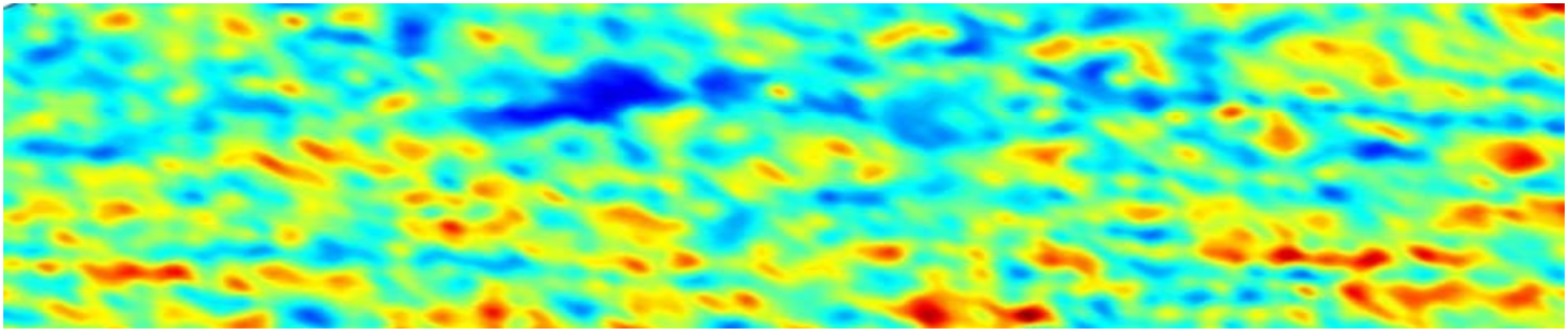
Coherent X-ray Diffraction Imaging of Phase Defects in Magnetically and Electronically Ordered Materials



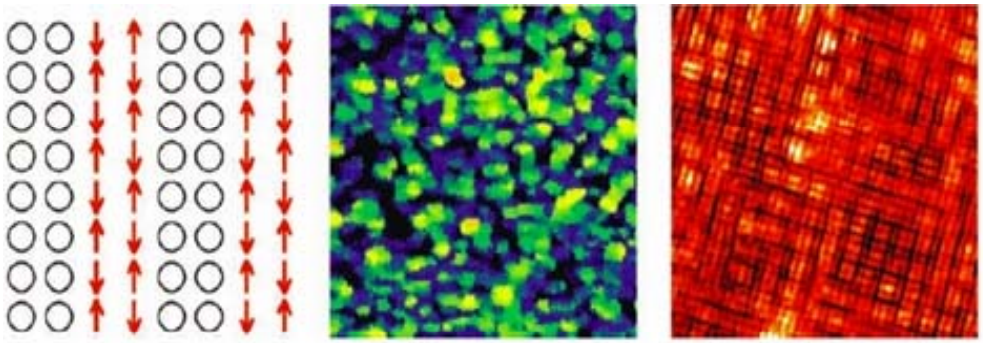
Oleg Shpyrko
University of California San Diego

X-ray Contrast mechanisms:

- Electron density (atomic density)
  - Elemental sensitivity (John Miao)
- Electron density variations
  - Charge ordering, Charge Density Waves (CDW)
  - Strain fields (Ian Robinson)
- Spin ordering (e.g. Antiferromagnets)
  - Resonant (need convenient adsorption edges)
  - Non-resonant (weak scattering)
- Orbital ordering

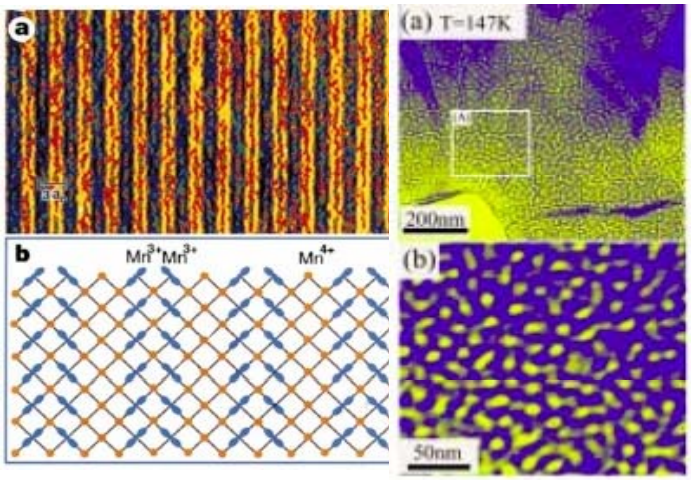
Stripes, checkerboards and zig-zags

High-Tc cuprates



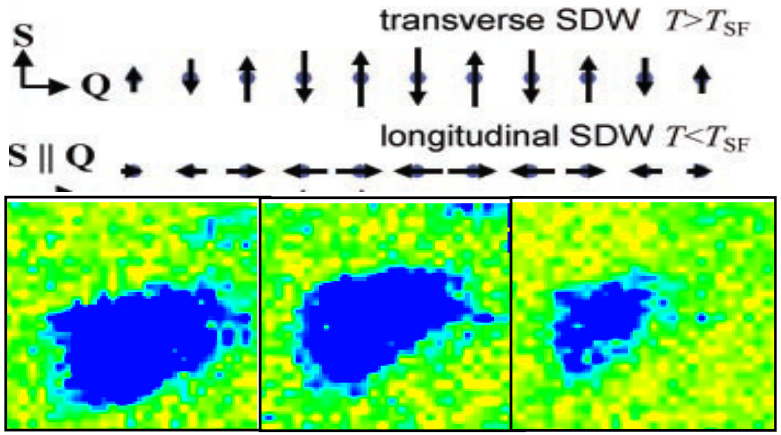
E. Dagotto, T. M. Rice, *Science* **271**, 618 (1996).
T. Hanaguri et al., *Nature* **430**, 1001 (2004).

CMR manganites

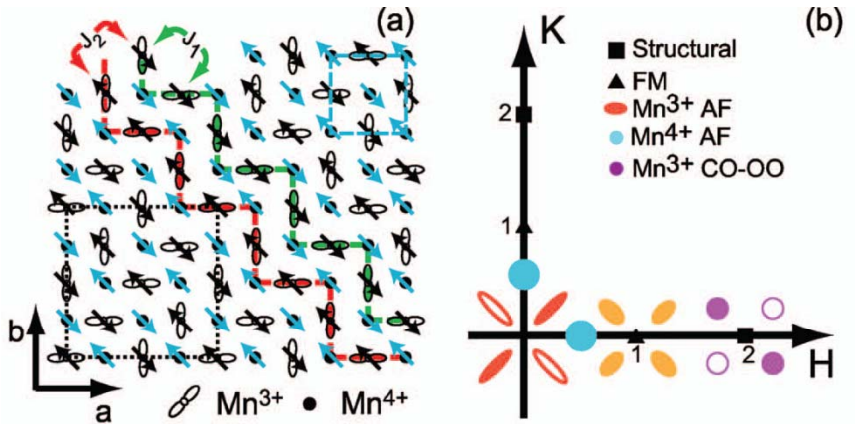


S. Mori et al., *Nature* **392**, 473 (1998)
M. Uehara et al., *Nature* **399**, 560 (1999)

AFM chromium

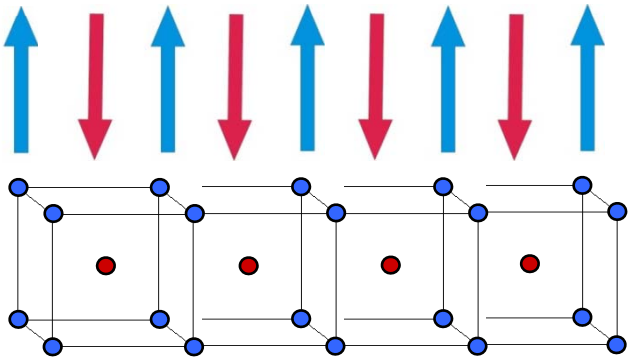


P. G. Evans et al., *Science* (2002)

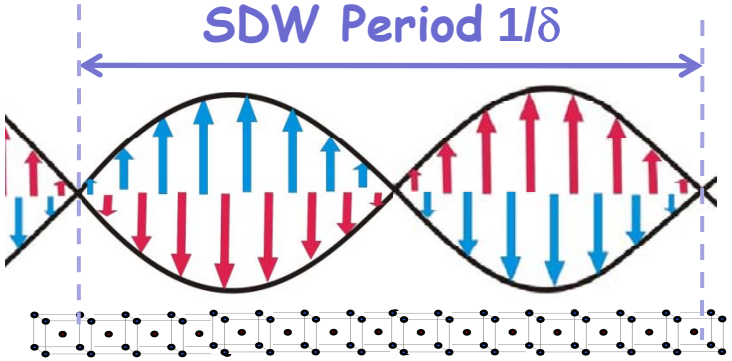


Spin Density Wave (SDW) in Chromium:

Commensurate Anti-ferromagnetic SDW (C-SDW)
Wave follows periodicity of underlying atomic lattice



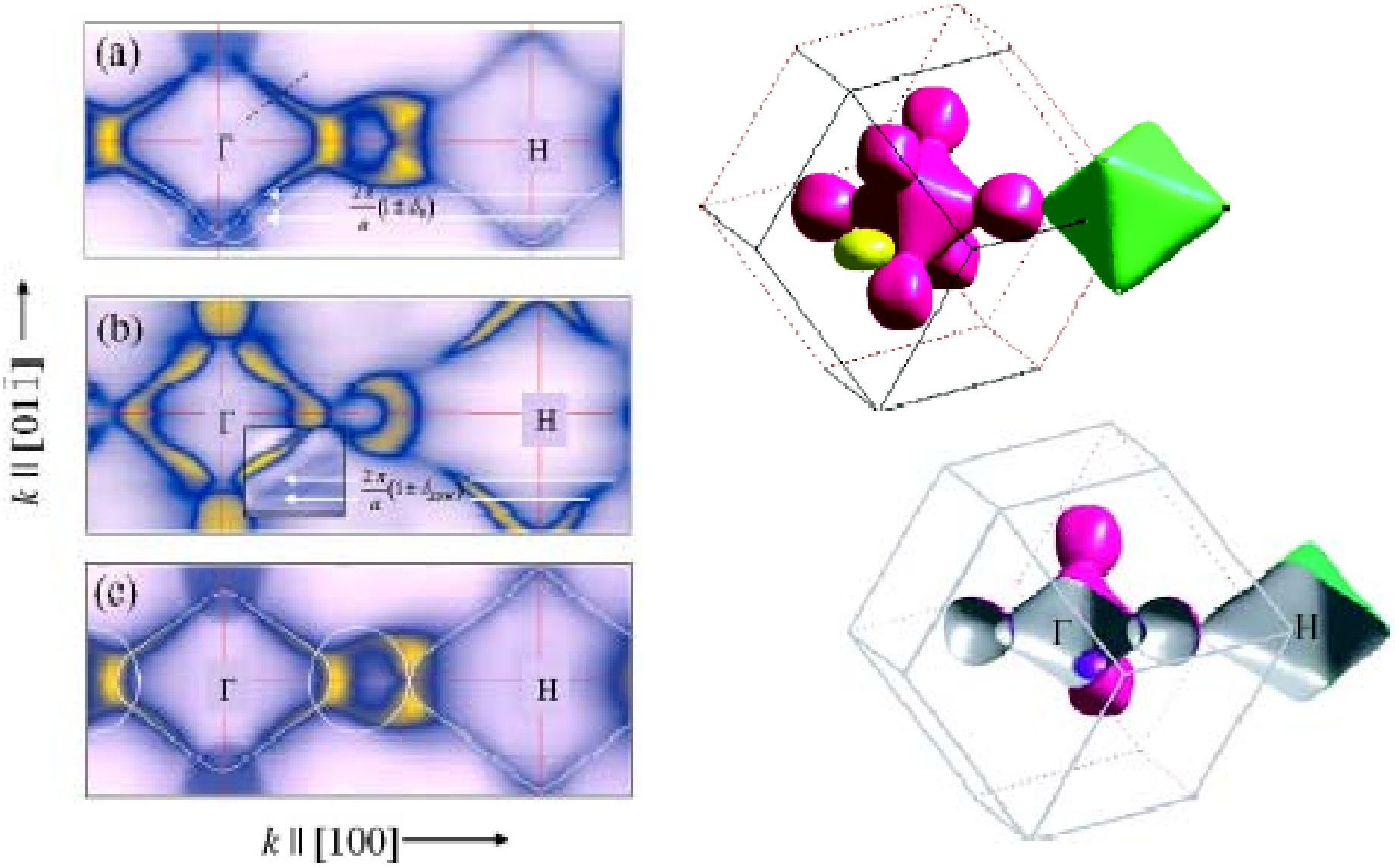
Incommensurate SDW (IC-SDW)
Modulation period incommensurate with lattice periodicity



For chromium incommensurability parameter is δ=0.038 at room T (period is δ^{-1}~26 times the lattice constant)

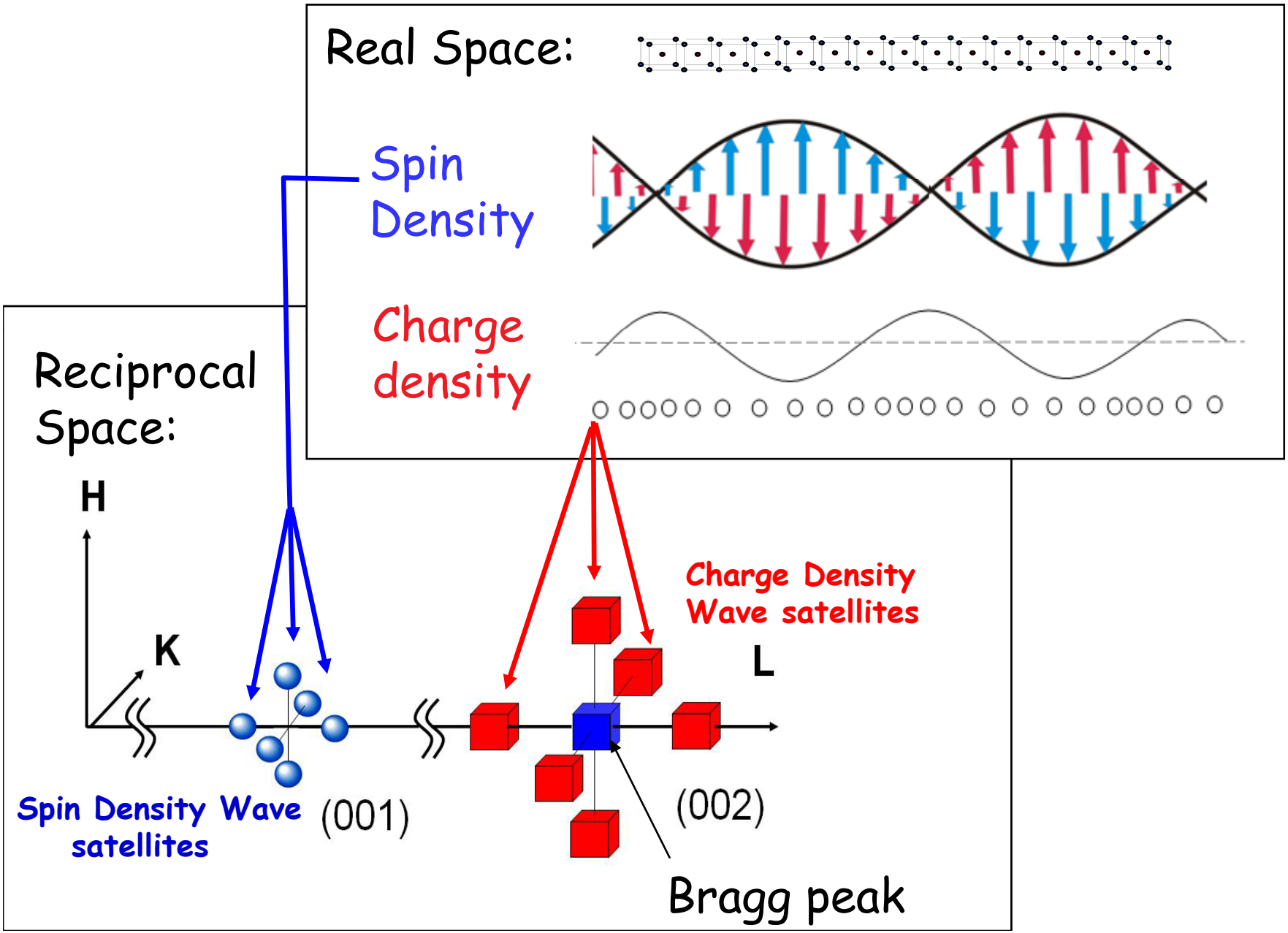
Scattering experiments typically measure Q=1-δ

SDW: nesting of Fermi Surface



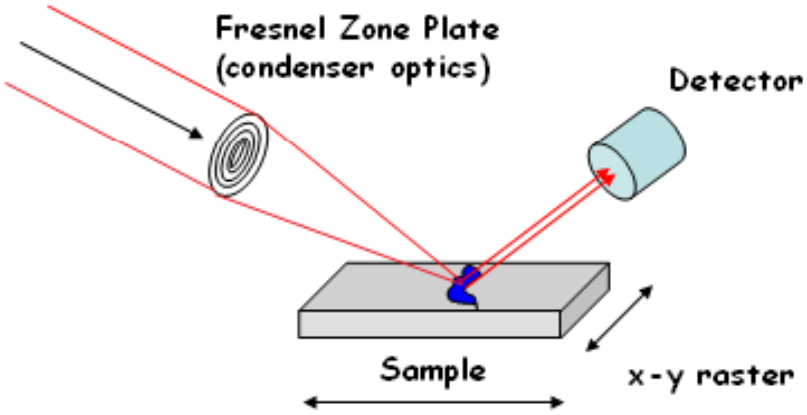
E. Rottenberg et al., *New Journal of Physics* 7, 114 (2005)

Charge, Spin and Lattice order parameters:



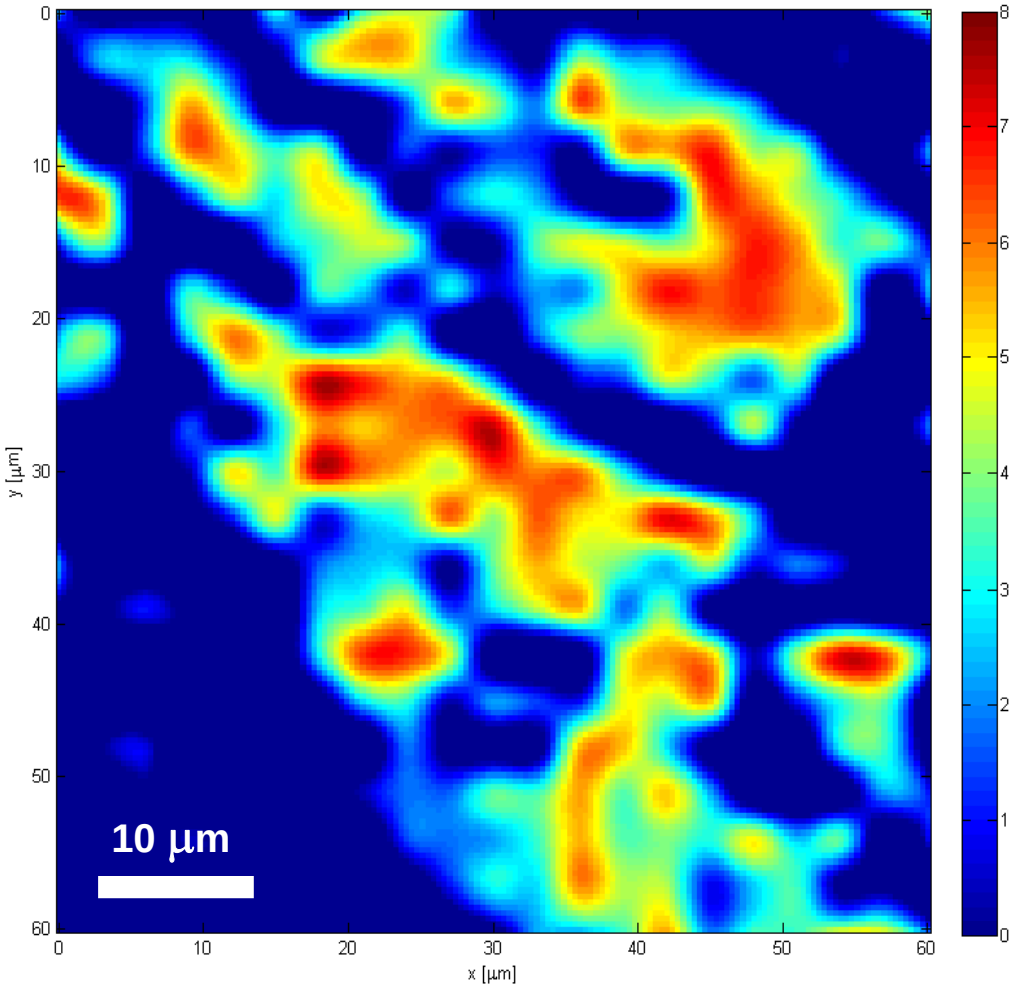
Microscopic SDW/CDW Domains in Chromium:

Scanning X-ray Microscopy:

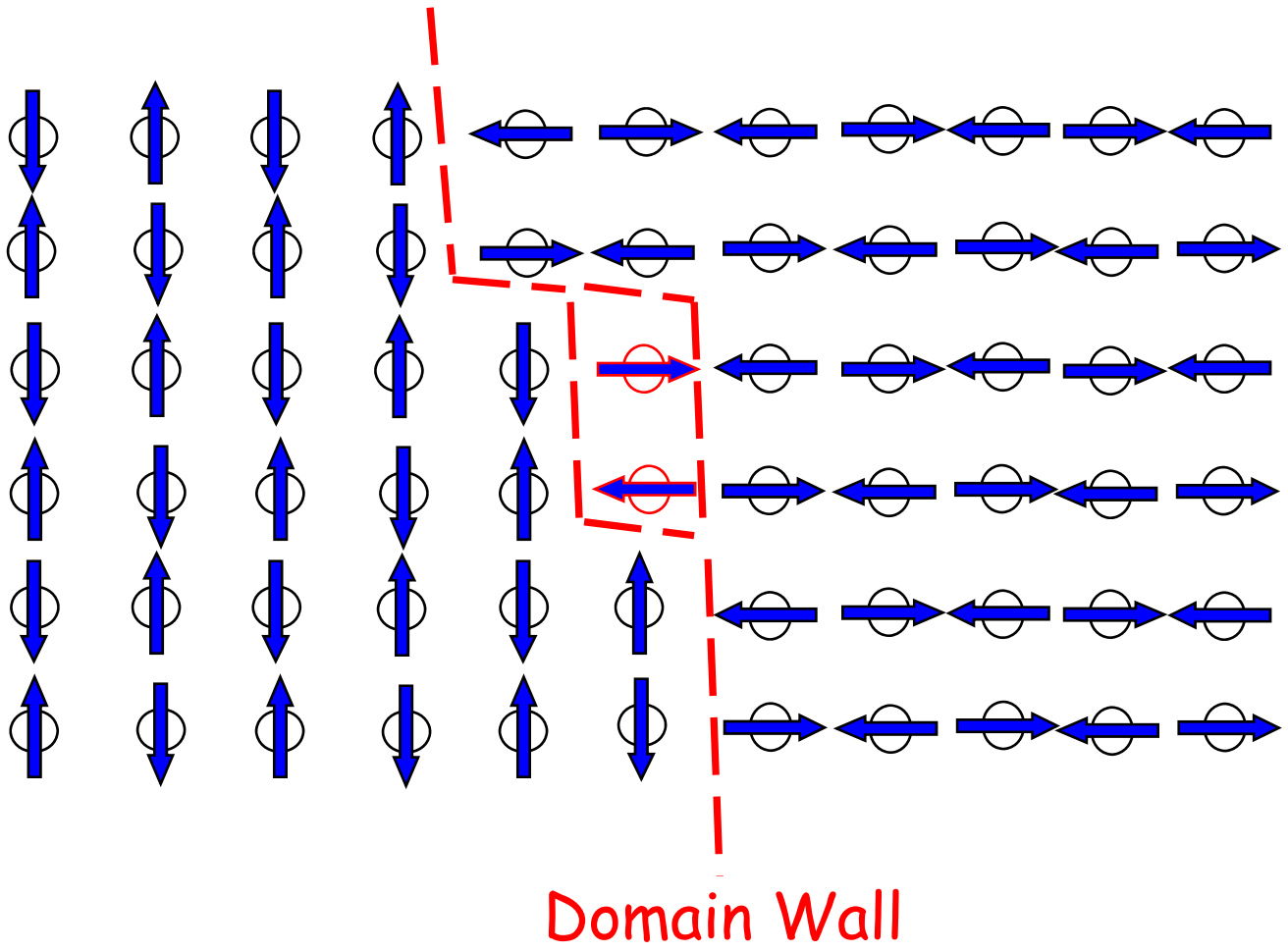


- bulk probe (micron-sized penetration depth)
- spin, charge, lattice and chemical sensitivity

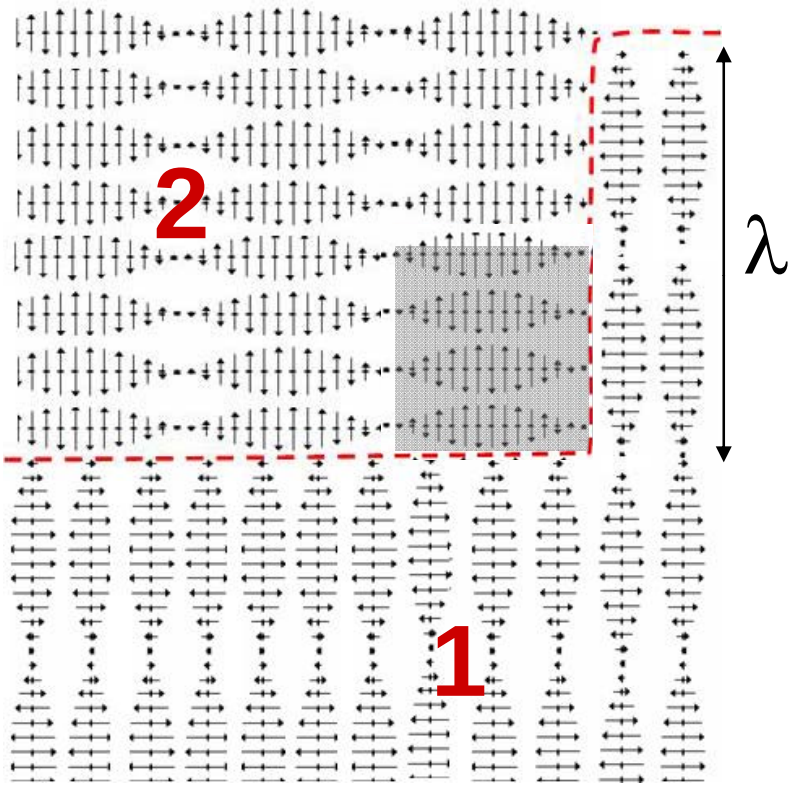
[0, 0, 2-2δ] Charge-density wave satellite

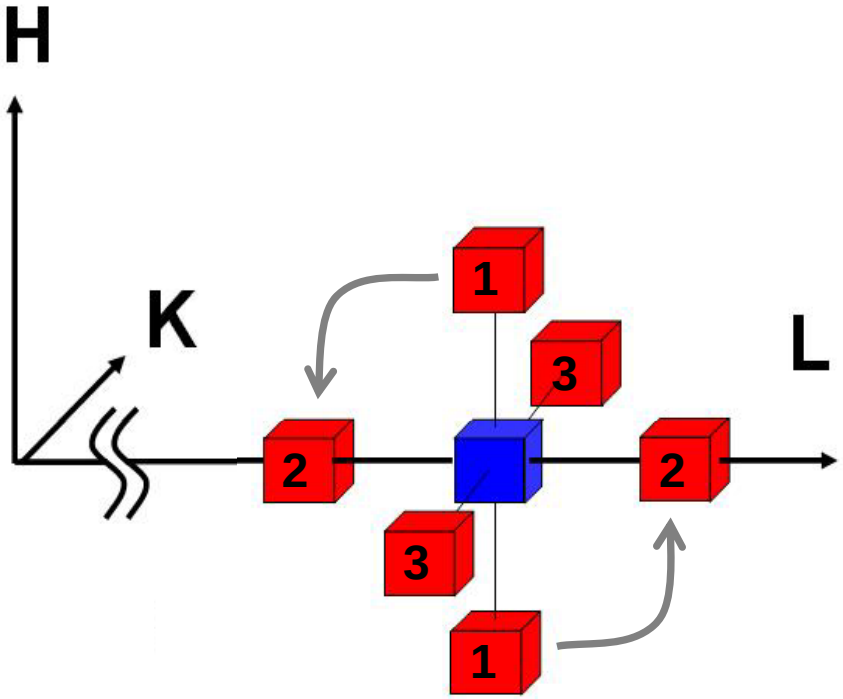


Domain Wall Fluctuations in Antiferromagnets



Magnetic domain wall fluctuations in real and reciprocal space:





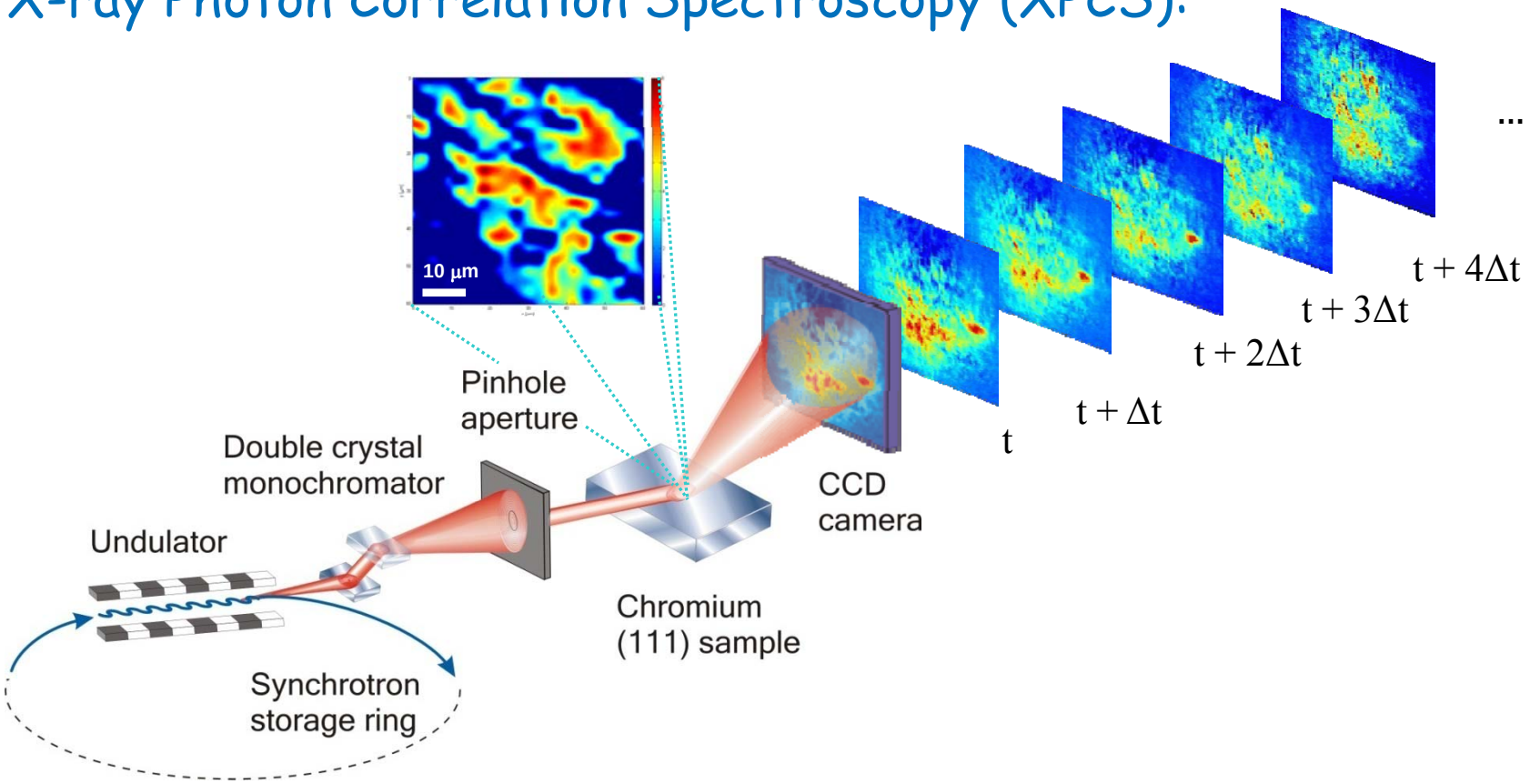
Real Space:

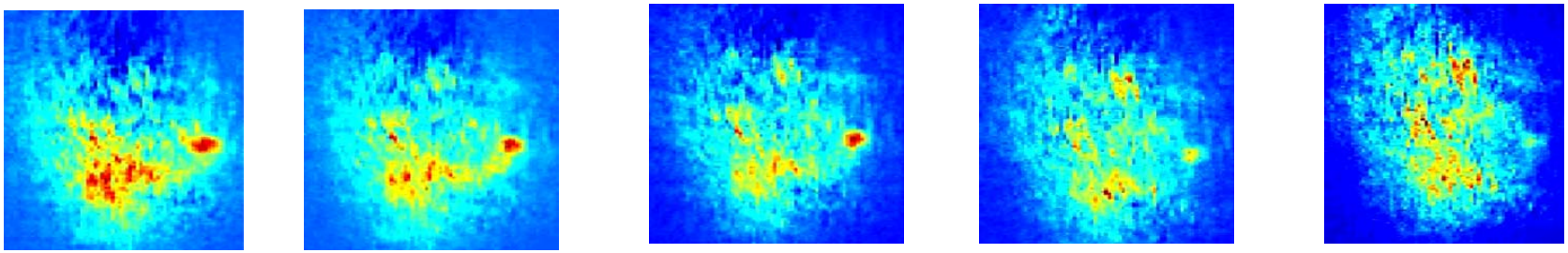
elemental switching block,
w/ volume $(\lambda/2)^3$, λ=3-4 nm

Momentum Space:

transfer of intensity from satellites 1 to 2 due to switch

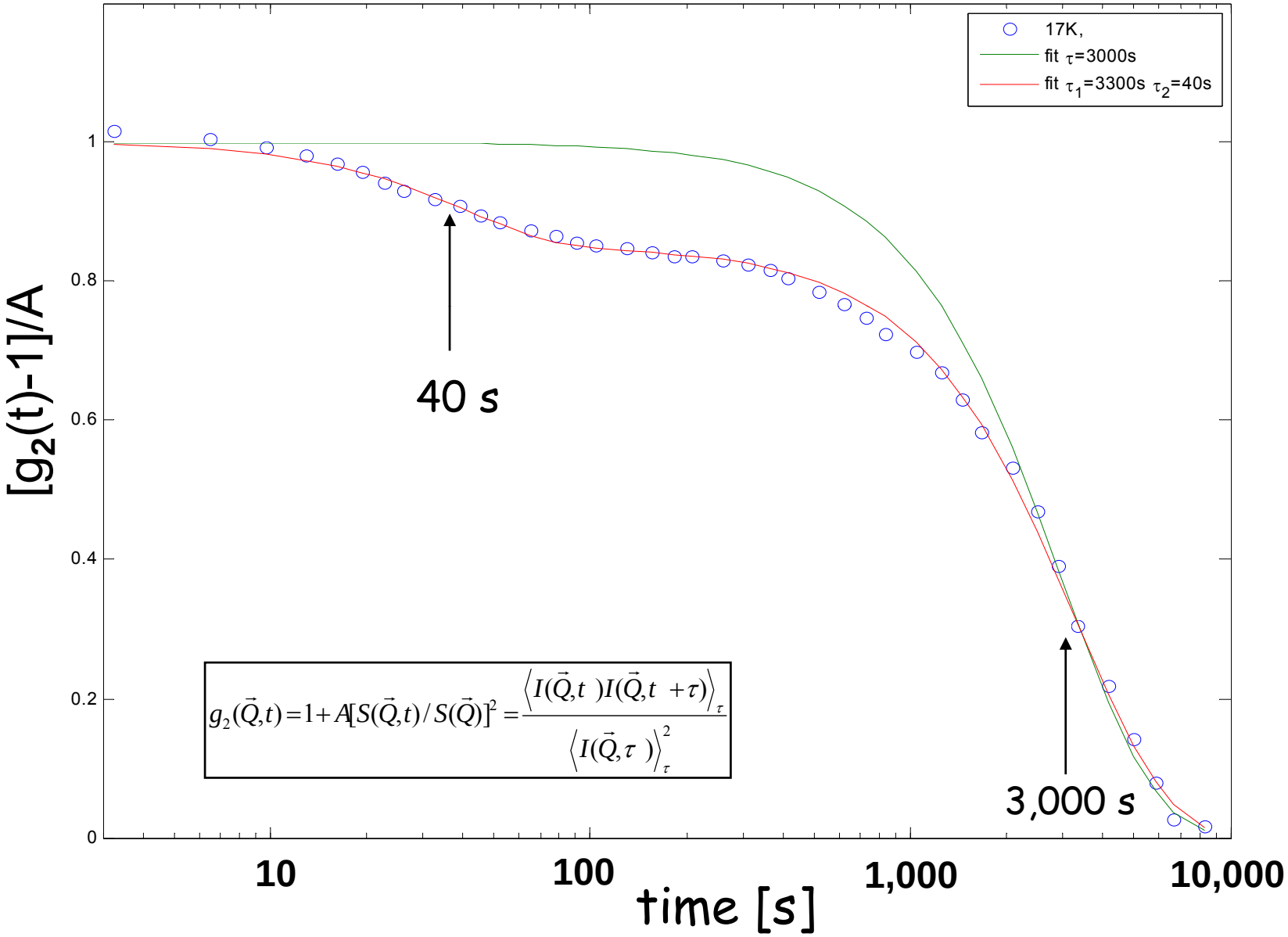
X-ray Photon Correlation Spectroscopy (XPCS):



