Imaging with future light sources

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Dictionary

aphorism

aph•o•rism |ˈafəˌrizəm|

noun

a pithy observation that contains a general truth, such as, “if it ain't broke, don't fix it.” See note at SAYING .

• a concise statement of a scientific principle, typically by an ancient classical author.

DERIVATIVES

aph•o•rist noun

aph•o•ris•tic |ˌafəˈristik| adjective

aph•o•ris•ti•cal•ly |ˌafəˈristik(ə)lē| adverb

aph•o•rize |-ˌrīz| verb

ORIGIN early 16th cent.: from French ***aphorisme*** or late Latin ***aphorismus***, from Greek ***aphorismos ‘definition,’*** from ***aphorizein ‘define.’***

Future light source aphorisms

- You don’t use dynamite to roast a turkey.
- Incoherence doesn’t keep one from success - even the Presidency!
- Even in the freezer, food doesn’t last forever.
- Tenfold is a useful gain; thousandfold is a revolution.
- The rich can afford to waste money.
- If it’s a once-in-a-lifetime experience, savor it.
- You can observe a lot by watching.
- What time is it? You mean now?

Future light source action: heating up!

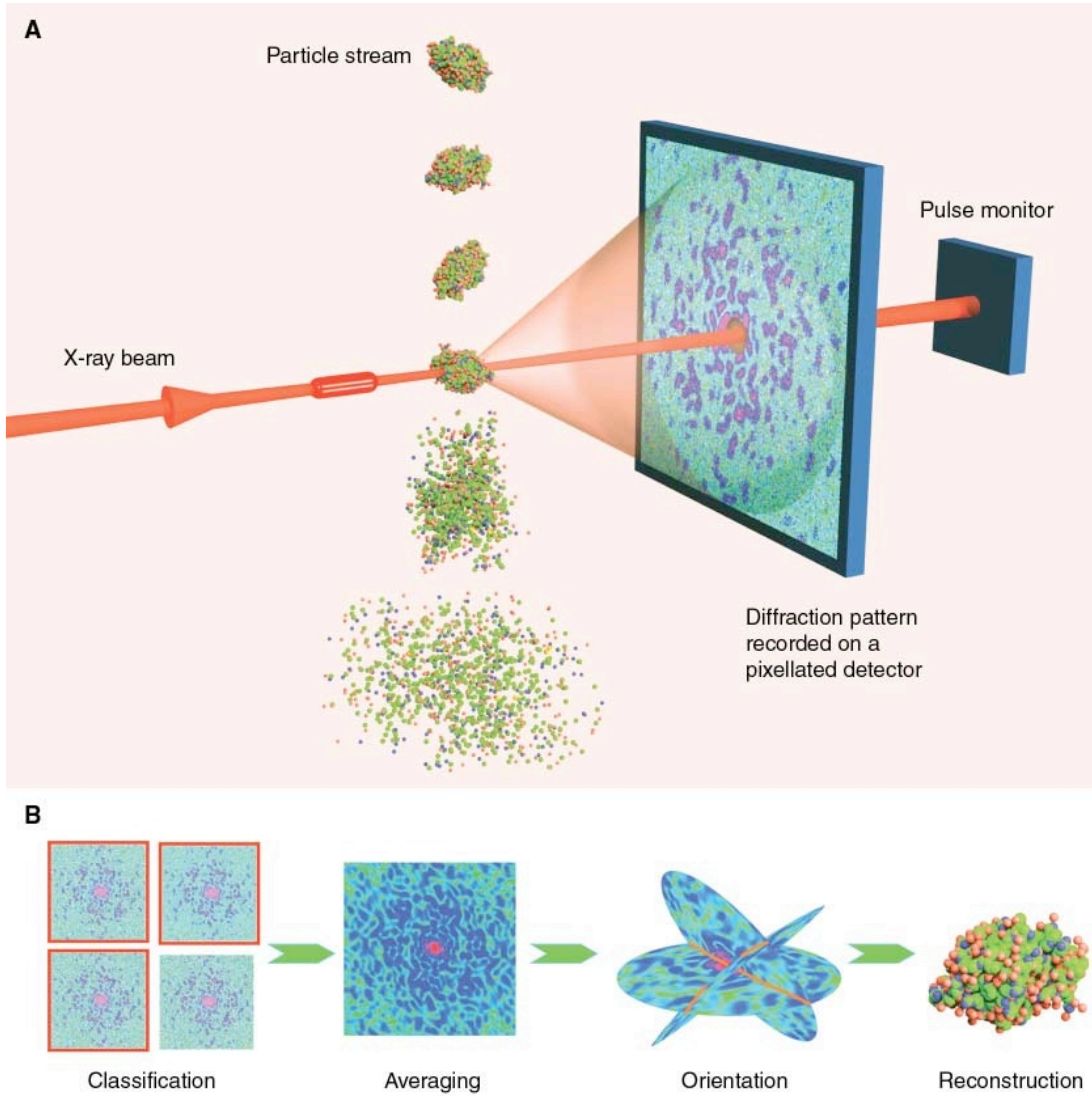
- High spatial resolution imaging demands lots of photons, like 10^5 per pixel or more!
- 10^5 photons incident on $(10\text{ nm})^3$ and no cooling:
  - H_20@500 eV ⇒ 2300K
  - H_20@3 keV ⇒ 2200K
  - Si@10 keV ⇒ 7300K
- What are our options?

Option 1: let it rip!

Bullet in cucumber (MIT strobe lab)

Exploding molecules

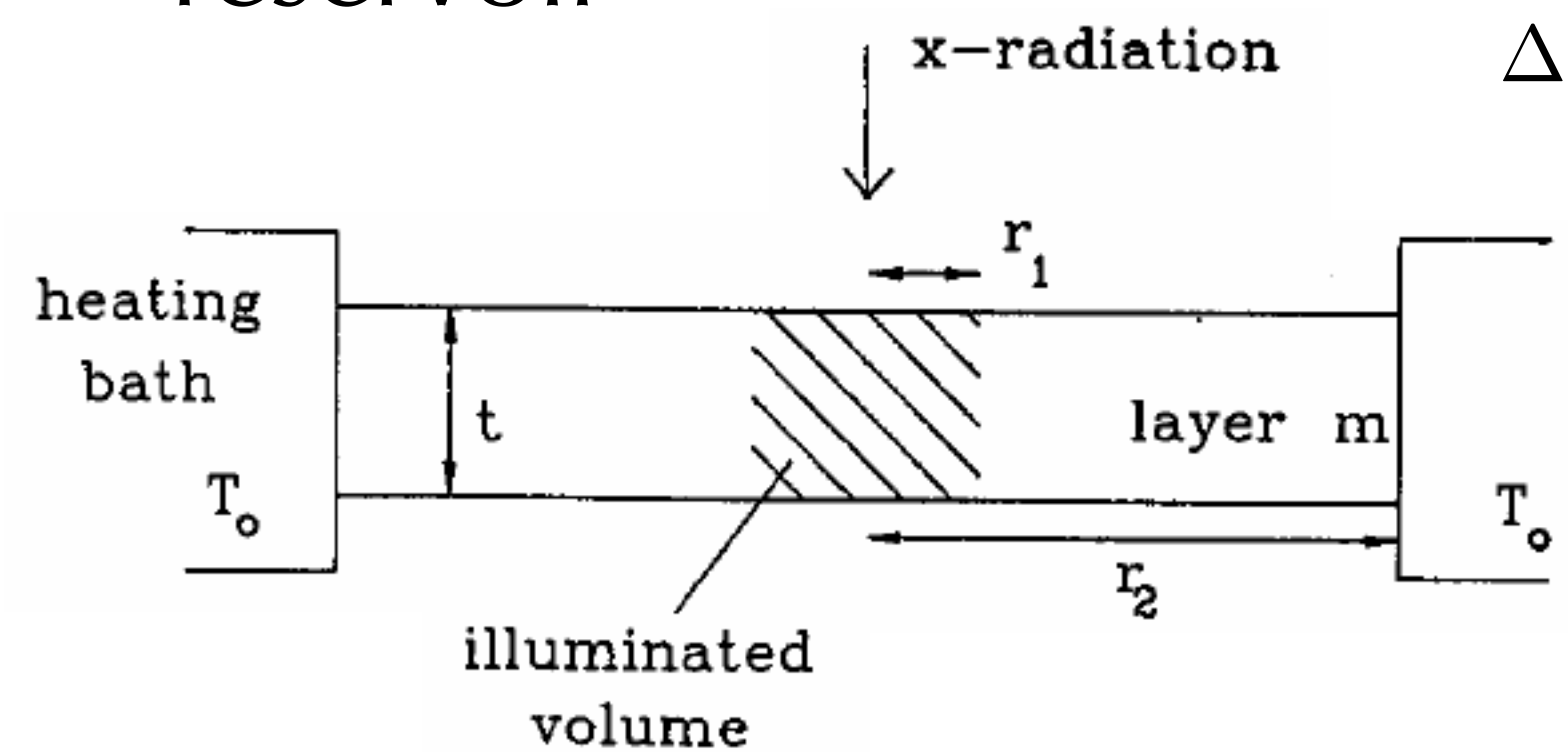
- Requires identical objects (rigid viruses, molecules)
- To trace amino acid sequence into electron density, you need ~3 Å resolution.
- R. Neutze *et al.*, *Nature* **406**, 752 (2000); Gaffney and Chapman, *Science* 316, 1445 (2007)



Option #2: keeping cool with a focused beam

- Scanned probes benefit from a thermal reservoir

$$\Delta T = \frac{N}{t}\,\frac{h\nu \cdot \mu}{4\pi k}\left(1 + 2\ln\frac{r_2}{r_1}\right)$$

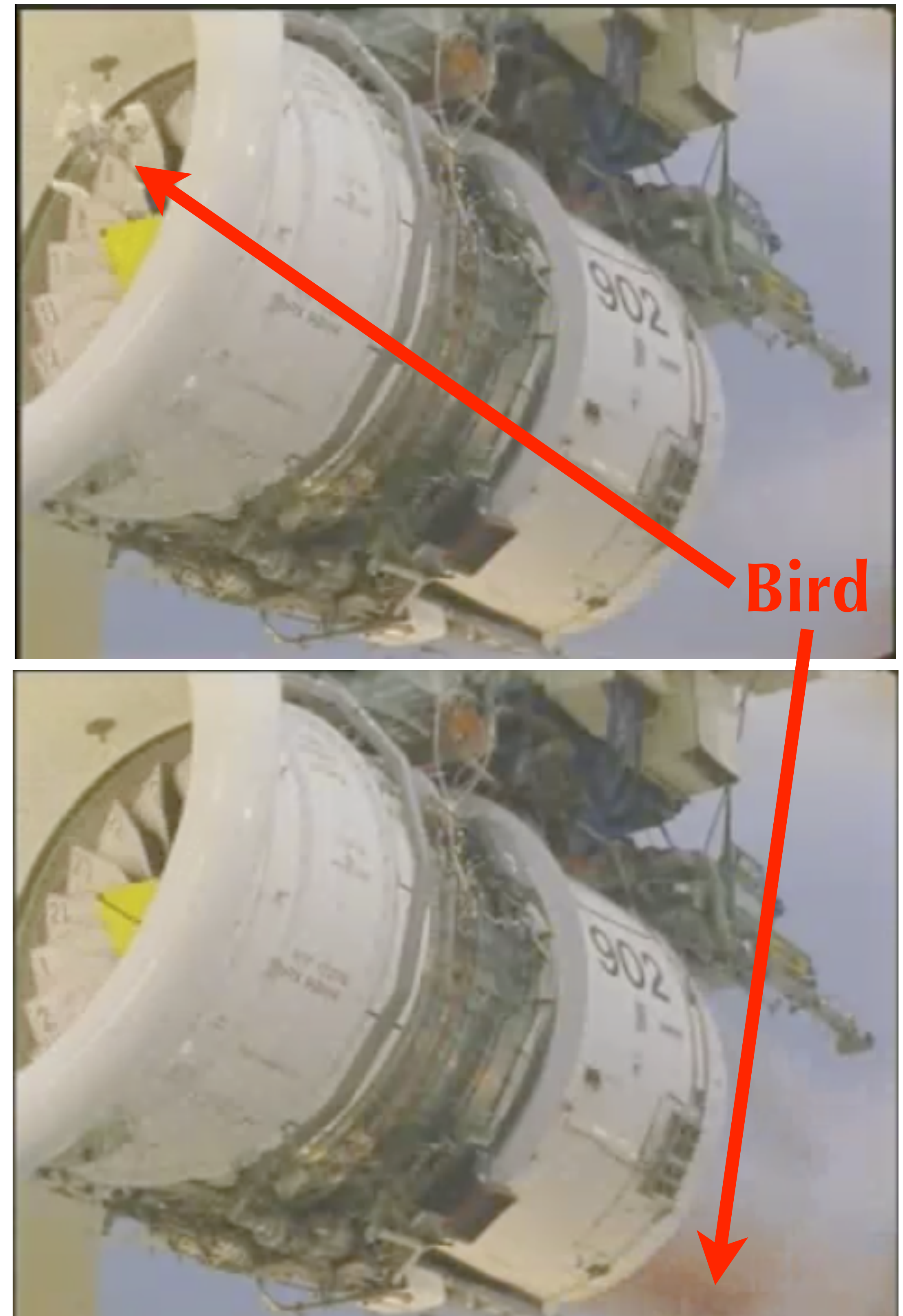


Greinke and Gölz, XRM 1991

- Photon flux for ΔT=1K in 10 nm wide spot:
  - H_20@500 eV: 4×10^{10} photons/sec
  - Si@10 keV: 2×10^{12} photons/sec

