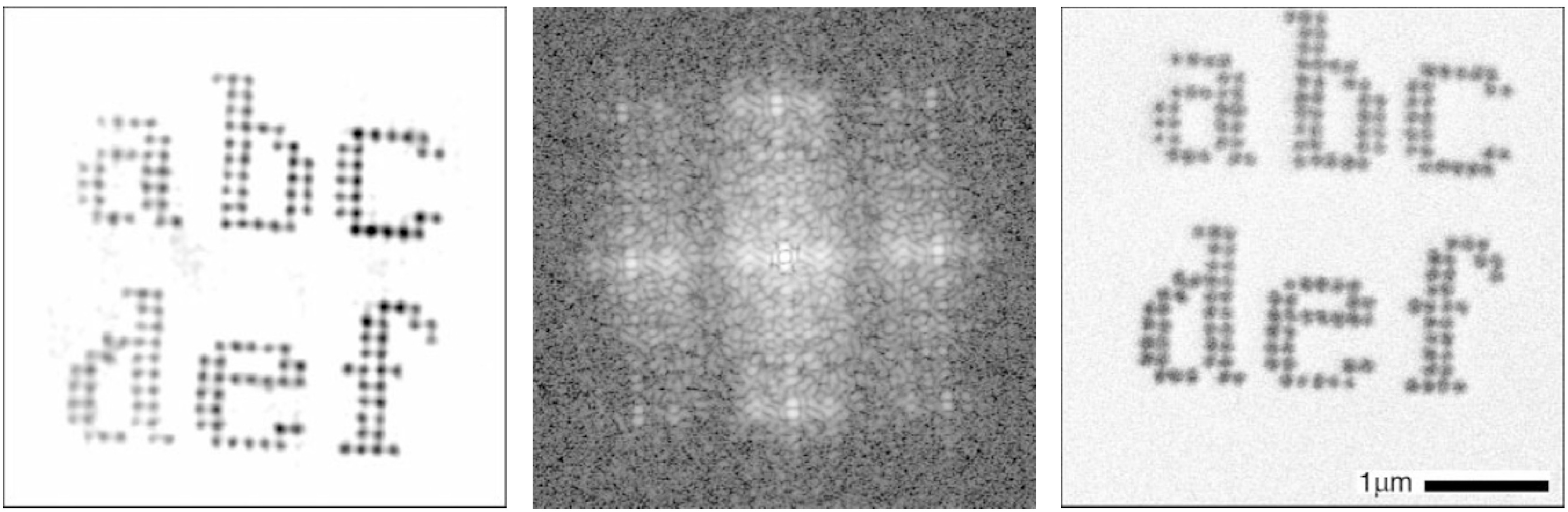


Jianwei Miao, Nature (1999)

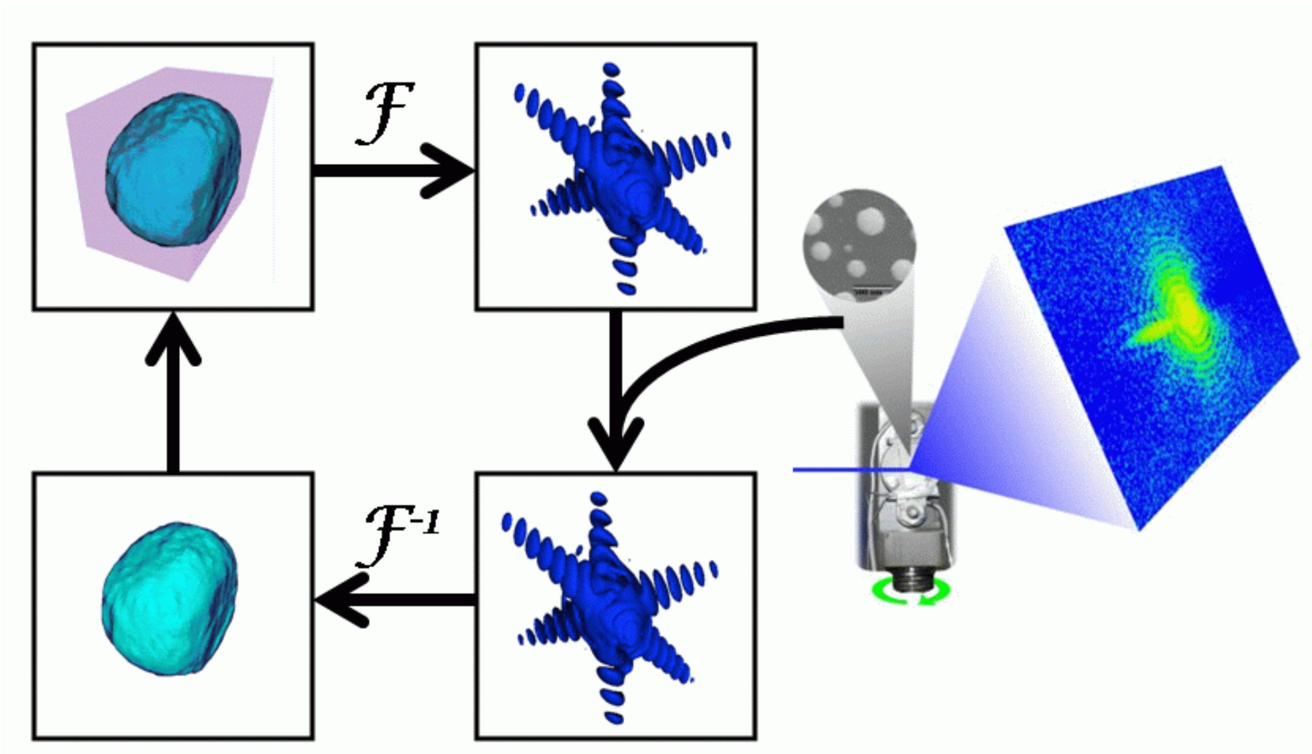
Extending the methodology of X-ray crystallography to allow imaging of micrometre-sized non-crystalline specimens

Jianwei Miao*, Pambos Charalambous†, Janos Kirz* & David Sayre*‡

** Department of Physics and Astronomy, State University of New York, Stony Brook, New York 11794-3800, USA*
† Kings College, Strand, London WC2R 2LS, UK



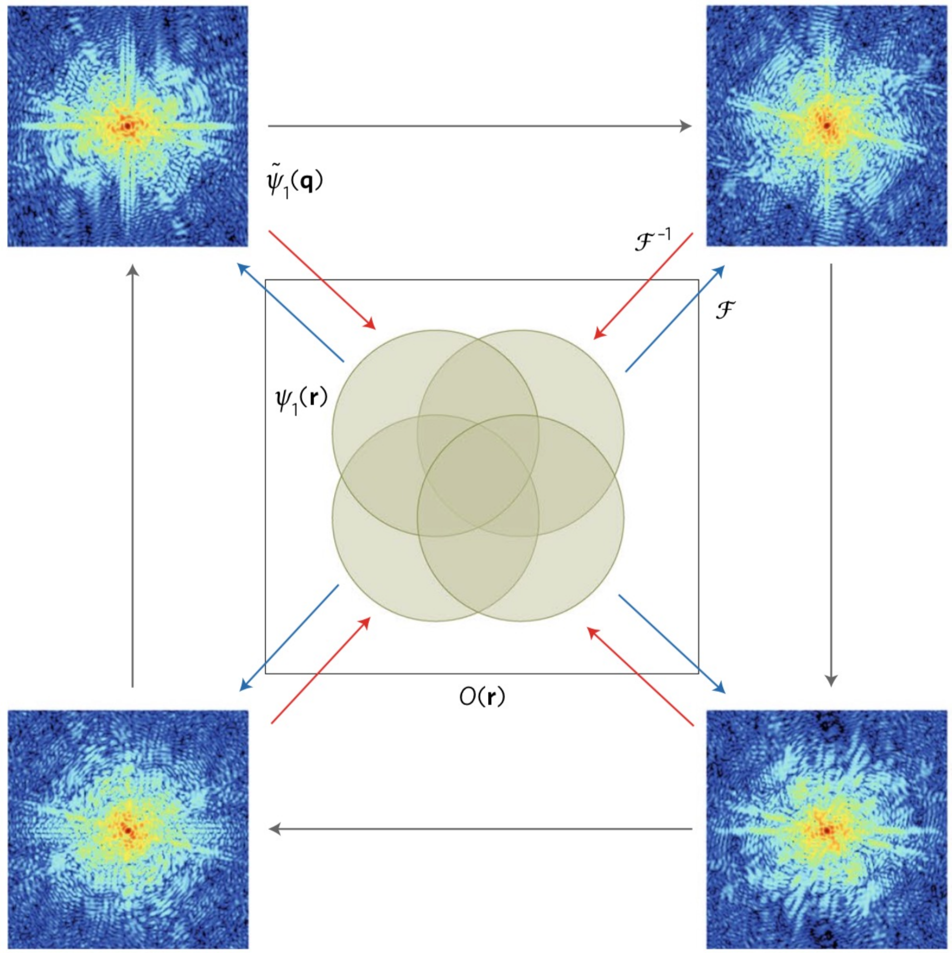
Support-based "Error Reduction" method



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

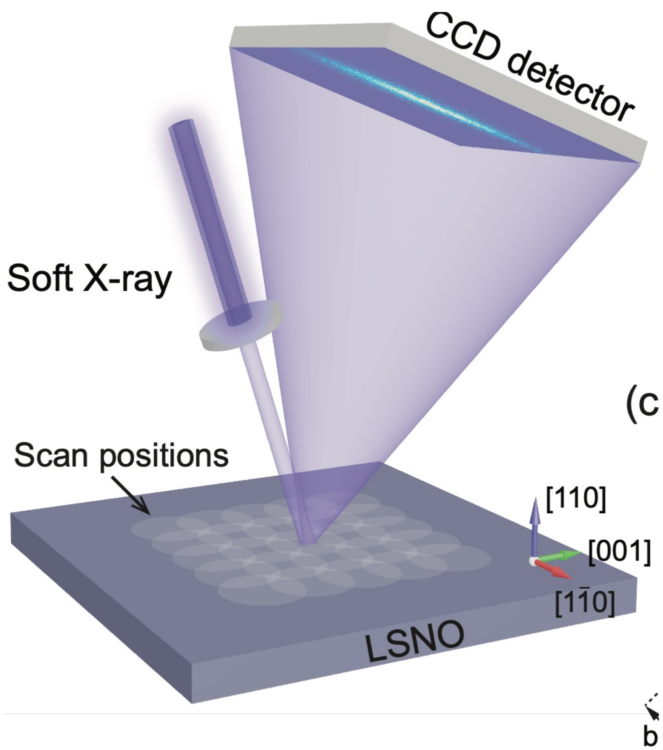
Ptychography Method

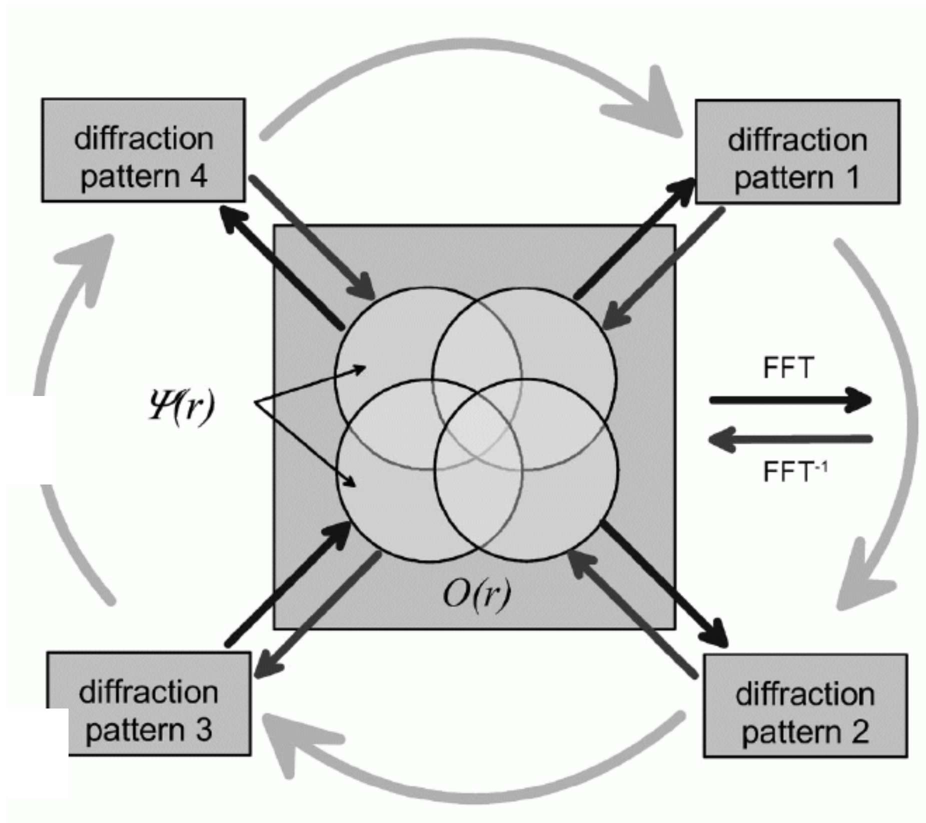
Franz Pfeiffer
Nature Photonics
12 9 (2018)