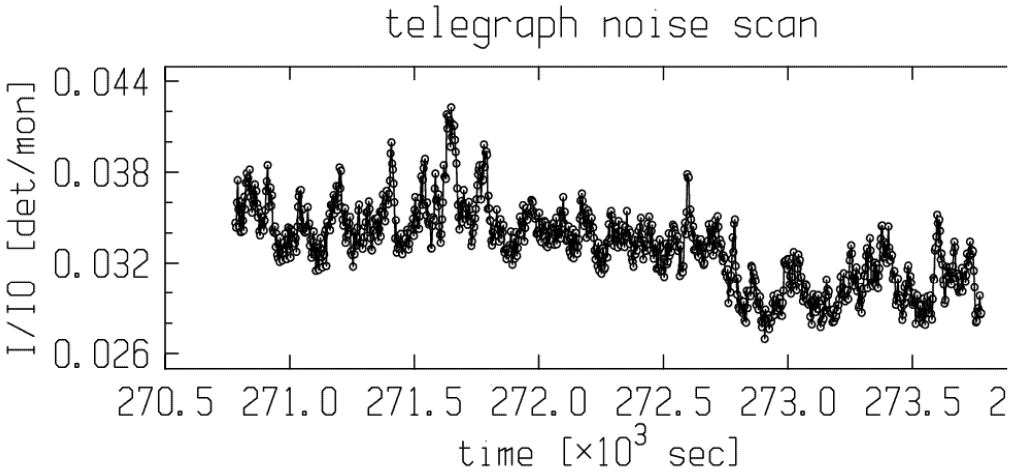


O. G. Shpyrko et al., *Nature* **447**, 68 (2007)

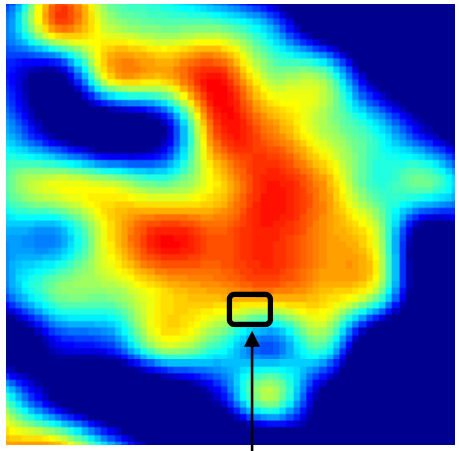
Autocorrelation function $g_2(t)$: Multiple relaxation timescales



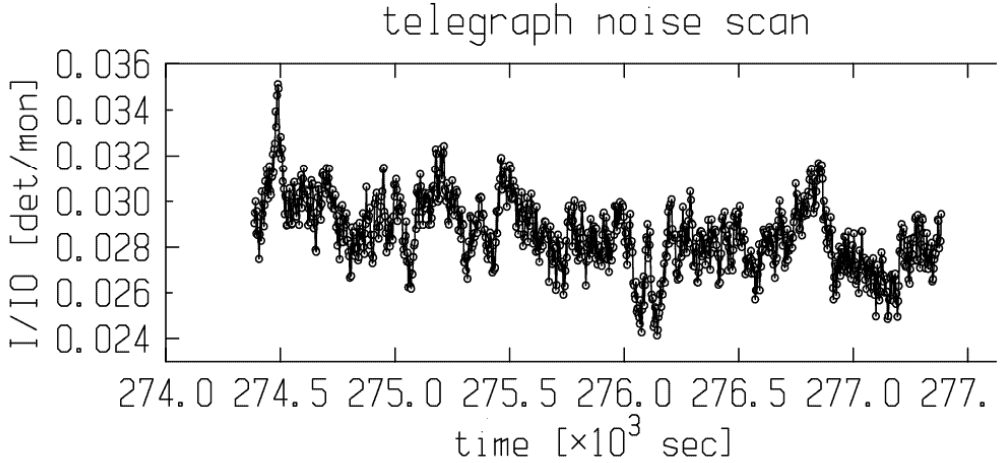
Random Telegraph Noise measurements:
Focus on the Domain Wall



~100 nm

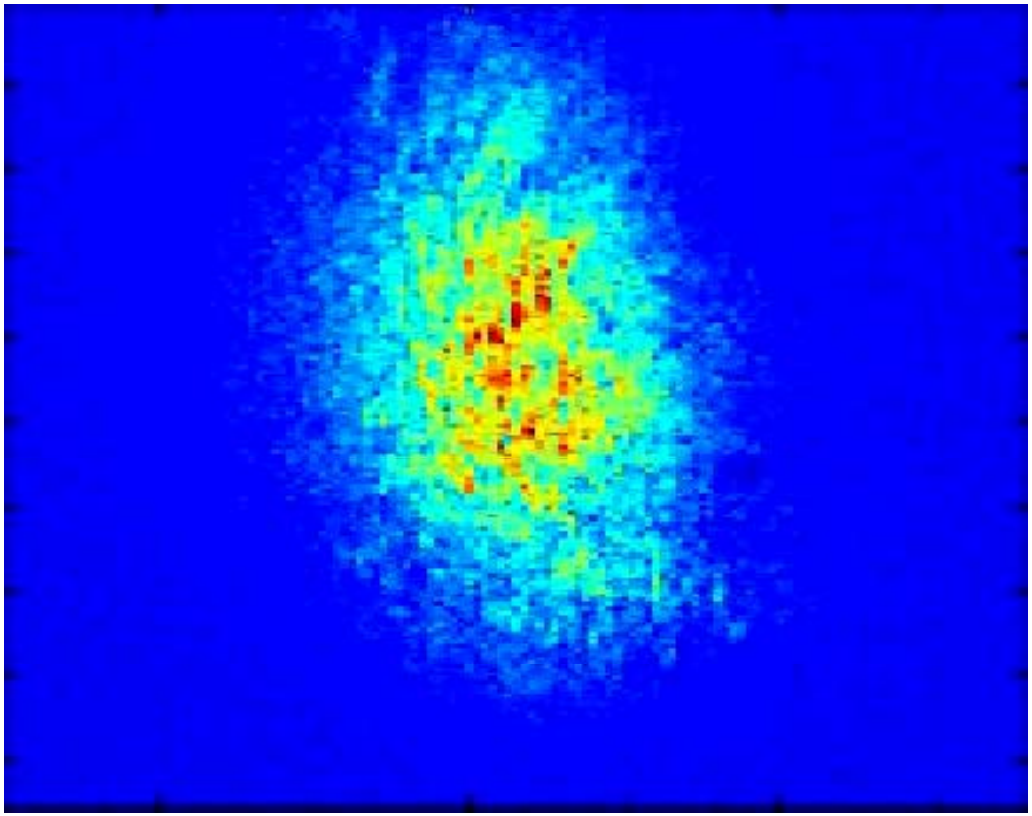


focused x-ray beam (0.5 μm)

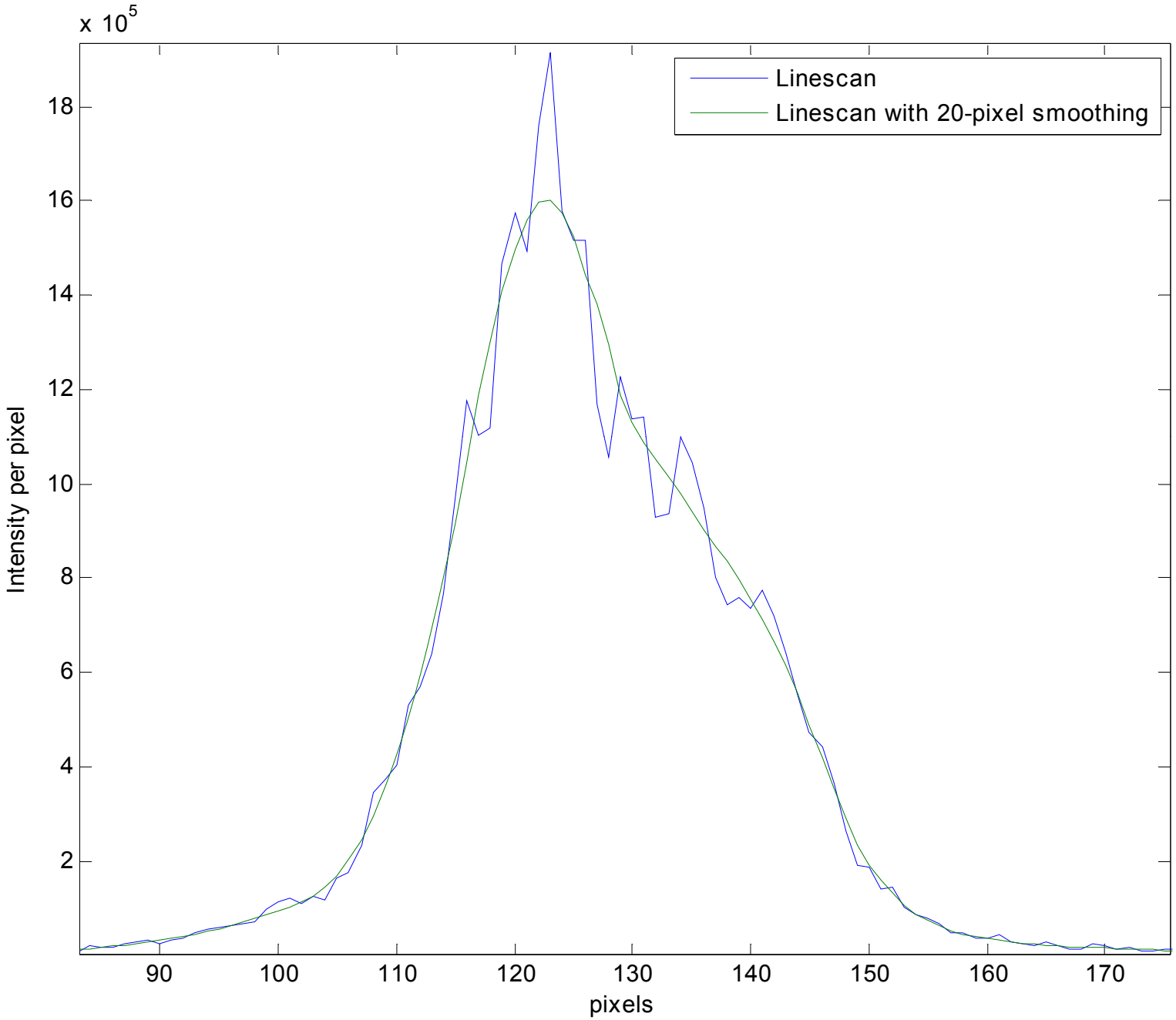


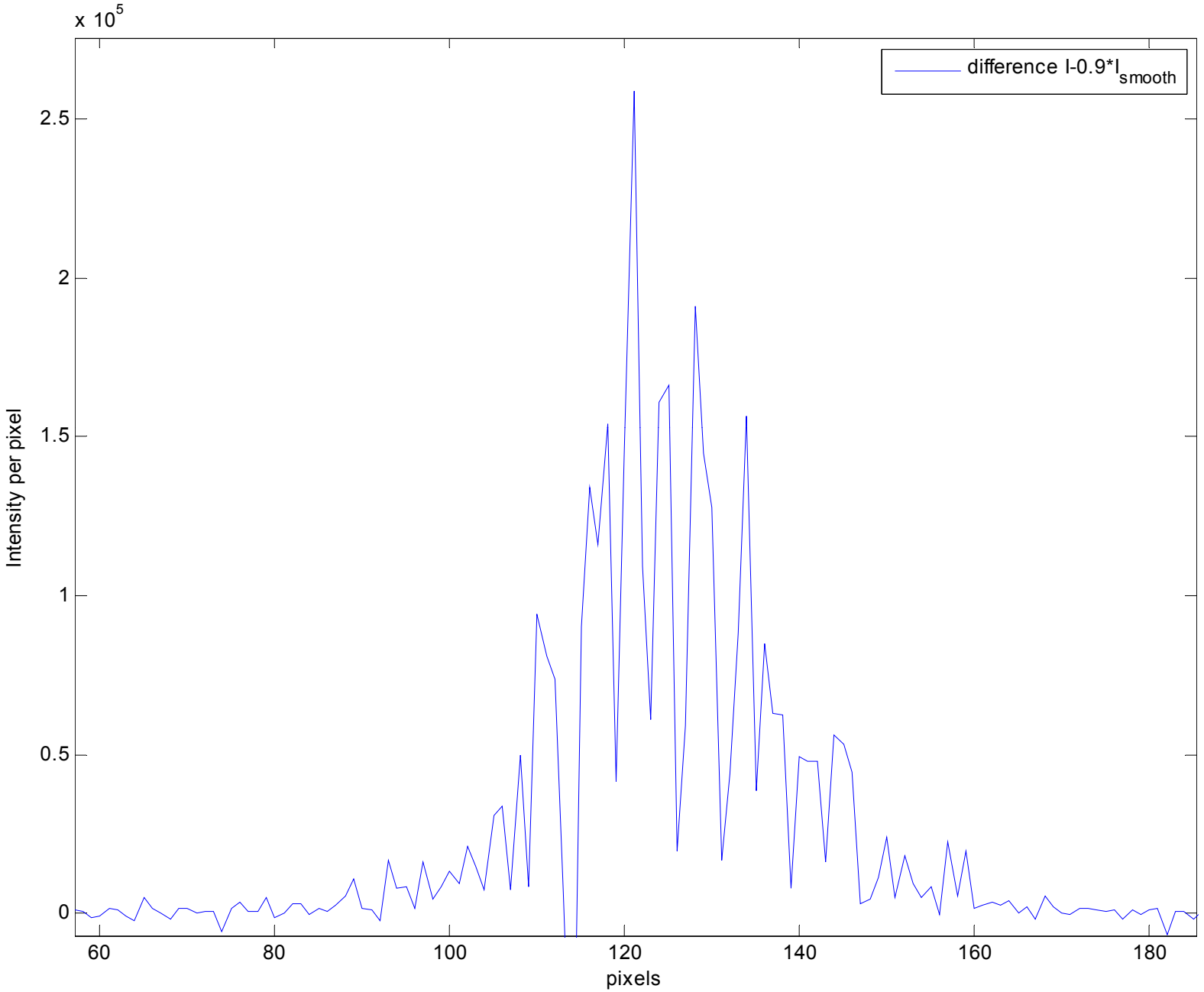
~100 nm

Why is the CDW speckle so "speckly"?

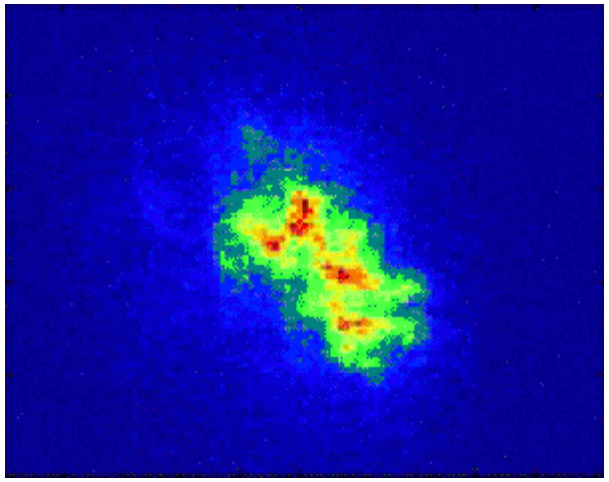


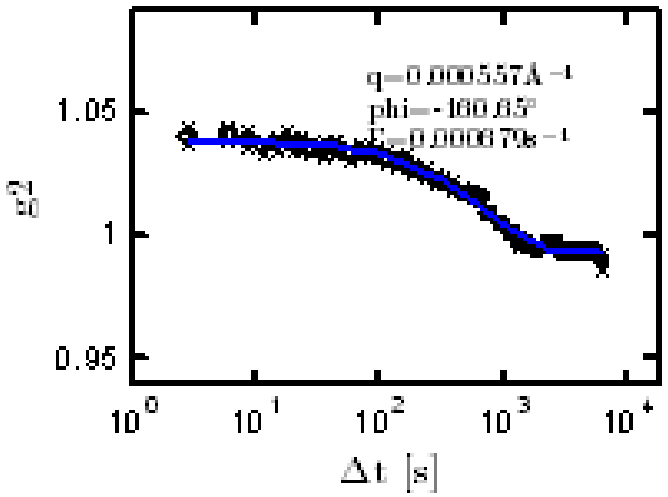
Number of speckles ≈ Number of coherent volumes

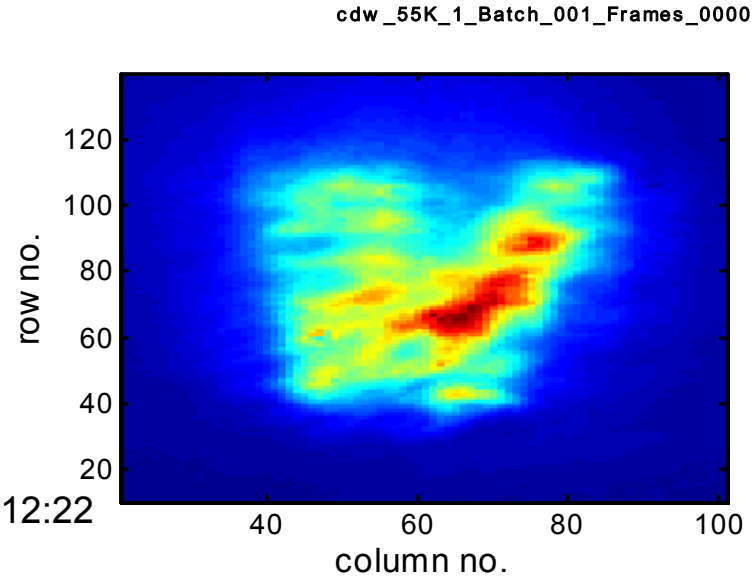

x 10^5
18
16
14
12
10
8
6
4
2
Intensity per pixel
90
100
110
120
130
140
150
160
170
pixels
Linescan
Linescan with 20-pixel smoothing

