

# Opportunities for Advanced Materials and Nanotechnology

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LCLS

PAL-XFEL

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UK X-ray FEL Science Case

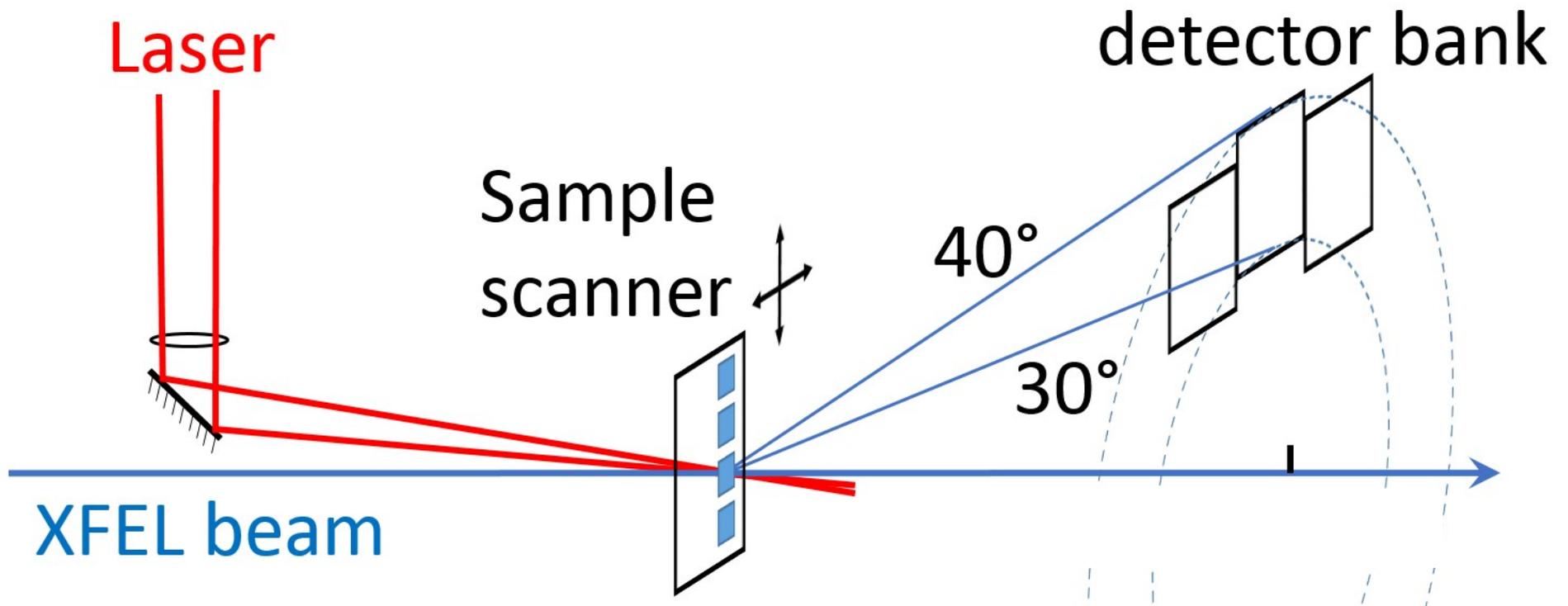
The Royal Society

London, July 2019

# Outline

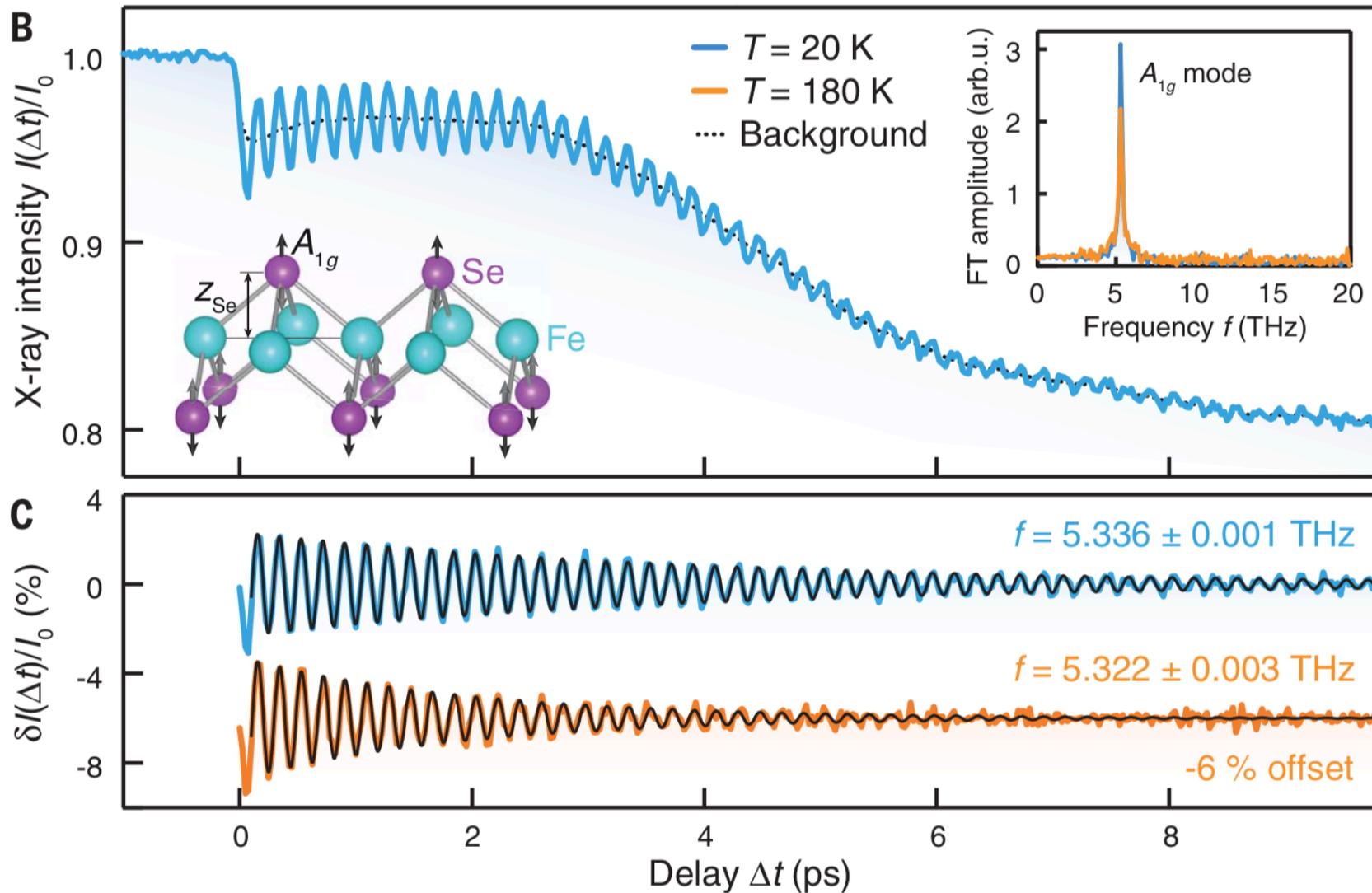
- Pump-probe method
- Excitations in the time domain
- Bragg Coherent Diffraction Imaging
- Evolution of nanoparticle strain
- Ultrafast melting of gold films

# Pump-probe Method using Sample Scanner



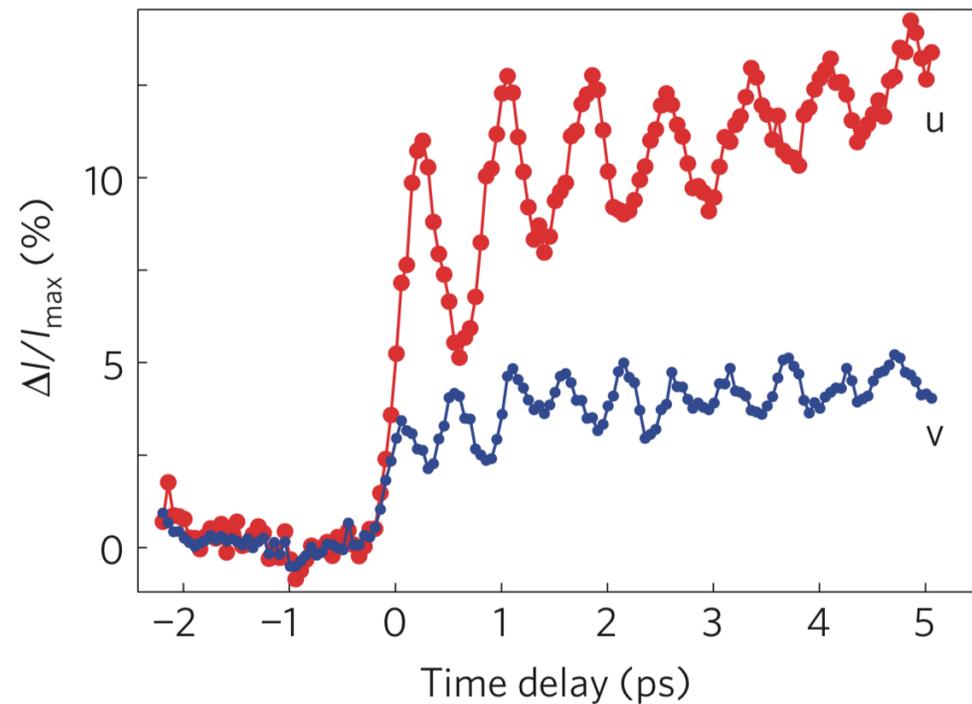
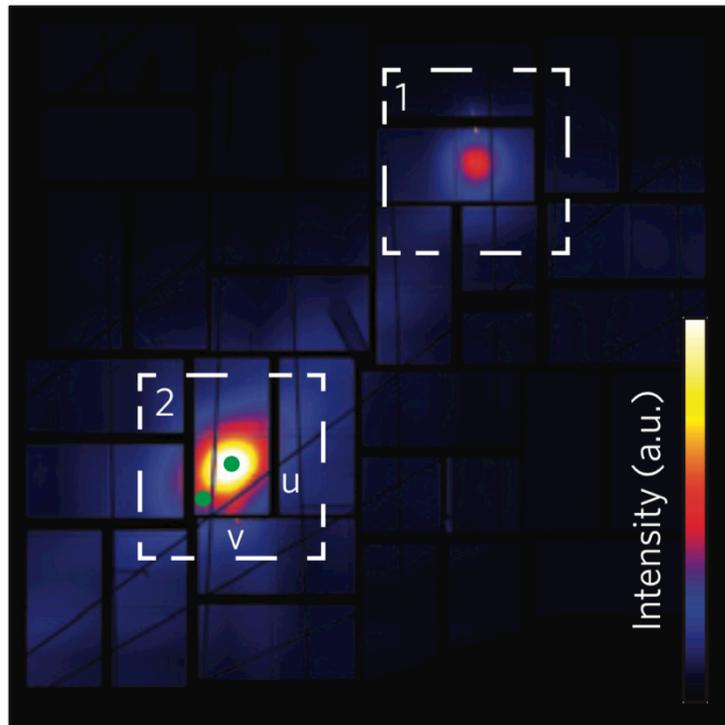
# Zone-Centre Optical Phonon in FeSe