X-ray Bragg Pytchography

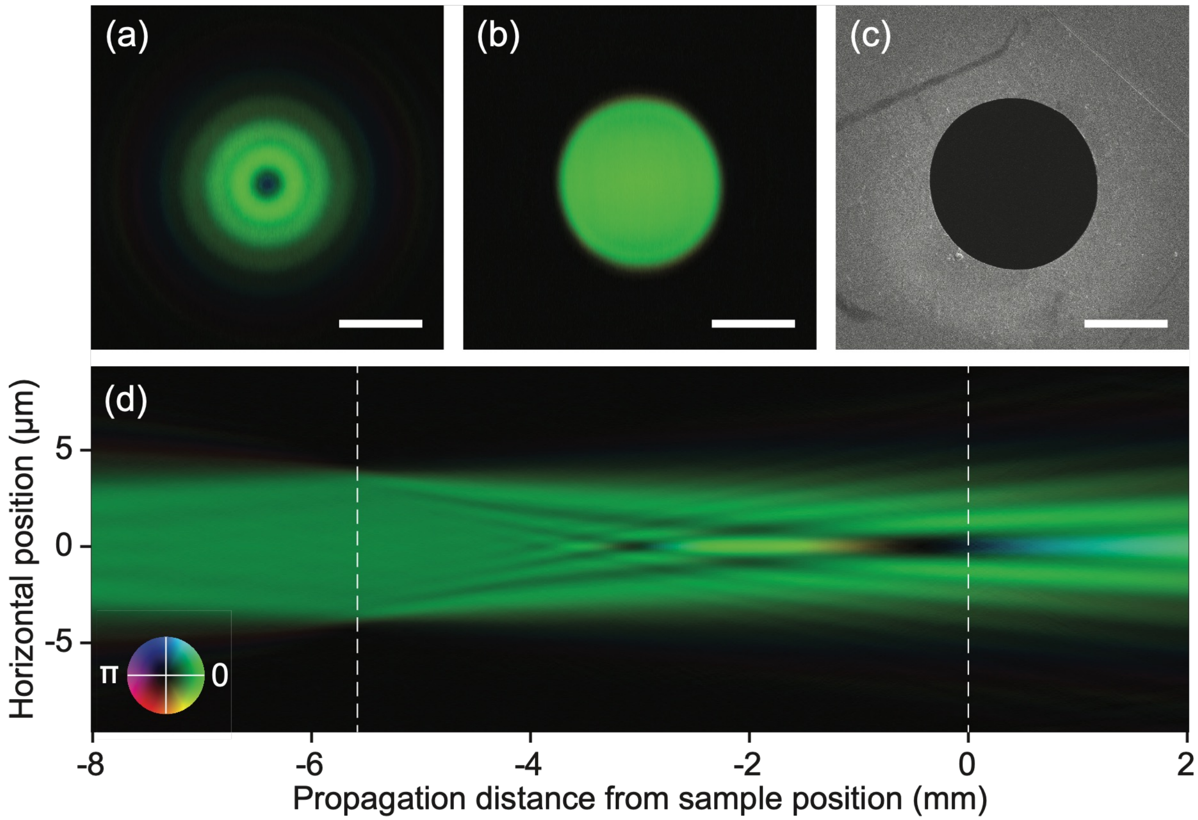
J. Rodenburg et al, PRL 98, 034801 (2007)





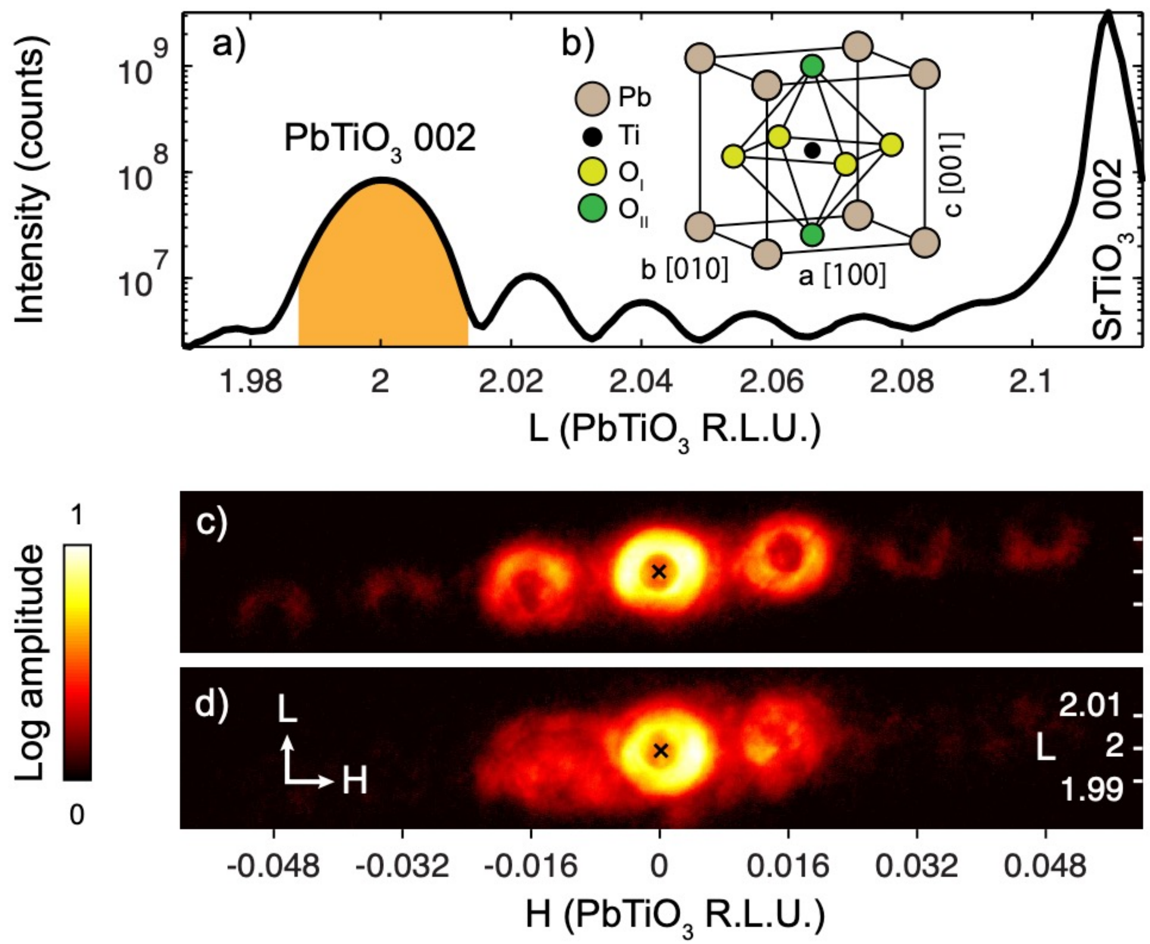
FIB-polished 8μm Pinhole

Longlong Wu, Yao Shen, et al Phys. Rev. Letts 127 275301 (2021)



$PbTiO_3$ thin film imaging by Bragg Ptychography

S. O. Hruszkewycz, et al Phys. Rev. Lett. 110, 177601 (2013)



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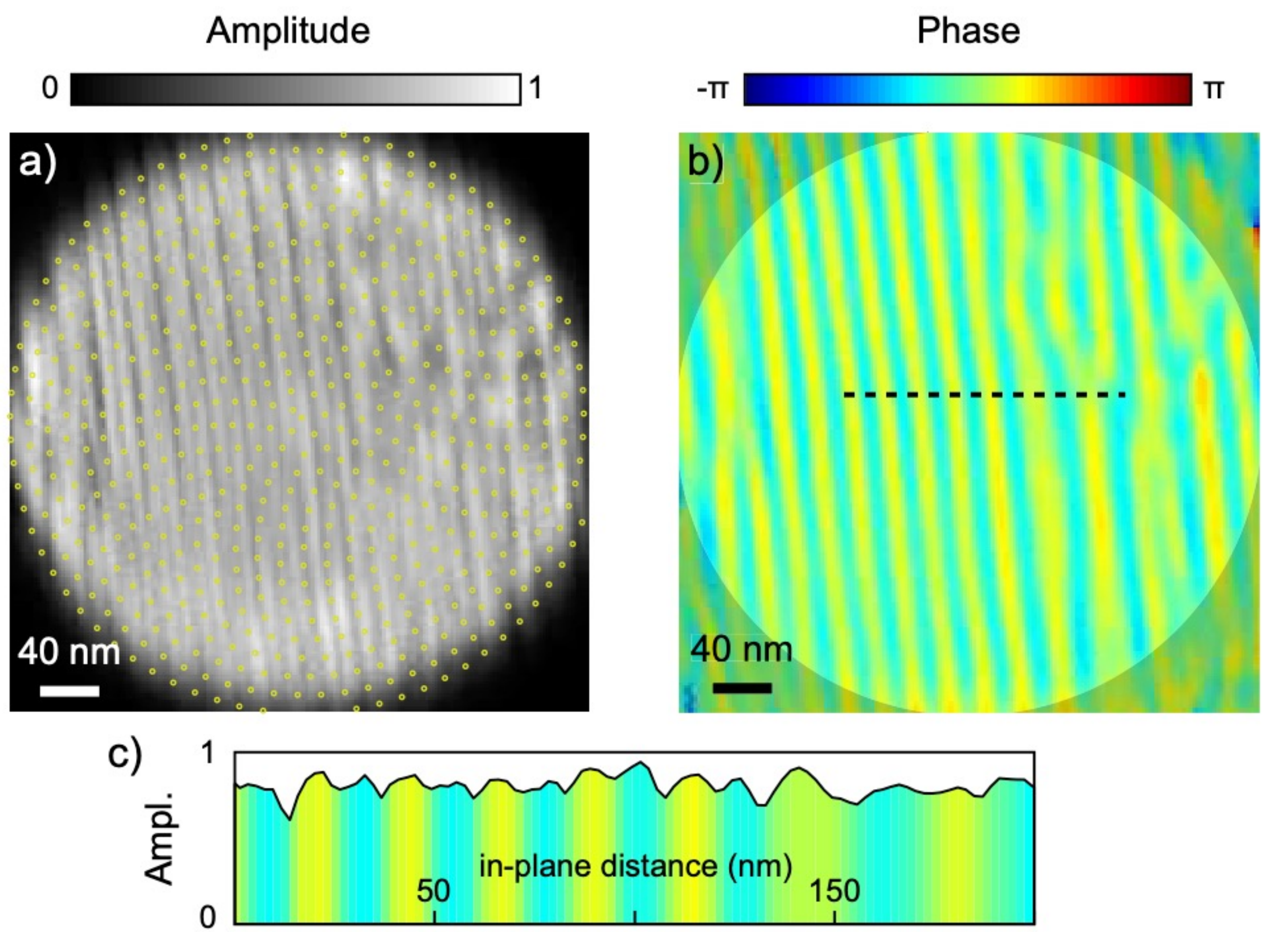