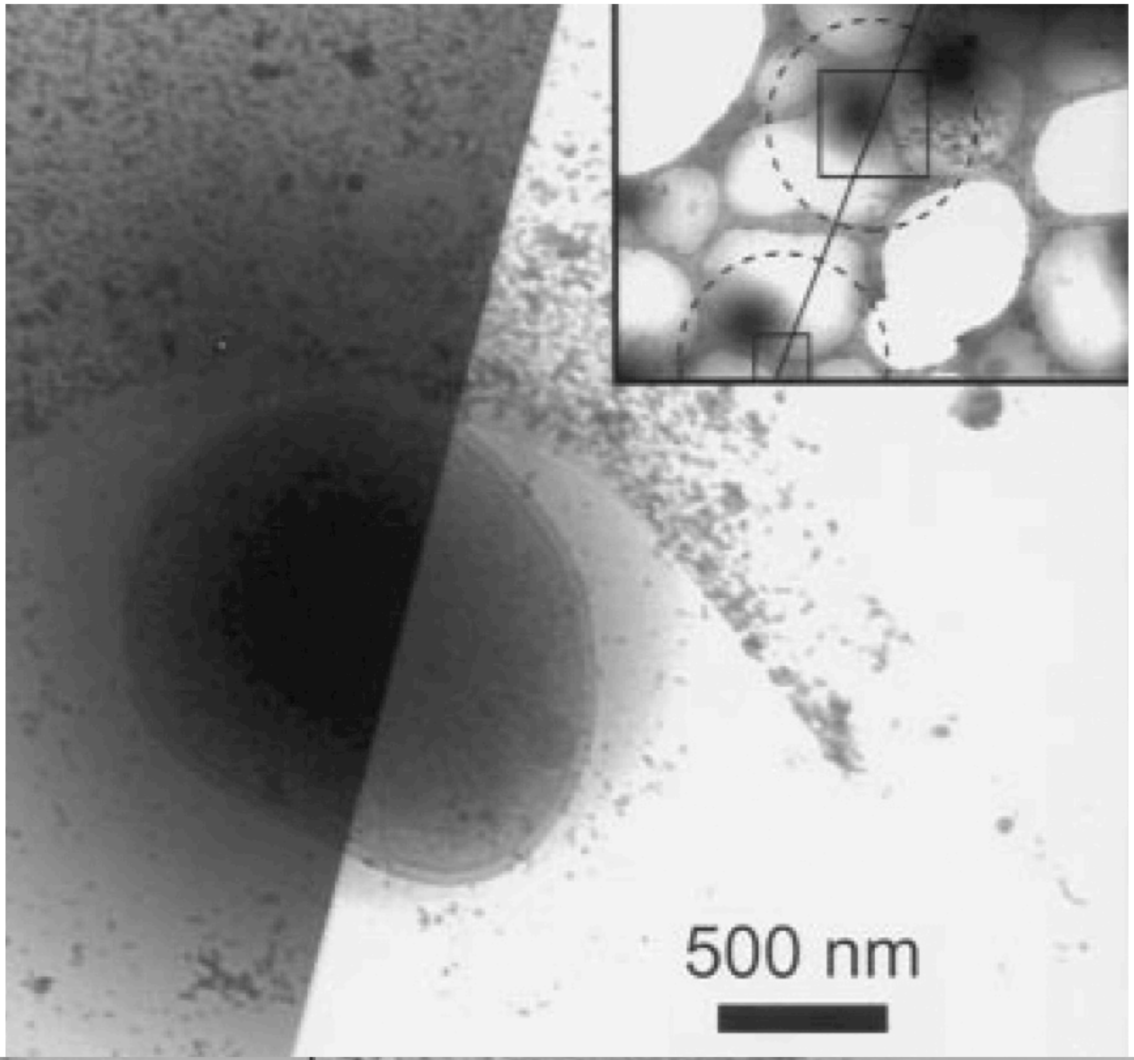
(r_2=100 μm)

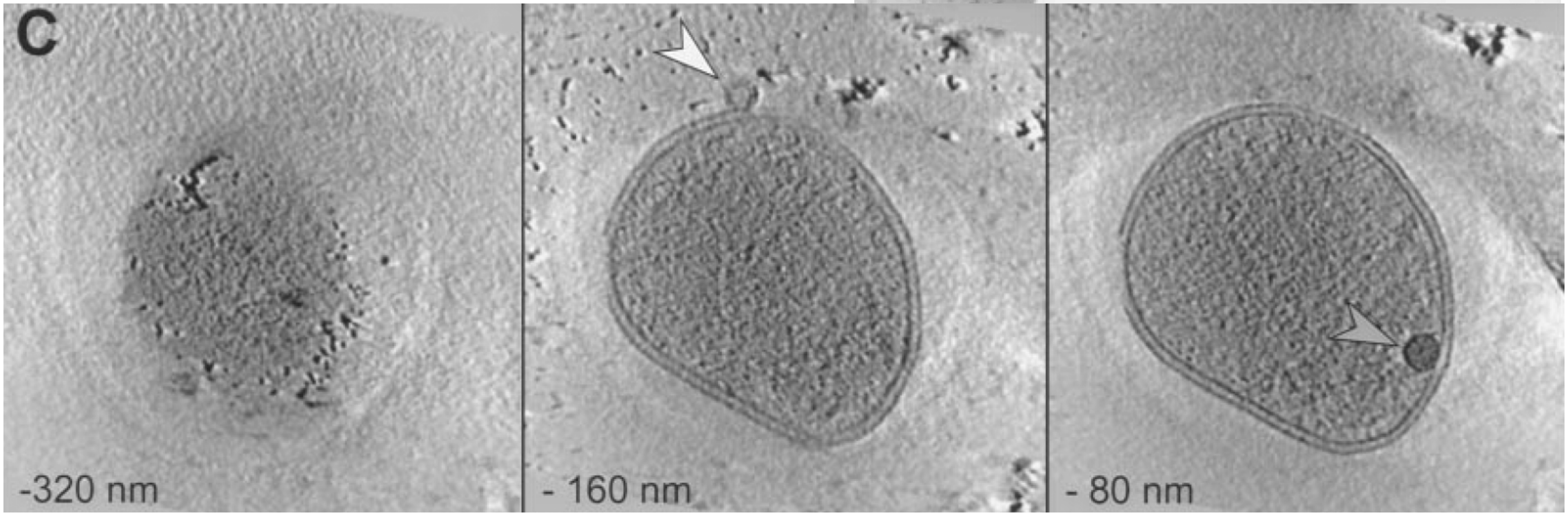
You don’t use dynamite to roast a turkey



Slow is good #1

- 3D imaging of complex objects: slices from tomography are *much* more revealing than single projections.
- Tomography requires multiple views of unchanged specimen.

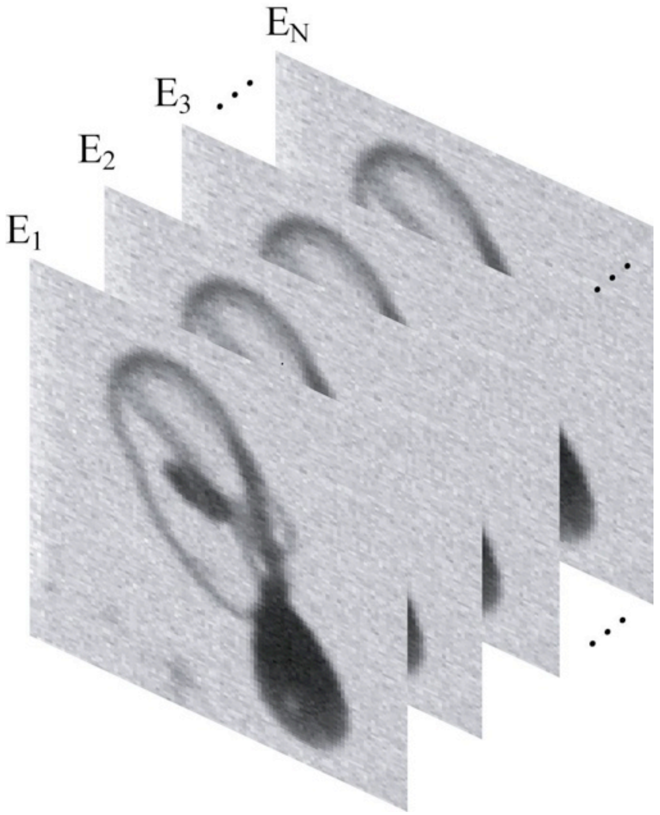


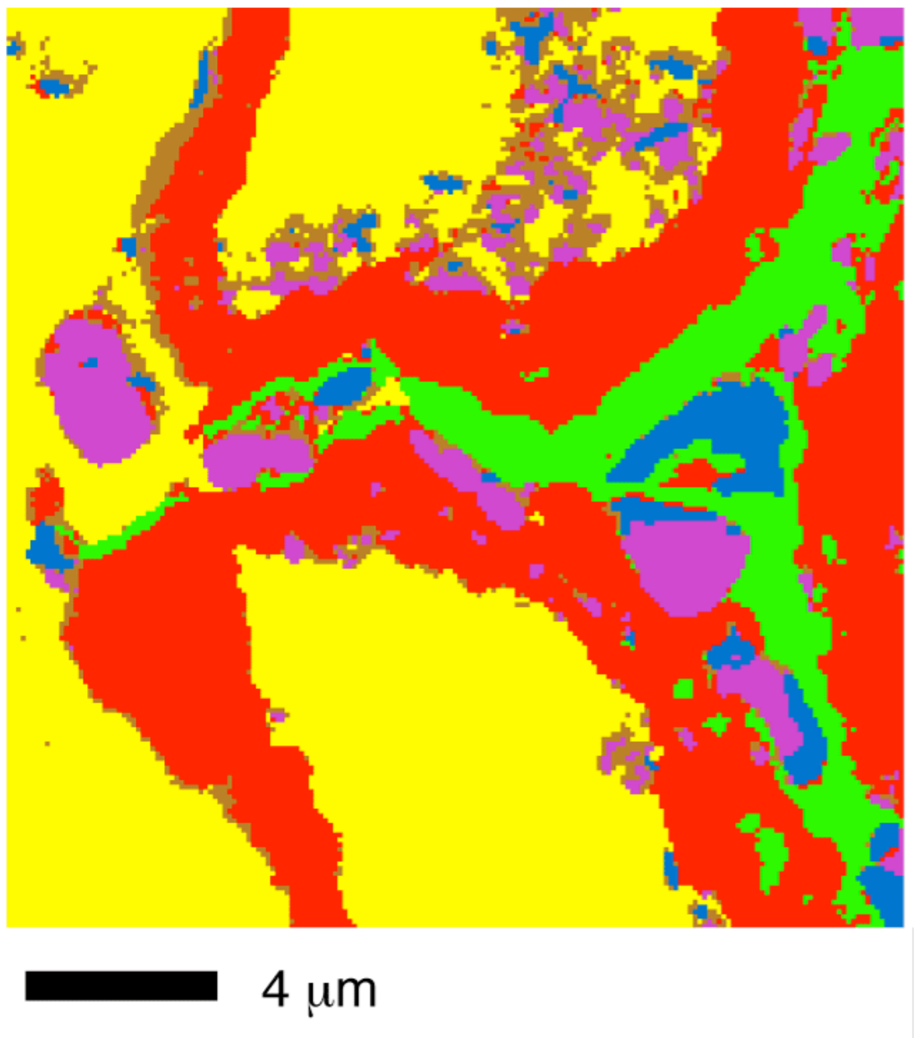


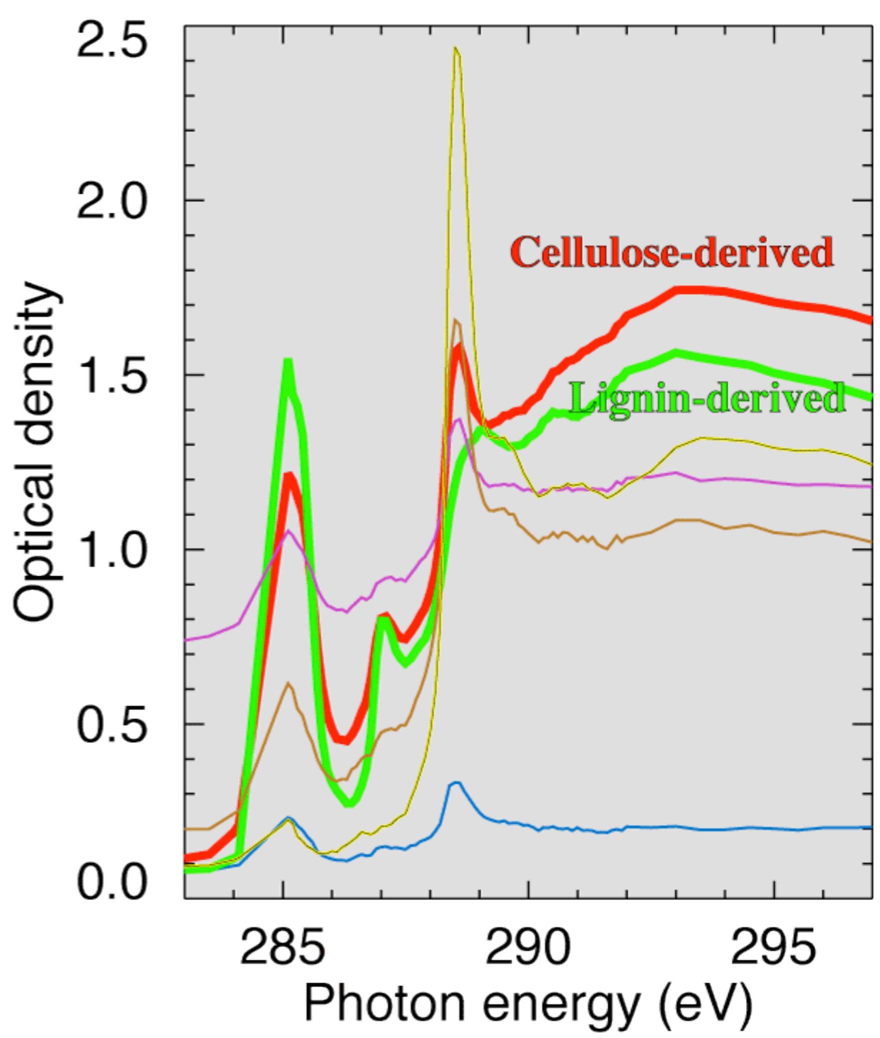
Grimm *et al.*, *Biophys. J.* **74**, 1031 (1998).

Slow is good #2

- Spectromicroscopy: learn about chemical speciation.
- Requires unchanged sample at multiple photon energies (or pink beam and spectrometer)







Lignin and cellulose in 400 million year old chert: Boyce *et al.*, *Proc. Nat. Acad. Sci.* **101**, 17555 (2004), with subsequent pattern recognition analysis by Lerotic *et al.*, *Ultramicroscopy* **100**, 35 (2004).

When slow is good

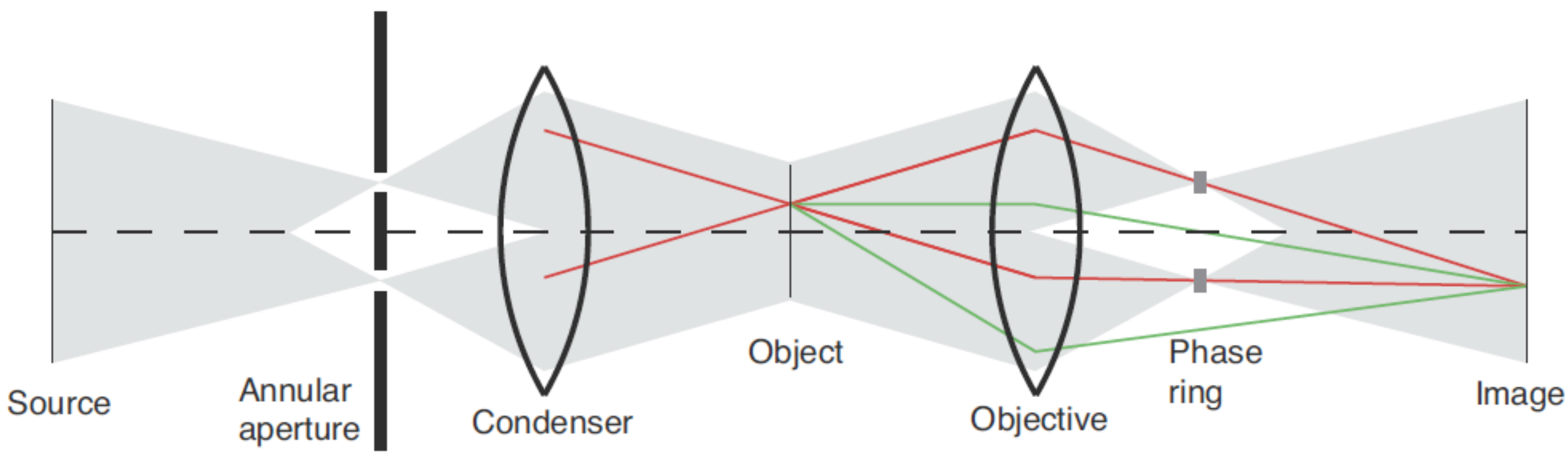
- Sometimes high repetition rate, and fewer photons per pulse, is better.
- You can’t explode the sample if you want to do tomography or spectromicroscopy.
- For ultrafast studies, are strobe lights sometimes better than nuclear weapons?