S. Gerber et al., Science 357 71–75 (2017)

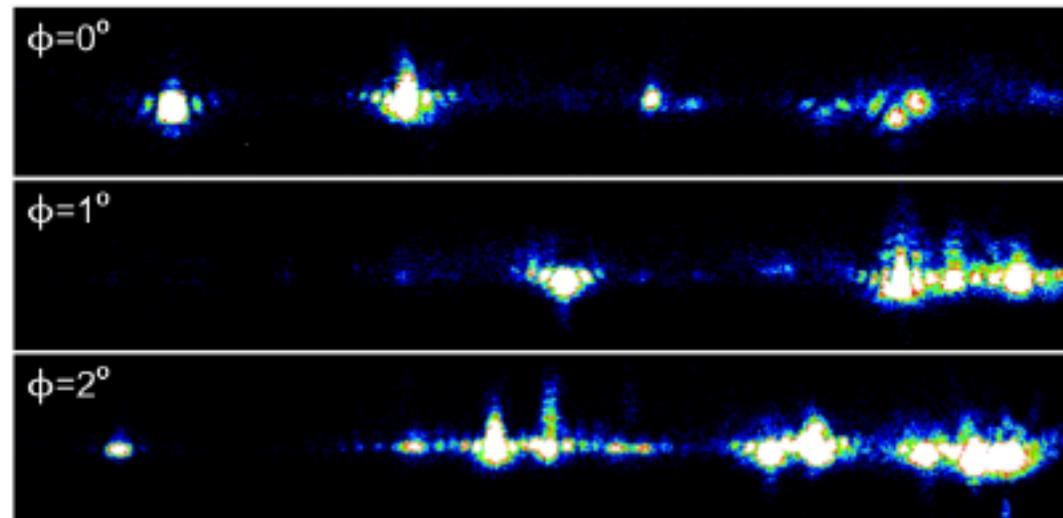
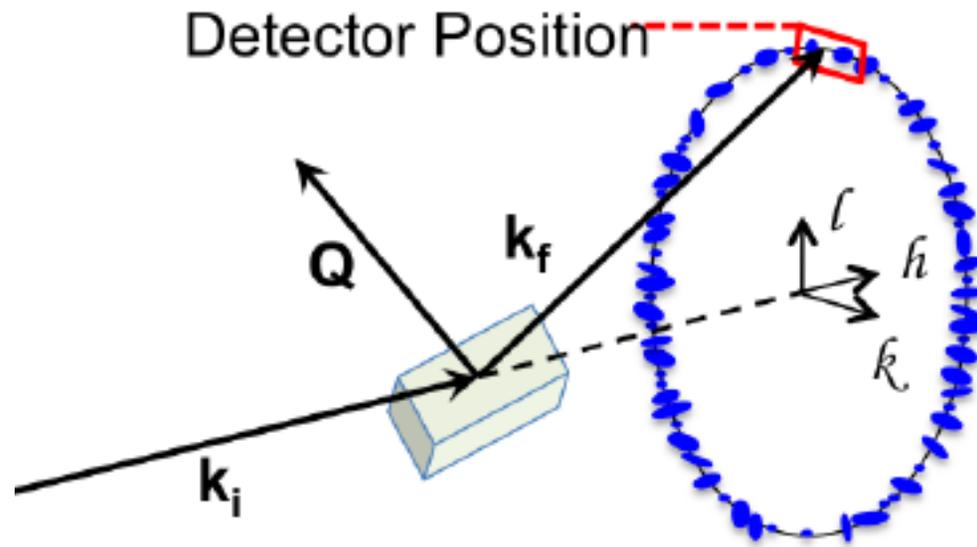


# Phonon Dispersion in Ge by FT-IXS

M. Trigo et al, Nat. Phys. 9 790 (2013)

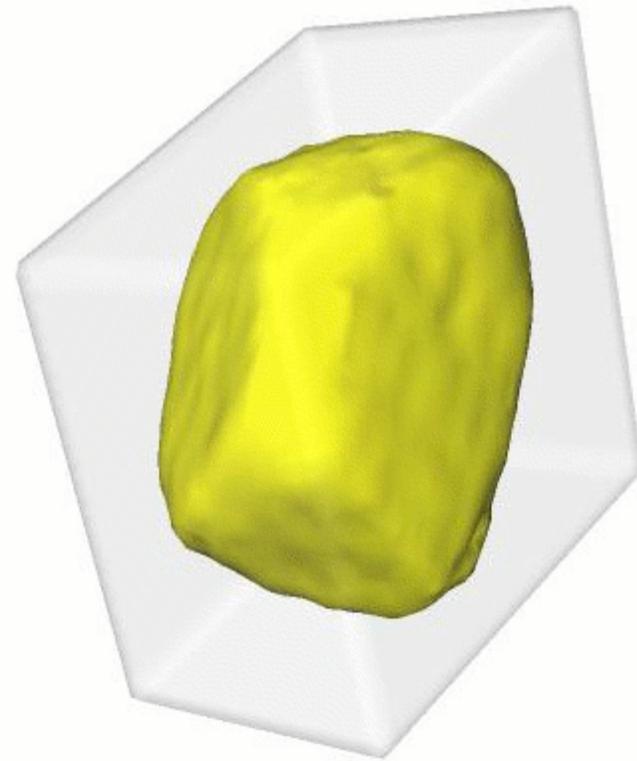
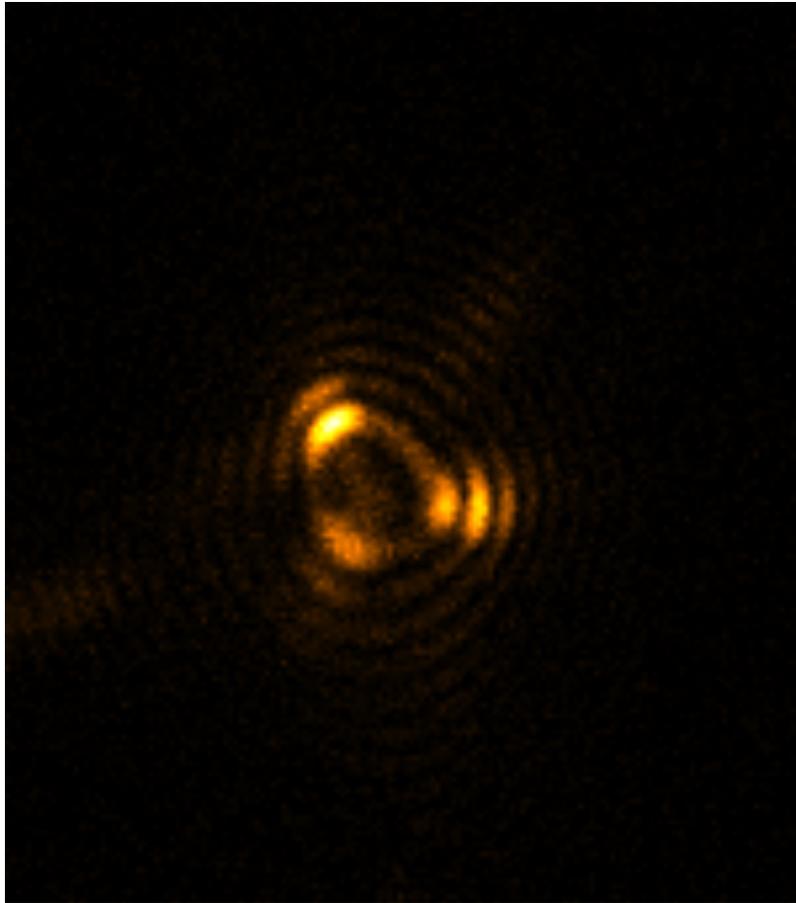