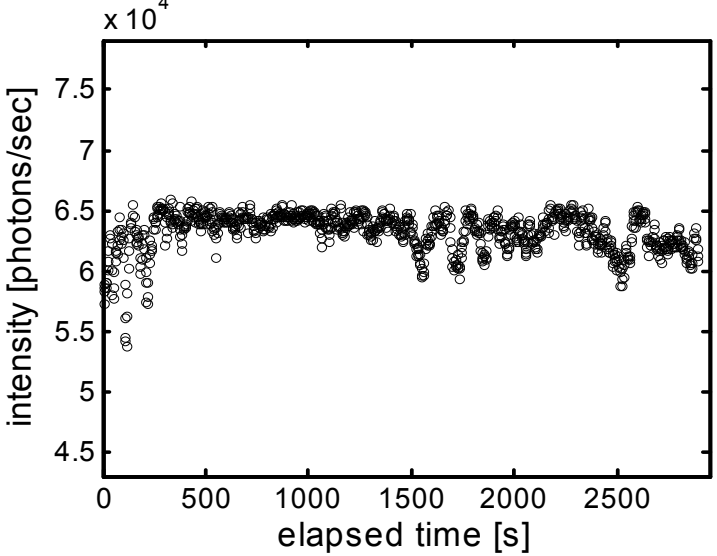

x 10^5
difference I-0.9*I_smooth
2.5
2
1.5
1
0.5
0
Intensity per pixel
60
80
100
120
140
160
180
pixels

Speckle with microfocused (0.5x2) μm beam

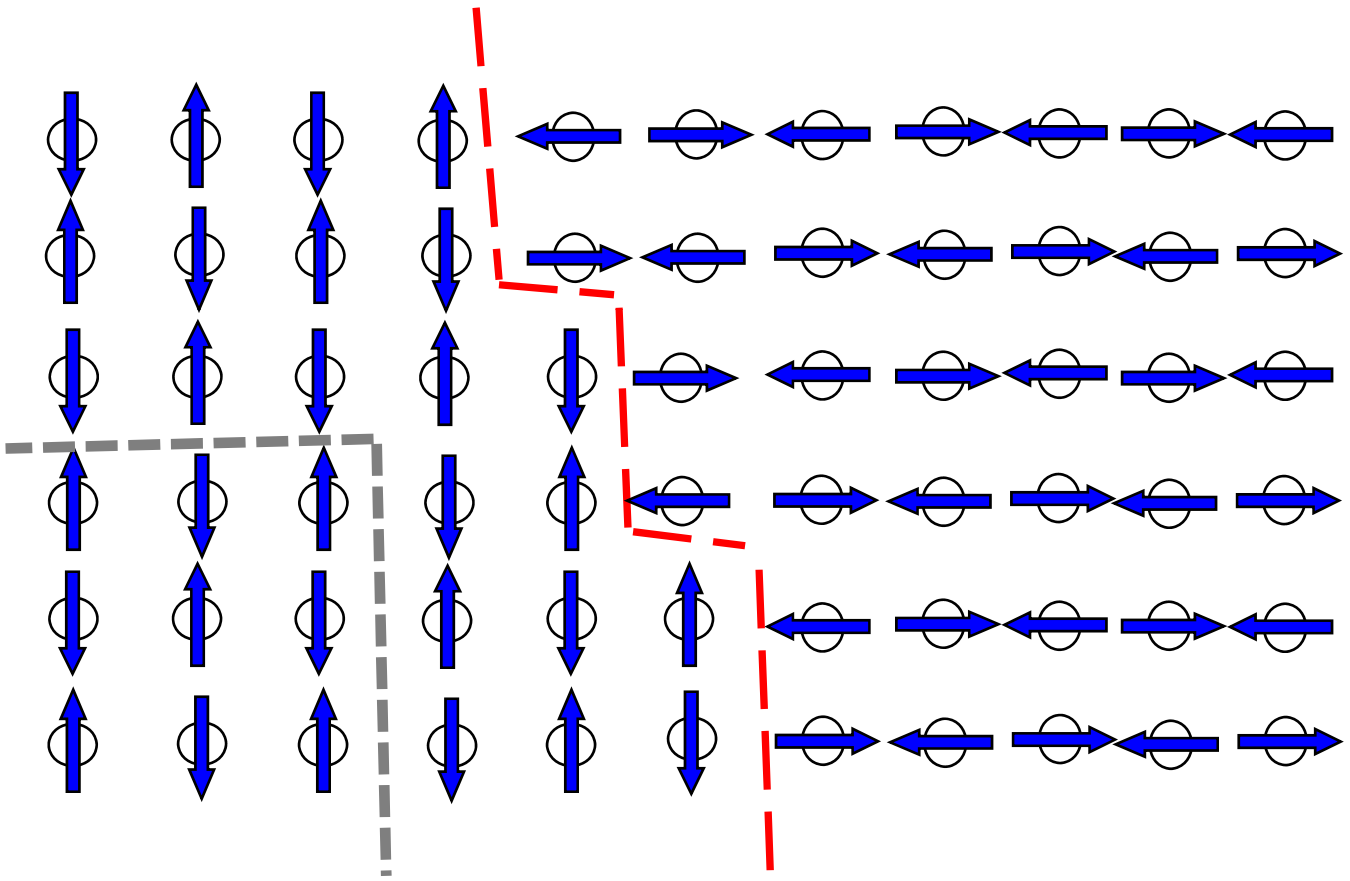








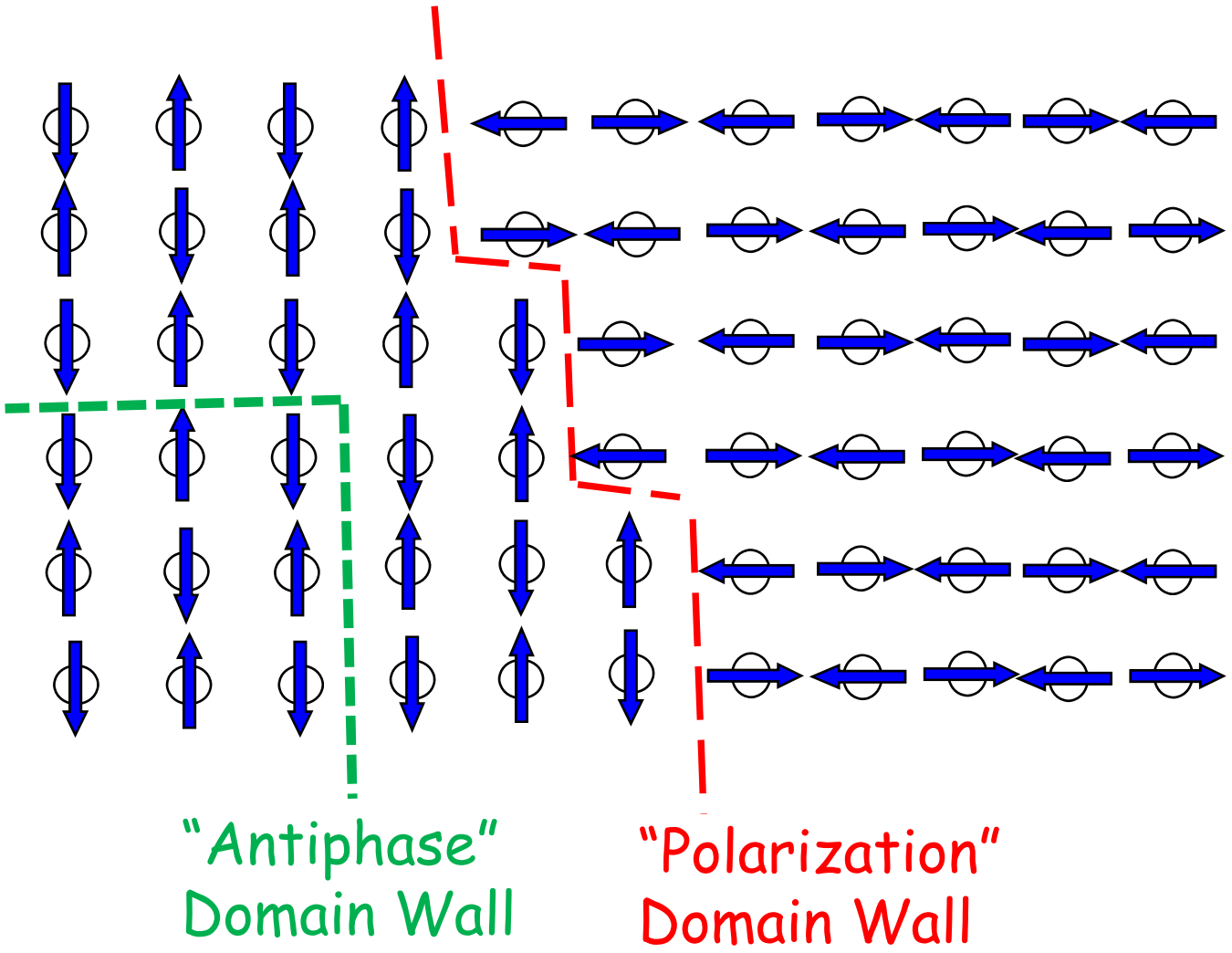
Domain Wall Fluctuations in Antiferromagnets



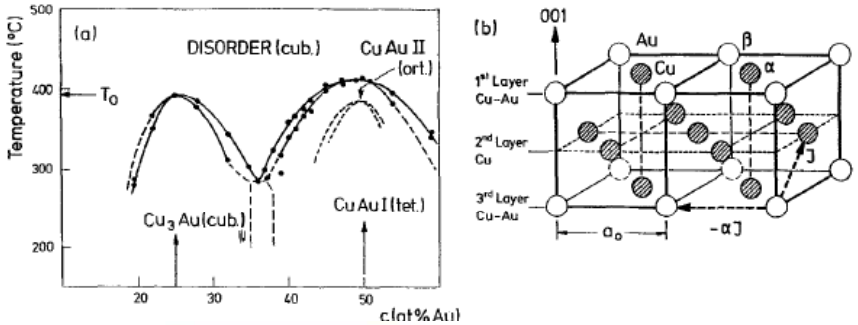
Flip all spins by 180 deg

Domain Wall

Phase vs. Polarization domain walls:

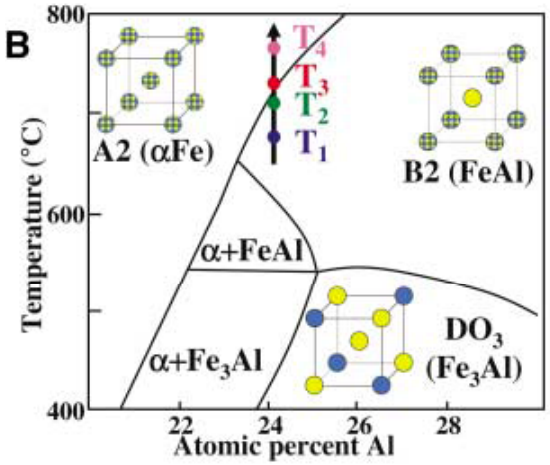


Antiphase domains in binary alloys:



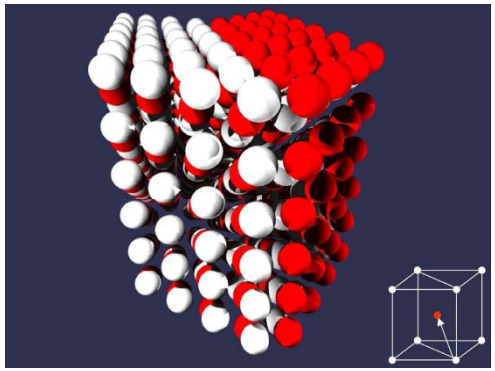
Cu_3Au

Sutton et al., Nature 1991, PRL 2005



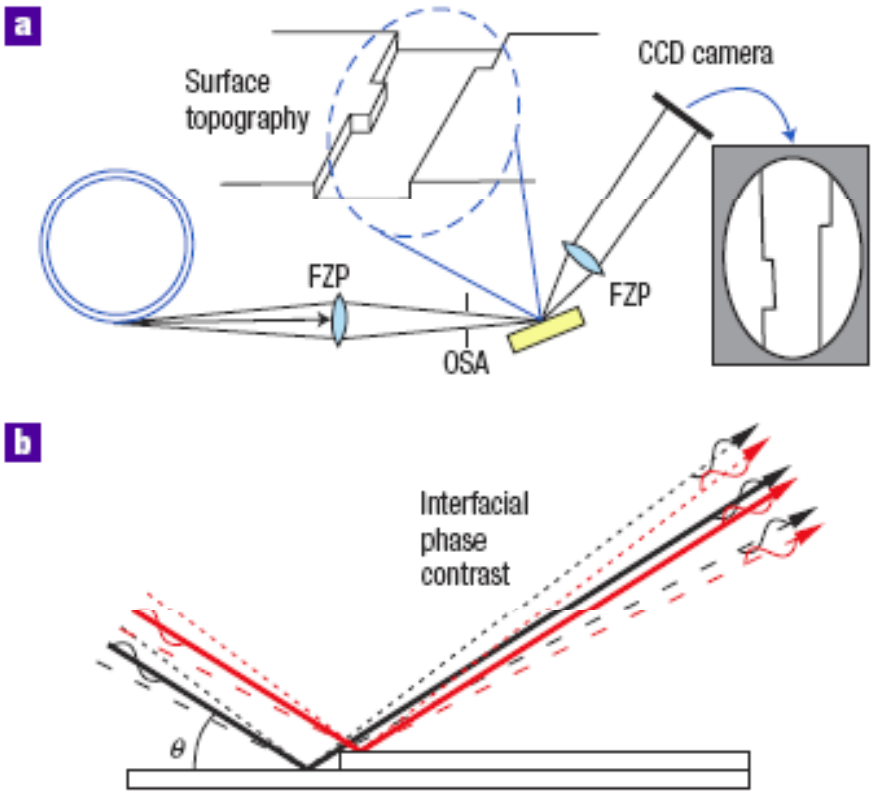
Fe_3Al

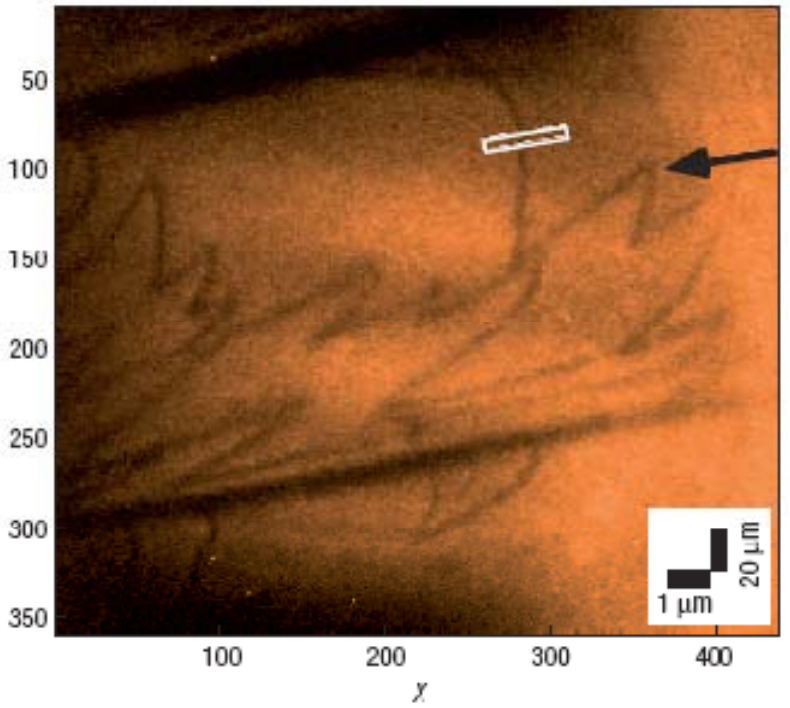
Brauer et al., PRL 1995
Mocuta et al., Science 2002



CoGa, AlLi, AlZn, AlAg

Stadler et al. 2004-2007

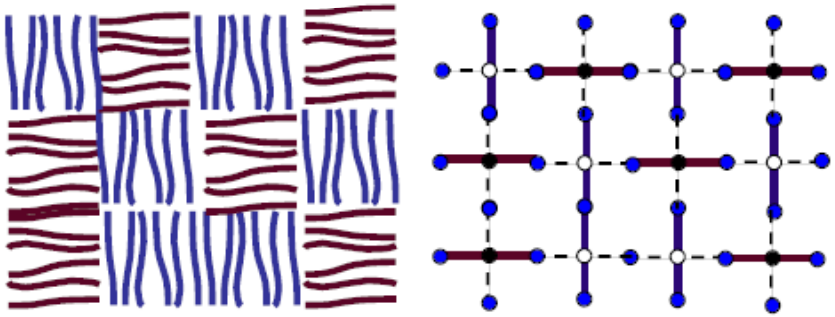


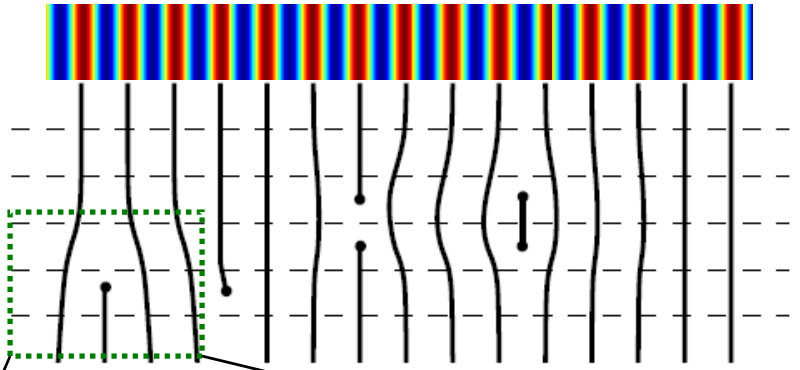


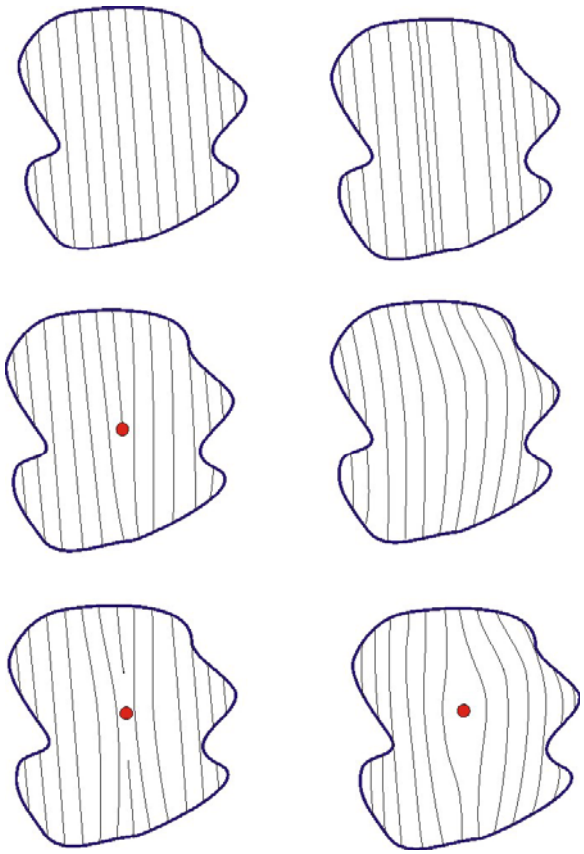
P. Fenter et al., *Nature Phys.* **2**, 700 (2006)