Incoherence doesn't keep one from success - even the Presidency!

Fig. 6-14 of Goodman, *Introduction to Fourier Optics* (McGraw Hill, 1968)

Zernike phase contrast with *incoherent* light

- Annular stop, annular phase ring at respective back focal planes
- "Reference" wave (illumination) is phase shifted
- Object scatters waves, most of which then miss the phase ring.



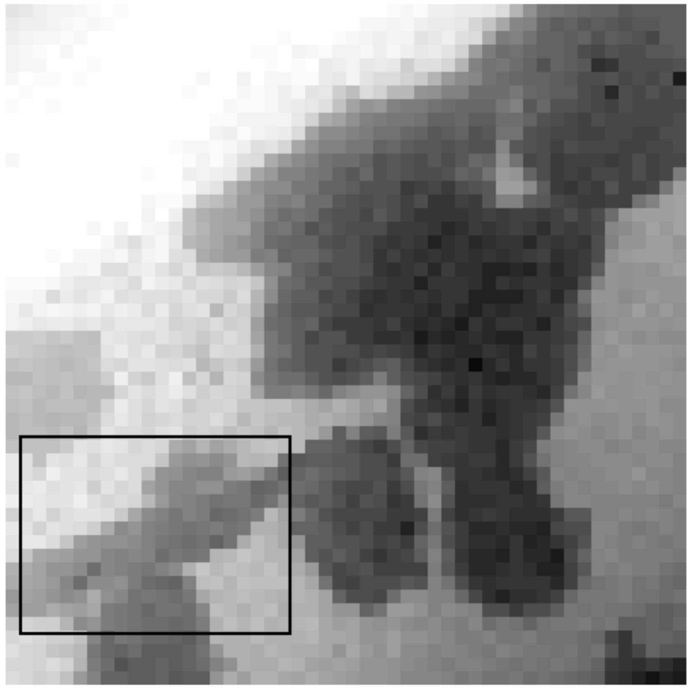
F. Zernike, 1935. Nobel Prize 1953

Even in the freezer, food doesn't last forever

- Cryo is important for high resolution imaging.
- Cryo reduces but does not remove radiation damage.

Radiation damage on (initially) living cells

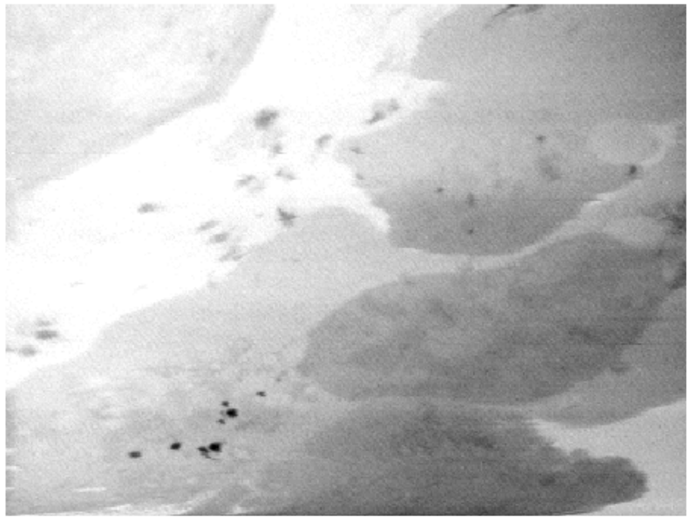
- Chick embryo fibroblasts. Reflux of culture medium every 20 min to keep unexposed cells alive.
- Makes it hard to view living cells!



10 μm

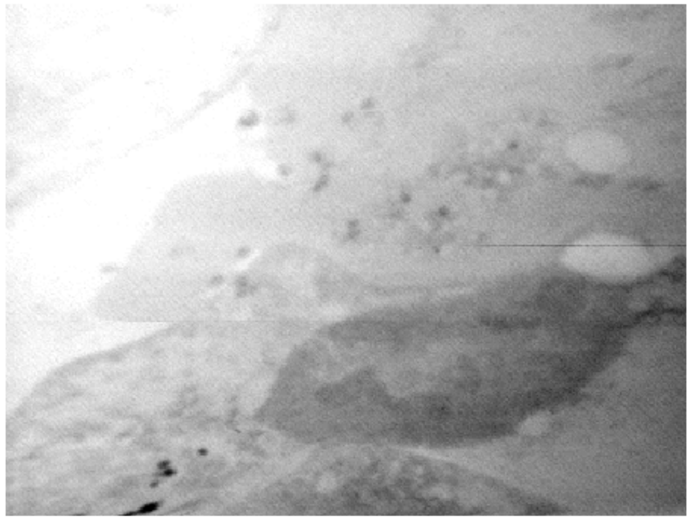
$6.0 \cdot 10^2$ Gray, ET=2 min.

Experiment by V. Oehler, J. Fu, S. Williams, and C. Jacobsen, Stony Brook using specimen holder developed by Jerry Pine and John Gilbert, CalTech. Never properly published, but see Kirz *et al*, *Q. Rev. Biophys.* **28**, 33 (1995)



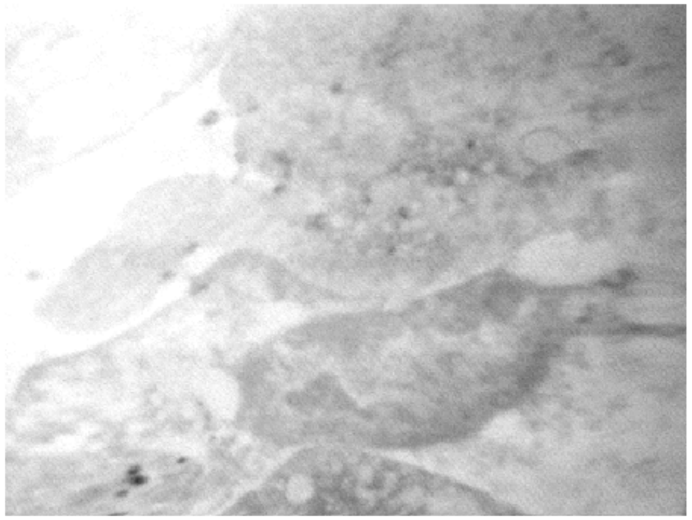
5 μm

$1.2 \cdot 10^5$ Gray, ET=9.5 min.



5 μm

$2.4 \cdot 10^5$ Gray, ET=17 min.



5 μm

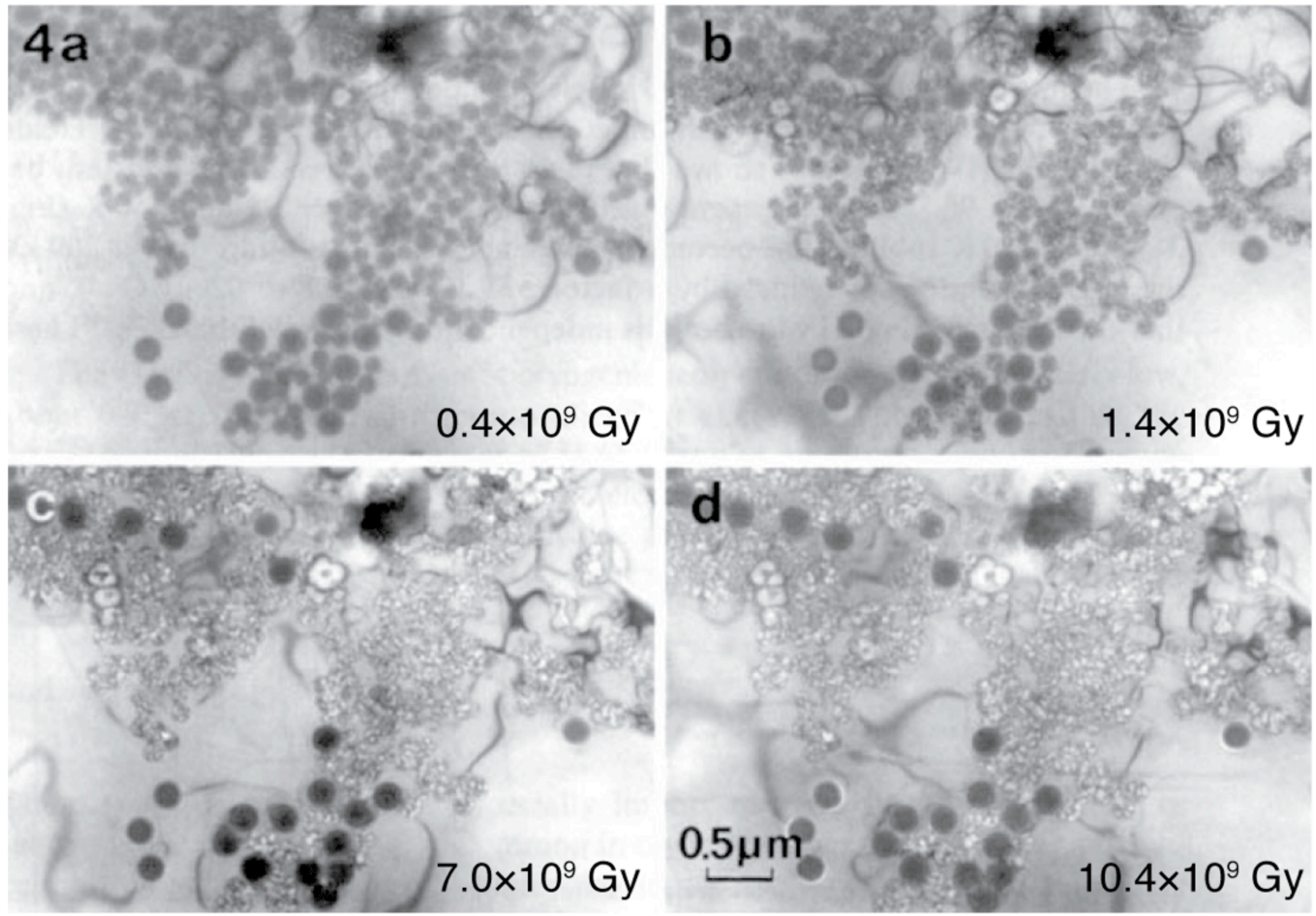
$3.7 \cdot 10^5$ Gray, ET=24.5 min.

Electrons: frozen hydrated

Polymer spheres in amorphous ice viewed with low dose rate at 100 keV

- Smaller spheres: PMMA
- Larger spheres: PS

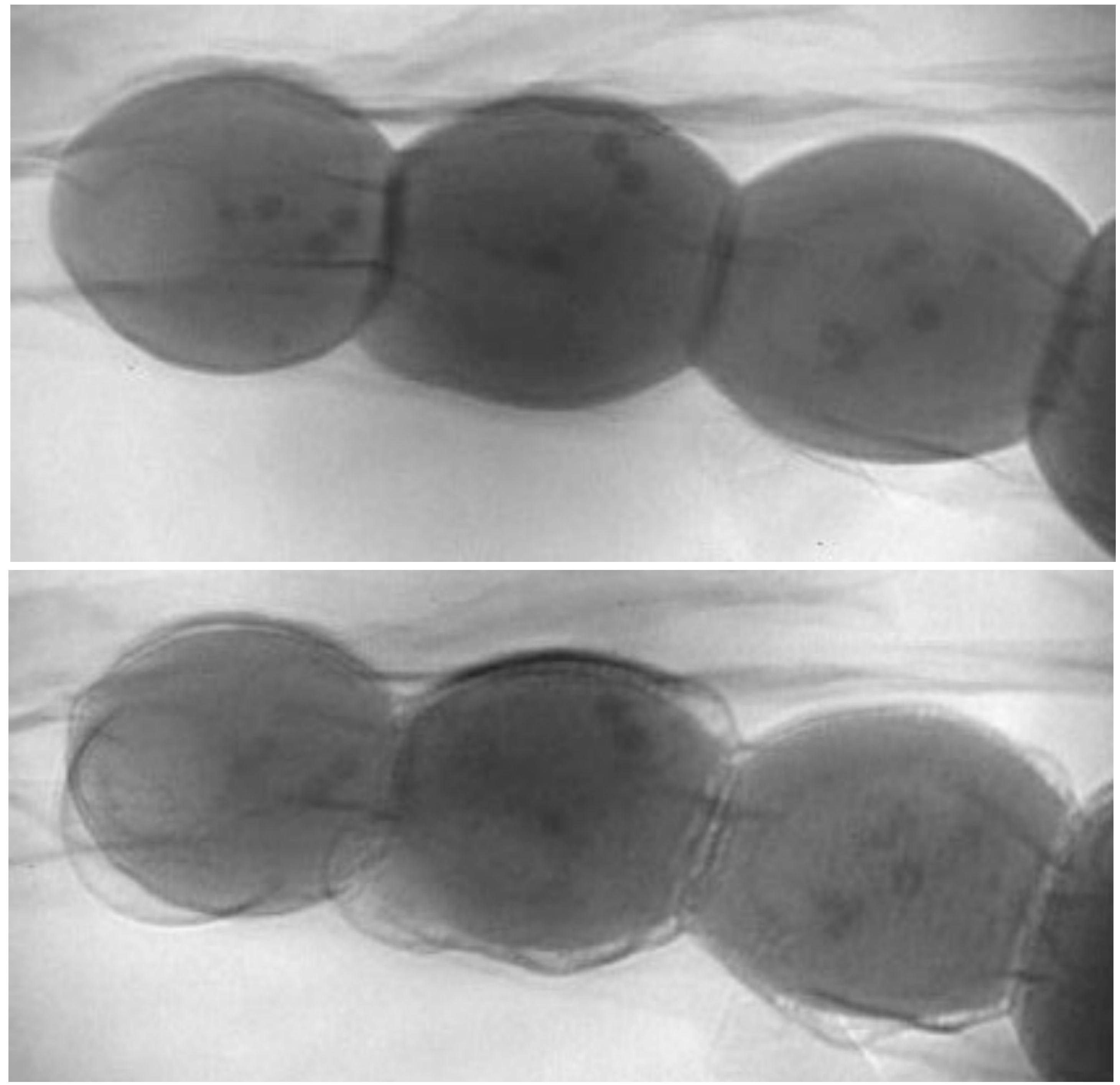
From Y. Talmon, in Steinrecht and Zierold, **Cryotechniques in Biological Electron Microscopy** (Springer, 1987)