# Bragg Coherent Diffraction Imaging (BCDI)

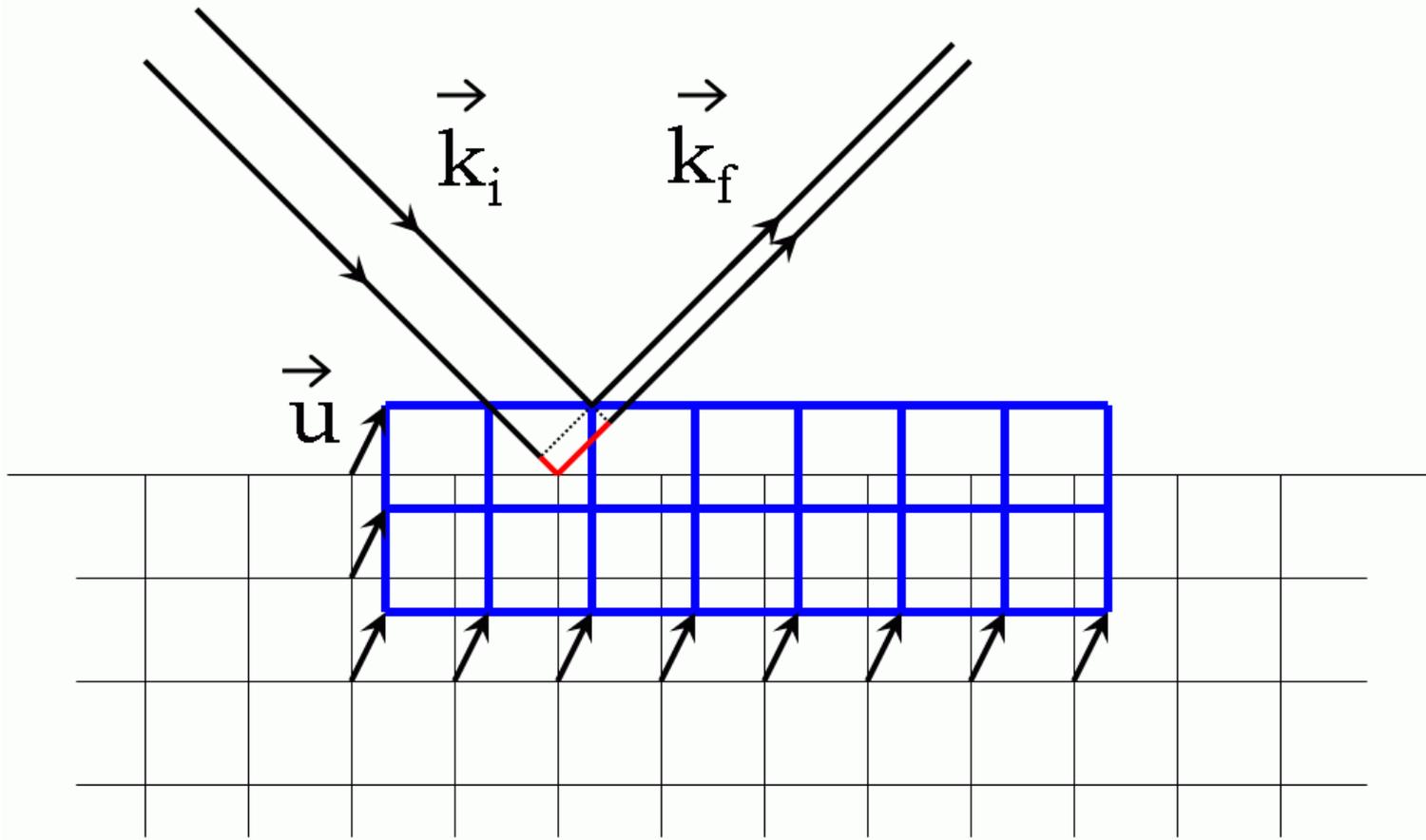


# Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER

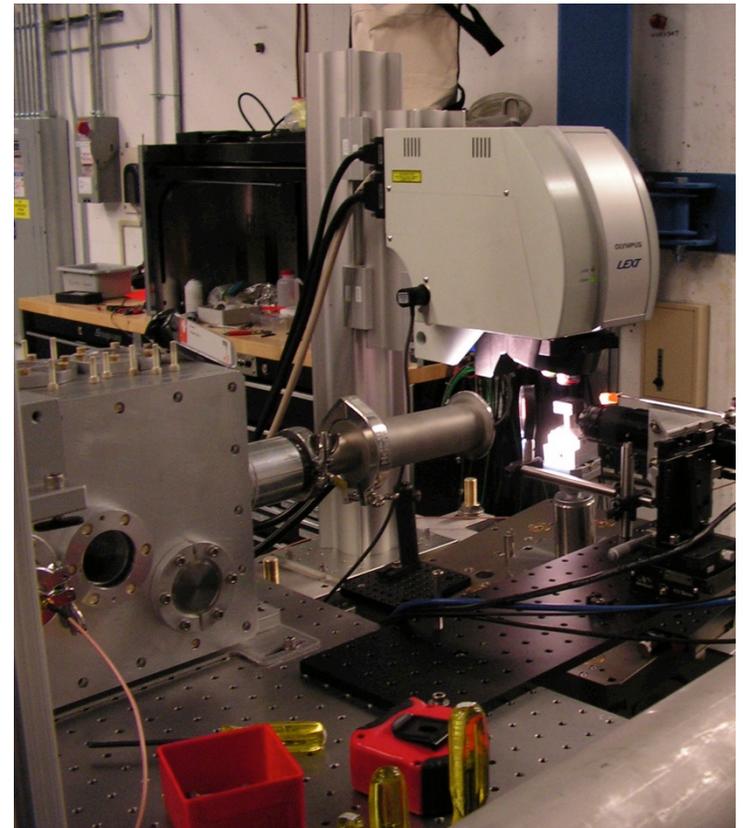
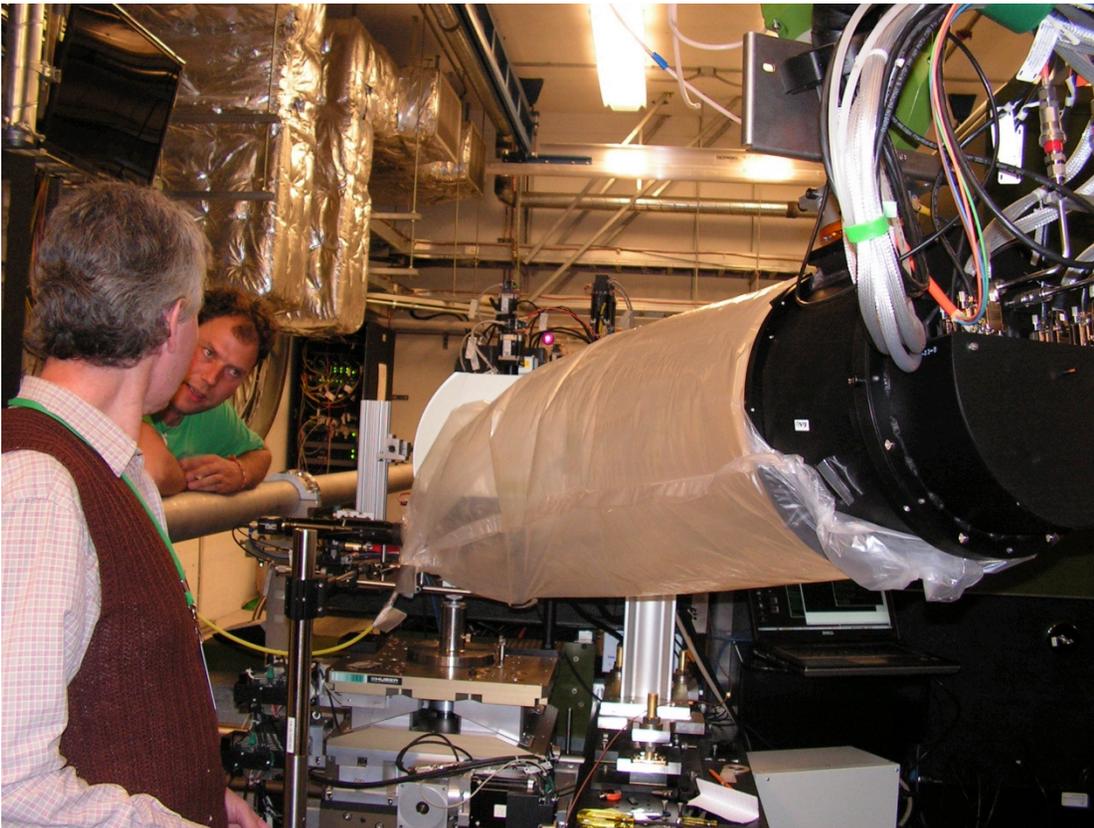


# Sensitivity to strain

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


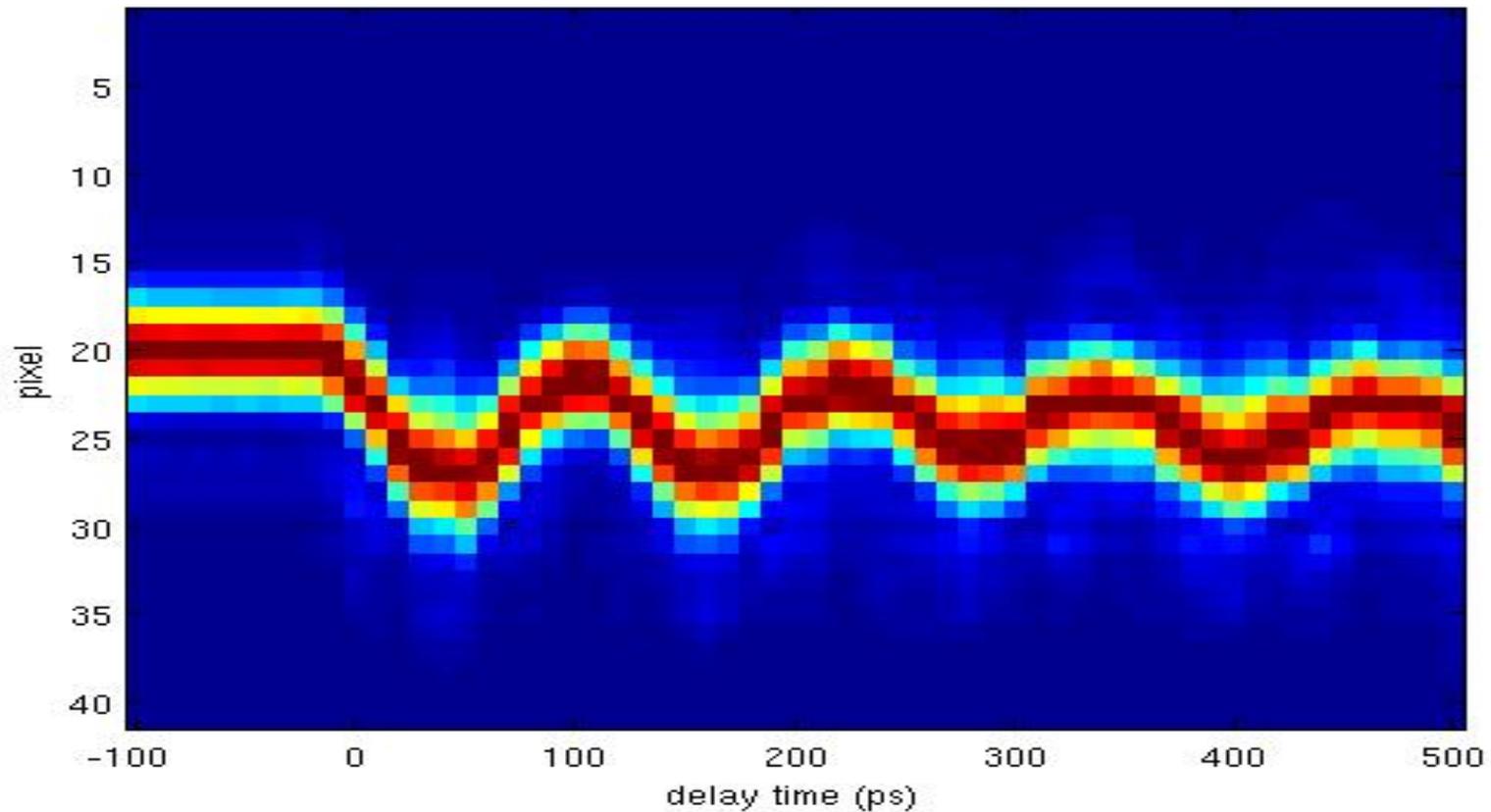
# Pump-probe at LCLS (XPP)