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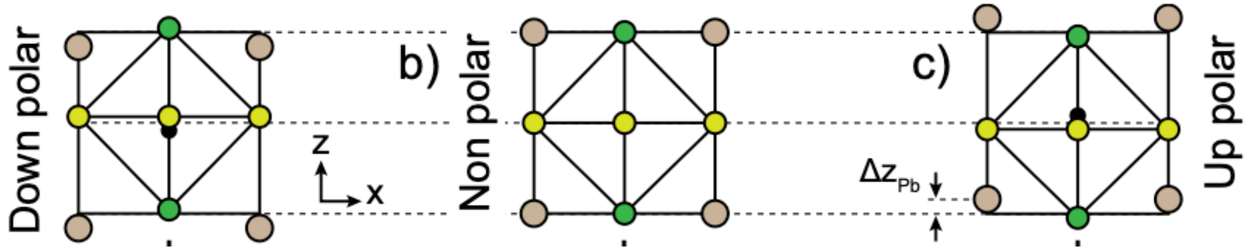
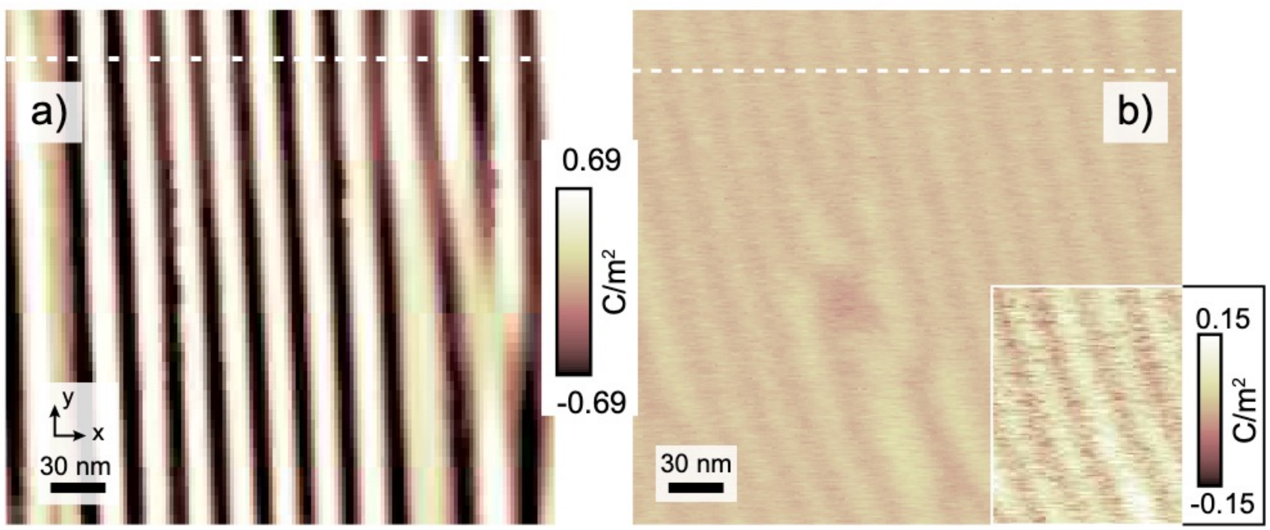
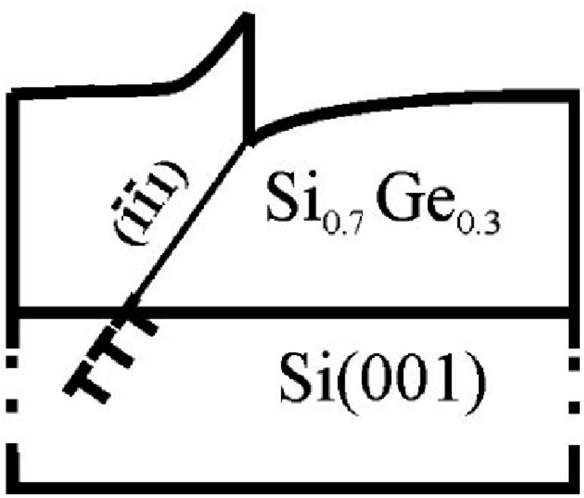
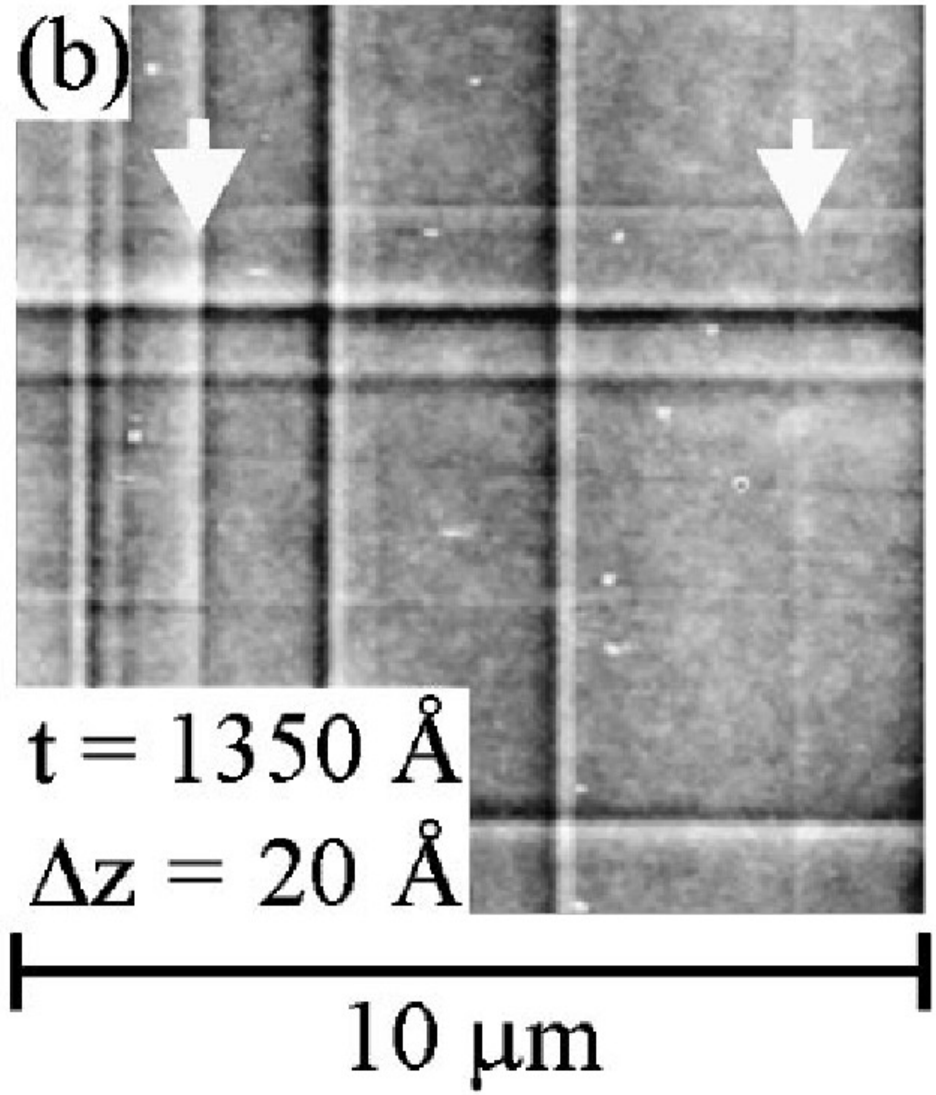




Ge$_{0.3}$Si$_{0.7}$/Si(100) thin films grown by CVD

T. Spila et al J. Appl. Phys 93 1918 (2003)





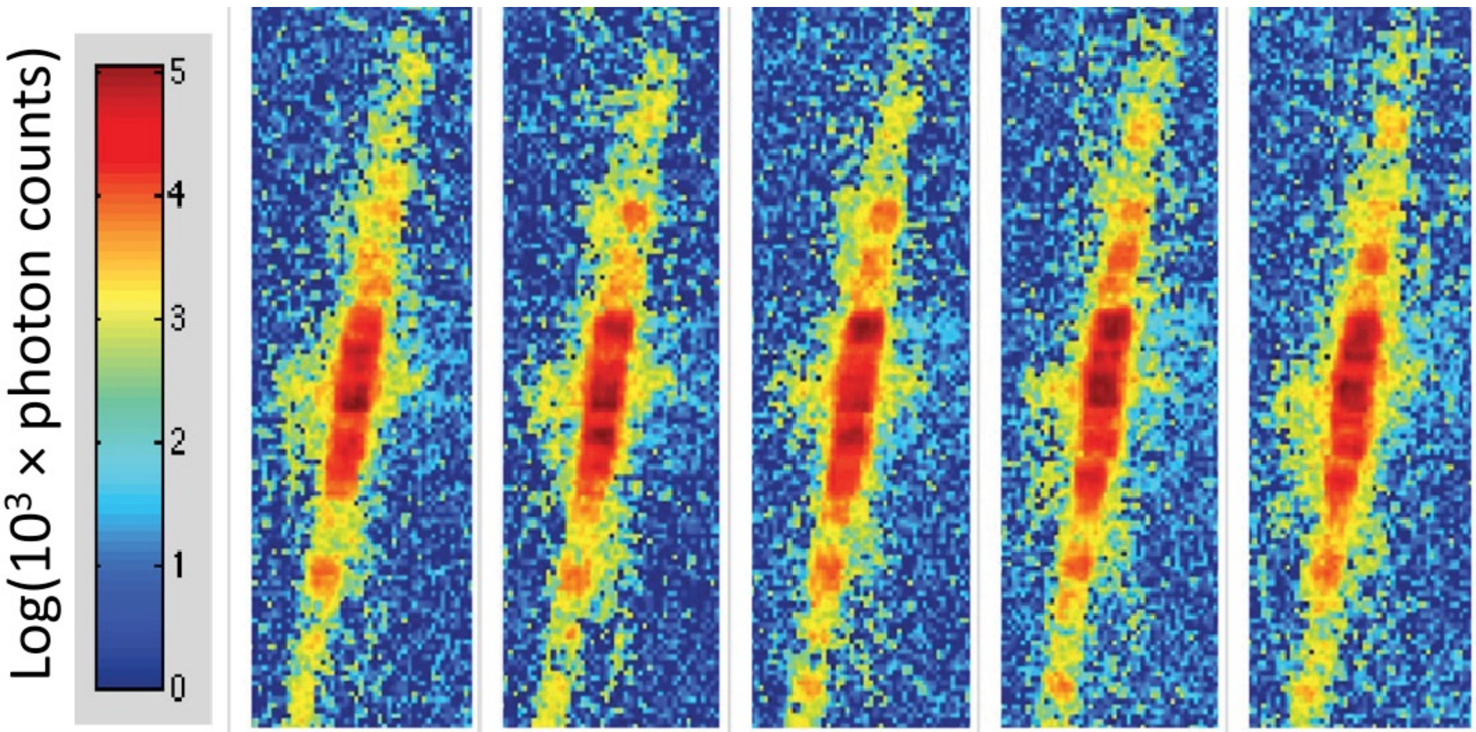
I. K. R

Ptychographic x-ray imaging of surfaces on crystal truncation rod

Chenhui Zhu … Hoydoo You, Appl Phys Lett 106 101604 (2015)