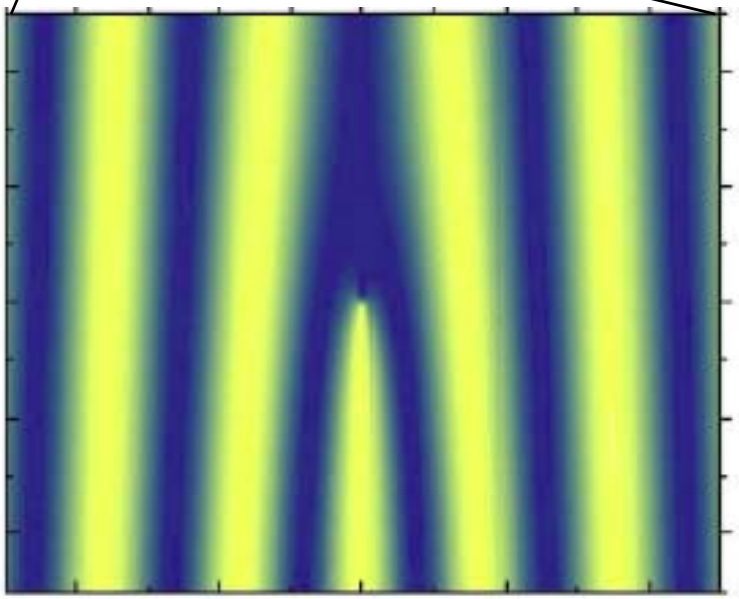
In-situ growth, surface defects, reactions at buried interfaces

Phase defects in nematic-like order parameter:



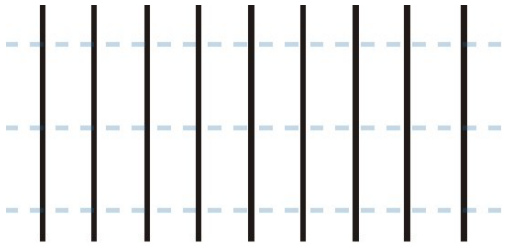




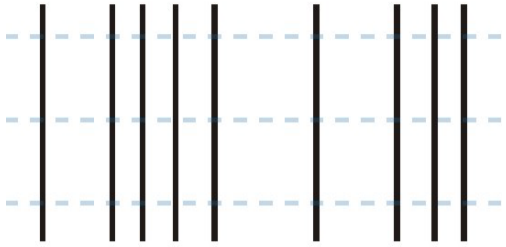


Phase defects of SDW/CDW

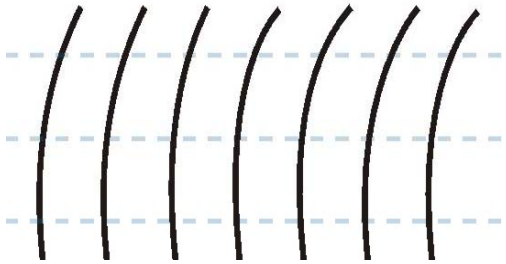
Phase strain:



periodic phase

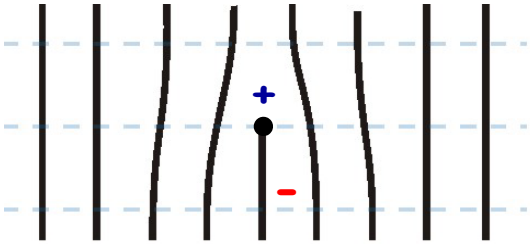


compression, dilatation

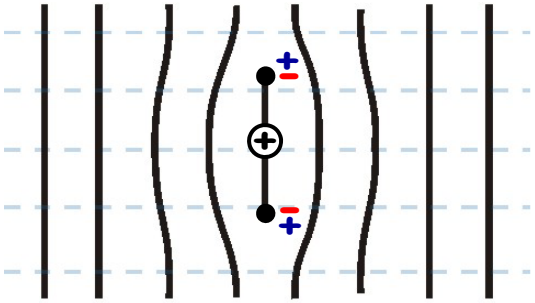


shear

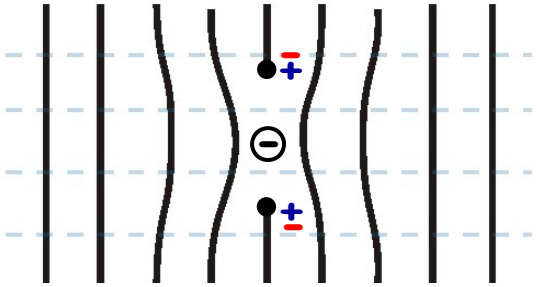
Edge dislocations:



electrical dipole

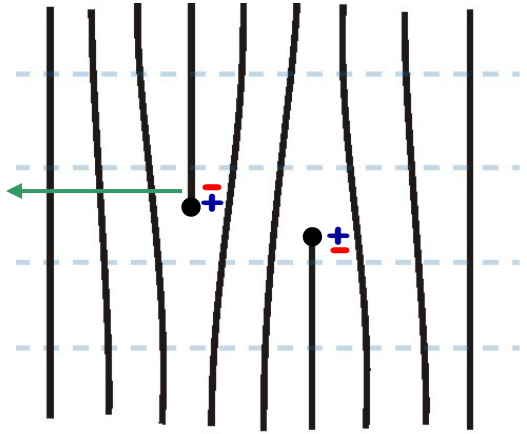


positive charge defect

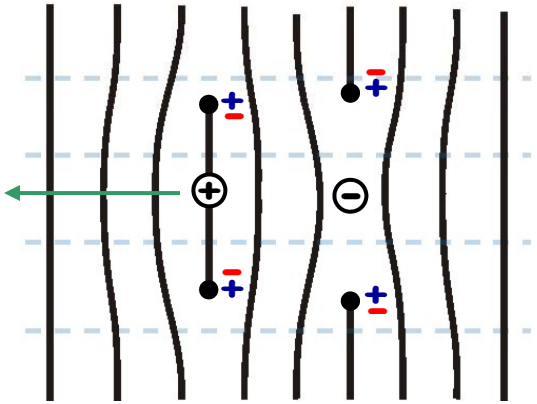


negative charge defect

Nucleation and growth of edge dislocations:

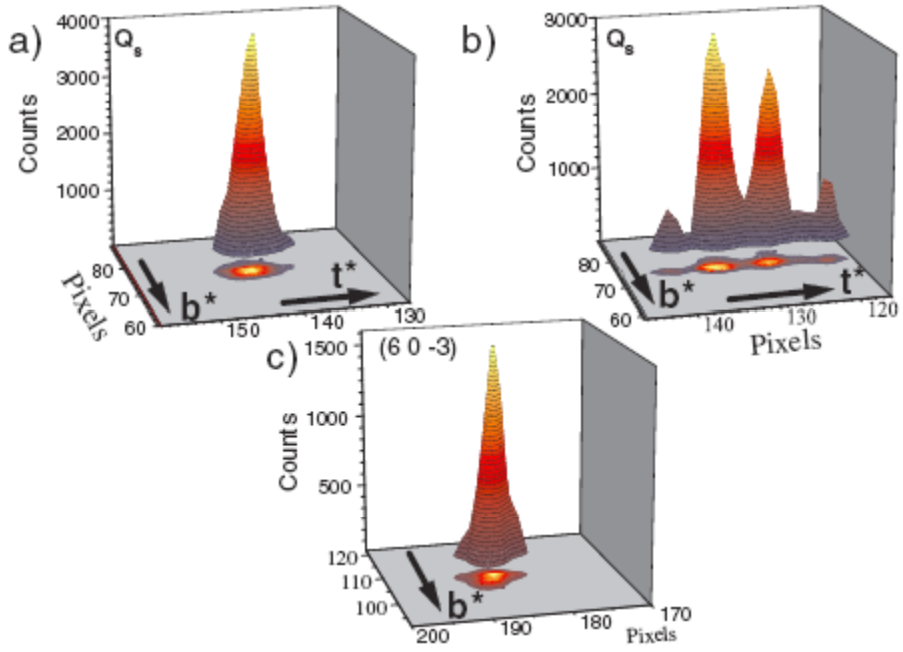


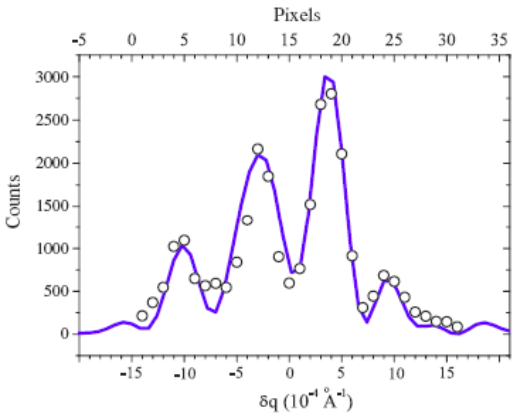
dislocation glide

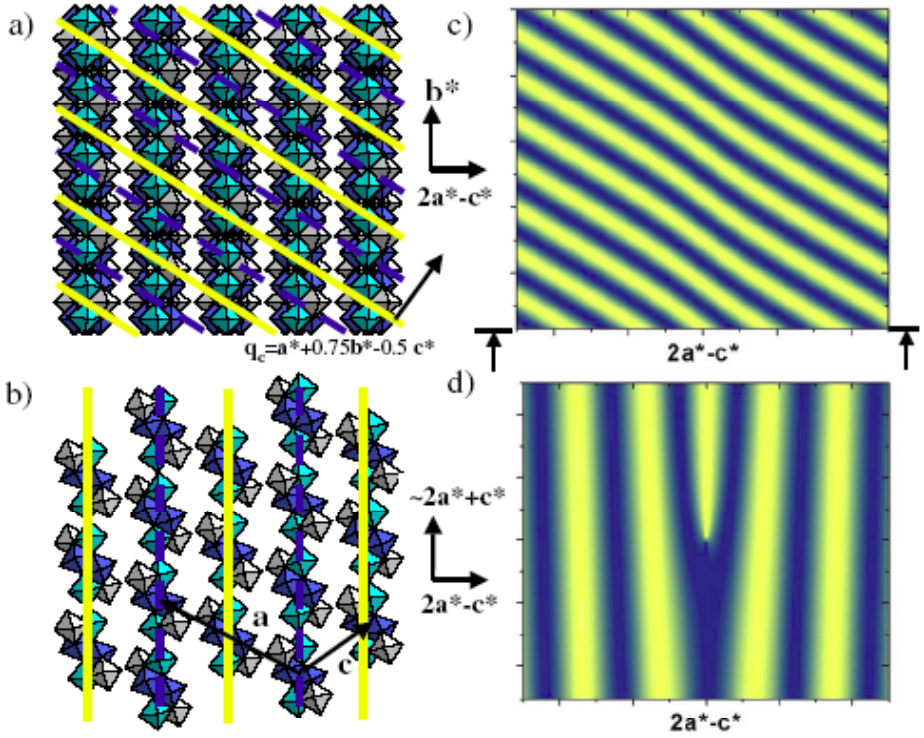


dislocation climb

X-ray Speckle Imaging of dislocations in electronic (CDW) crystals







D. LeBolloc'h et al., PRL **95**, 116401 (2005)

Interactions of SDW/CDW with defects

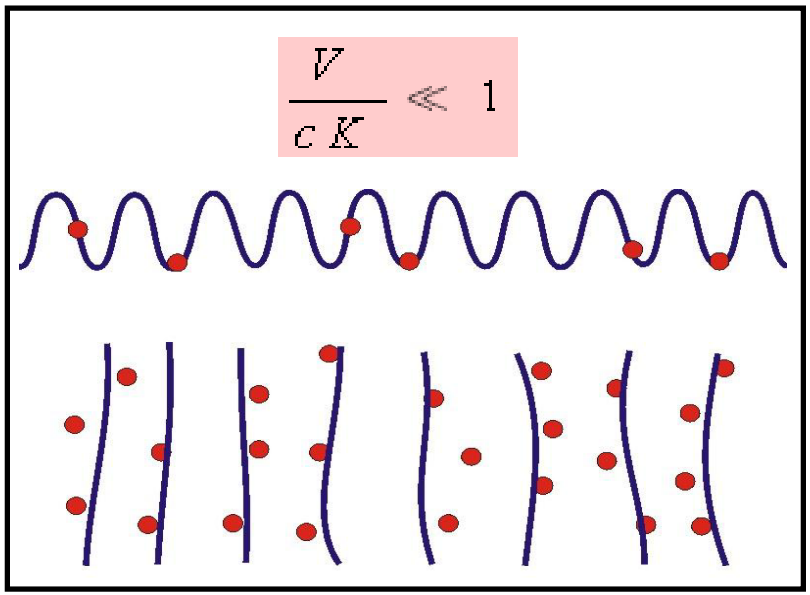
$$E = \int dx \left\{ \tfrac{1}{2} K [\nabla \varphi(x) - q]^2 + V \sum_i \cos[Qx + \varphi(x)] \delta(x - R_i) \right\}$$

Phase elasticity

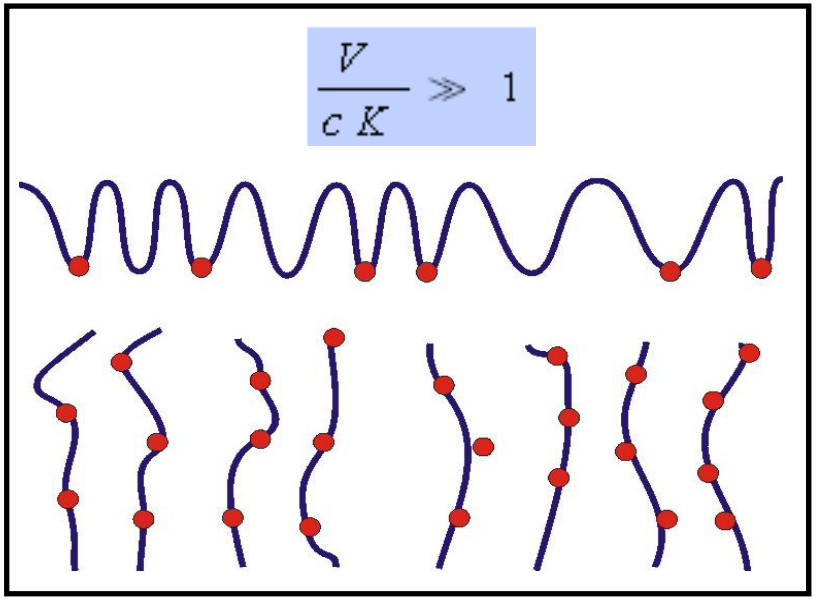
Pinning potential

H. Fukuyama and P. A. Lee, Phys. Rev. B 17, 535 (1978)
P. Littlewood and T. M. Rice, Phys. Rev. Lett 48, 44 (1982)

V – pinning potential, ***c*** – concentration of defects, ***K*** – phase elasticity of SDW/CDW

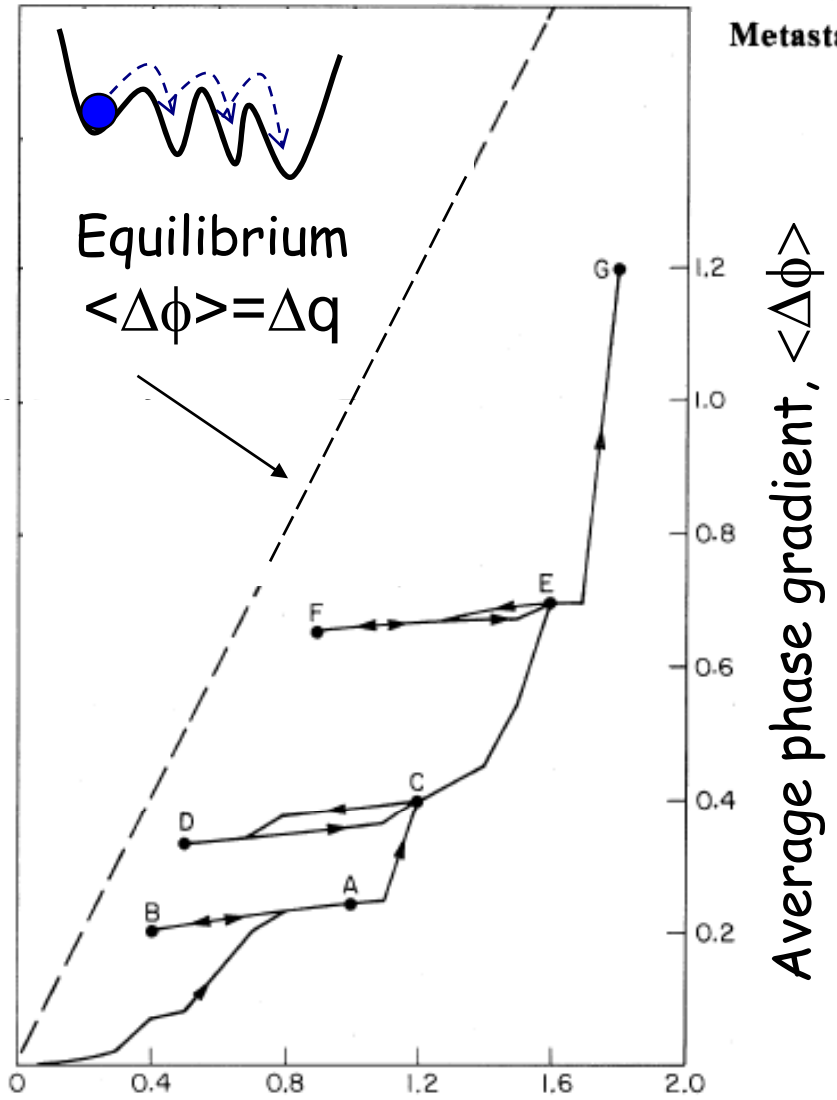


Weak Pinning



Strong Pinning

Metastability and glassiness of pinned SDW in Cr



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Metastability of the *Q* Vector of Pinned Charge- and Spin-Density Waves