J. N. Clark, L. Beitra, G. Xiong, A. Higginbotham, D. M. Fritz, H. T. Lemke, D. Zhu, M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder, A. M. Korsunsky, J. S. Wark and I. K. Robinson, *Science* **341** 56 (2013)



# Pump-probe at LCLS (XPP)

Justin Wark, Loren Beitra, Alexander Korsunsky, Ross Harder, David Fritz ,  
Sebastien Boutet, **Jesse Clark**, Garth Williams, Brian Abbey, Andy Higginbotham,  
Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt



# “Two-temperature” model

I.K. Robinson et al, Journal of Optics **18** 054007 (2016)

J.K. Chen et al, Int J. Heat Transfer **49** 307 (2006)

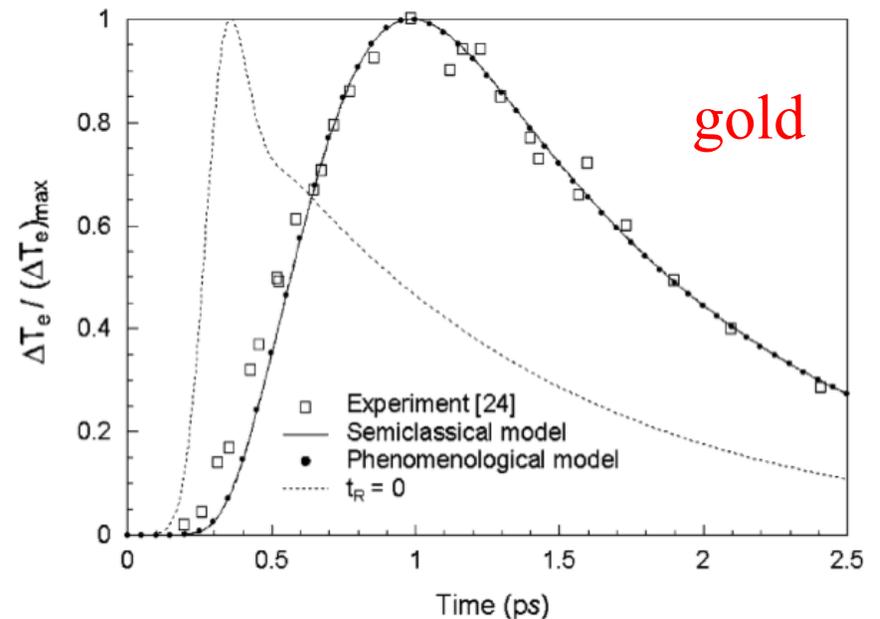
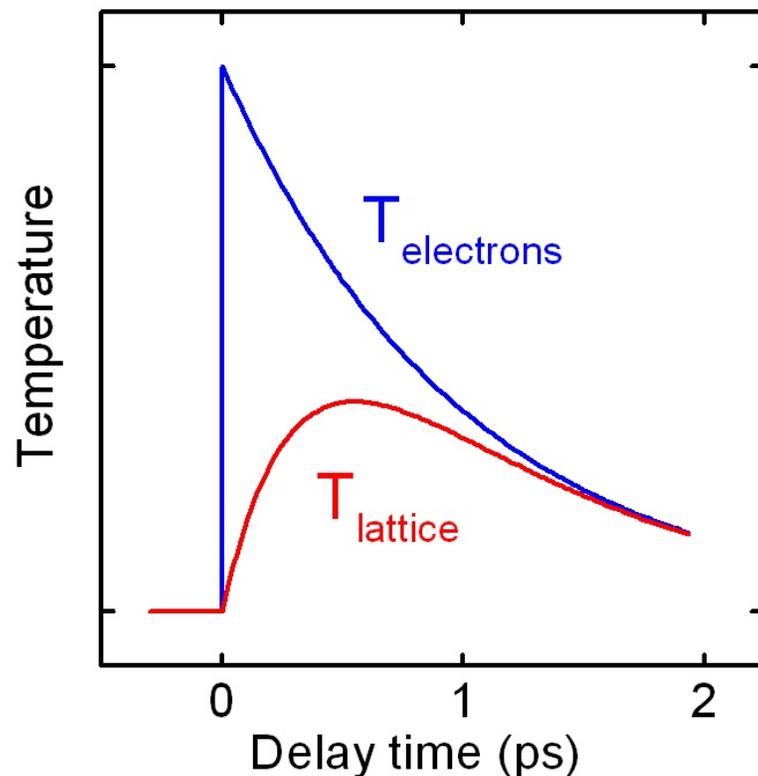
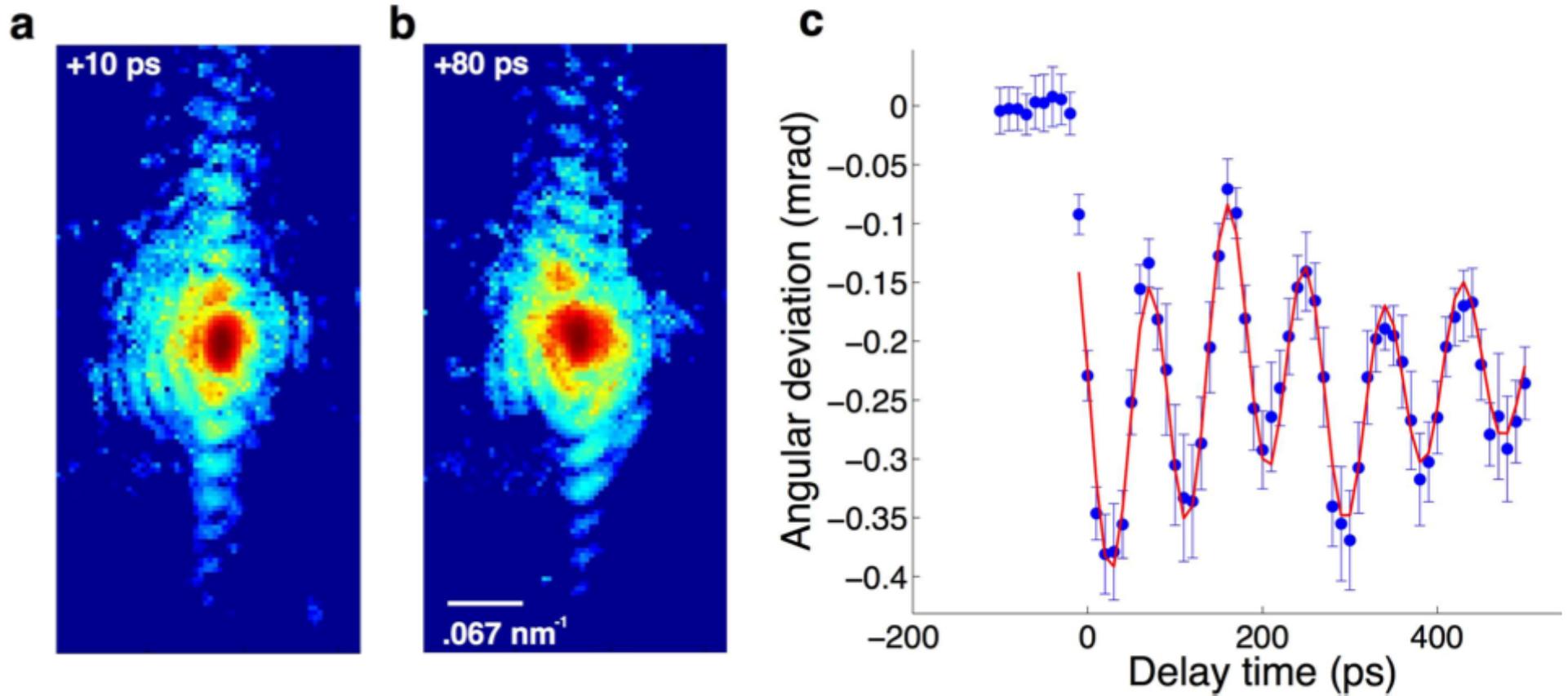


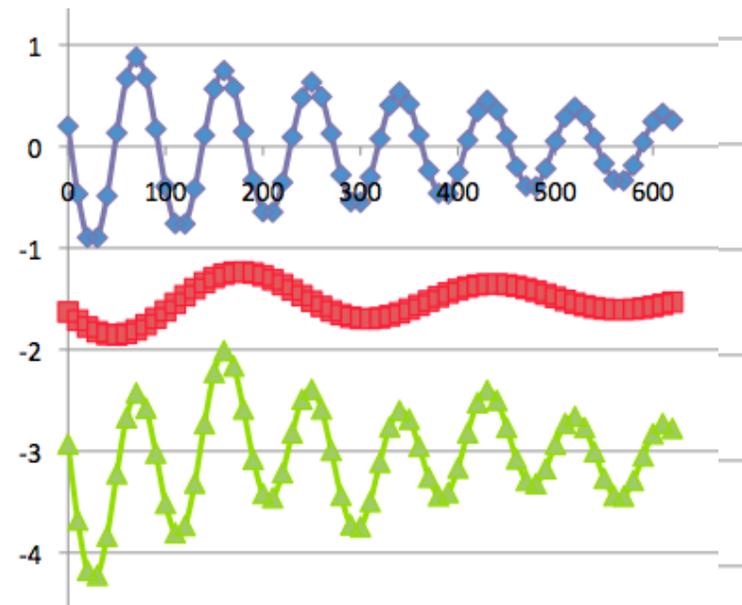
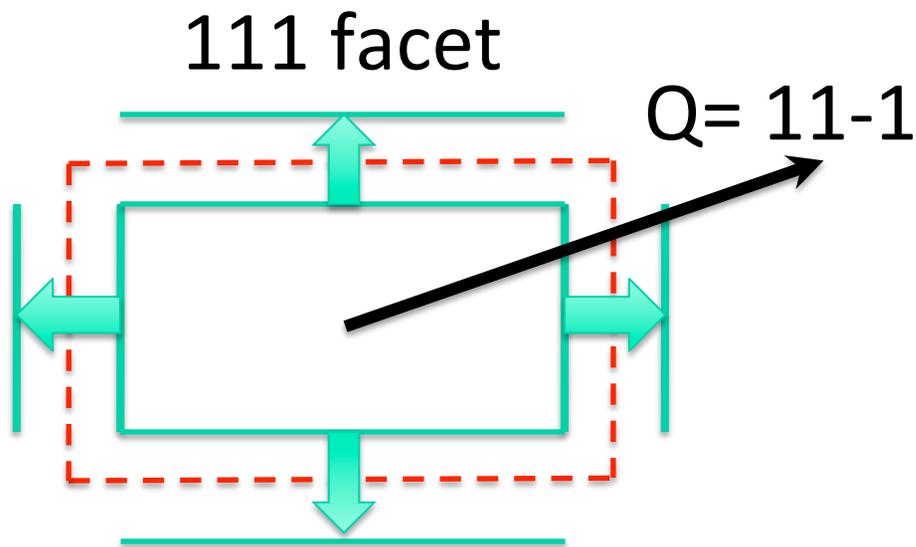
Fig. 2. Comparison of the change in electron temperature at the front surface of an 80-nm gold film irradiated by a 2.8 mJ/cm<sup>2</sup>, 800 nm, 150-fs laser pulse.