Pt(111) crystal with steps measured at [0, 0,1.5]

34-ID-C
83 positions
100 s expos



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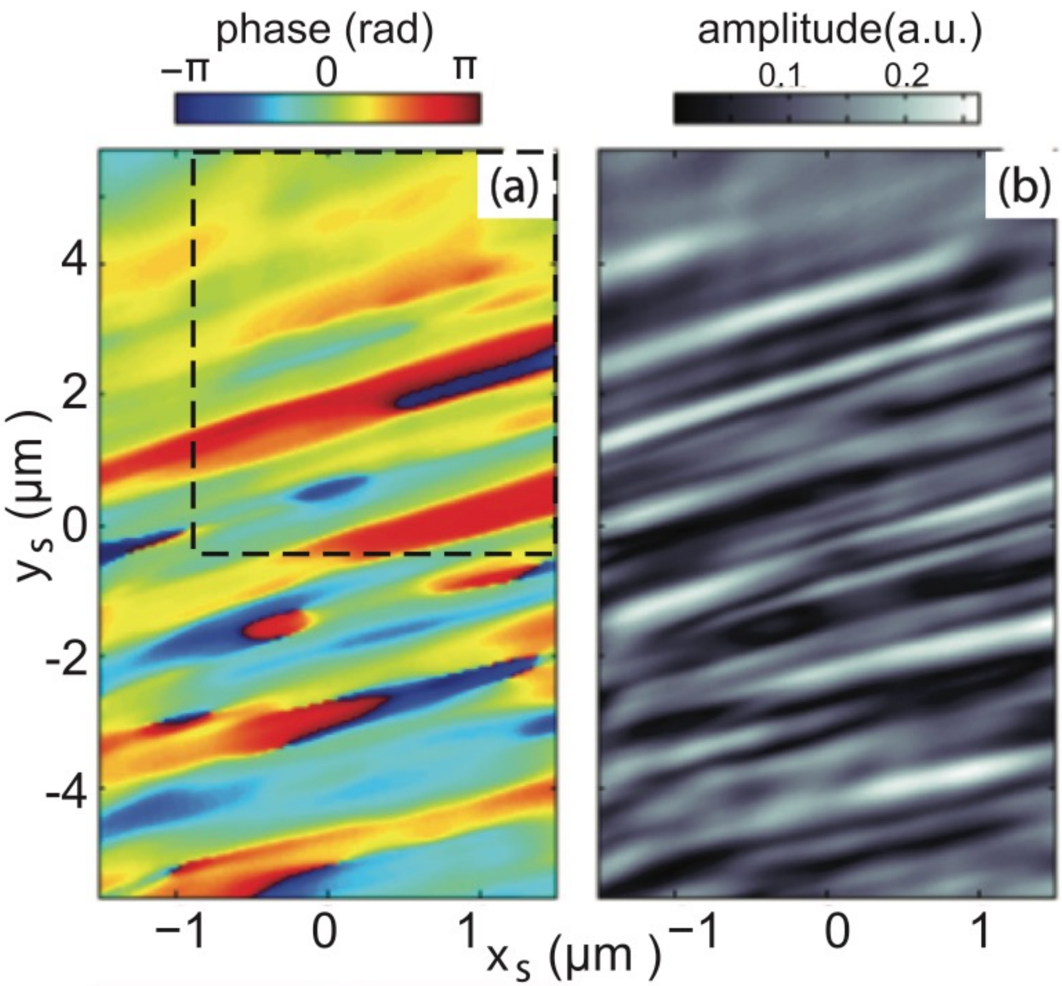
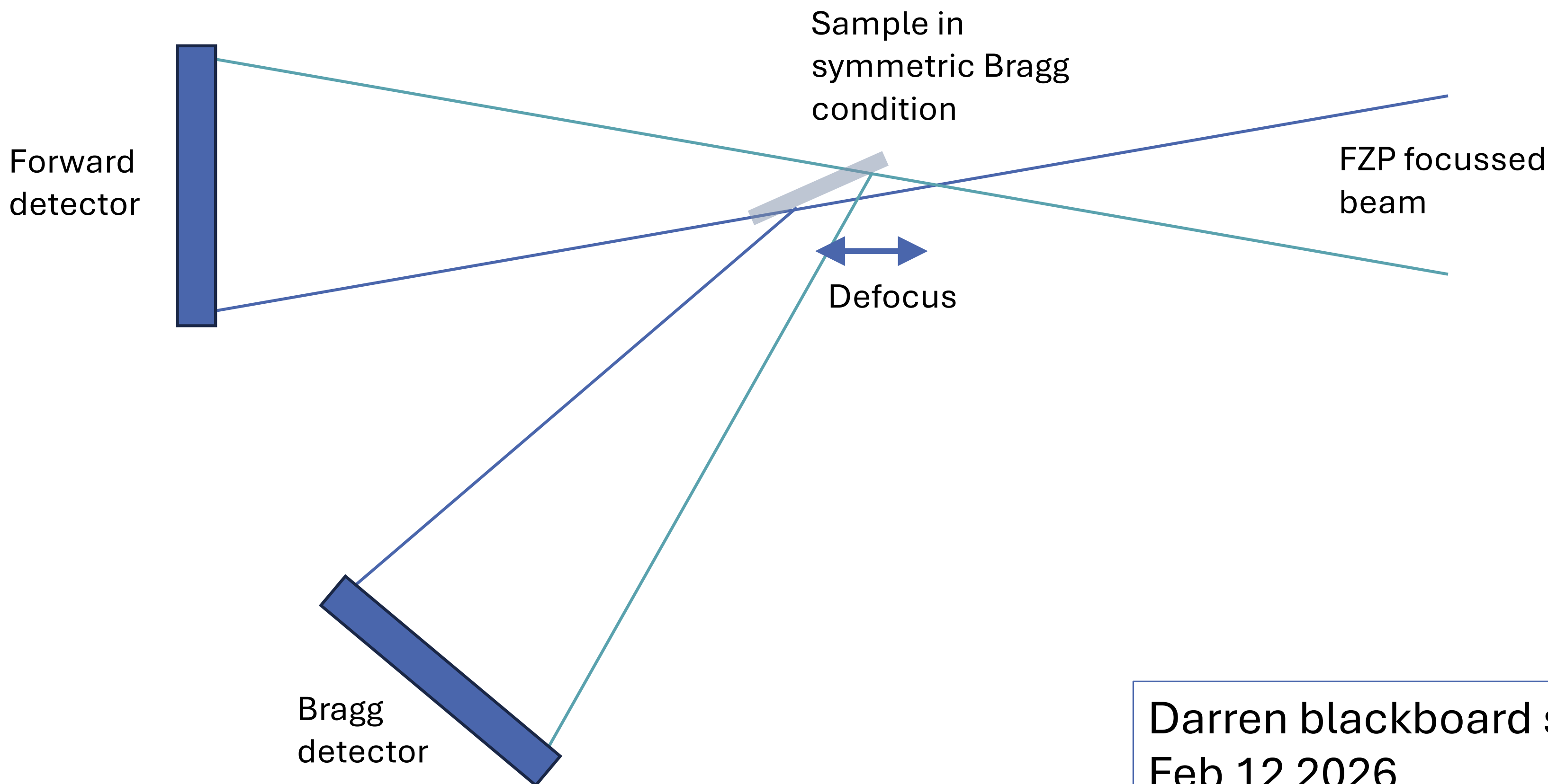
Appl Phys Lett
106 101604 (2015)

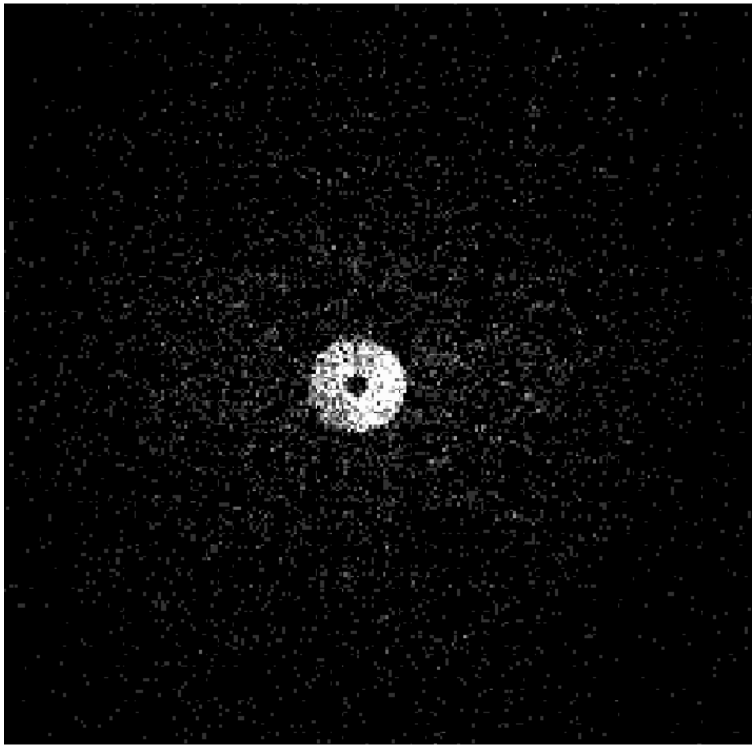


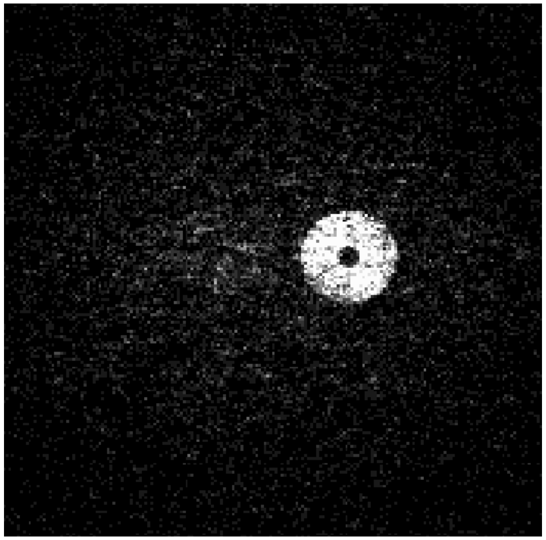
I-13 ptychography setup at Diamond Light Source



Darren blackboard sketch
Feb 12 2026

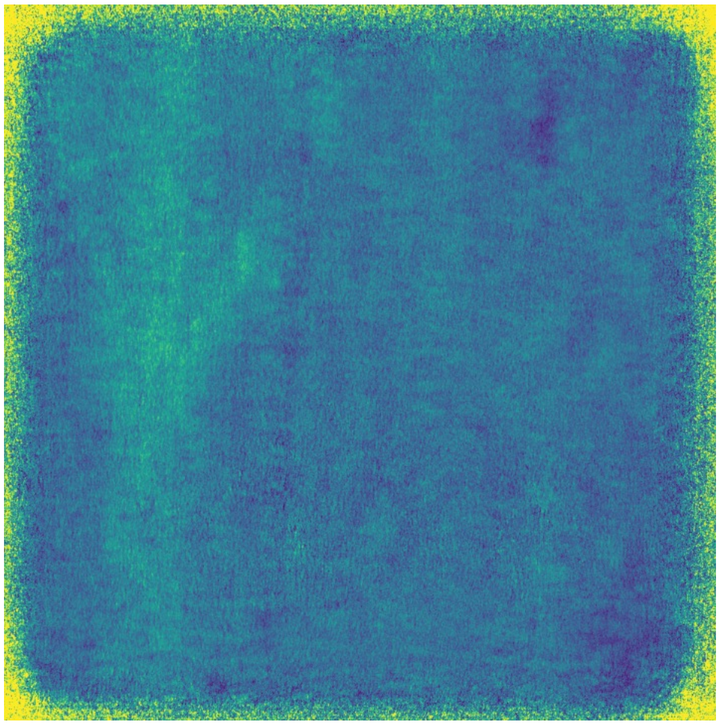
30 nm La_2CuO_4 thin film by atomic layer epitaxy
Two-component Diffraction Patterns