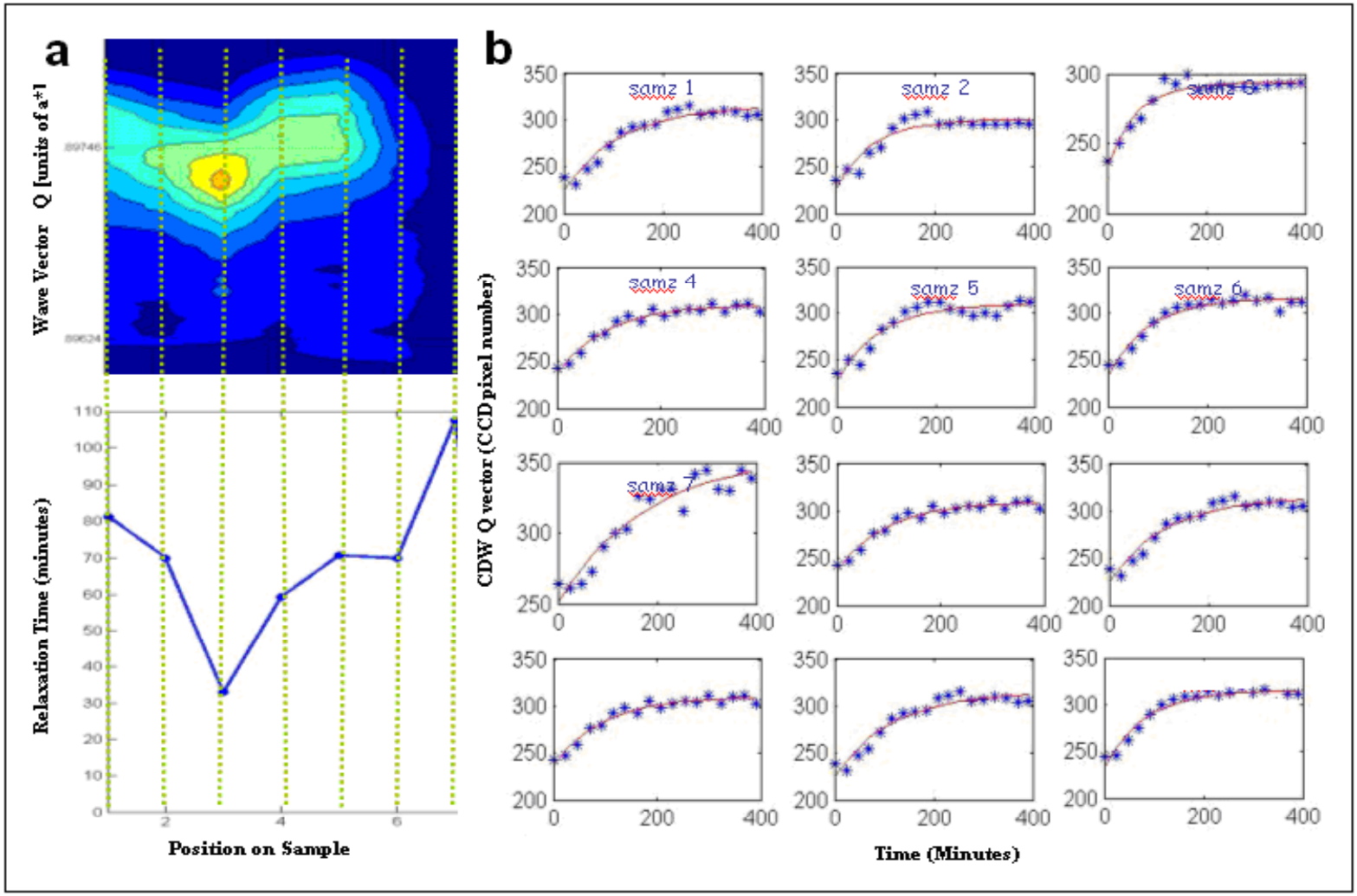
P. B. Littlewood and T. M. Rice[a]
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 1 September 1981)

Computer simulations for Chromium (weak pinning)

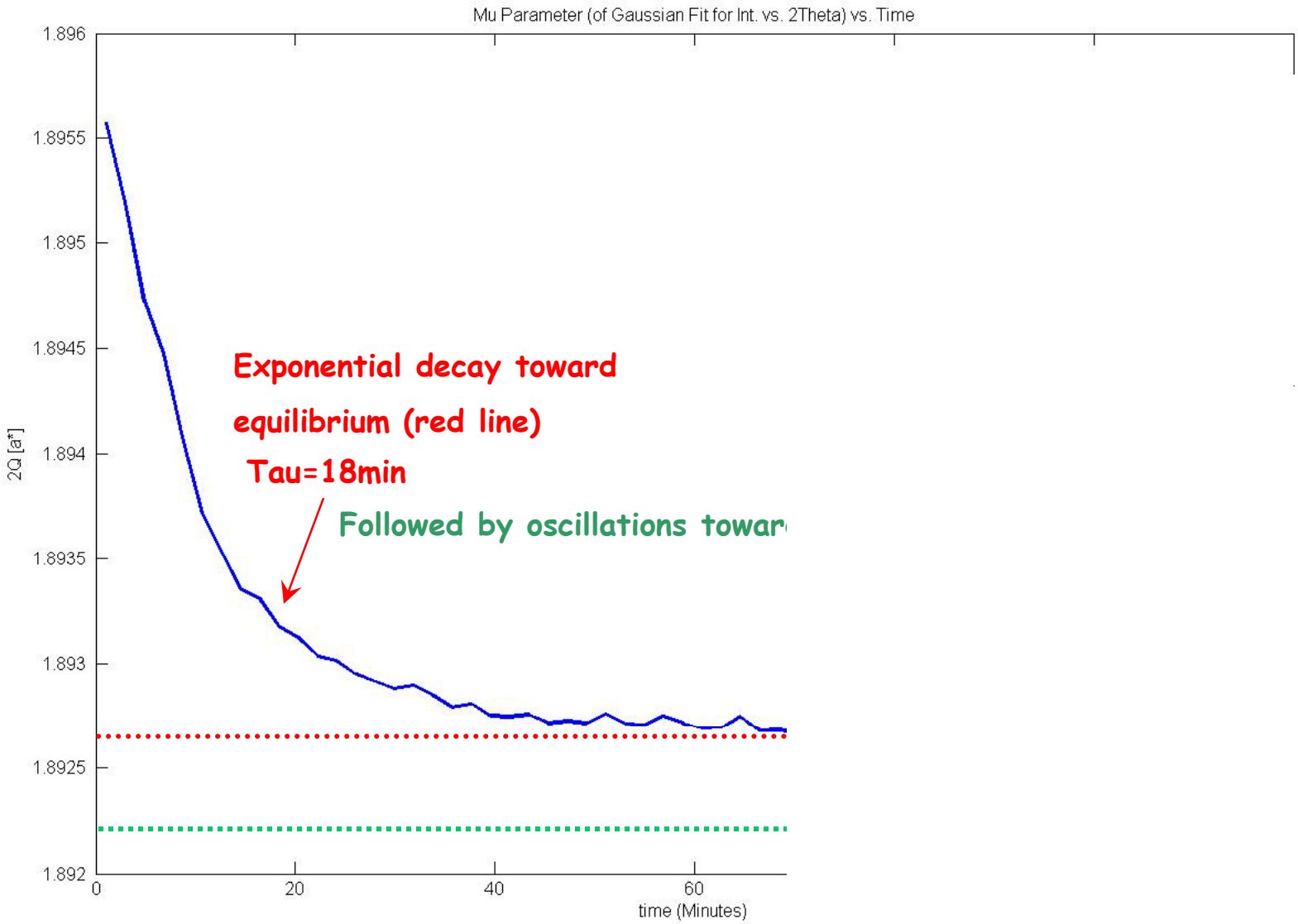
- Average phase gradient lags significantly behind wavevector change
- System "stuck" in metastable state – relaxation of phase gradient happens through nucleation of solitons
- Hysteretic behavior and slow "glassy" relaxation towards equilibrium

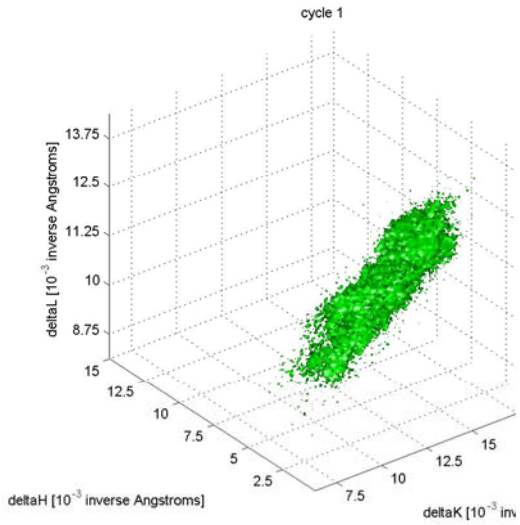
P. Littlewood and T. M. Rice,
Phys. Rev. Lett. **48**, 44 (1982)

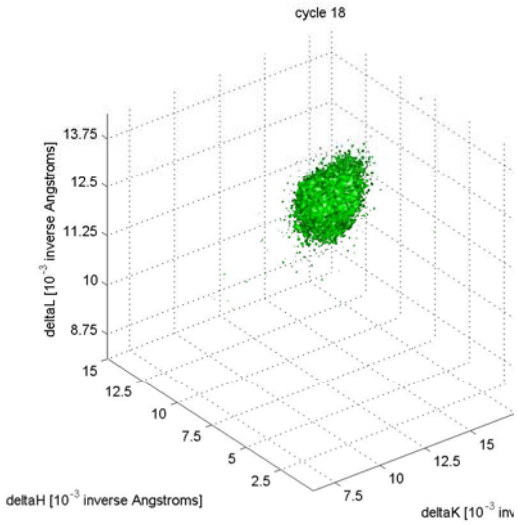
Q-value relaxation, measured by X-ray microdiffraction:

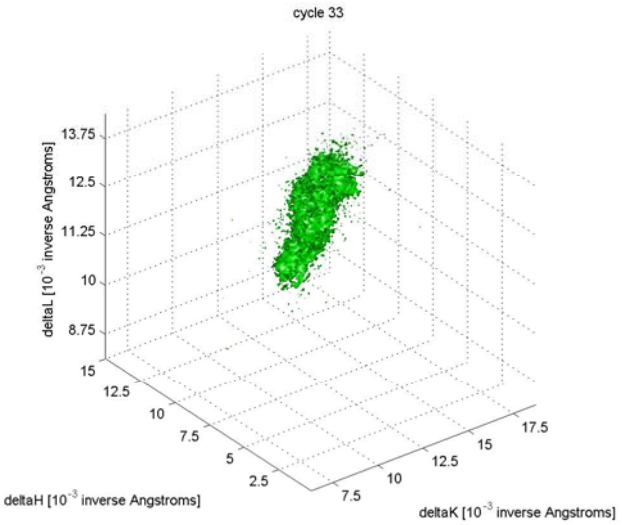


Avalanches in Q-relaxation

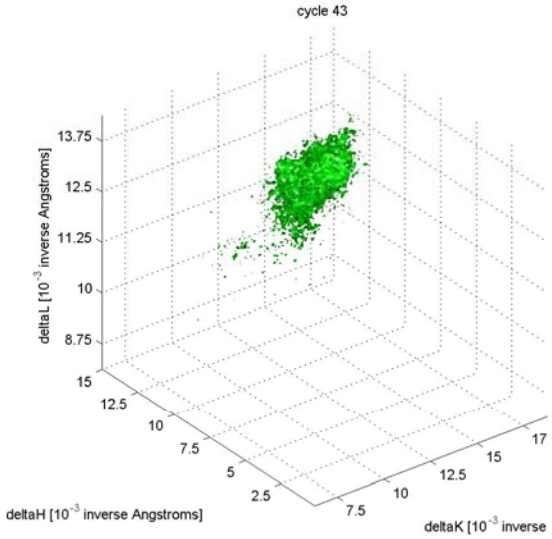


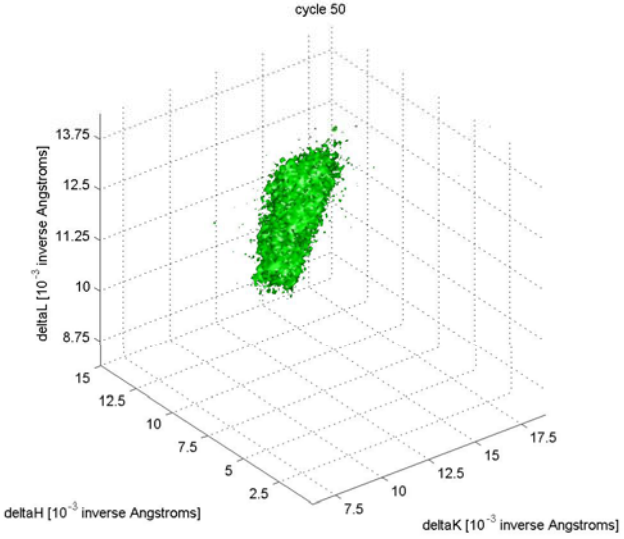


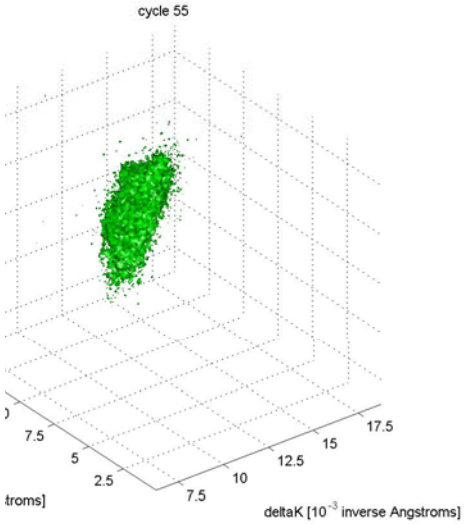


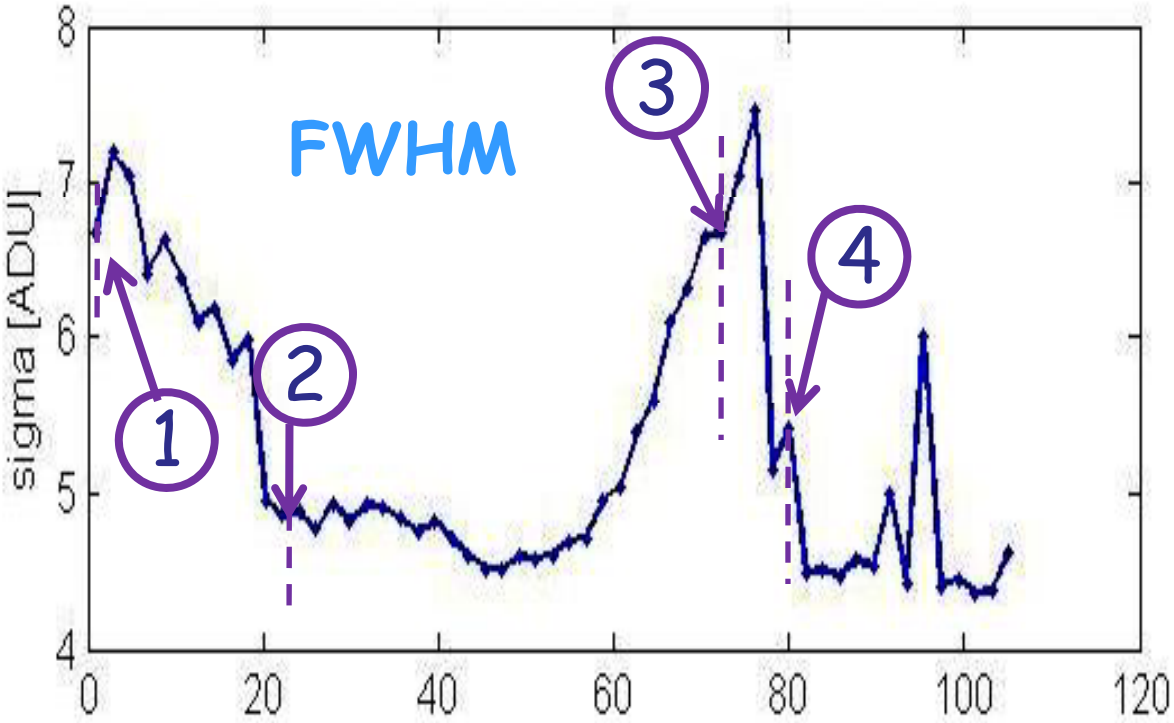


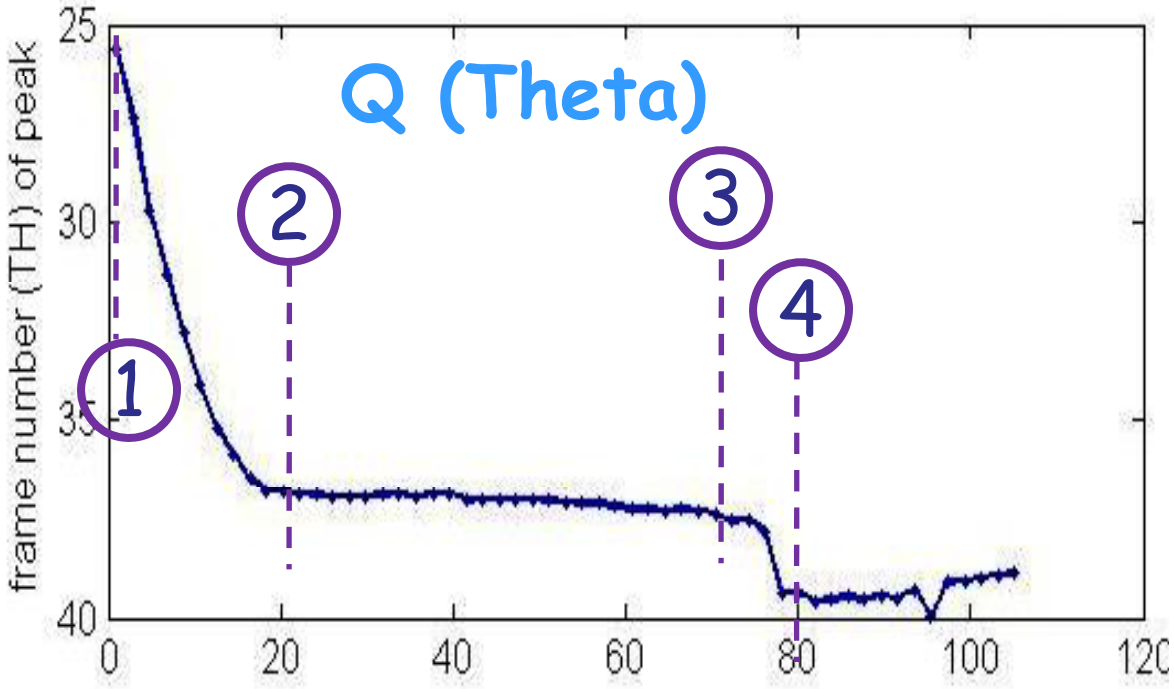
Correlation lengths (shear, compression-dilatation of Q) during pinning-depinning