# Time resolved Bragg peak position



# Two Normal Modes of Vibration

$$S(\tau) = \sum_{n=1}^N A_n \exp[-(\tau/\tau_{d,n})^2] \cos(\omega_n \tau + \varphi_{0,n})$$



$$T_1 = 90\text{ps} \quad h_1 = 145\text{nm} \quad c_S = 3240 \text{ m/s}$$

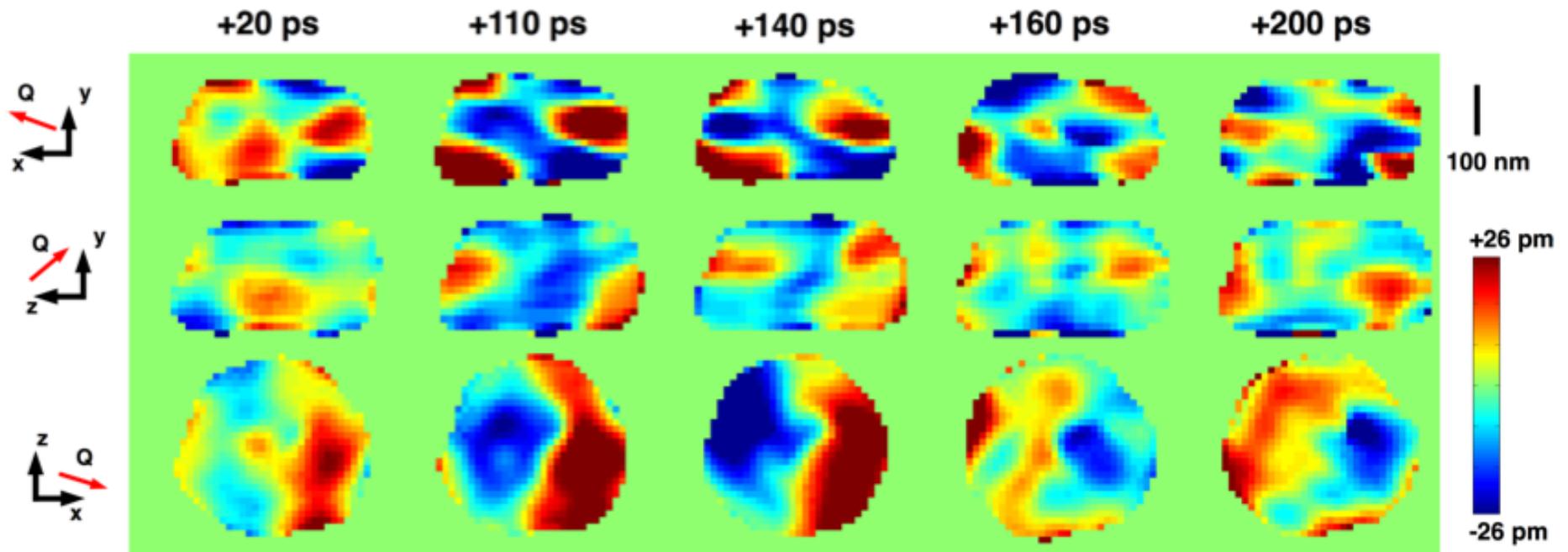
$$T_2 = 259\text{ps} \quad h_2 = 420\text{nm}$$

# Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

1000 frames averaged at each point of rocking curve

Jesse Clark et al, Science **341** 56 (2013)

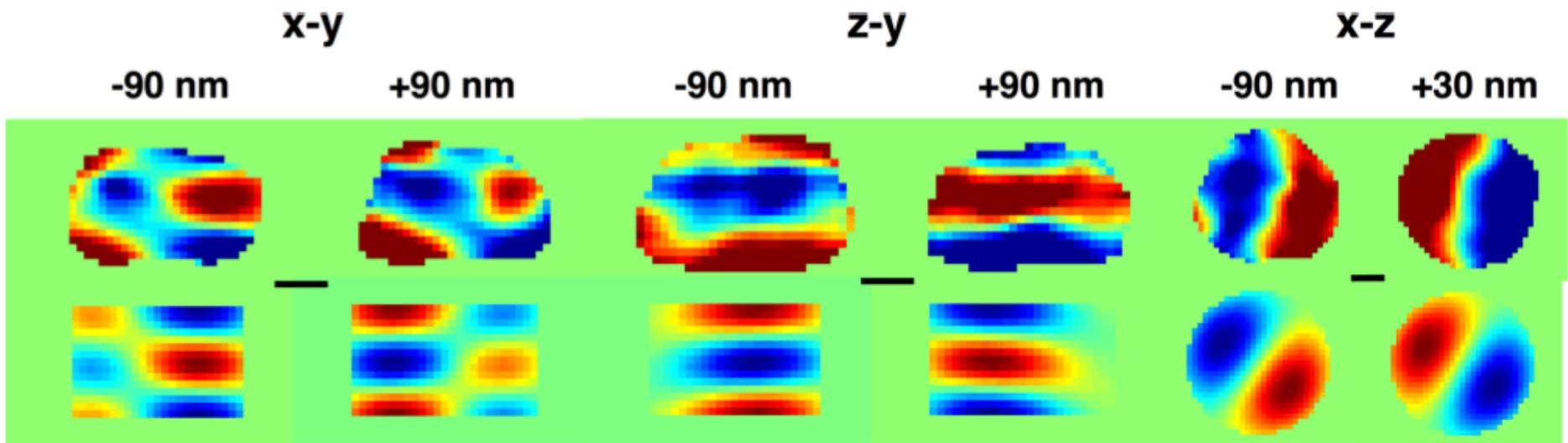


# Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

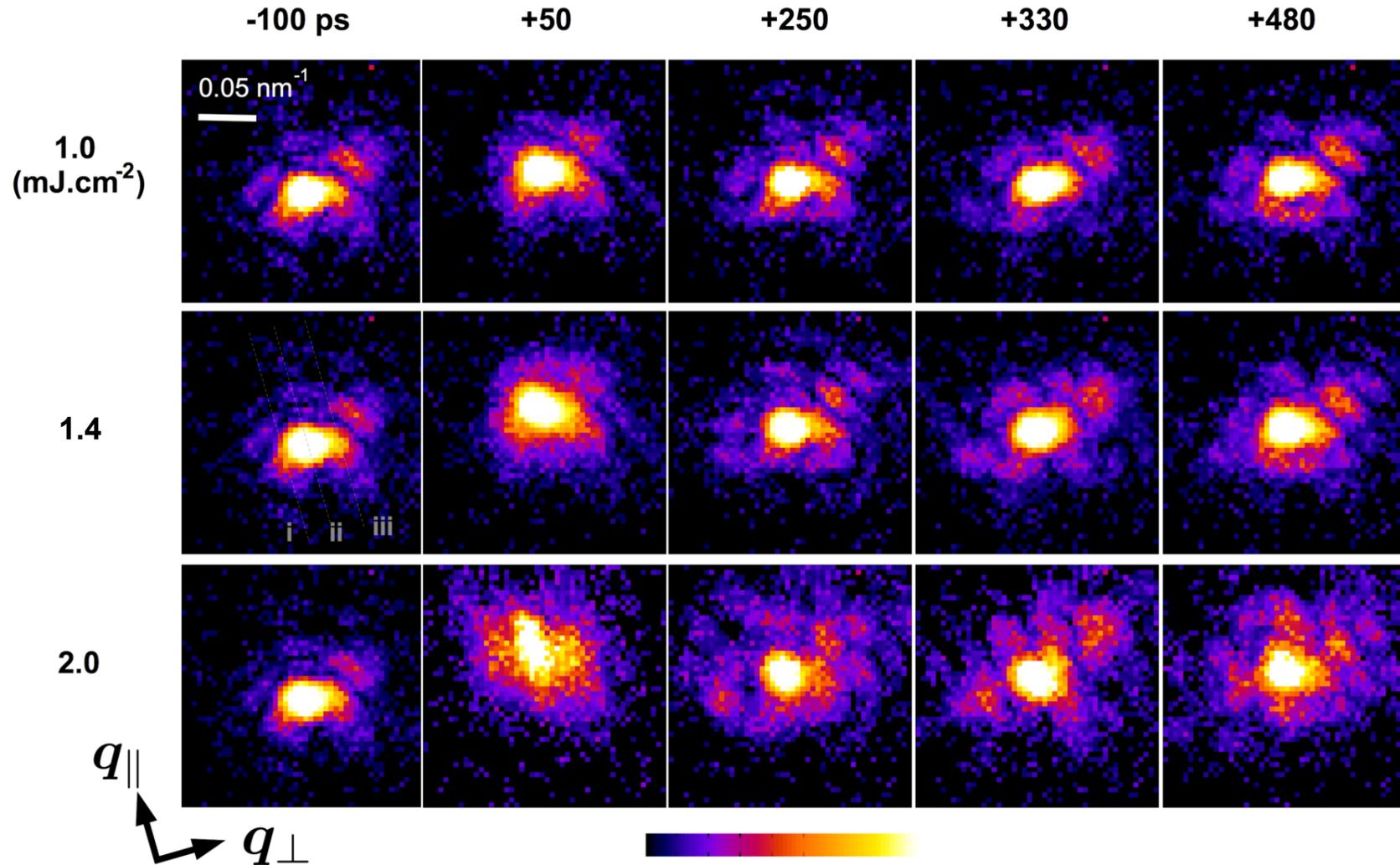
Comparison with (1,1) normal mode of cylinder