"Bubbling" dose in cryo electron microscopy: ~1000 e-/nm^2 or about 3x10^7 Gray. Bubbles: hydrogen gas [Leapman, *Ultramic.* **59**, 71 (1995); Sun *et al.*, *J. Mic.* **177**, 18 (1995)]

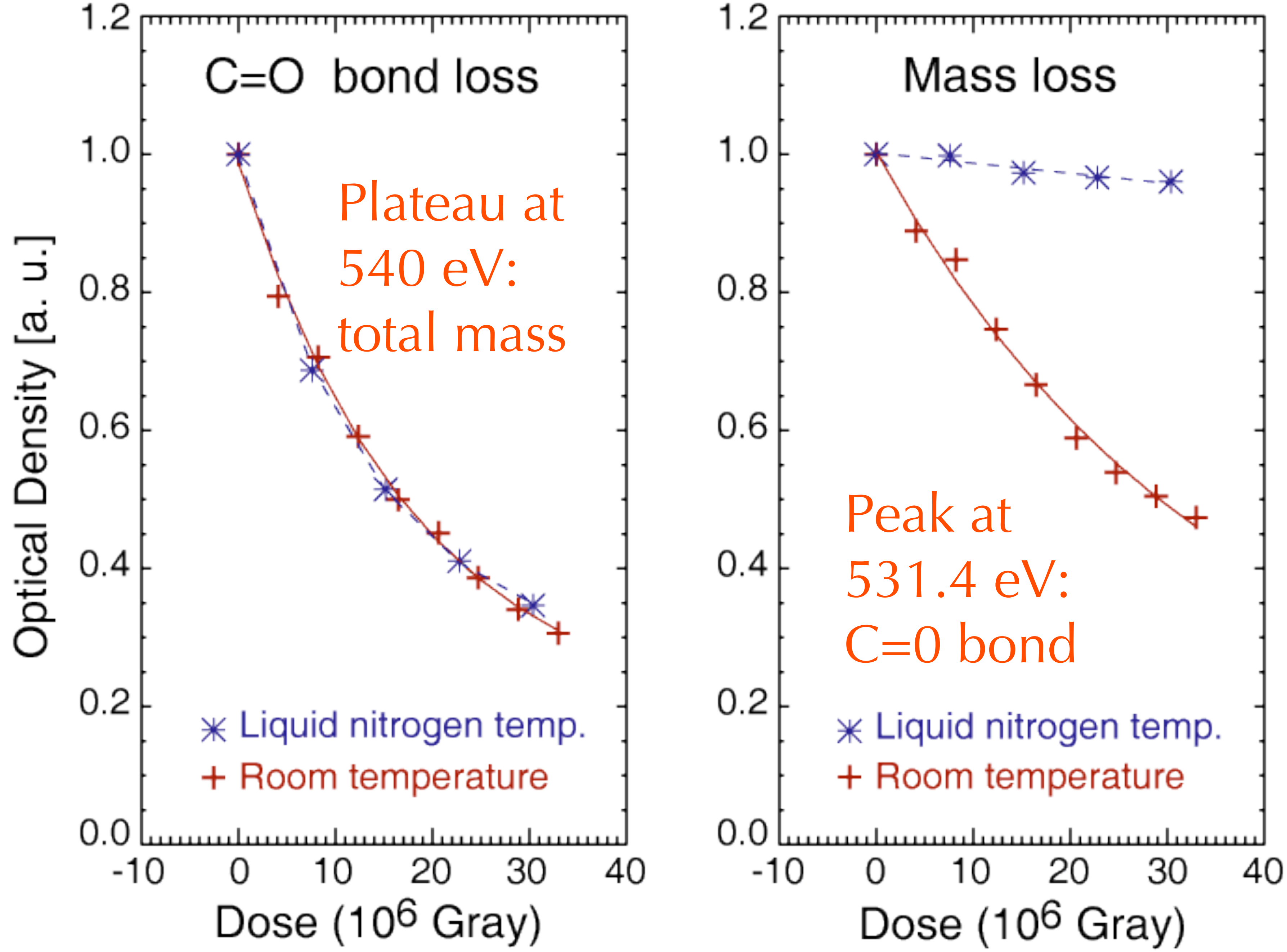
New cryo TXM at BESSY II

- Images before and after a high-dose series
- Stony Brook (Nelson, Holzner, Steinbrener, Jacobsen) and Helmholz (Guttmann, Heim, Schneider)



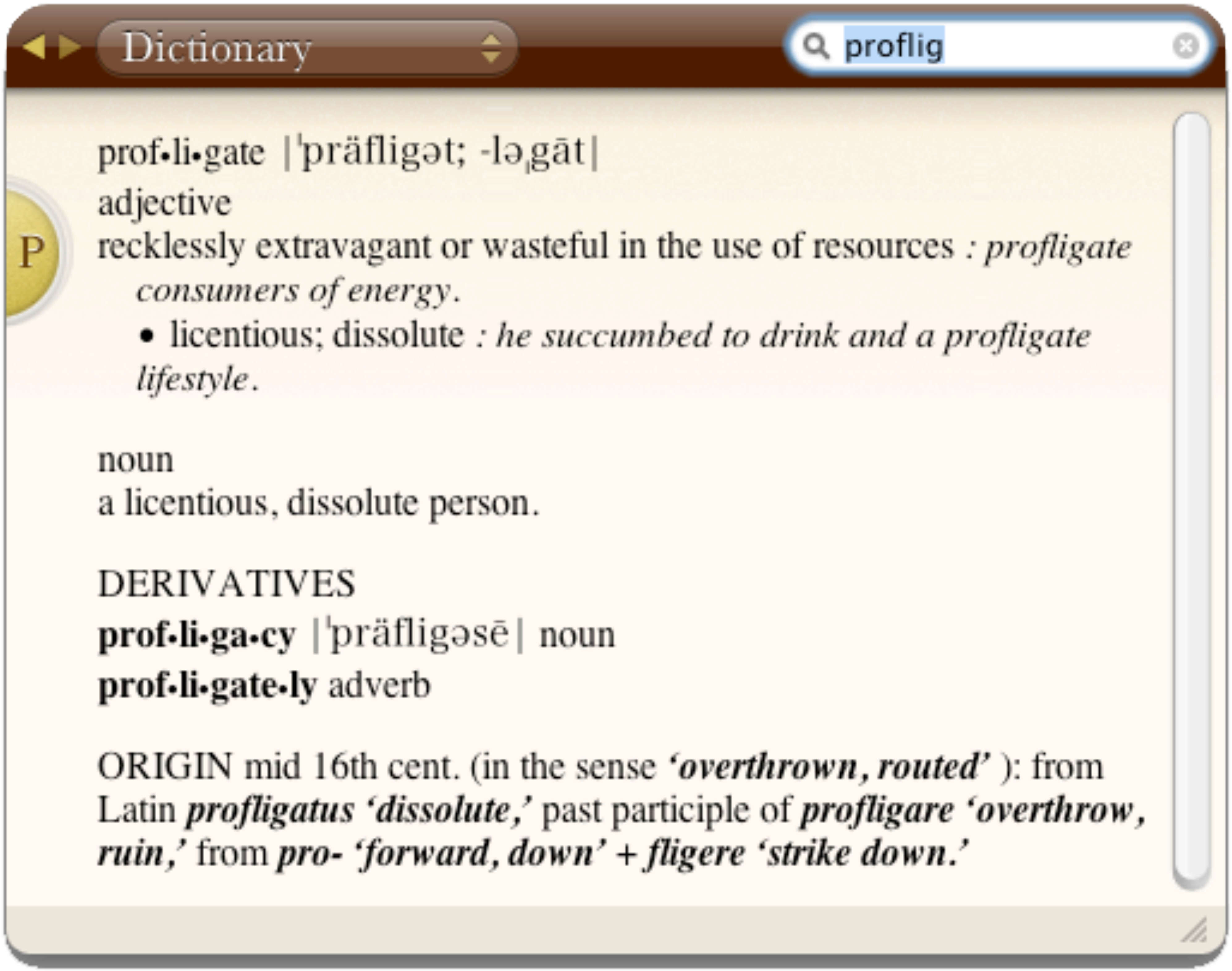
Cryo and chemistry

LN_2 temp: protection against mass loss, but not against breaking bonds (at least C=0 bond in dry PMMA)



Beetz and Jacobsen, *J. Synchrotron Radiation* **10**, 280 (2003)

The rich can afford to waste money



Dictionary

proflig

prof•li•gate |ˈpräfligət; -ləˌgāt|

adjective

recklessly extravagant or wasteful in the use of resources : *profligate consumers of energy*.

- licentious; dissolute : *he succumbed to drink and a profligate lifestyle*.

noun

a licentious, dissolute person.

DERIVATIVES

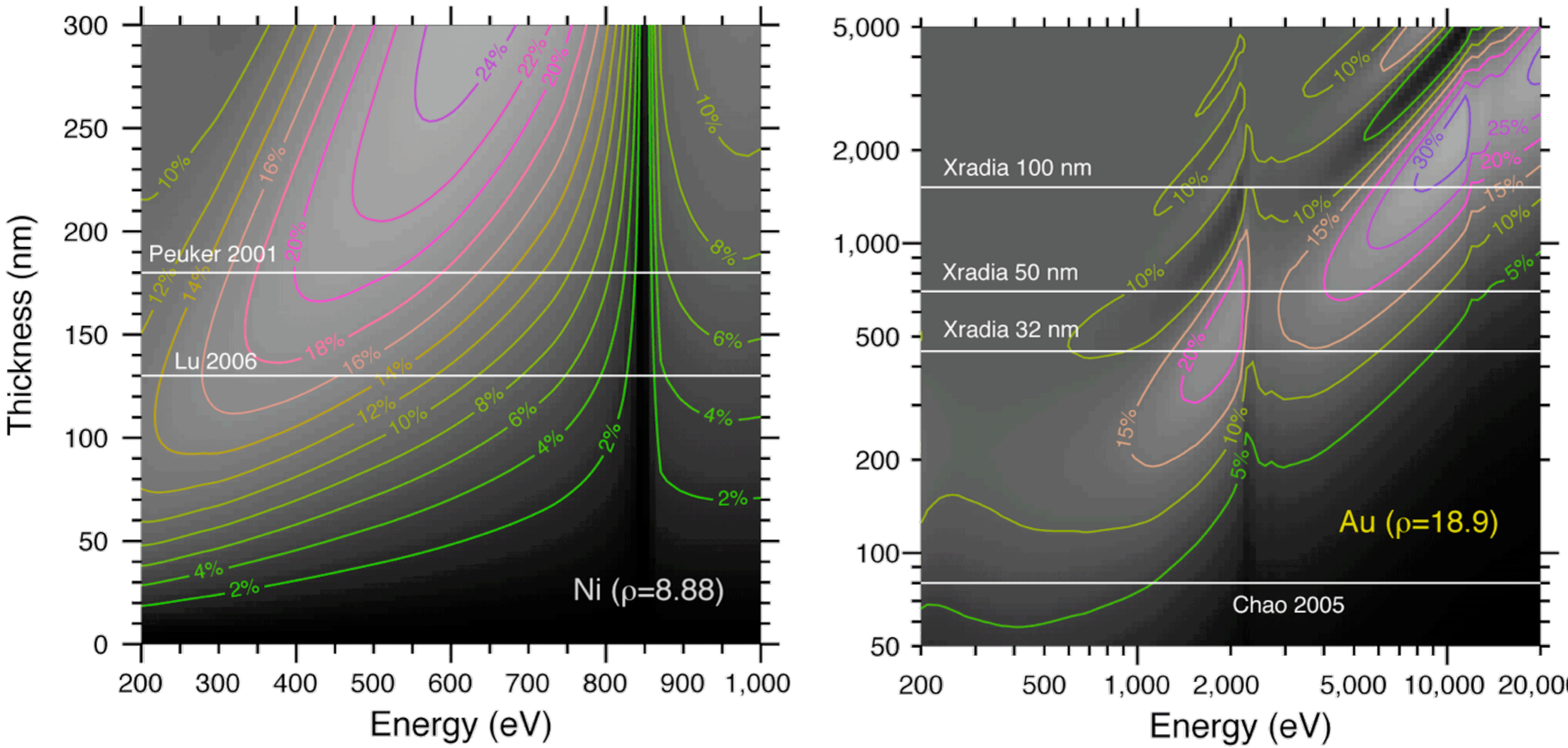
prof•li•ga•cy |ˈpräfligəsē| noun

prof•li•gate•ly adverb

ORIGIN mid 16th cent. (in the sense ***'overthrown, routed'***): from Latin ***profligatus* 'dissolute,'** past participle of ***profligare* 'overthrow, ruin,'** from ***pro-* 'forward, down'** + ***fligere* 'strike down.'**

Zone plate efficiency and thickness

For binary zones, first diffraction order, 1:1 mark:space ratio.
See Kirz, *J. Opt. Soc. Am.* **64**, 301 (1974)



Demonstration of 12 nm Resolution Fresnel Zone Plate Lens based Soft X-ray Microscopy

Weilun Chao,[1,*] Jihoon Kim,[2] Senajith Rekawa,[1] Peter Fischer,[1] and Erik H. Anderson[1]

[1]*Center for X-ray Optics, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA*
[2]*NSF ERC for Extreme Ultraviolet Science & Technology, University of California, Berkeley, CA 94720, USA*
**wlchao@lbl.gov*