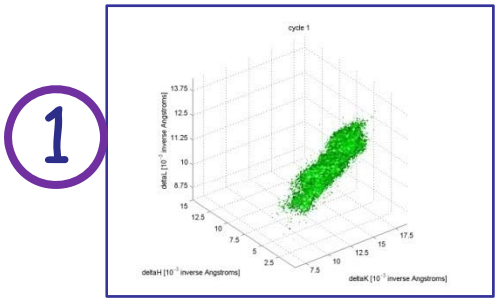


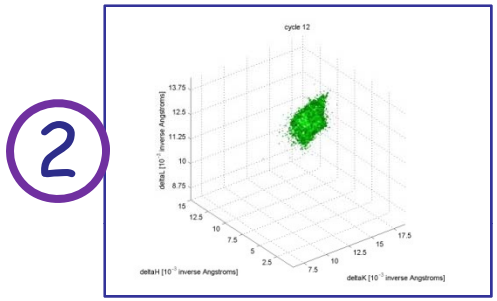


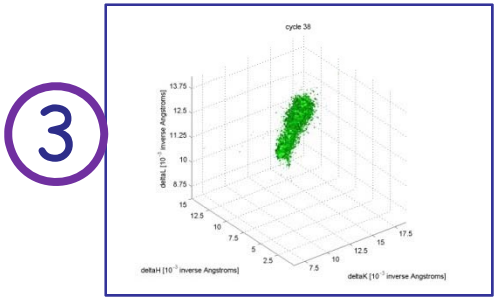


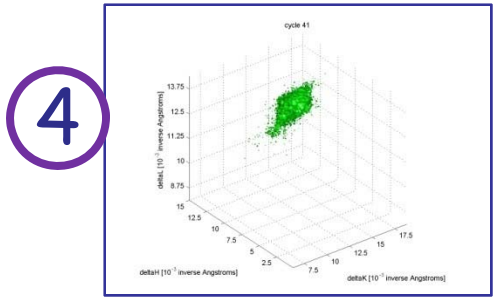

FWHM
sigma [ADU]
1
2
3
4


Q (Theta)
frame number (TH) of peak
1
2
3
4


1


2


3


4

mini-Summary:

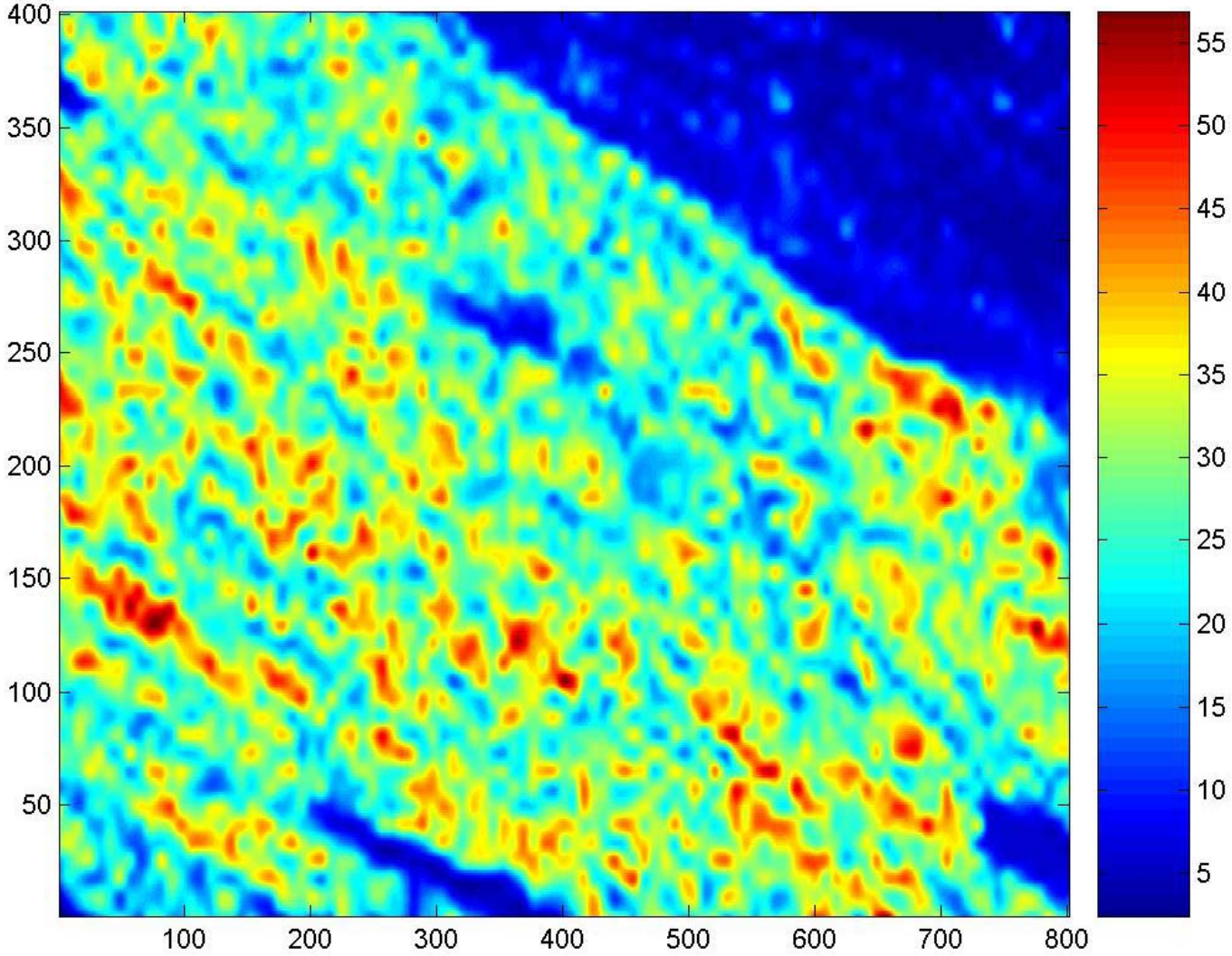
Currently can measure change in correlation length of CDW order parameter
(ensemble average over ~1 micron sized beam spot)

NEXT:

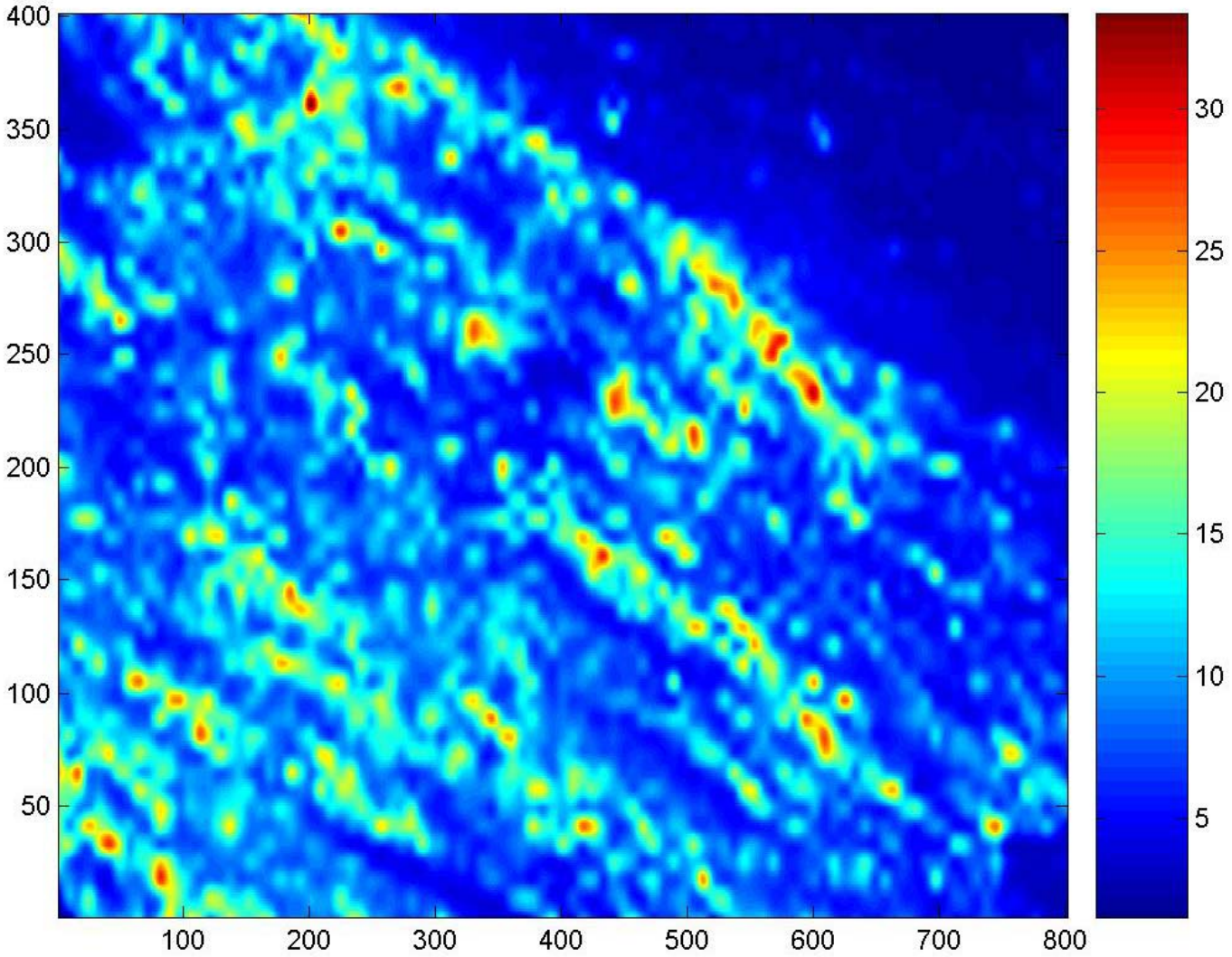
We want to "see" CDW defects, their (collective?) dynamics, relationship to crystalline defects

Resolution ~ 10 nm may be sufficient!

Equilibrium Q(T=4K) Value map: after 6 hr of "aging" at 4K

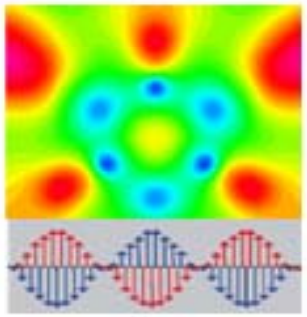


"Old" Q (T=150K) map at 4K
isolated pinned domains – "memory" of 150K persists

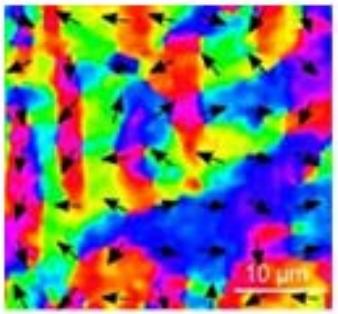


Collective dynamics of elastic media in presence of quenched disorder:

Charge-, Spin-density waves (10^{-10}-10^{-7} m)



Magnetic domains (10^{-8}-10^{-4} m)

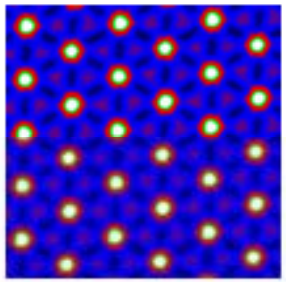


Sandpiles (10^{-3}-10 m)

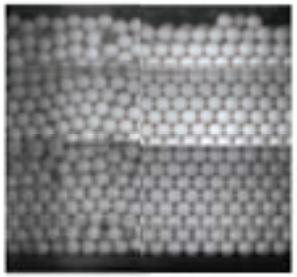
tectonic plates (10^{2}-10^{6} m)

1 nm — 1 mm — 1 km

1 Å — 1 mm — 1 m — 100km

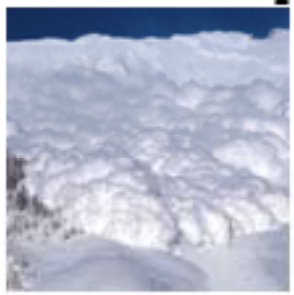


Abrikosov vortex lattice (10^{-7} m)



Jamming, shear flow in granular materials, colloids (10^{-6}–10^{-2} m)

Liquid droplets pinned on rough substrates (10^{-4} – 10^{-2} m)



Avalanches (10-10^{3} m)

12:22

What/where are the pinning centers?
(CXD provides phase information!)

- Need to image defects in order parameter

(charge, spin, orbital ordering)

- Classify domain walls/defects

(polarization vs. phase defects: dislocations, shear, etc.)

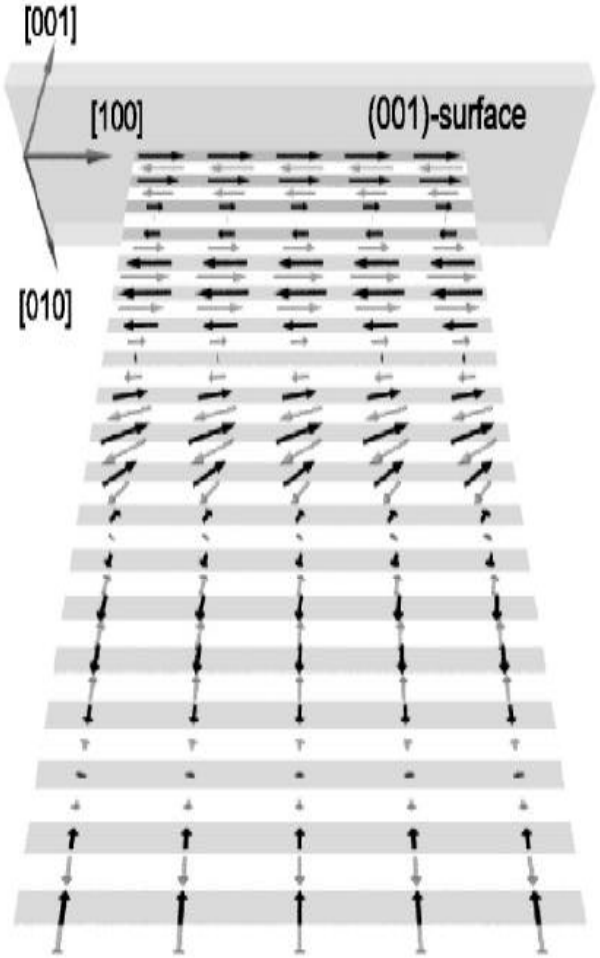
- Is there correlation to atomic lattice defects

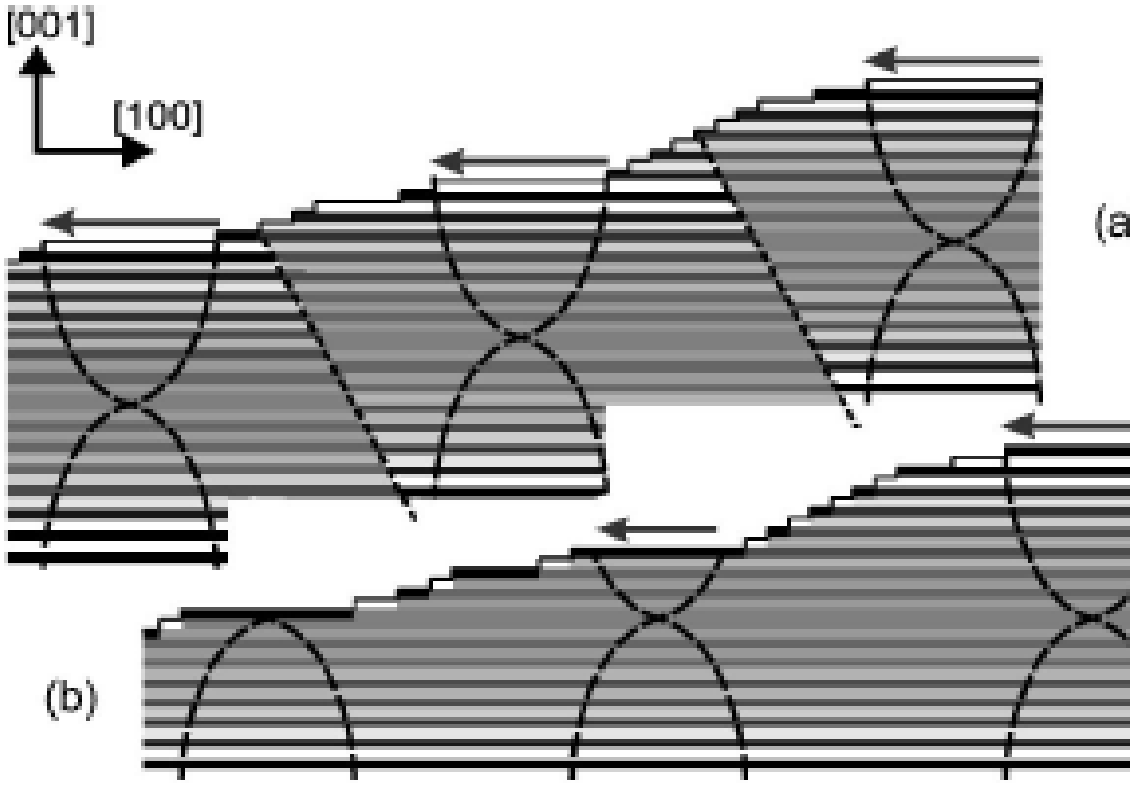
(strain, lattice dislocations, etc.)

- Surface vs. Bulk pinning?

- Can we engineer pinning?