Jesse Clark et al, Science **341** 56 (2013)



# Dependence on Laser Fluence

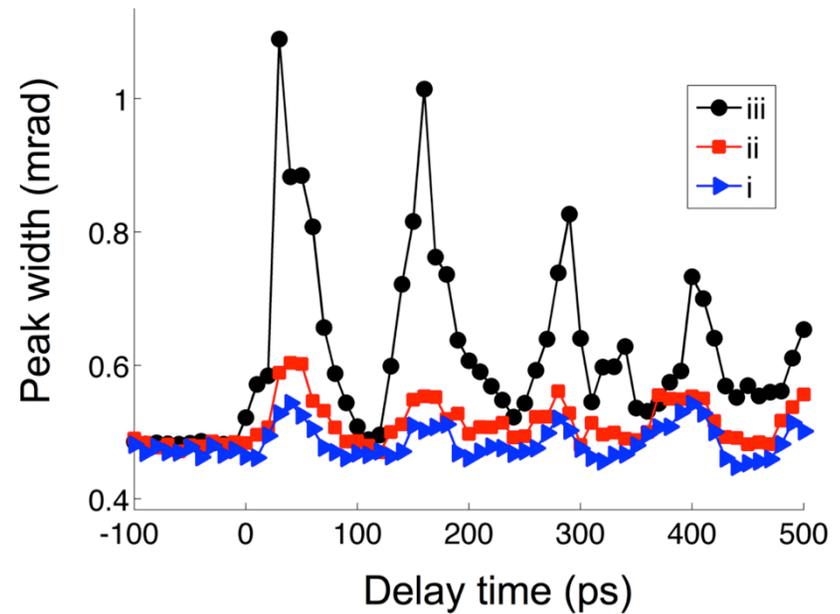
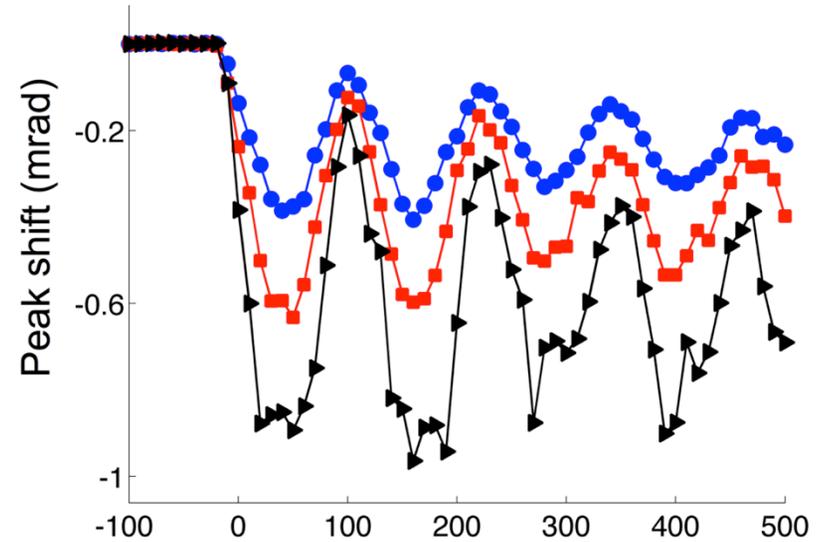
Jesse Clark et al, PNAS 112 7444-8 (2015)



# Dependence on Laser Fluence

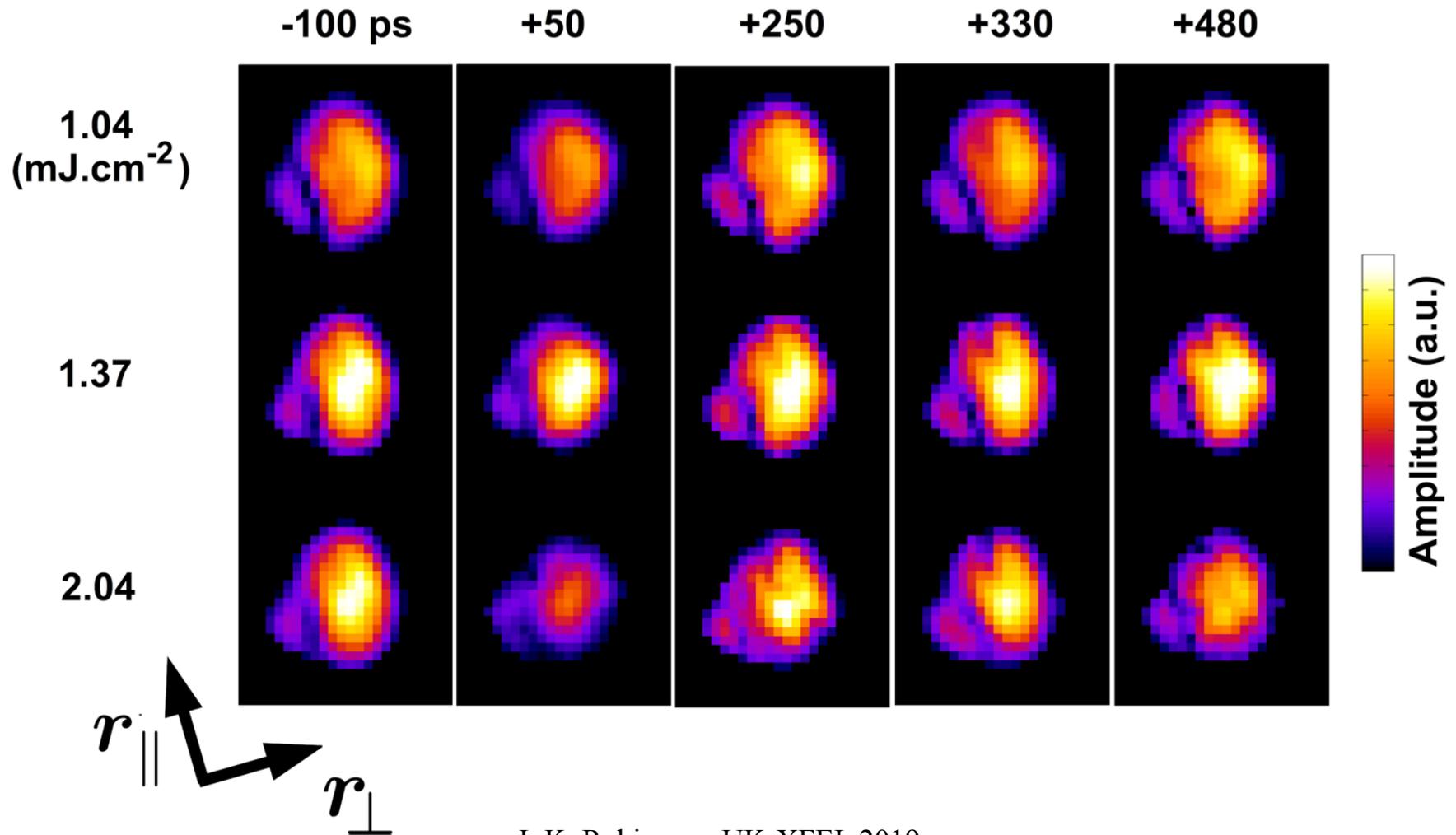
Jesse Clark et al, PNAS  
112 7444-8 (2015)

1.0 mJ cm<sup>-2</sup>  
1.4 mJ cm<sup>-2</sup>  
2.0 mJ cm<sup>-2</sup>

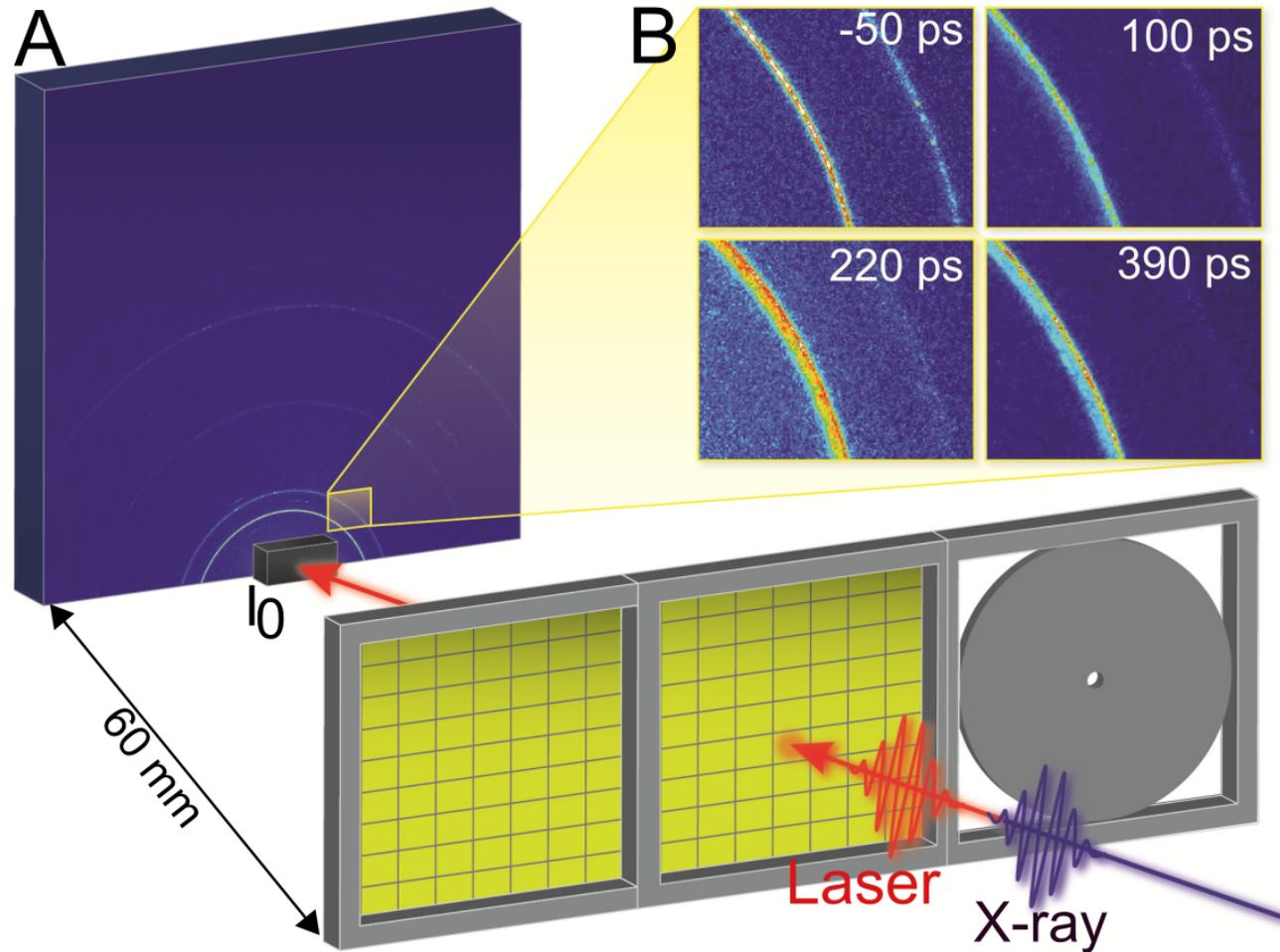


# Dependence on Laser Fluence

Jesse Clark et al, PNAS 112 7444-8 (2015)