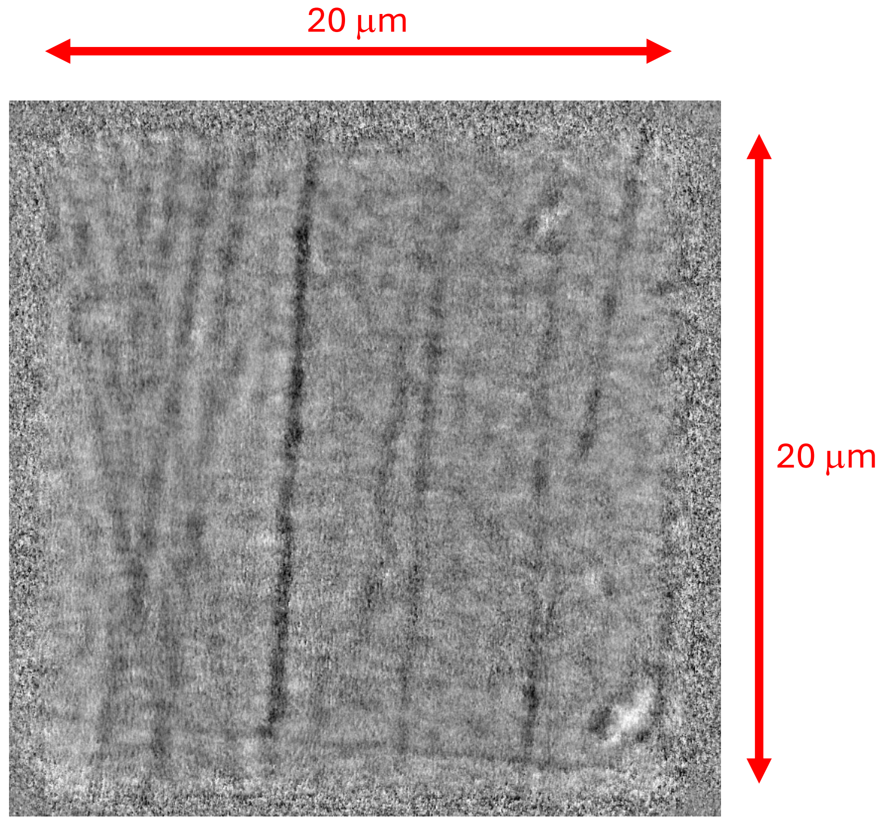




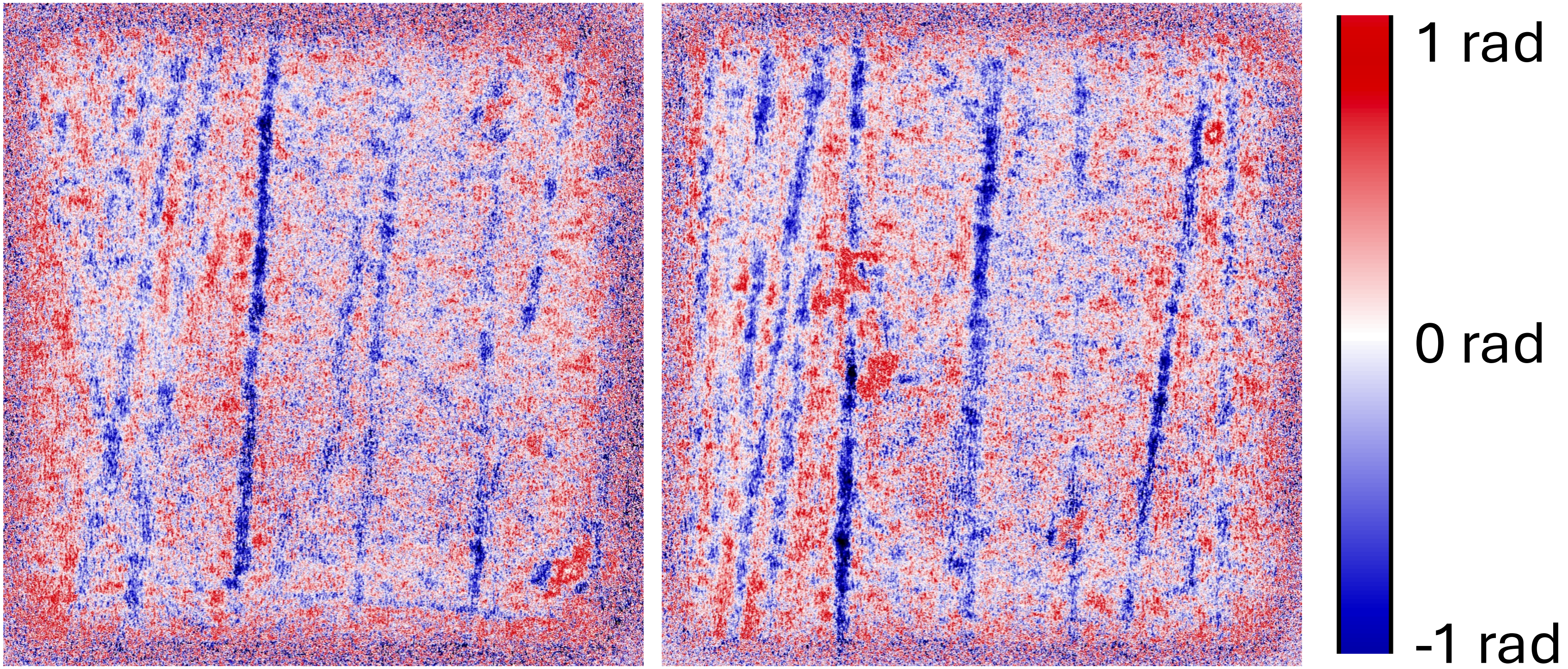
30 nm La_2CuO_4 thin film amplitude and phase

Image in forward forward direction

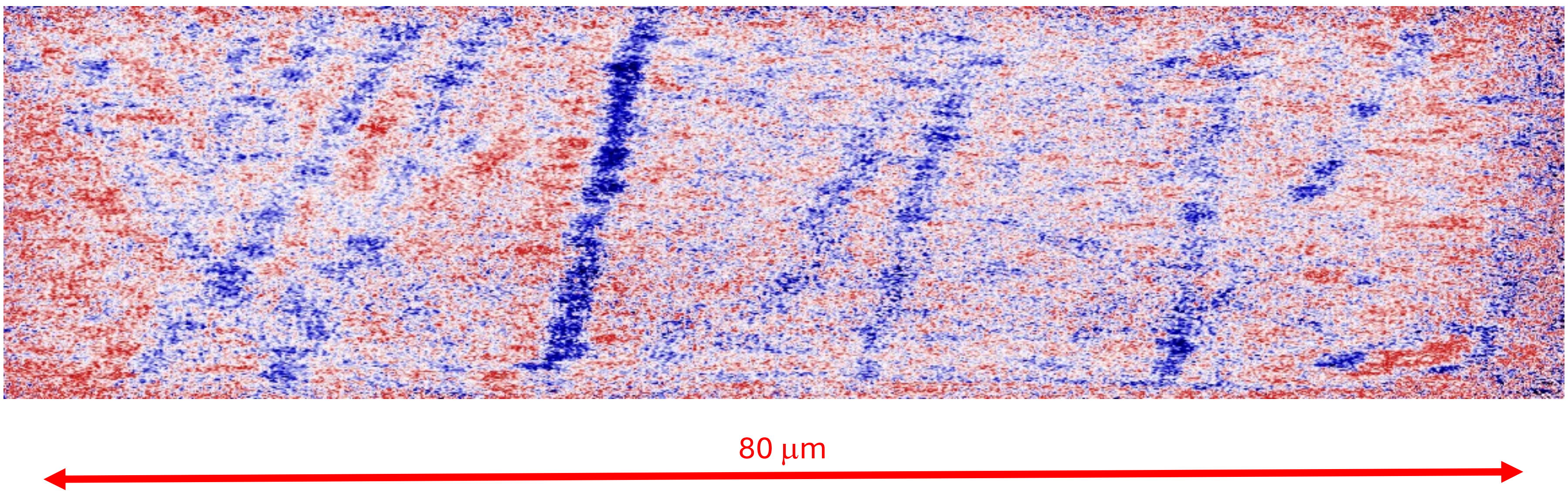




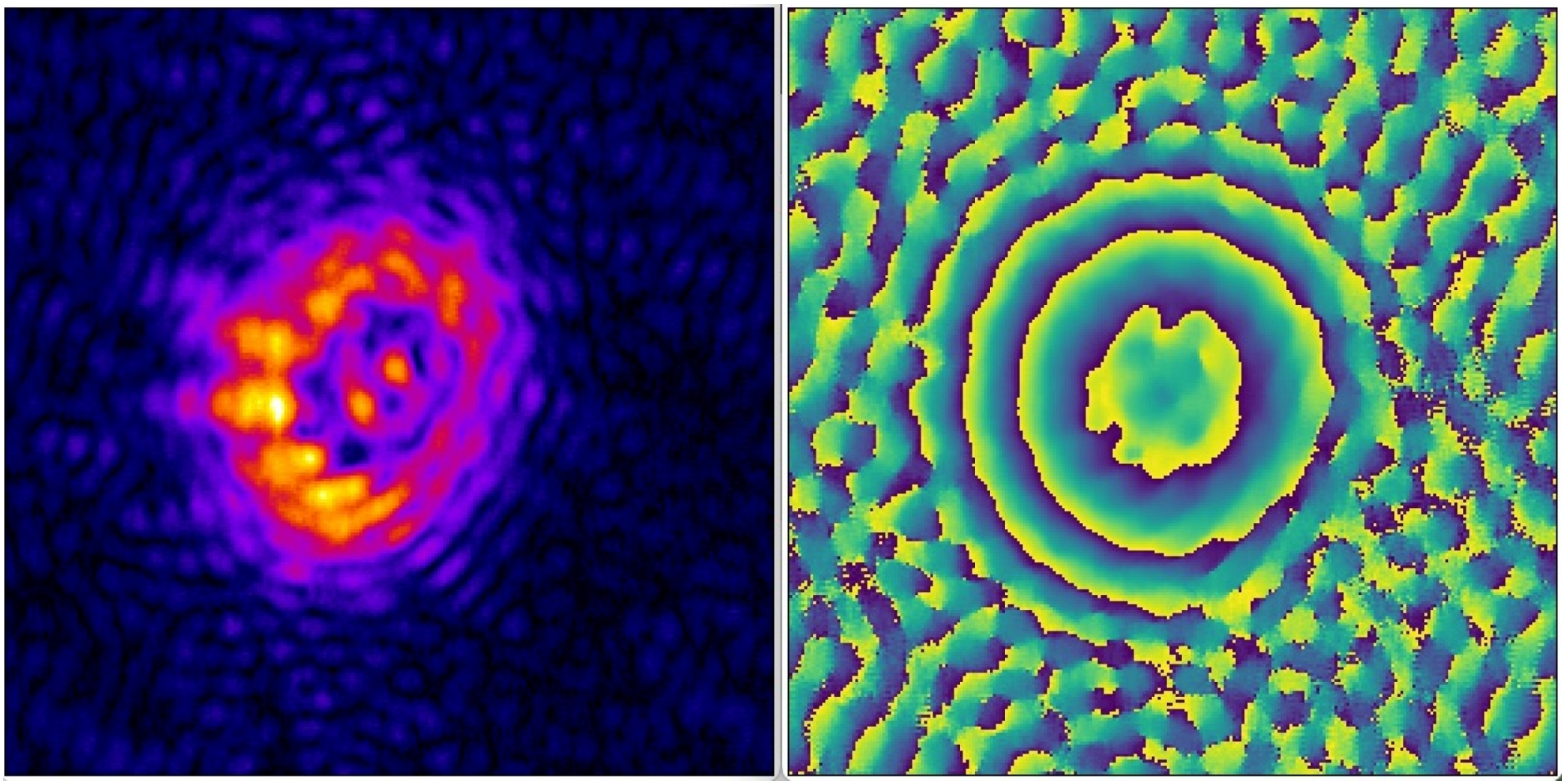
30 nm La_2CuO_4 thin film regions phase images