Surface vs. Bulk phase diagram for Cr

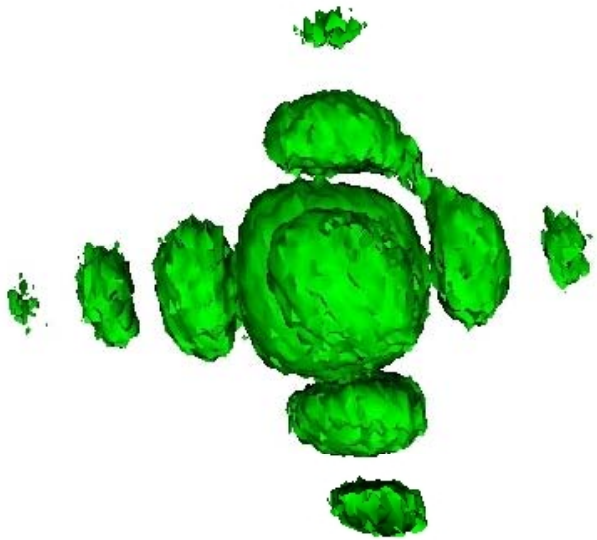




Hänke, T. et al., *Phys. Rev. B* **71**, 184407 (2005)

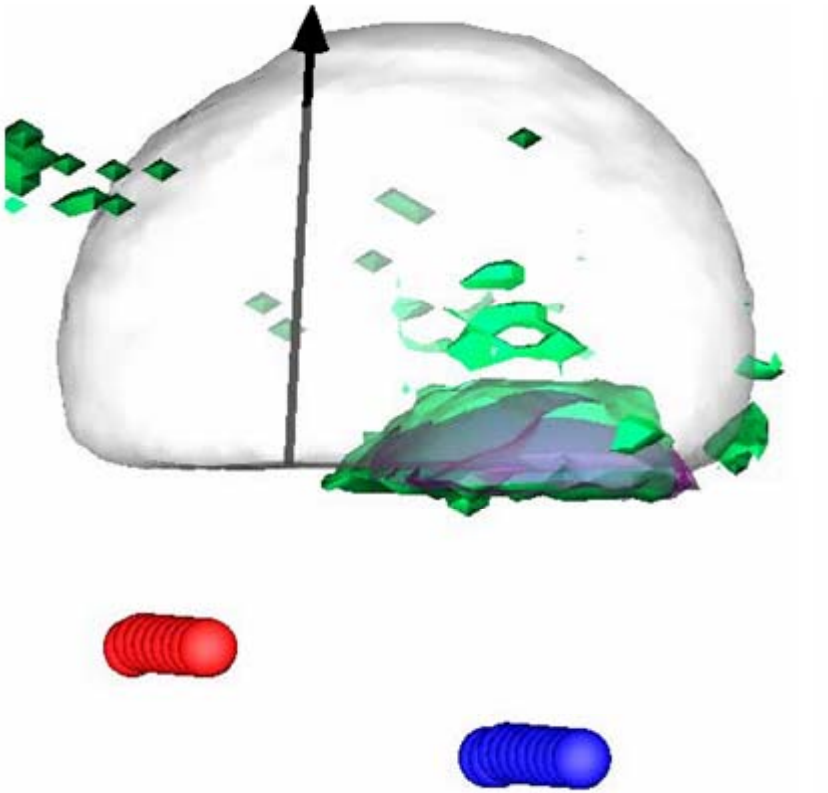
Coherent X-ray Diffraction (Lens-less imaging):

Reciprocal (momentum) space 3D "speckle"



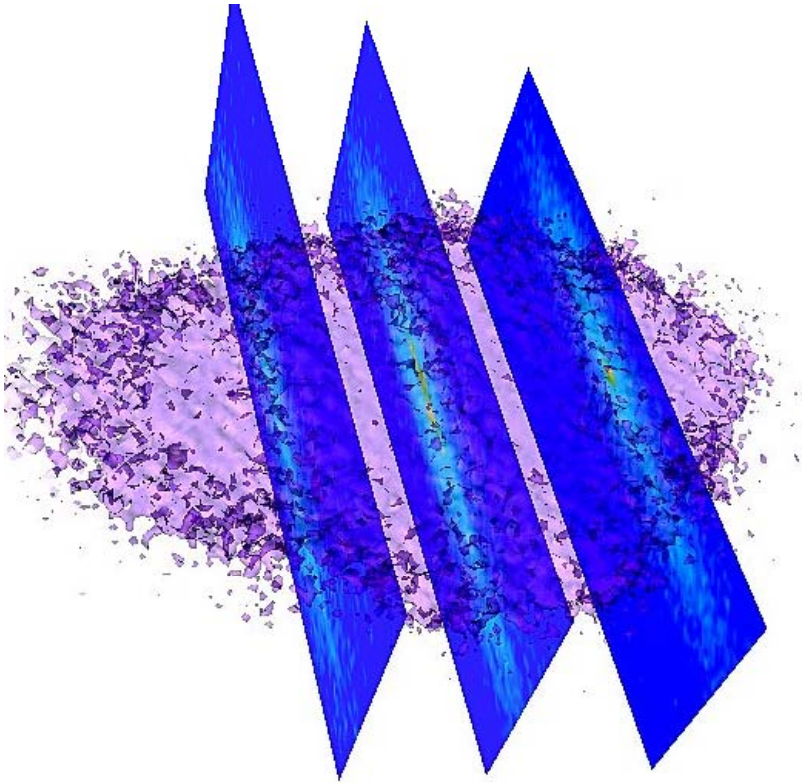
invert

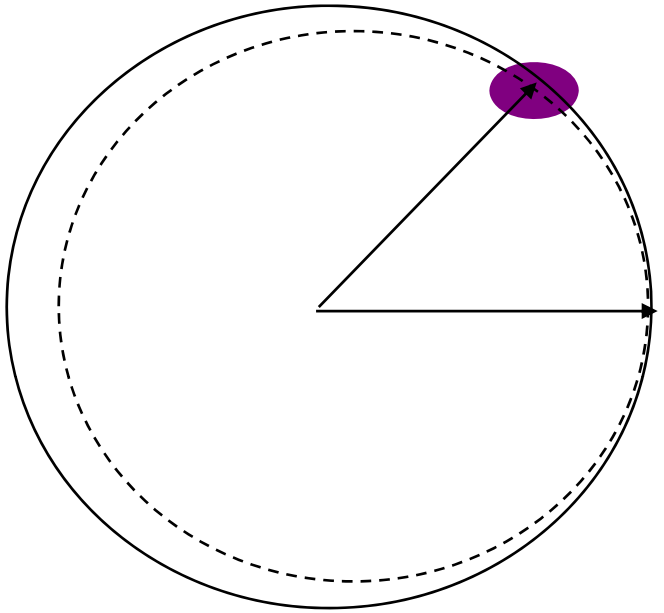
Real space object (phases and densities):



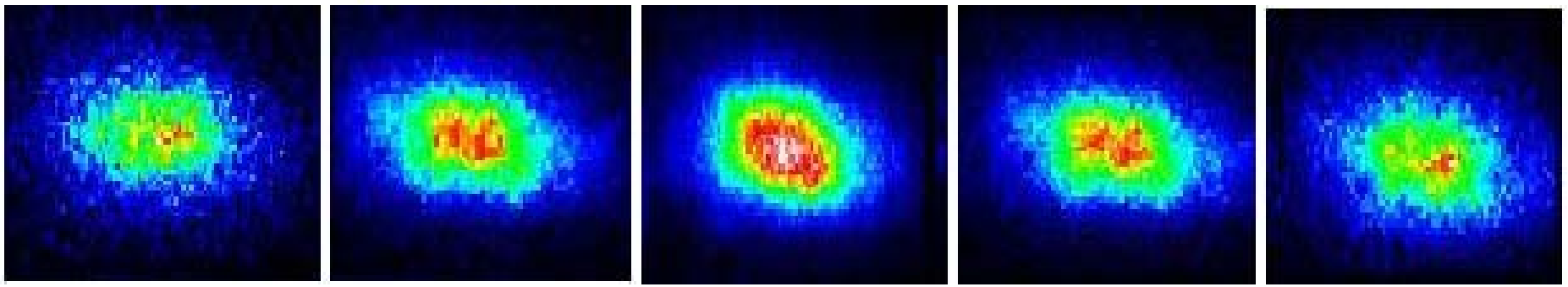
M. A. Pfeifer et al., *Nature* **442**, 63-66 (2006).

Lens-less imaging of defects



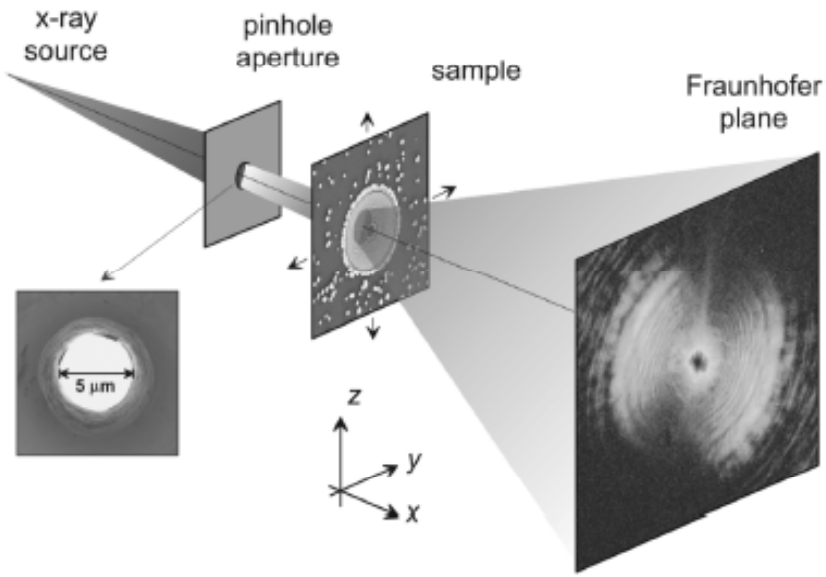


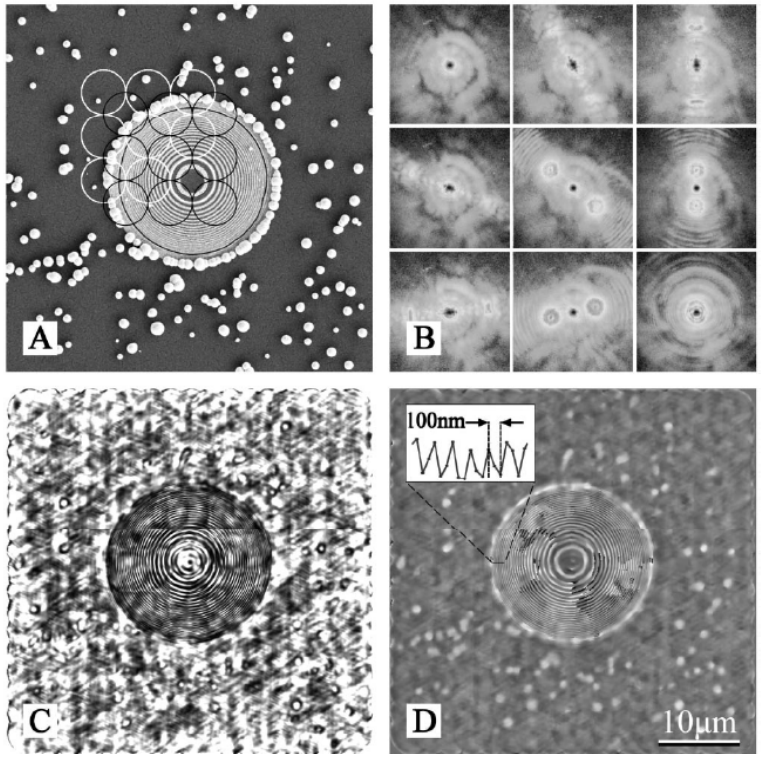
Scanning energy instead of rocking the sample theta



Ptychographical Iterative Engine (PIE)

(talk by Oliver Bunk earlier in the workshop)

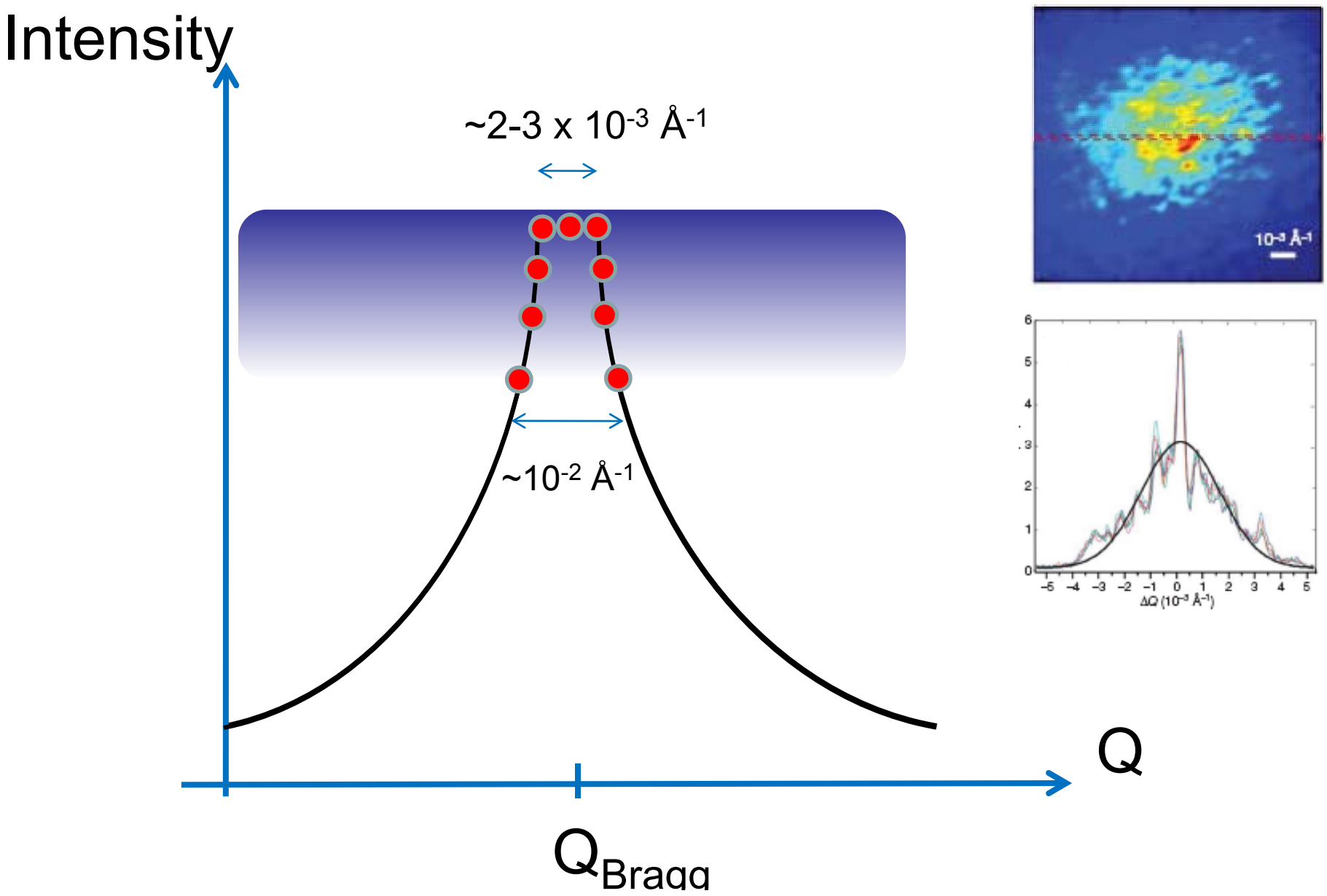


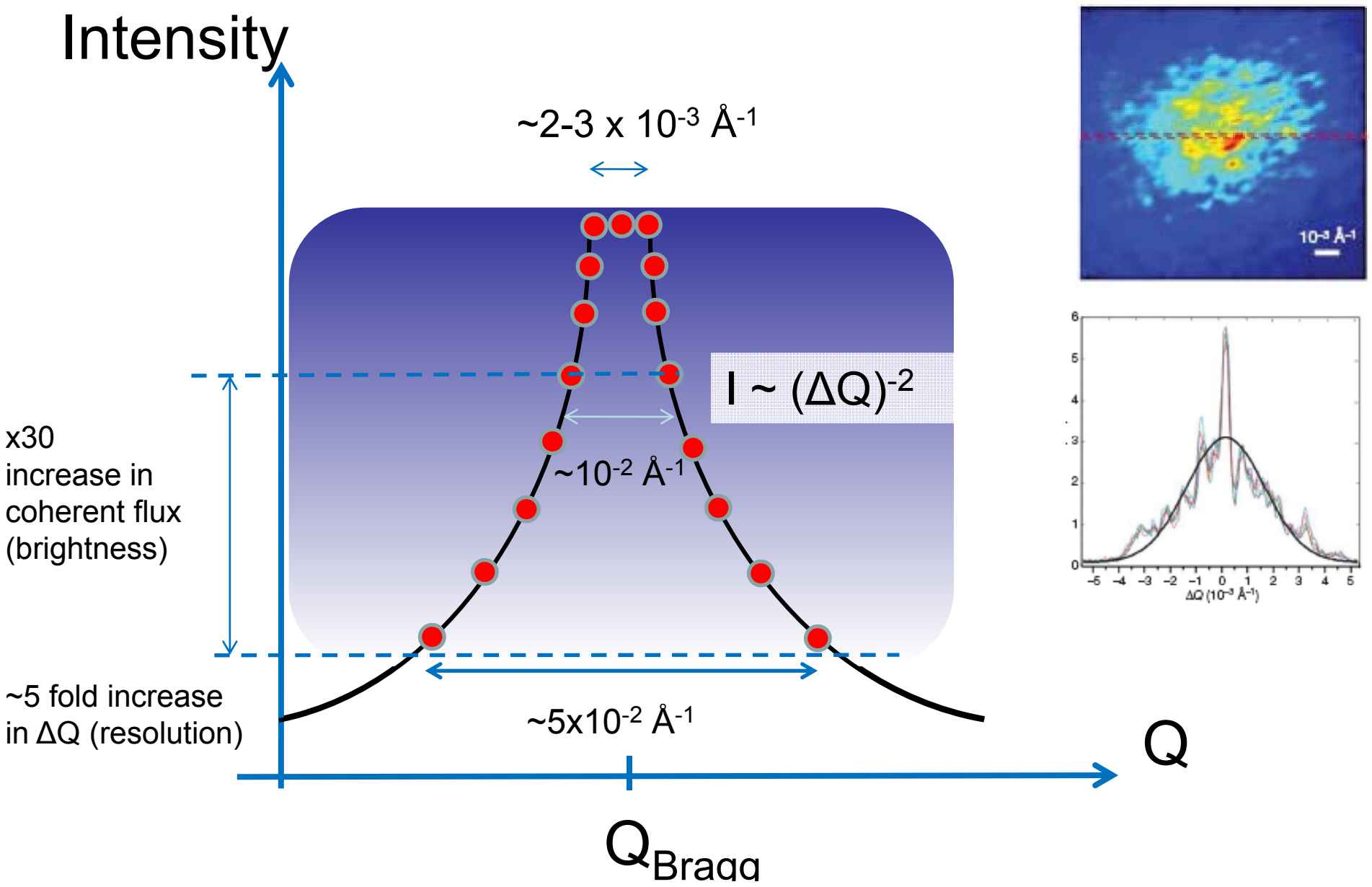


J. M. Rodenburg et al., *PRL* **98,** 034801 (2007)

Ptychographical Iterative Engine

- Complications arising from Bragg Diffraction (high-angle) geometry
- Precision of scanning
- Wavefront characterization
- Curved beam (?)
- Scanning Diffraction X-ray Microscopy + PIE


Intensity
~2-3 x 10-3 Å-1
~10-2 Å-1
Q
QBragg
10⁻³ Å⁻¹
ΔQ (10⁻³ Å⁻¹)



Instead of $\pi/10^{-2}$Å^{-1} ~30 nm, resolution becomes ~6 nm

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