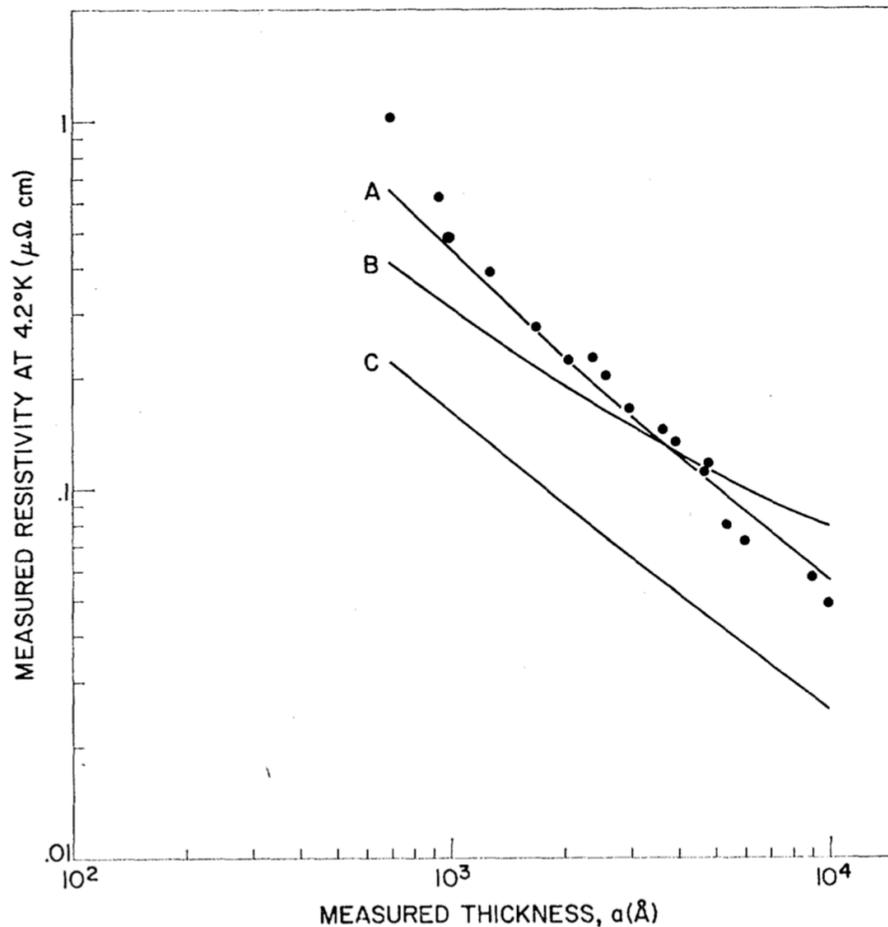


# Melt-front Dynamics in Gold Thin Films using PAL-XFEL



# Resistivity of Al Thin Films

A. F. Mayadas and M. Shatzkes, PRB 1 1382 (1970)

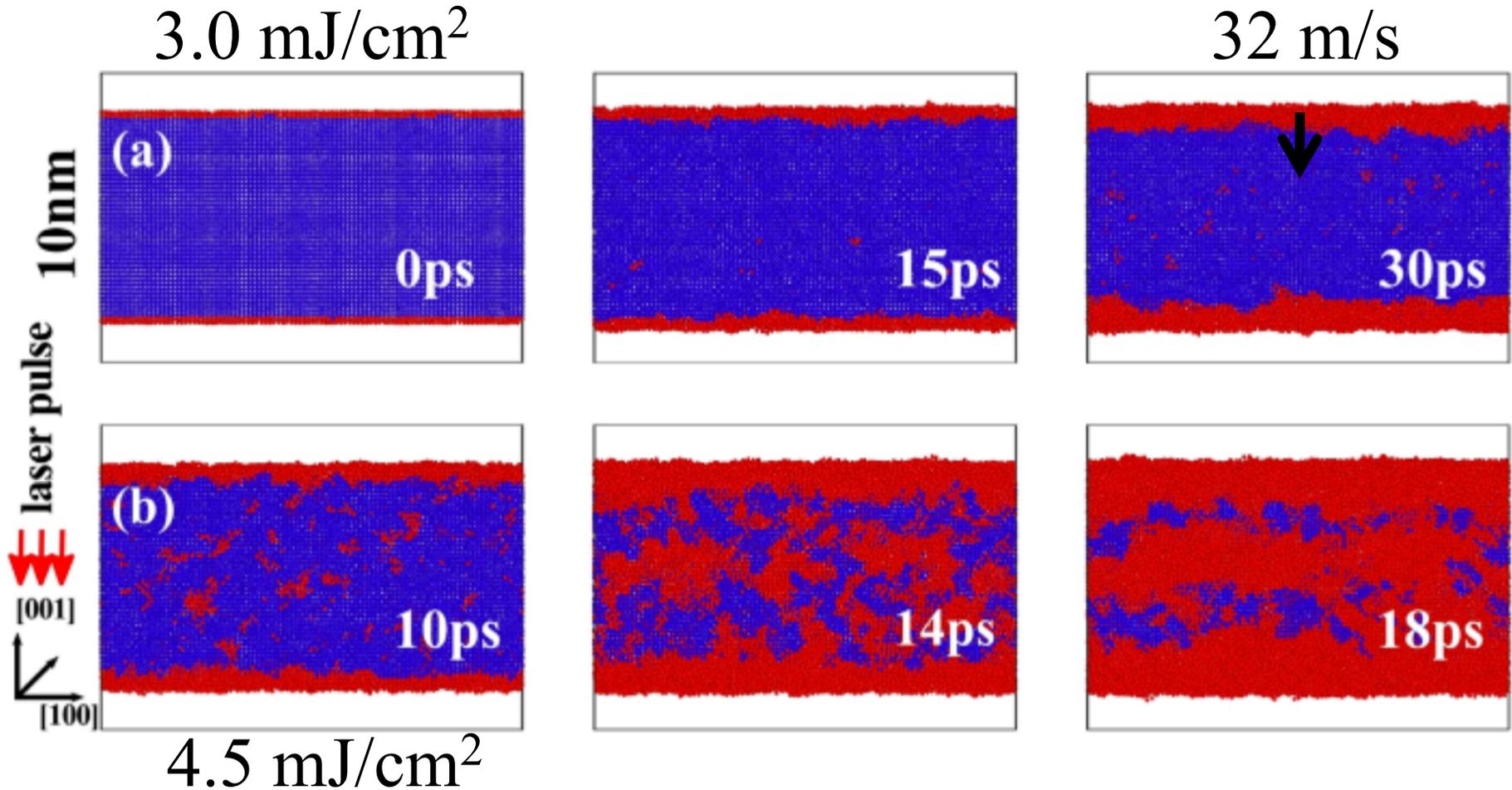


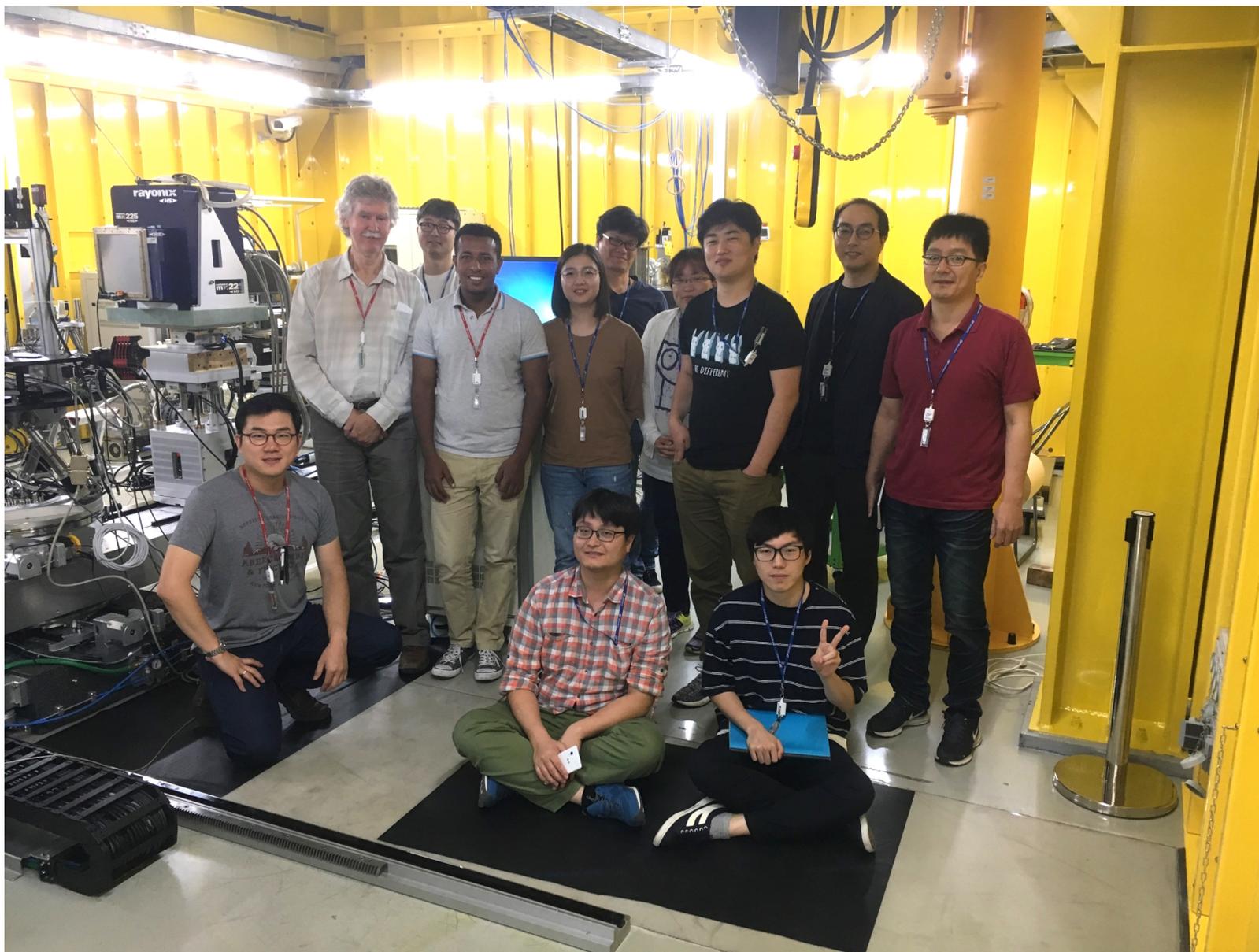
- “Universal curve” of MFP vs electron energy
- Thermal MFP removed at low temperature
- Grain size proportional to thickness (model)