Stretch 4x to transform to film coordinates



Refined Probe from BP data using ePIE

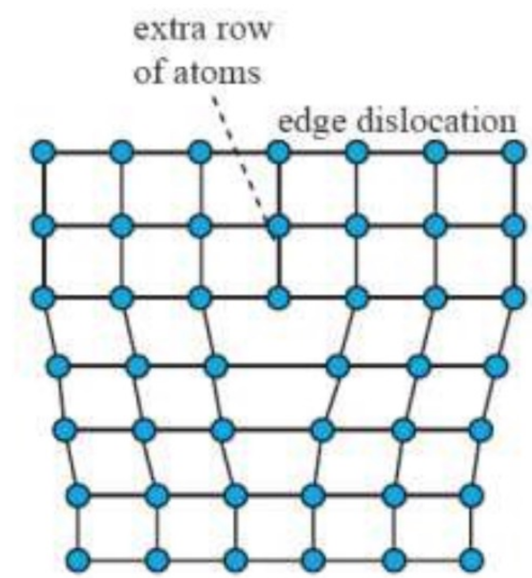


Edge dislocation. Plane inserted in y-direction

“Theory of Dislocations” J. P. Hirth and J. Lothe

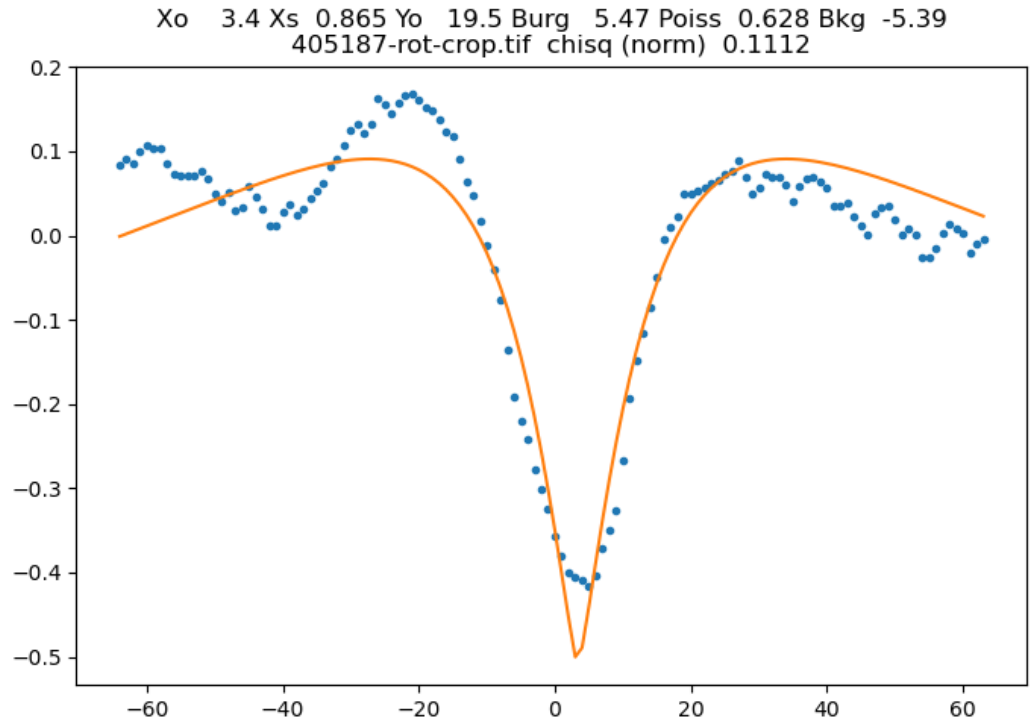
- **Displacement Field Formula:** The displacement u is given by with components:
  - $u_x = \frac{b}{2\pi}\left[\tan^{-1}\frac{y}{x} + \frac{xy}{2(1-\nu)(x^2+y^2)}\right]$
  - $u_y = -\frac{b}{2\pi}\left[\frac{1-2\nu}{4(1-\nu)}\ln(x^2+y^2) + \frac{x^2-y^2}{4(1-\nu)(x^2+y^2)}\right]$

  where ν is Poisson's ratio, and x, y are coordinates from the

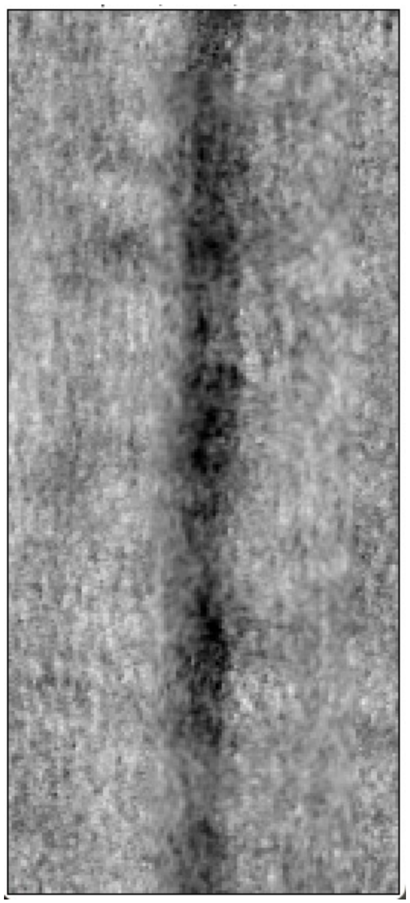


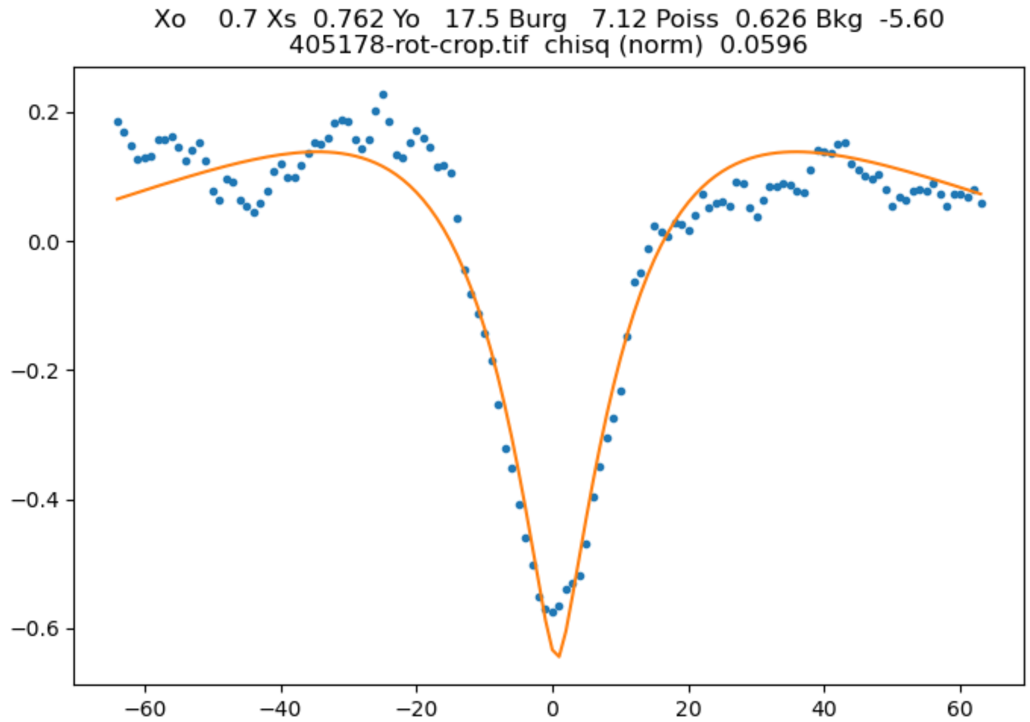
We fit the phase of sum(exp(iu_y)) over 60 layers in y
x is offset and scaled
y is offset, but starts near center of slab

Projection of $\exp(iQ.u_y)$ across film thickness

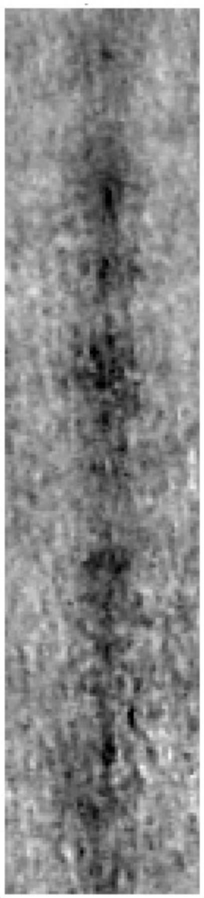


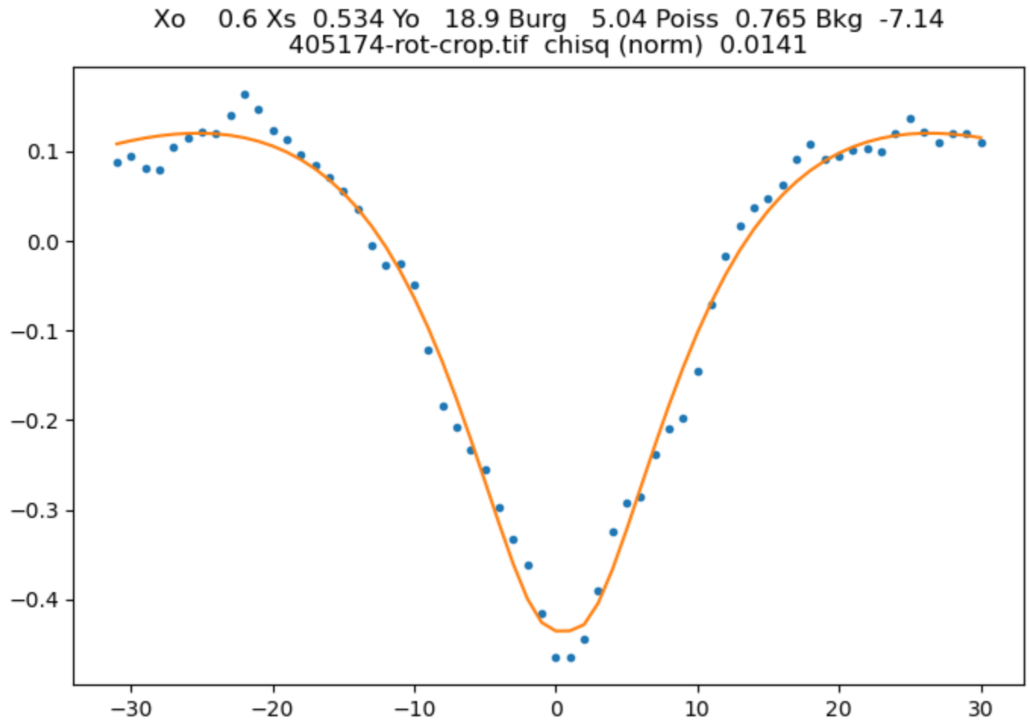
Projection of exp(iQ.u_y) across film thickness