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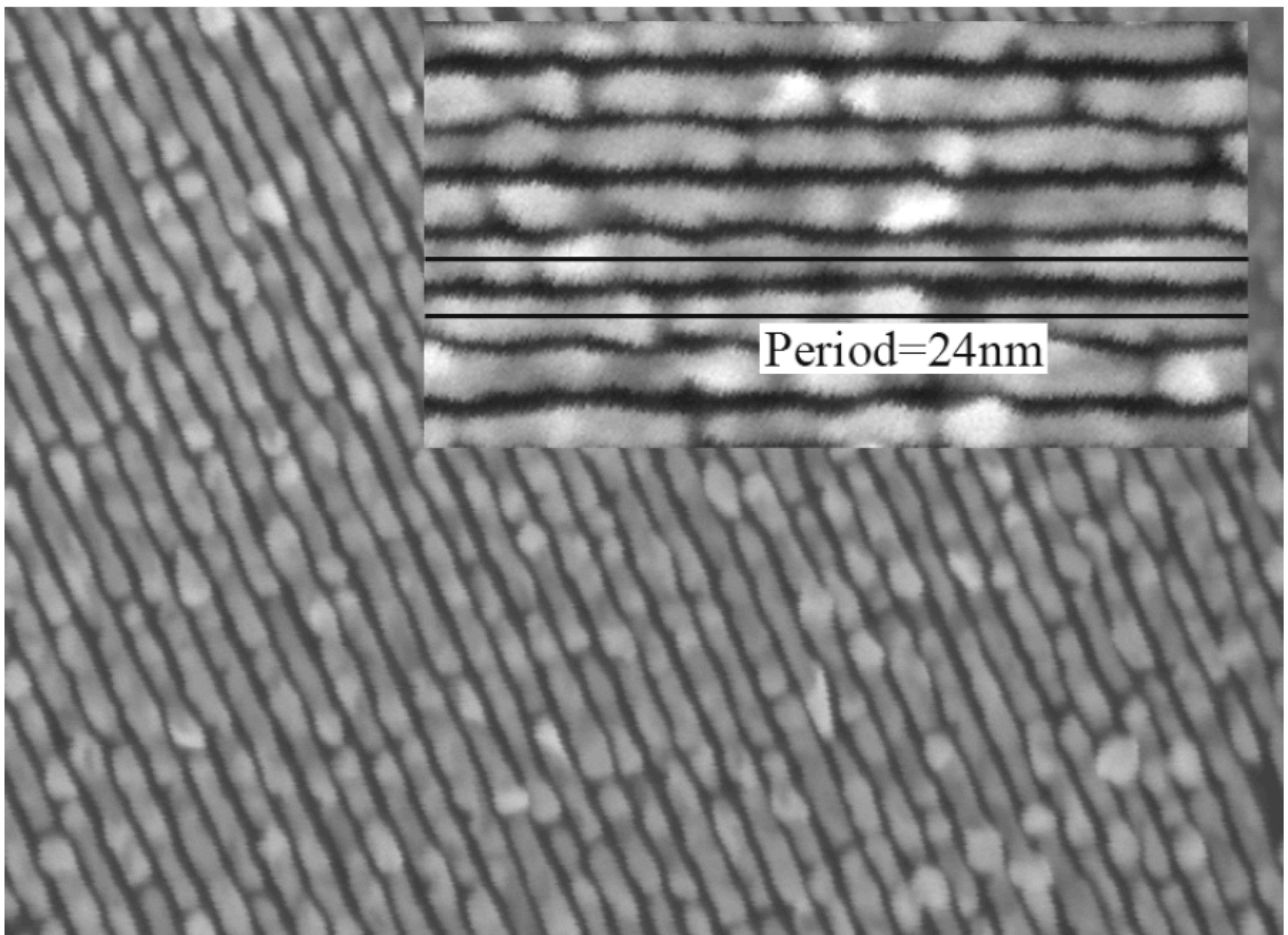
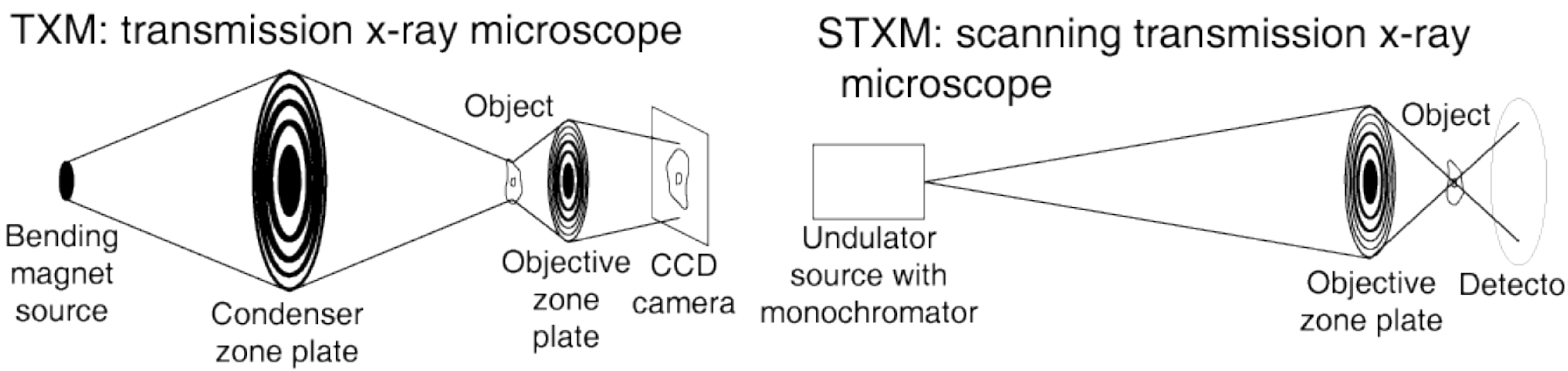


Efficiency: ~0.5%

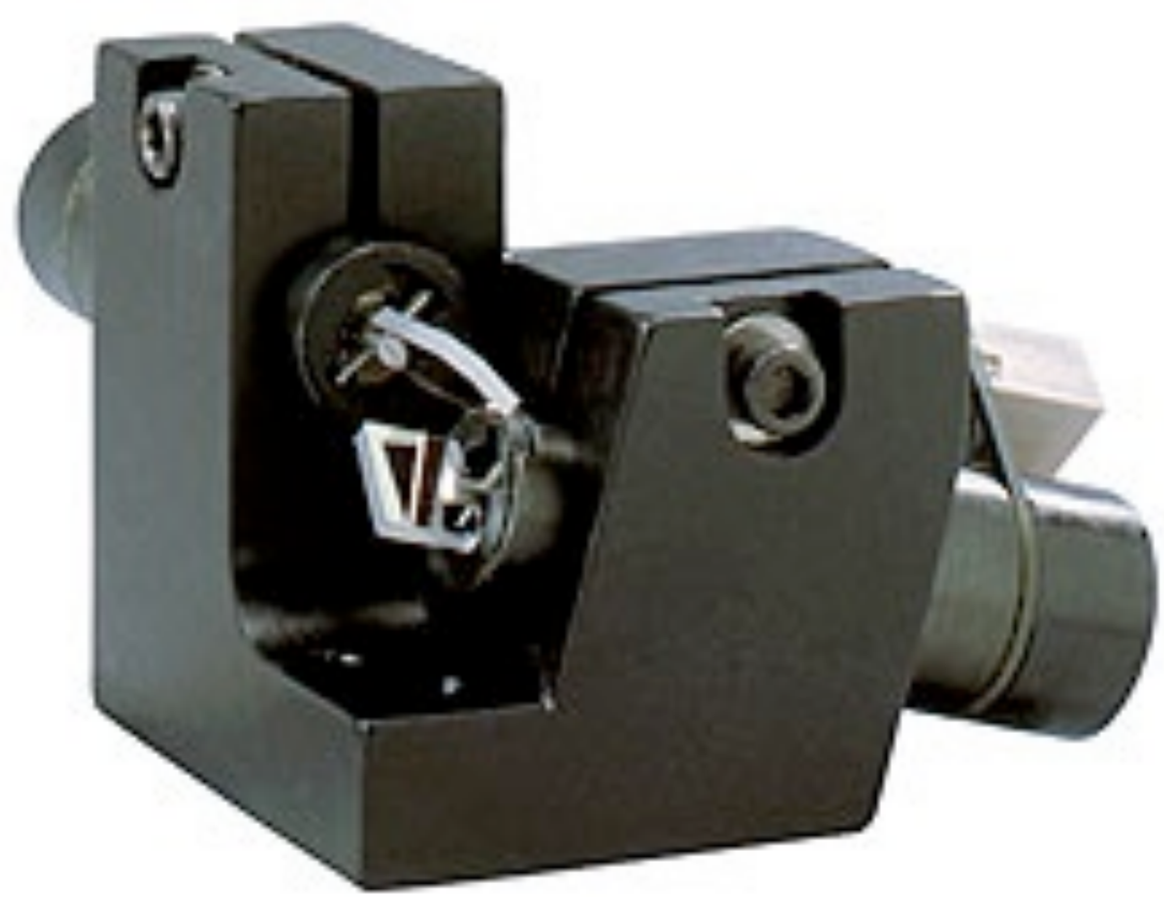
Scanning specimens

- Scanning: slower, but less dose to specimen and more modalities (fluorescence, simultaneous absorption and phase...)
- Example: NGLS rep rate 10^5 Hz, 10^3 pixels/scan line: 10 seconds/image, but serious shaking of specimen or zone plate!



Confocal laser scan microscopes

- They scan even faster.
- They don't scan the sample; they don't scan the objective lens.
- They use galvanometer-driven mirrors to scan the beam. Can we do this at grazing incidence with X rays, even if it's done in a lossy way?

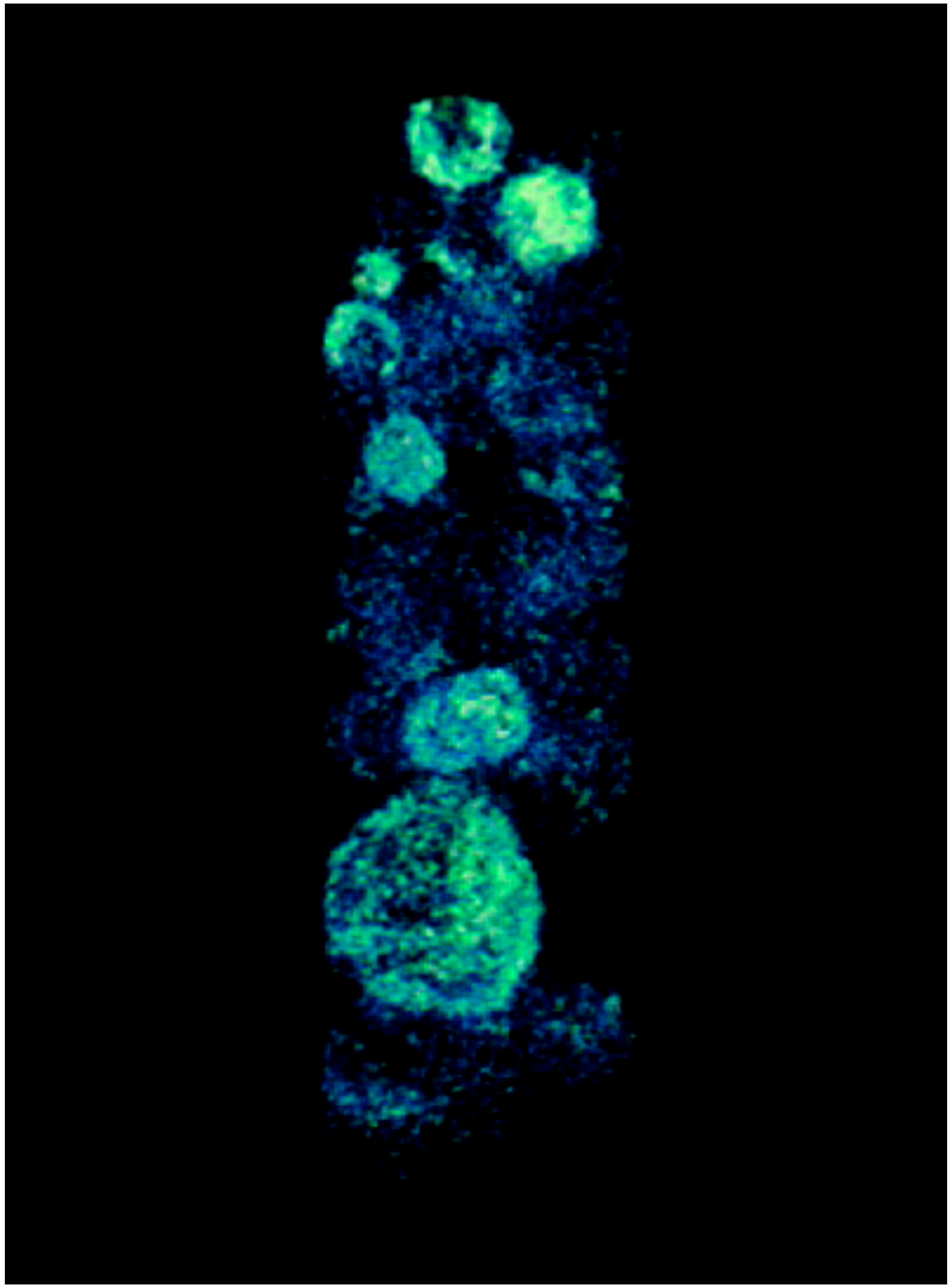


Tenfold is a useful gain; thousandfold is a revolution

- For soft X rays, factor of <10 brightness represents ALS to NSLS II: will certainly be helpful…
- Factor of 1000 means you can do completely new experiments. What would have taken a month now takes 45 minutes.
- Go from 2D to 3D (*xyz* tomography, *xyE* spectromicroscopy) to 4D (*xyzE* spectrotomography), or reciprocal space, or time…

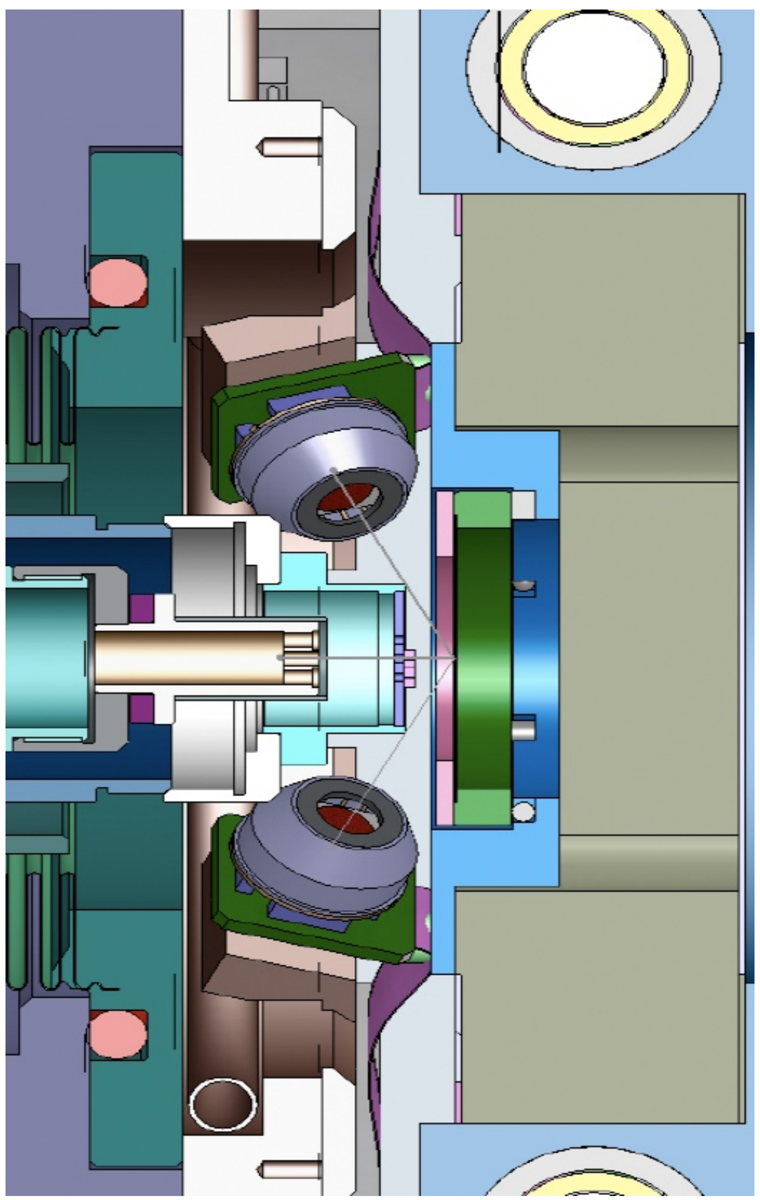
XANES tomography: chemical states in 3D

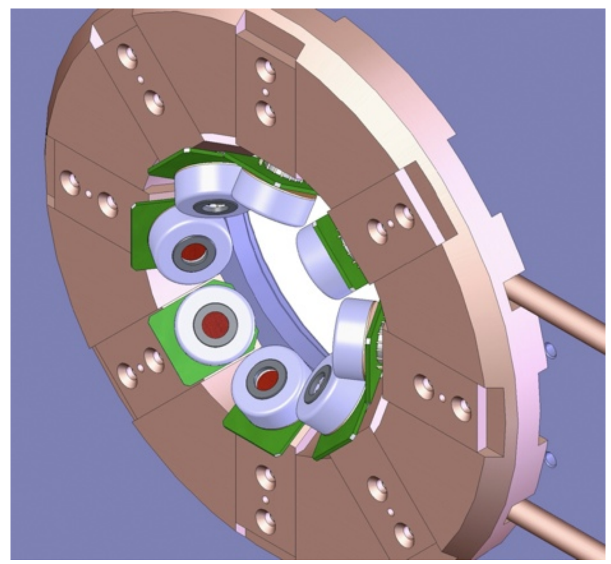
- Johansson, Hitchcock *et al.*, *J. Synch. Rad.* **14**, 395 (2007).
- This example: acrylates in polymer microspheres.
- Challenges: dose? Hegerl-Hoppe dose fractionation?