# 2TM-MD (EAM) simulation Au slab

Giret et al, APL 103 253107 (2013)

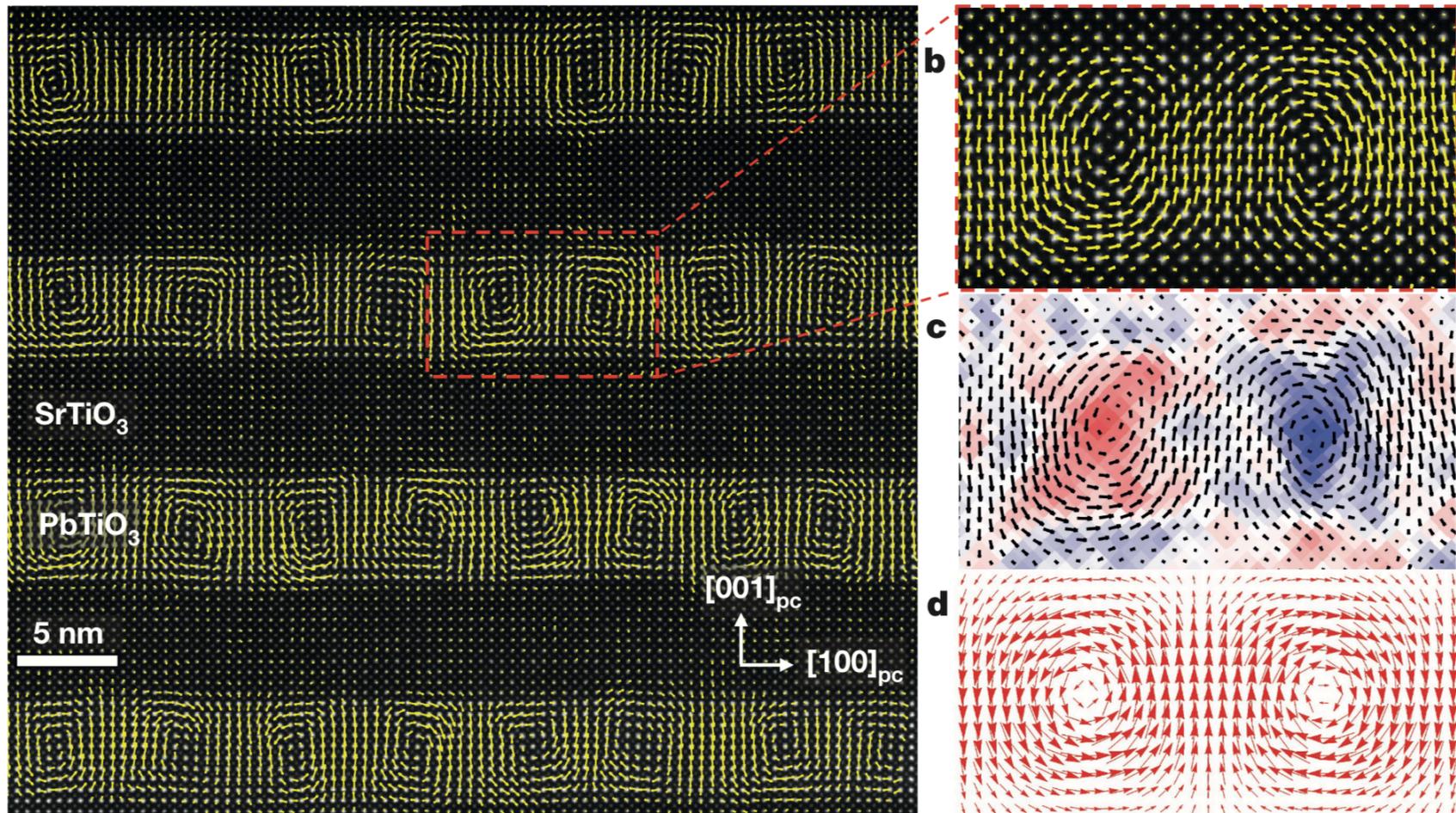




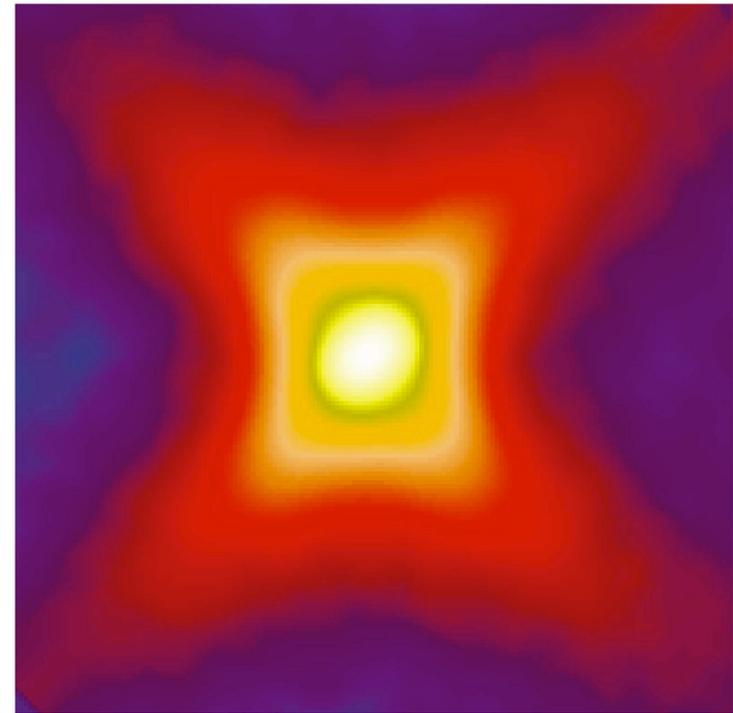
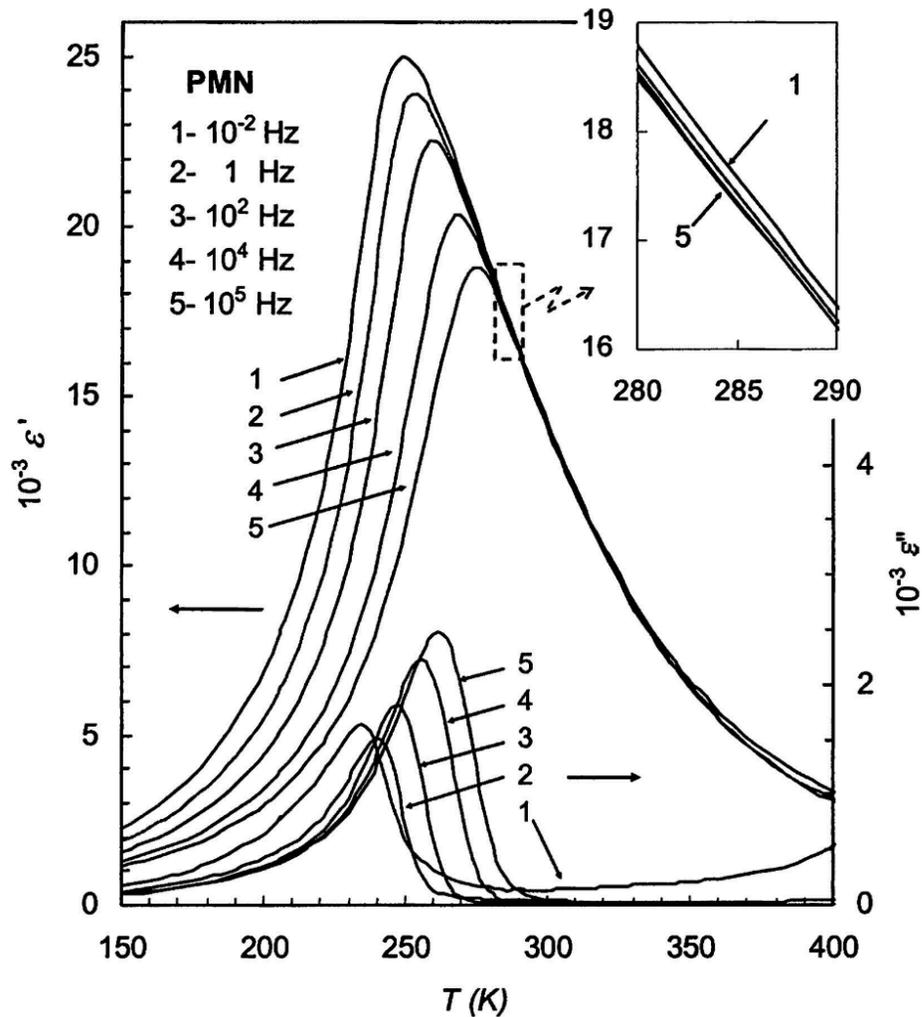
I. K. Robinson, UK-XFEL 2019

# Ferroelectric Polar Vortices

A. K. Yadav et al Nature 530 198 (2016)



# PbMg<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub> Relaxor Ferroelectric



A. A. Bokov et al J. Mat. Sci. 41 31 (2006)

G. Xu, G. Shirane, et al PRB 69 064112 (2004)

# Advanced Materials and Nanotechnology

- Pump-probe approach to excitations
- Bragg Coherent Diffraction Imaging (BCDI)
- New vibration mode of Au Nanoparticle
- Surface melting of Au Nanoparticle
- Melt-front picture of Ultrafast melting



# Acknowledgements



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