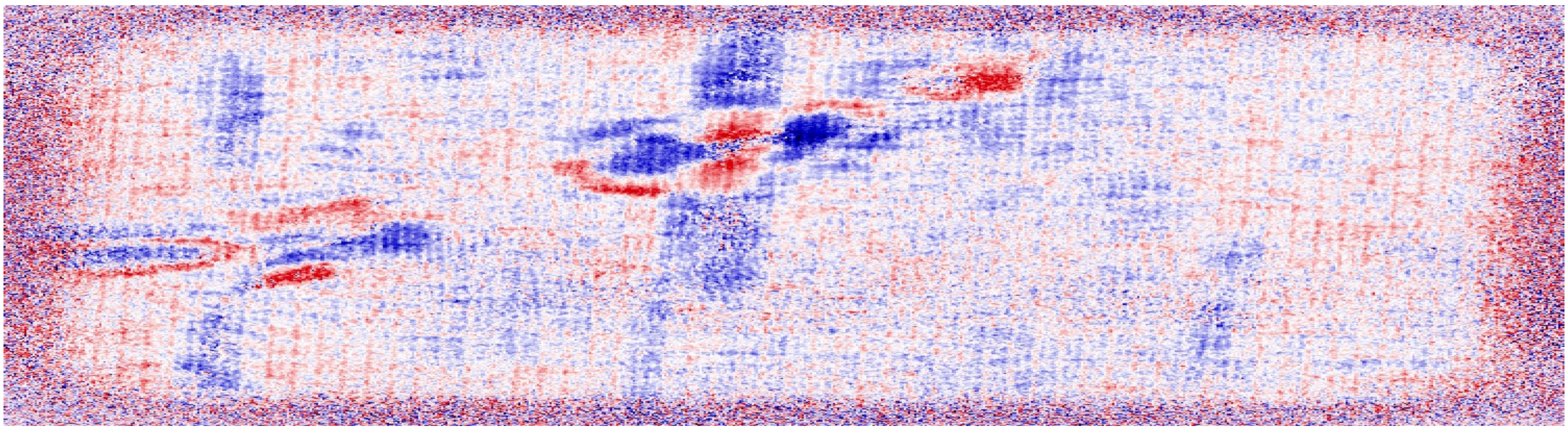


Projection of $\exp(iQ.u_y)$ across film thickness





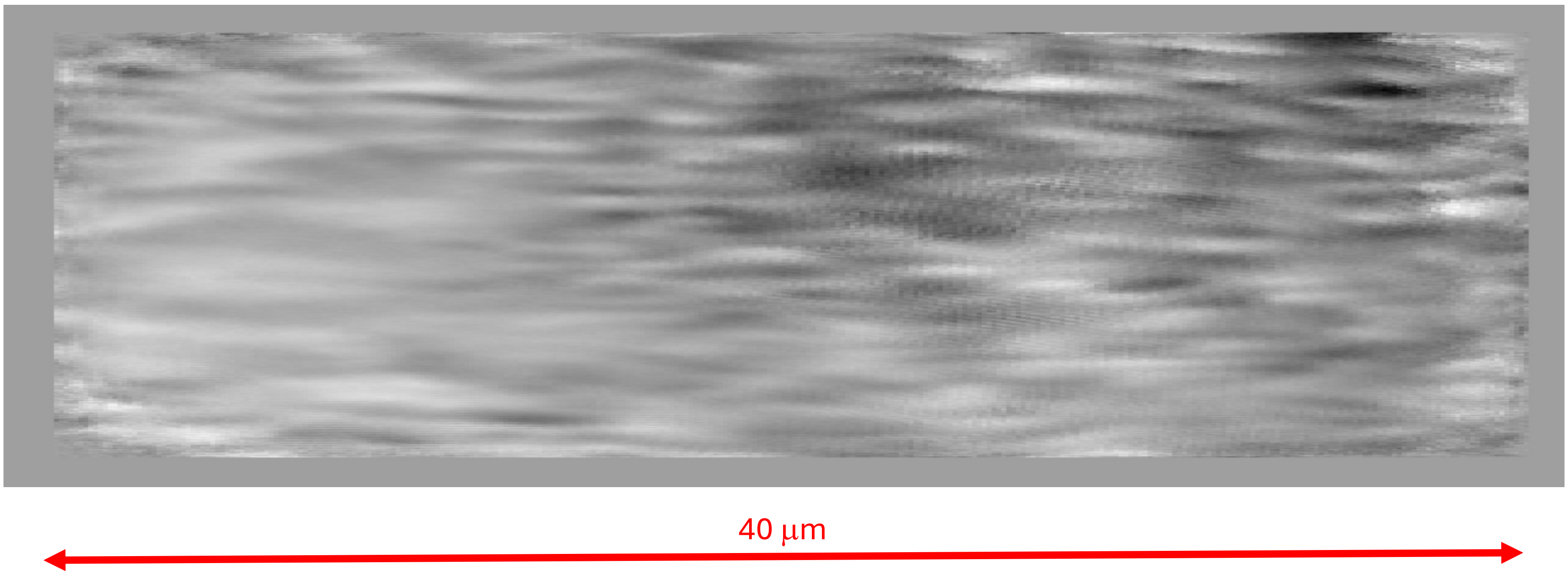
La_2CuO_4 thin film on LSAO substrate
- scan 405081 stretch 4x