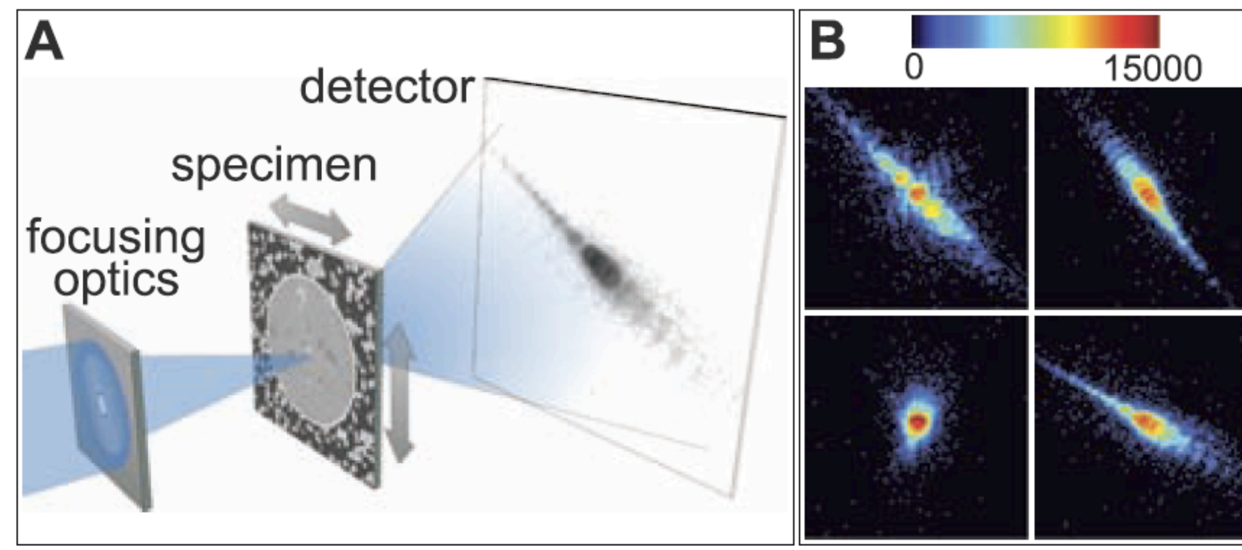
If it's a once-in-a-lifetime experience, savor it

- Multimode detection: transmission and fluorescence simultaneously.





Kaulich *et al.*,
TwinMic, Elettra



High-Resolution Scanning X-ray Diffraction Microscopy

Pierre Thibault,[1*] Martin Dierolf,[1] Andreas Menzel,[1] Oliver Bunk,[1] Christian David,[1] Franz Pfeiffer[1,2]

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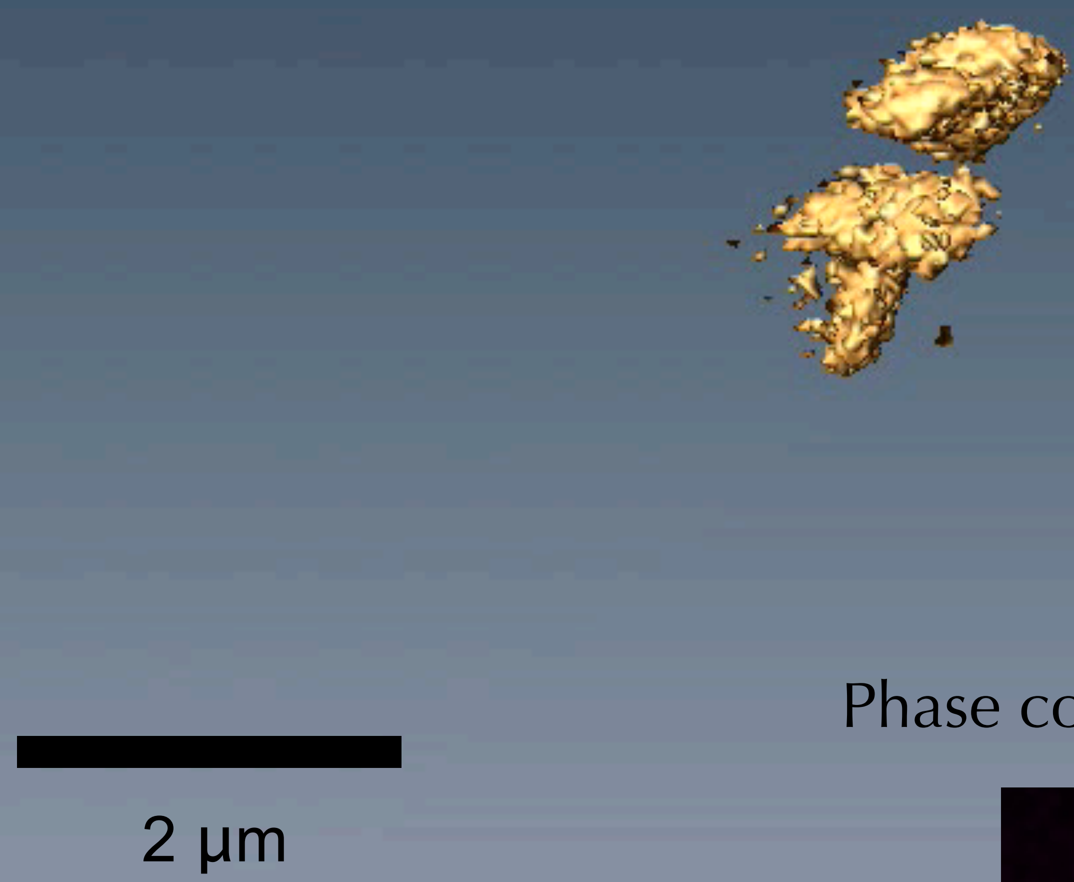
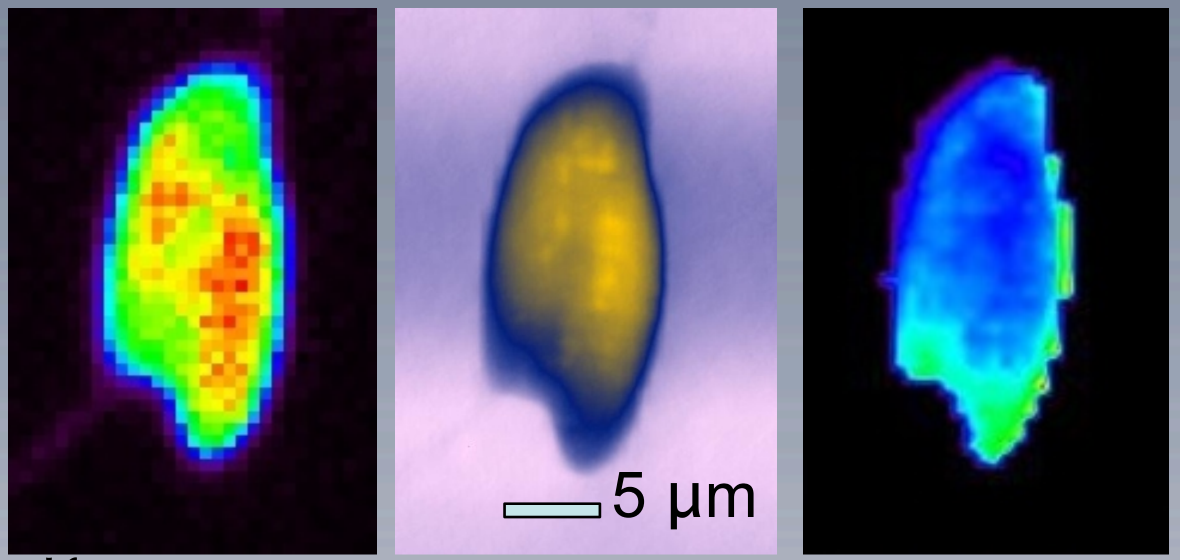
Phosphorous, Sulfur, Silicon



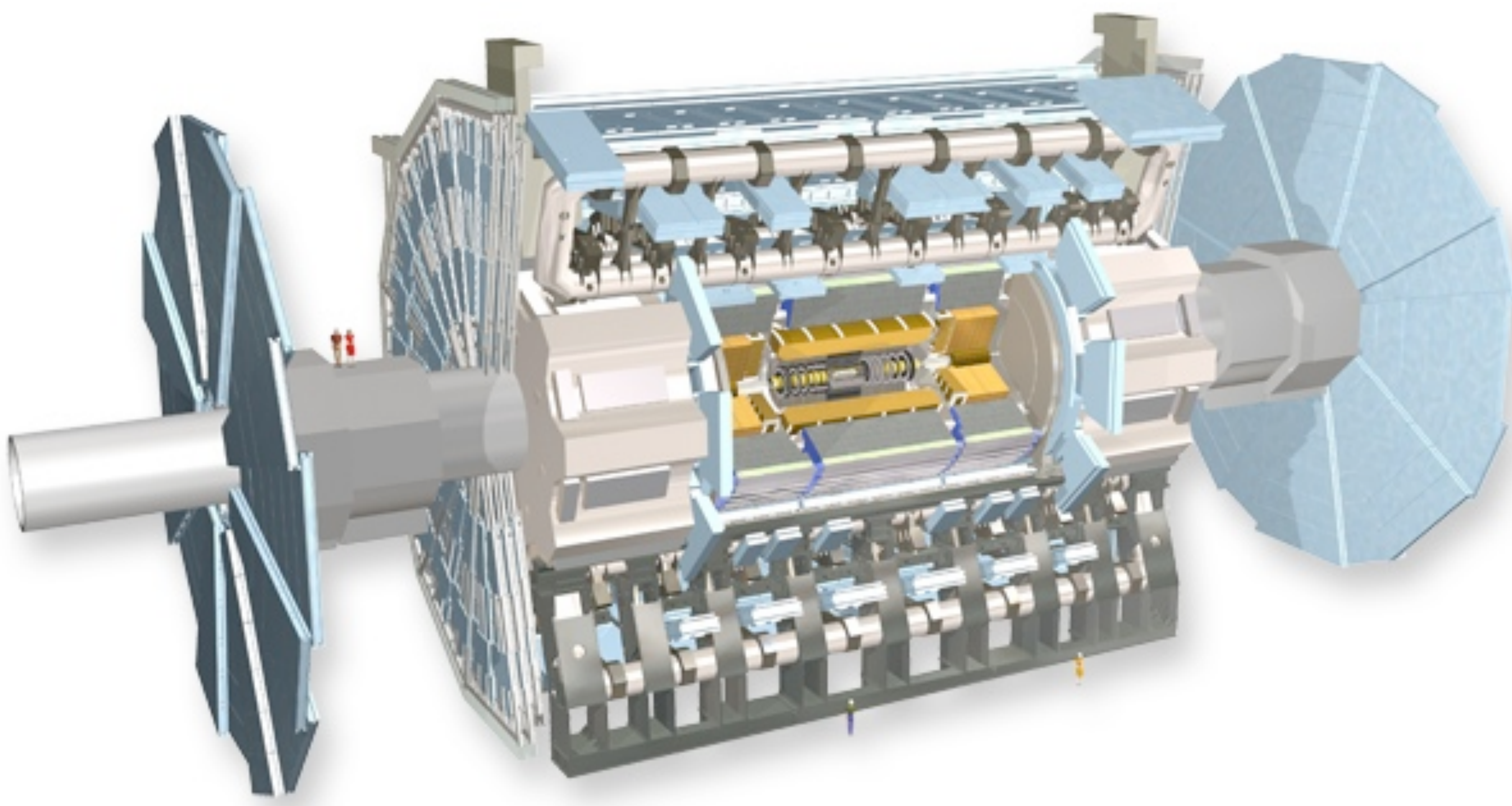
Phase contrast tomography of cyclotella (marine protist)



Sulfur content Protist mass Sulfur concentration

Phase contrast needed to align low-statistics fluorescence tilt series. de Jonge *et al.*, APS; Holzner *et al.*, Stony Brook

Back to the future: high energy physics?

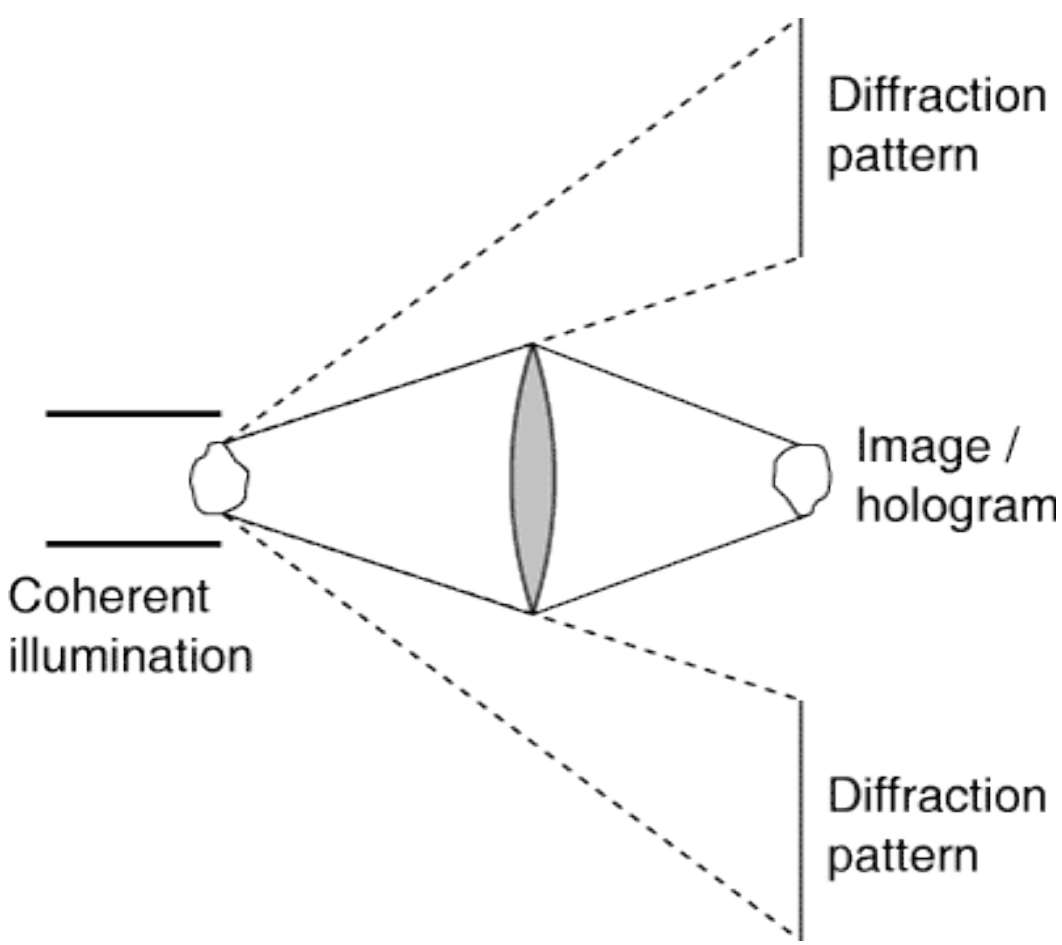


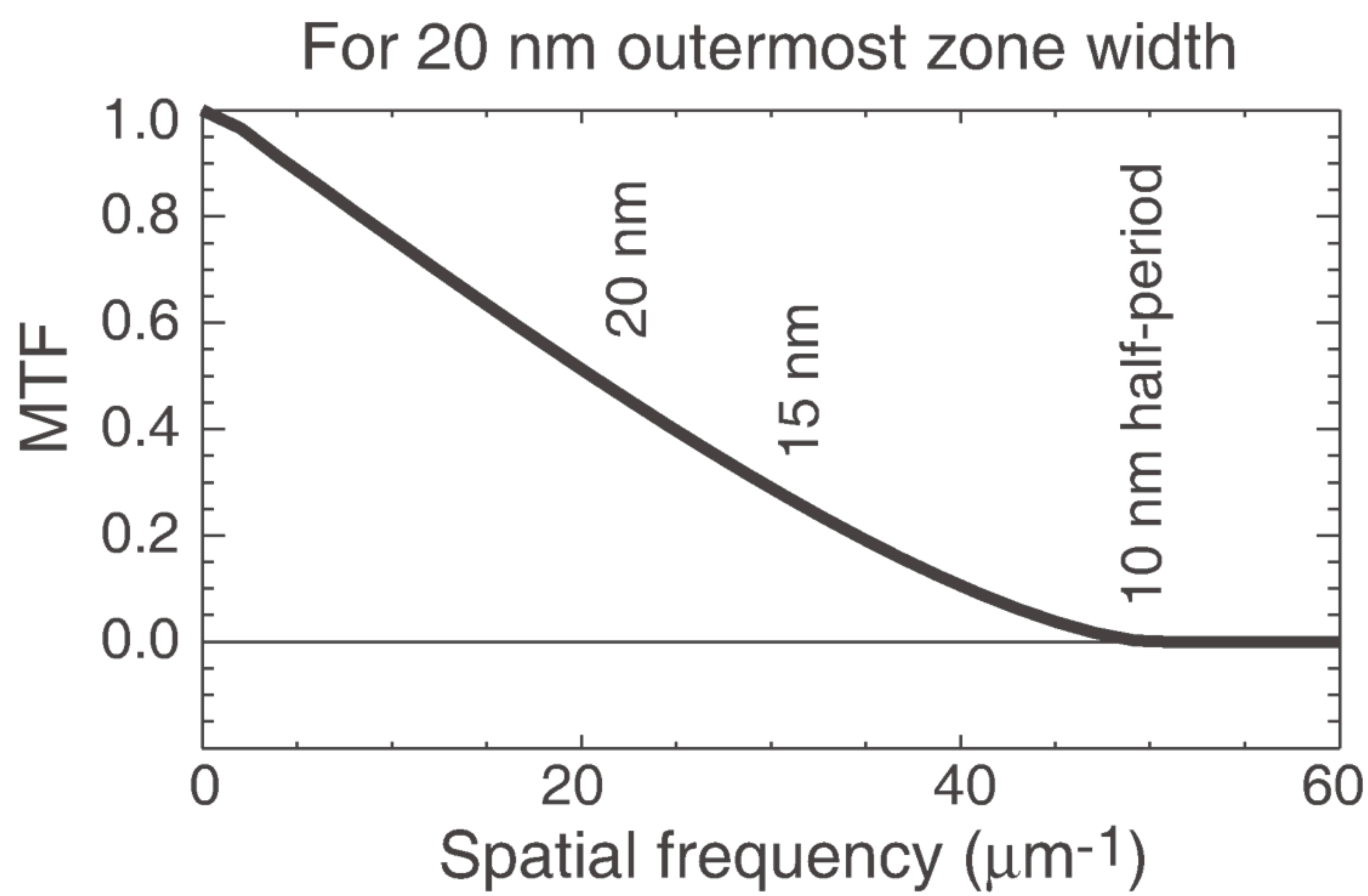
Make every photon count

- For many specimens, radiation damage sets the ultimate limit on achievable resolution.
- Lenses phase the signal, but lose the signal. Example: 20 nm zone plate with 10% efficiency, 50% window transmission, 20% modulation transfer function (MTF) for 15 nm half-period:

net transfer of 1% for high spatial frequencies

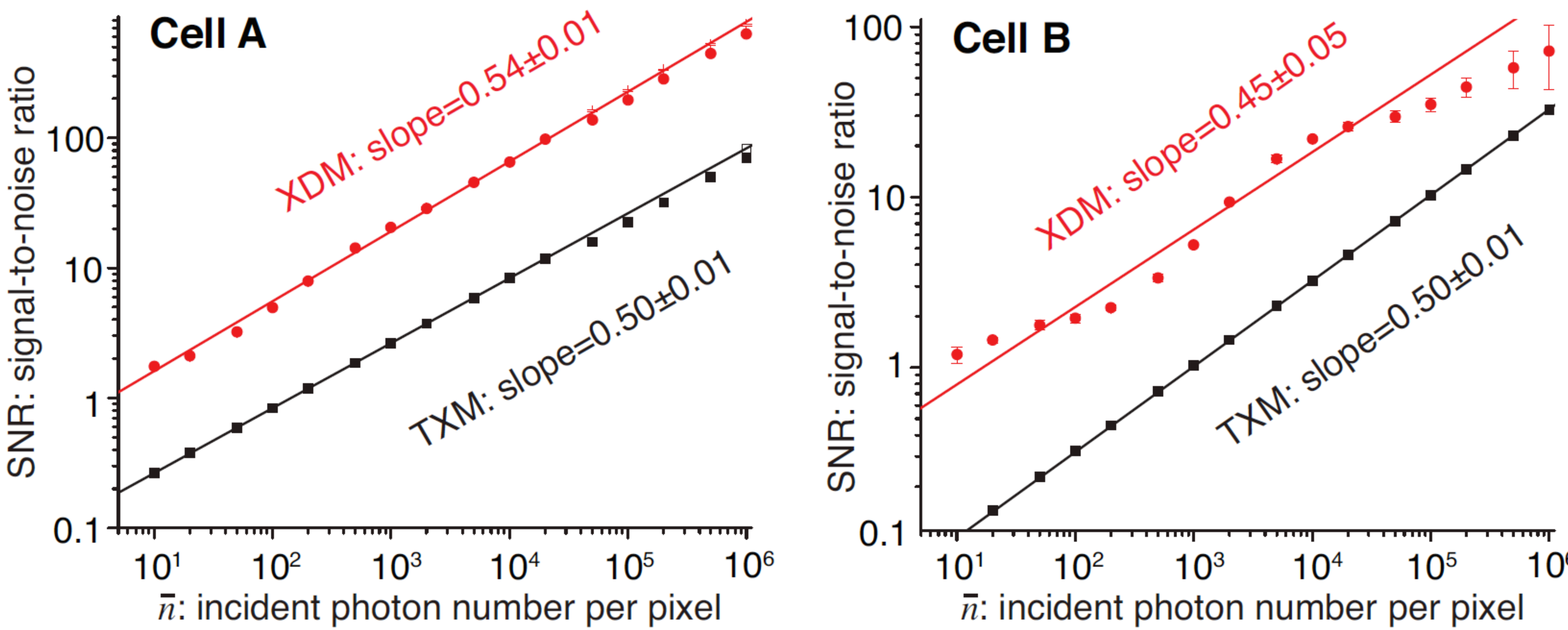
- Can we avoid this ~100x signal loss, and also go beyond numerical aperture limit of available optics?





SNR versus exposure: simulation results

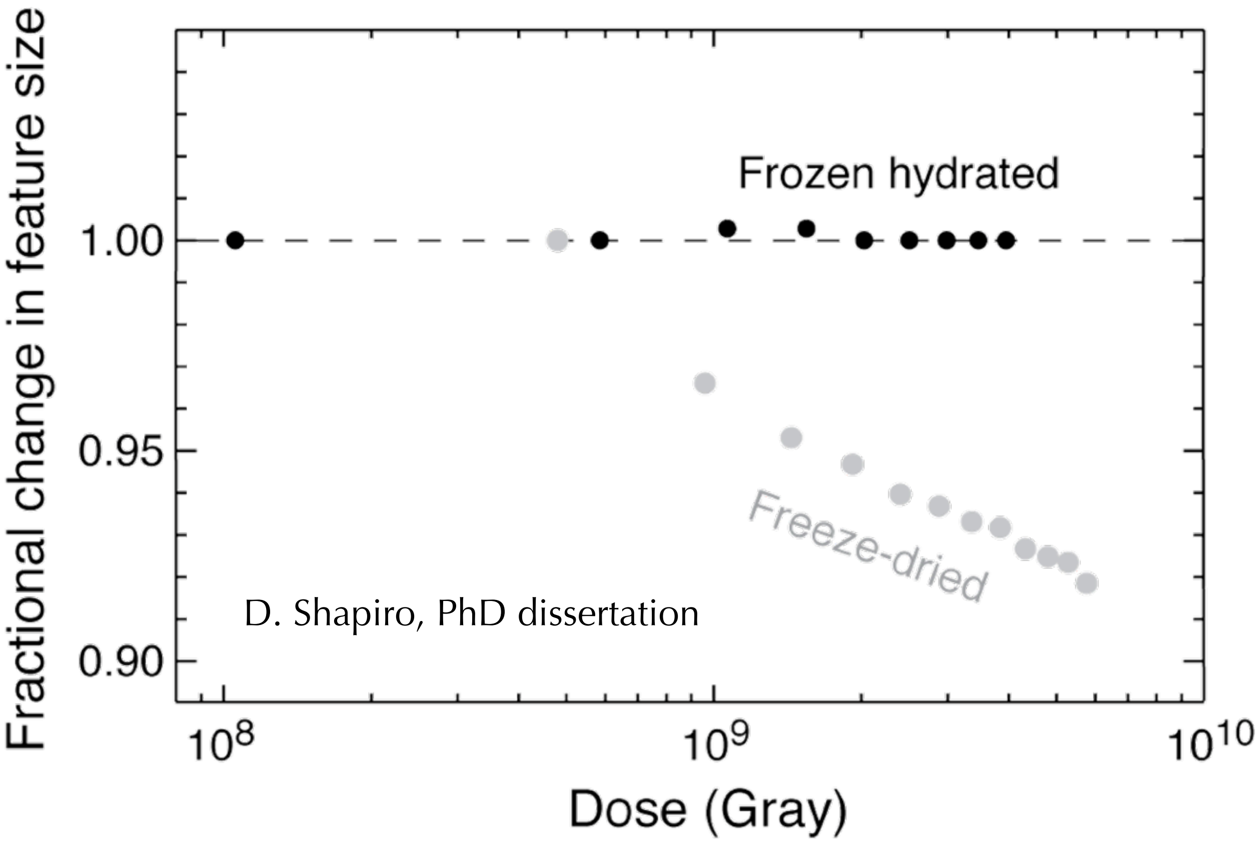
- Phasing in x-ray diffraction microscopy (XDM) does not introduce extra noise; potential signal gain versus transmission x-ray microscopy (TXM; here assuming 10% efficient 20 nm zone plate)