60 μm

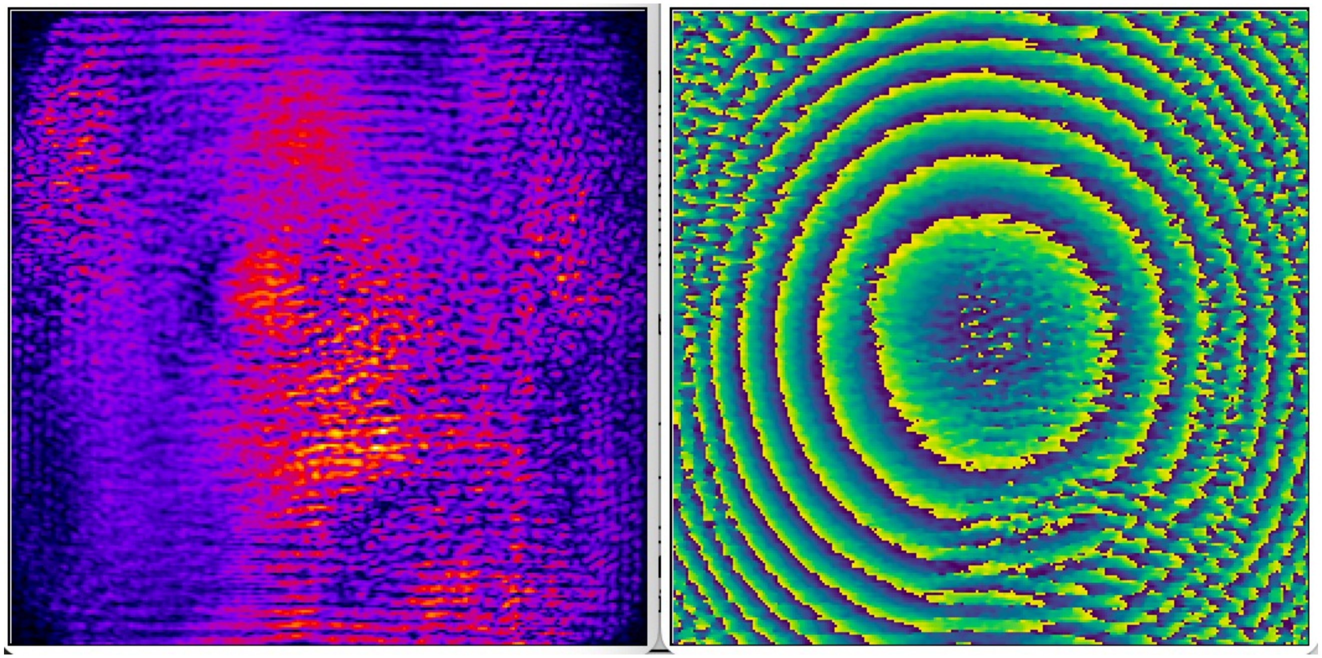
Nb(110) thin films on Sapphire by MBE

scan 404974

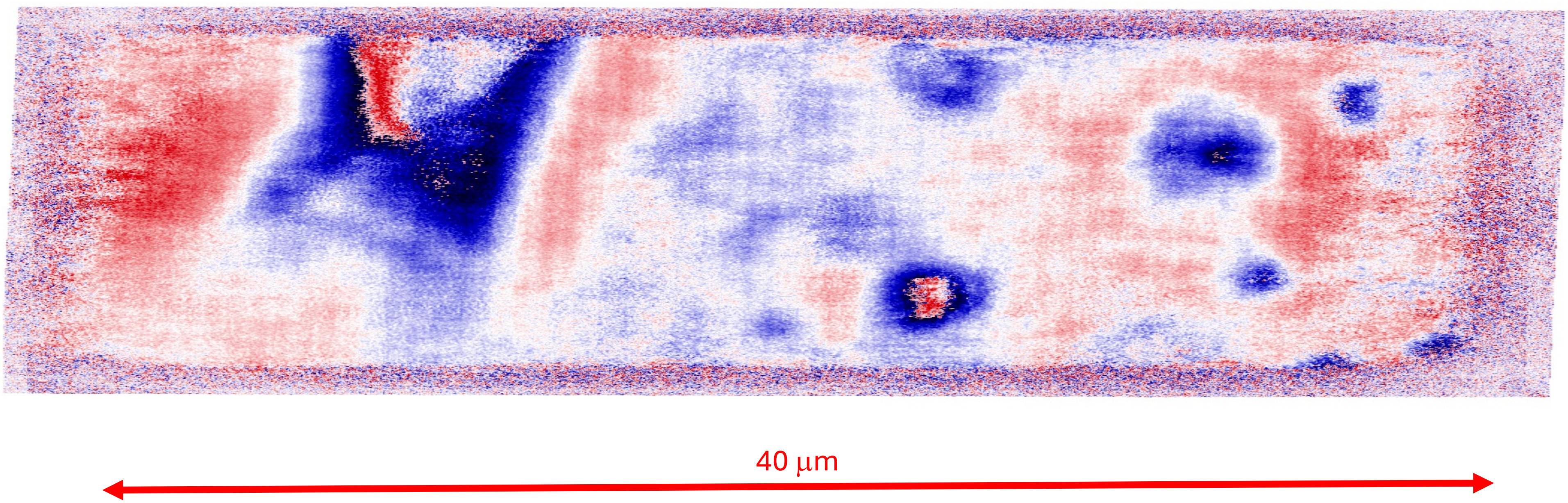


Nb(110) thin films on Sapphire by MBE

scan 404974



$La_{2-x}Sr_xCuO_4$ thin film on LSAO substrate
- scan 405065 stretch 4x



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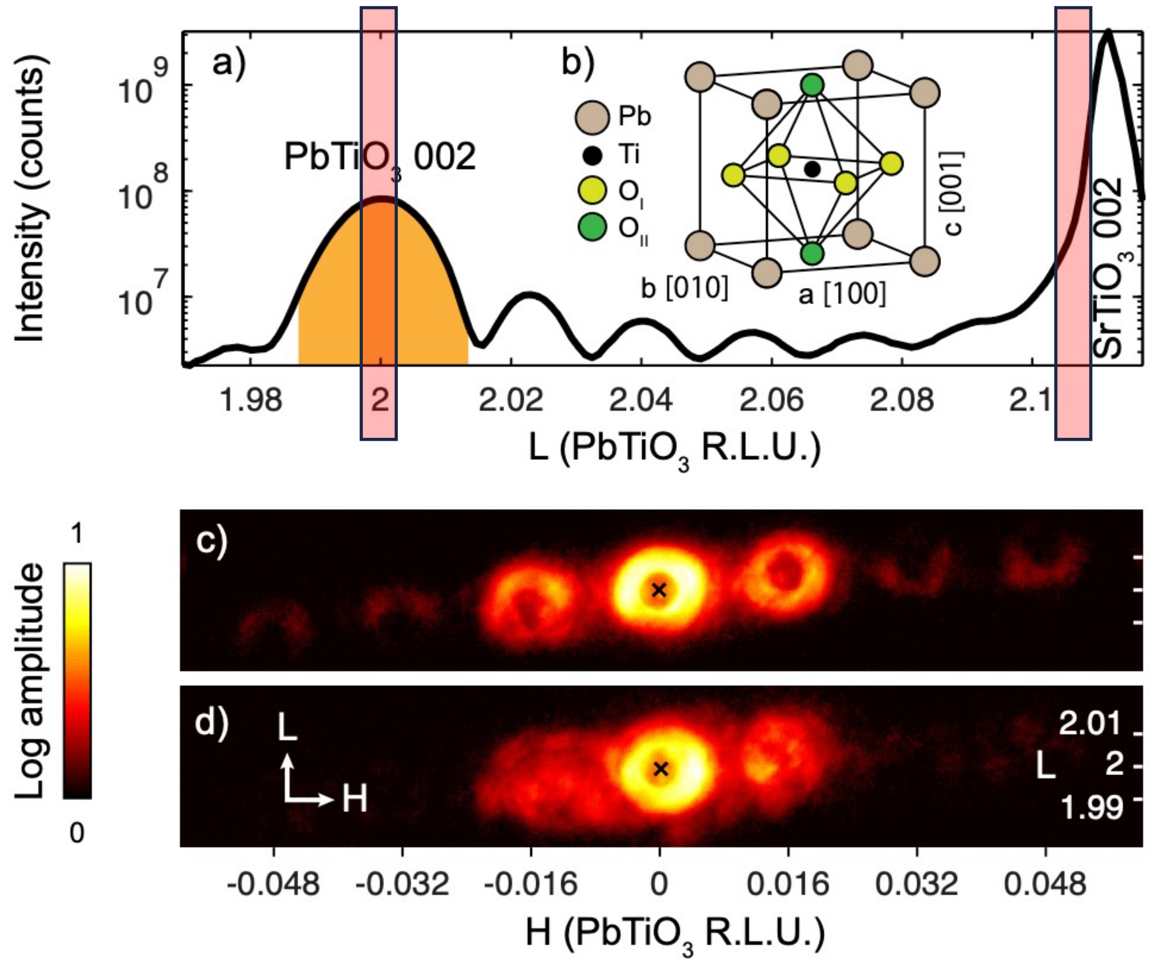
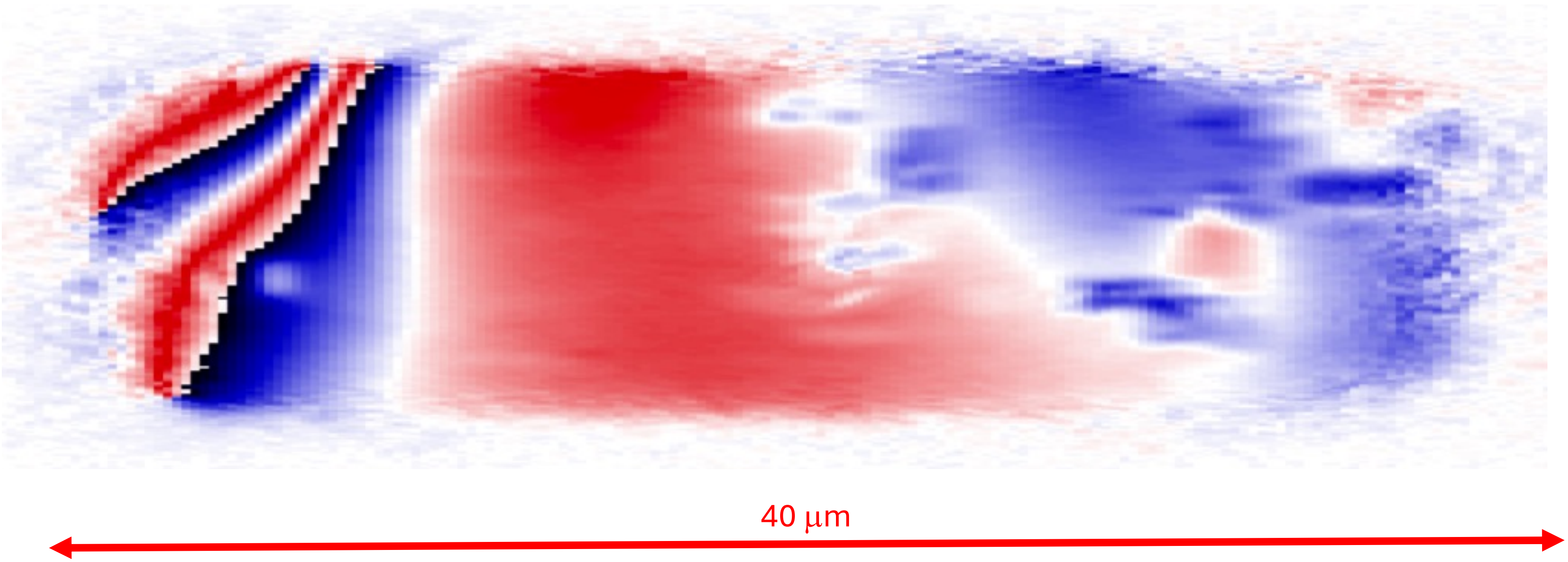
S. O. Hruszkewycz, et al Phys. Rev. Lett. 110, 177601 (2013)

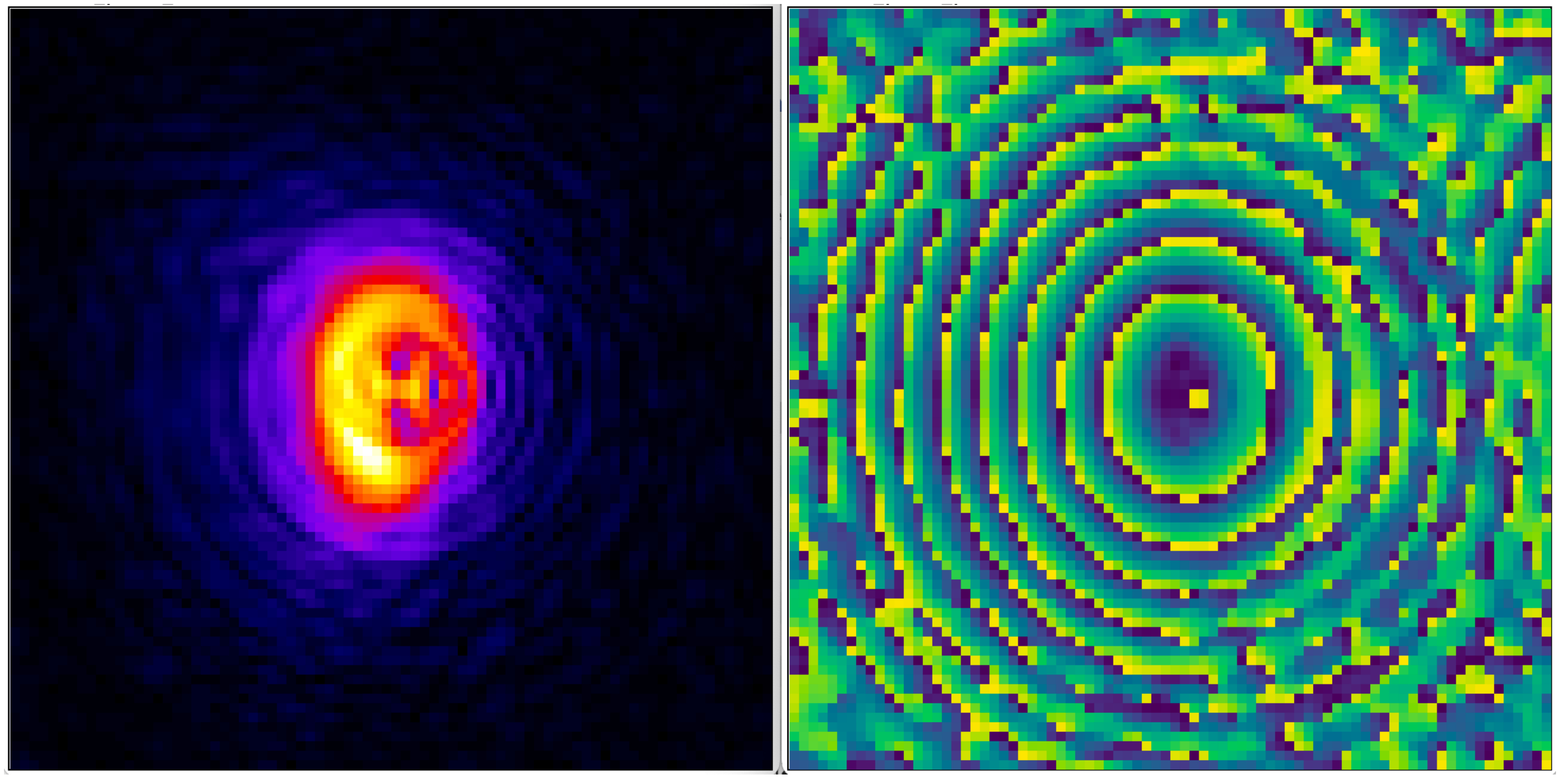


CTR of STO/La_2NiO_4 interface
- scan 405109



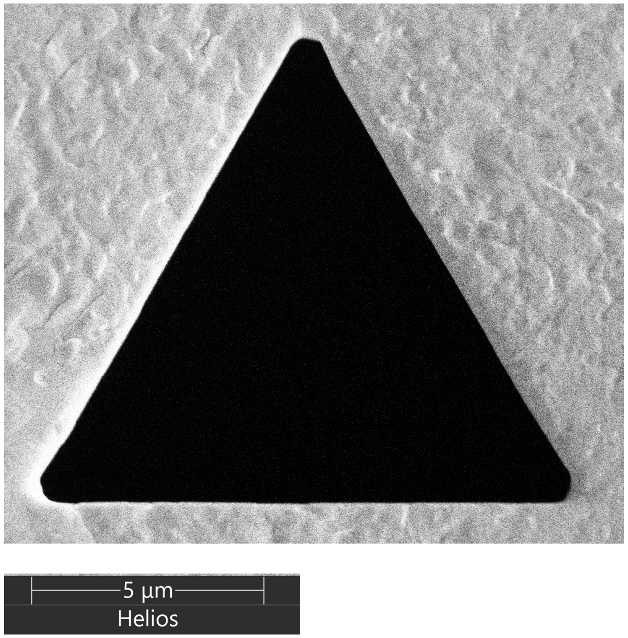
CTR of STO/La_2NiO_4 interface probe

- scan 405109



Future Directions of CTR imaging

- in-situ crystal growth
- Electrochemical cells
- Time domain study
- Single Shot imaging by BCDI



Conclusions

- Crystal Trucation Rods and SXNS
- Coherent Diffraction Imaging by Ptychography
- Bragg Ptychography
- Imaging of Thin Films and Interfaces
- Future applications to in-situ, time domain
- Future possiblity of Single Shot imaging.

Acknowledgements

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Office of Science

LCN LONDON CENTRE FOR NANOTECHNOLOGY

diamond

Brookhaven National Laboratory