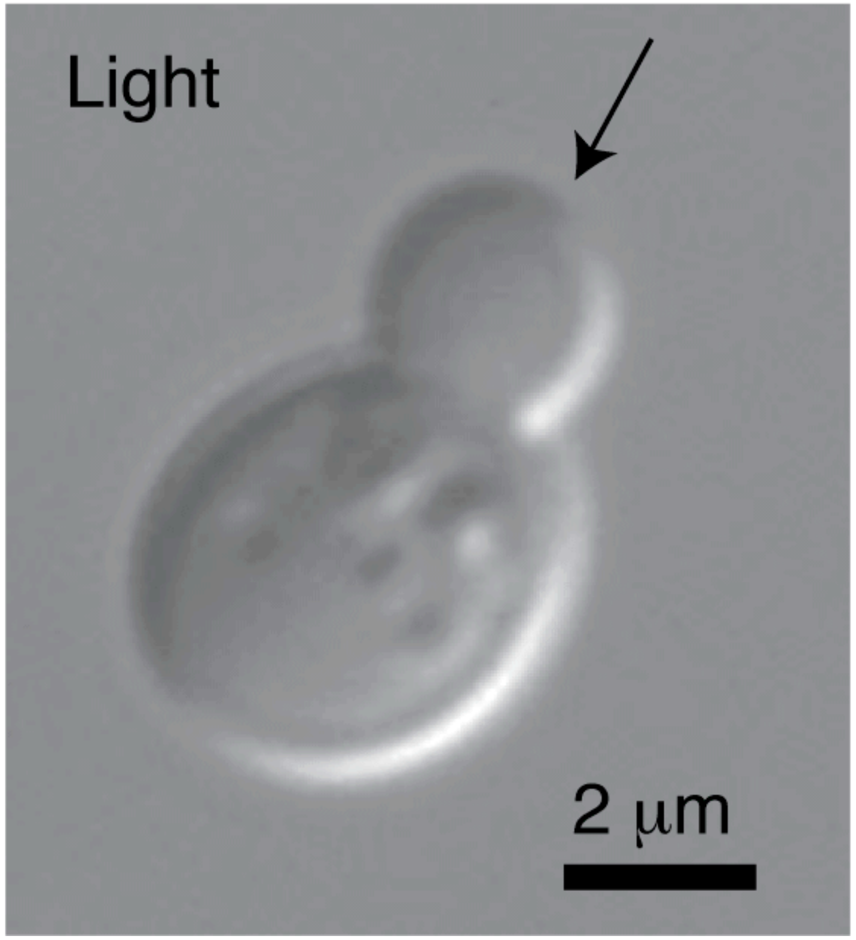


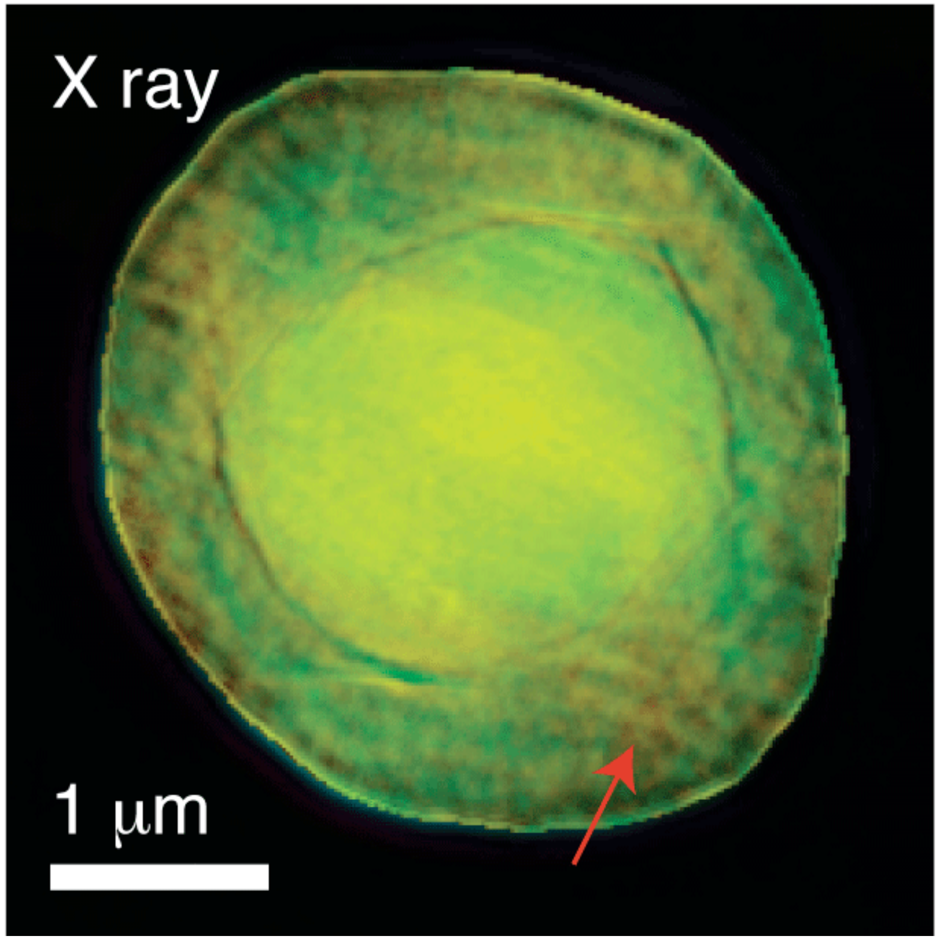
X. Huang *et al.*, *Optics Express* **17**, 13541 (2009)

Frozen hydrated yeast: present results

- X. Huang *et al.*, Stony Brook/ ALS. *Phys. Rev. Lett.* **103**, 198101 (2009)
- Also E. Lima *et al.*, images of *Deinococcus radiodurans* bacteria at ESRF, *Phys. Rev. Lett.* **103**, 198102 (2009)

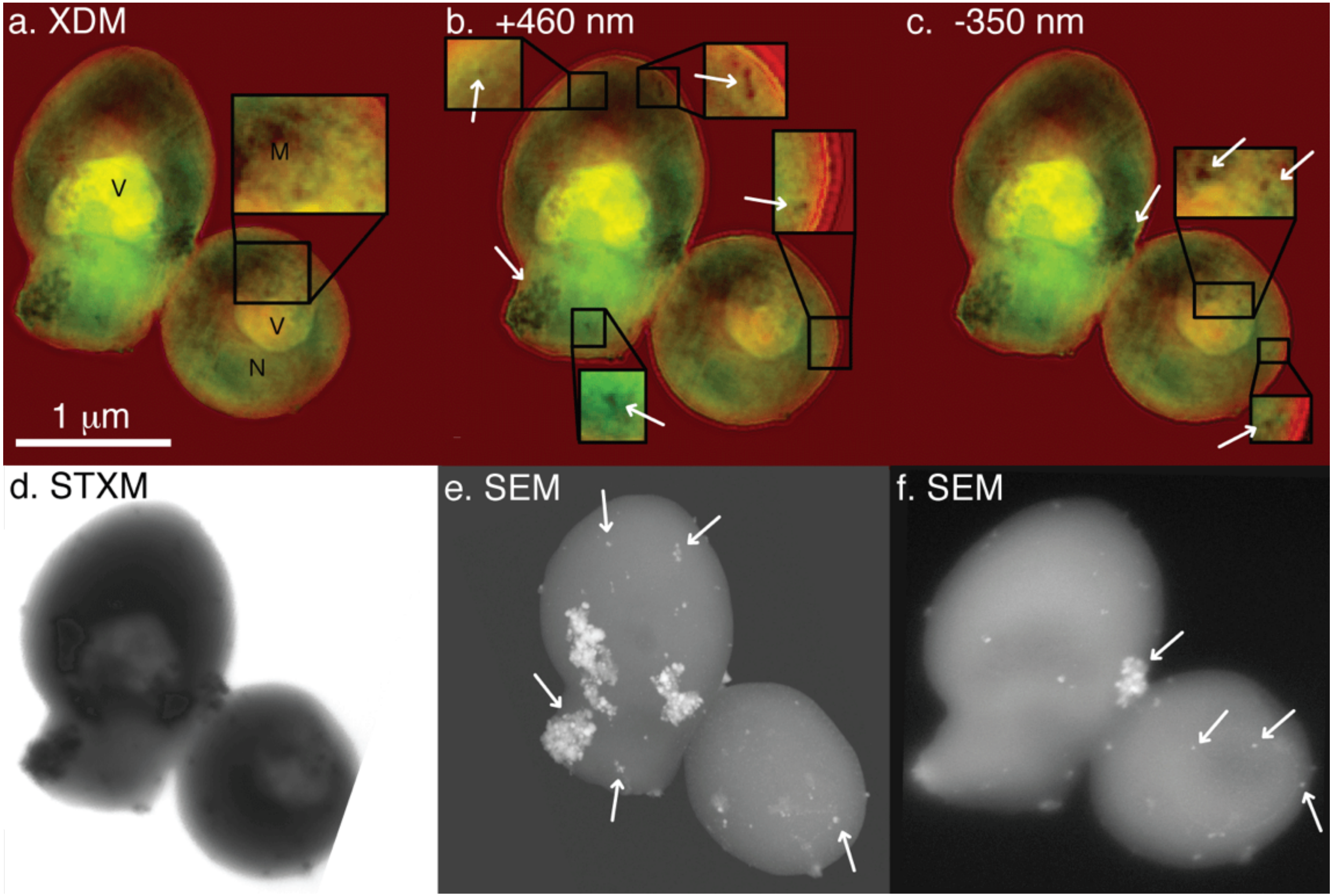






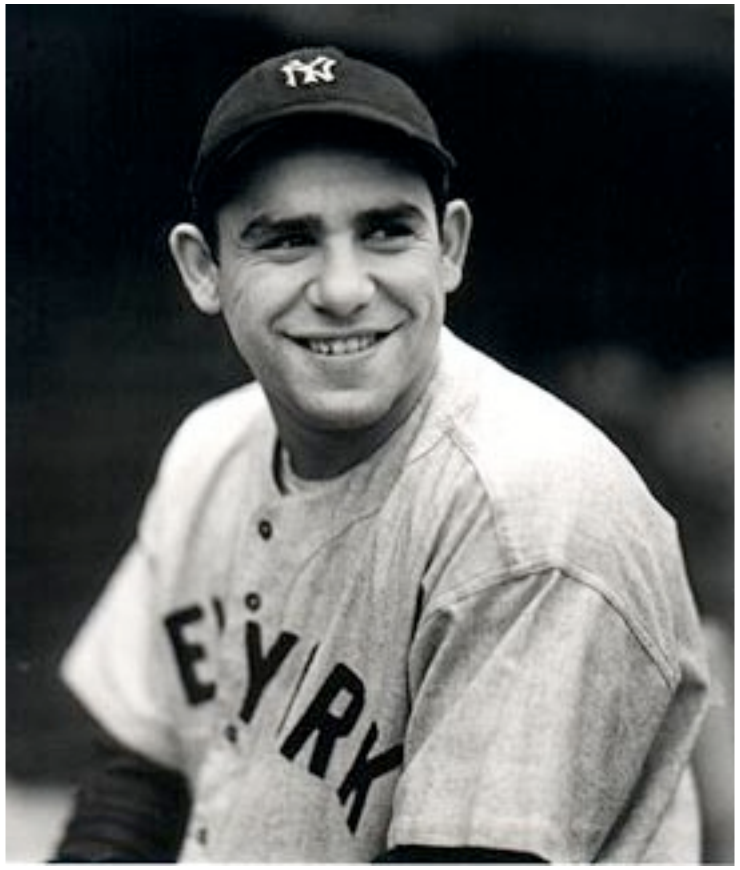
Gold-labeled yeast

Concanavalin A conjugated to 1.8 nm gold for labeling α-mannan, silver-enhanced, dehydrated: J. Nelson *et al.*, Stony Brook/ALS

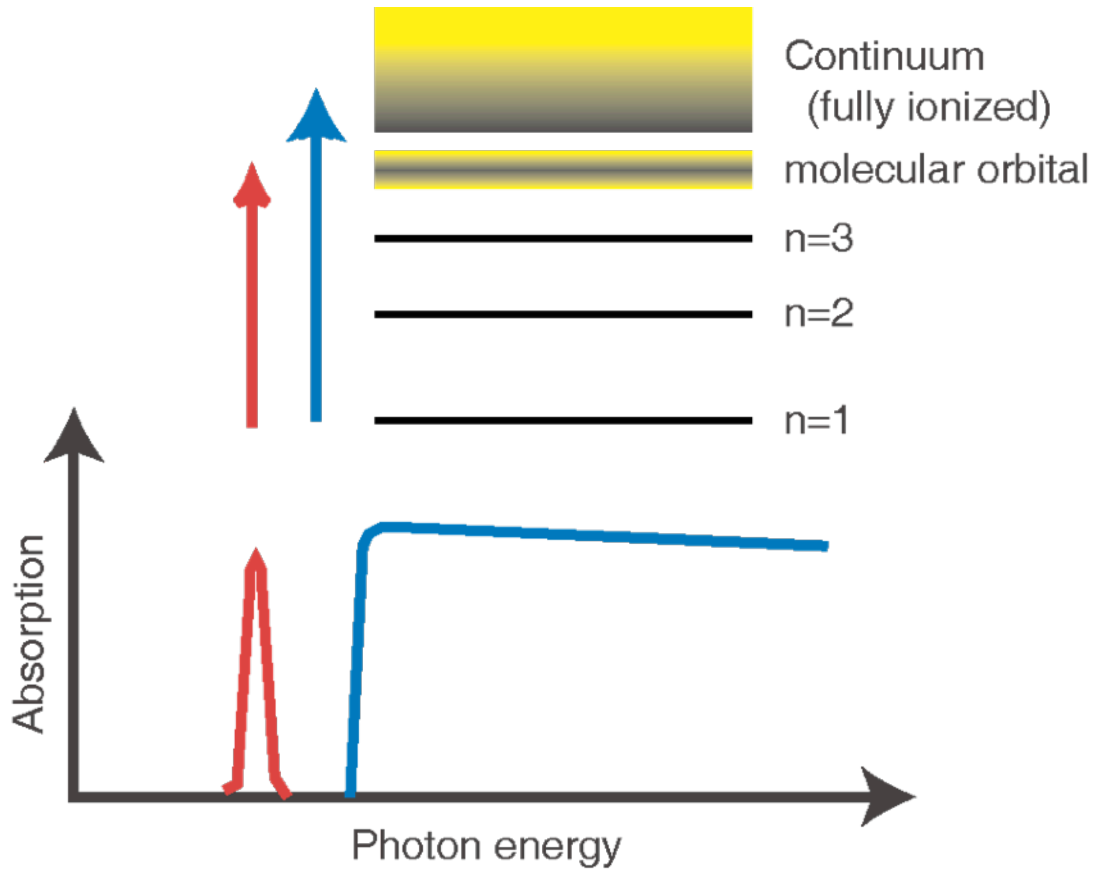


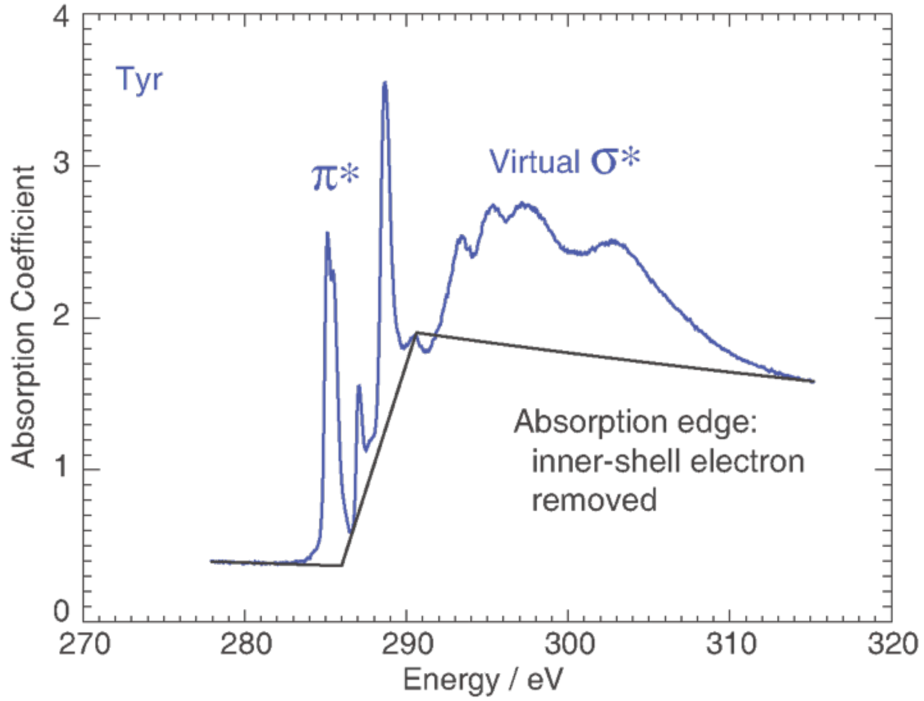
You can observe a lot by watching

- Chemical bond energies are 3-10 eV. Visible and UV photochemistry!
- XANES explores molecular orbital occupancy at these energies.



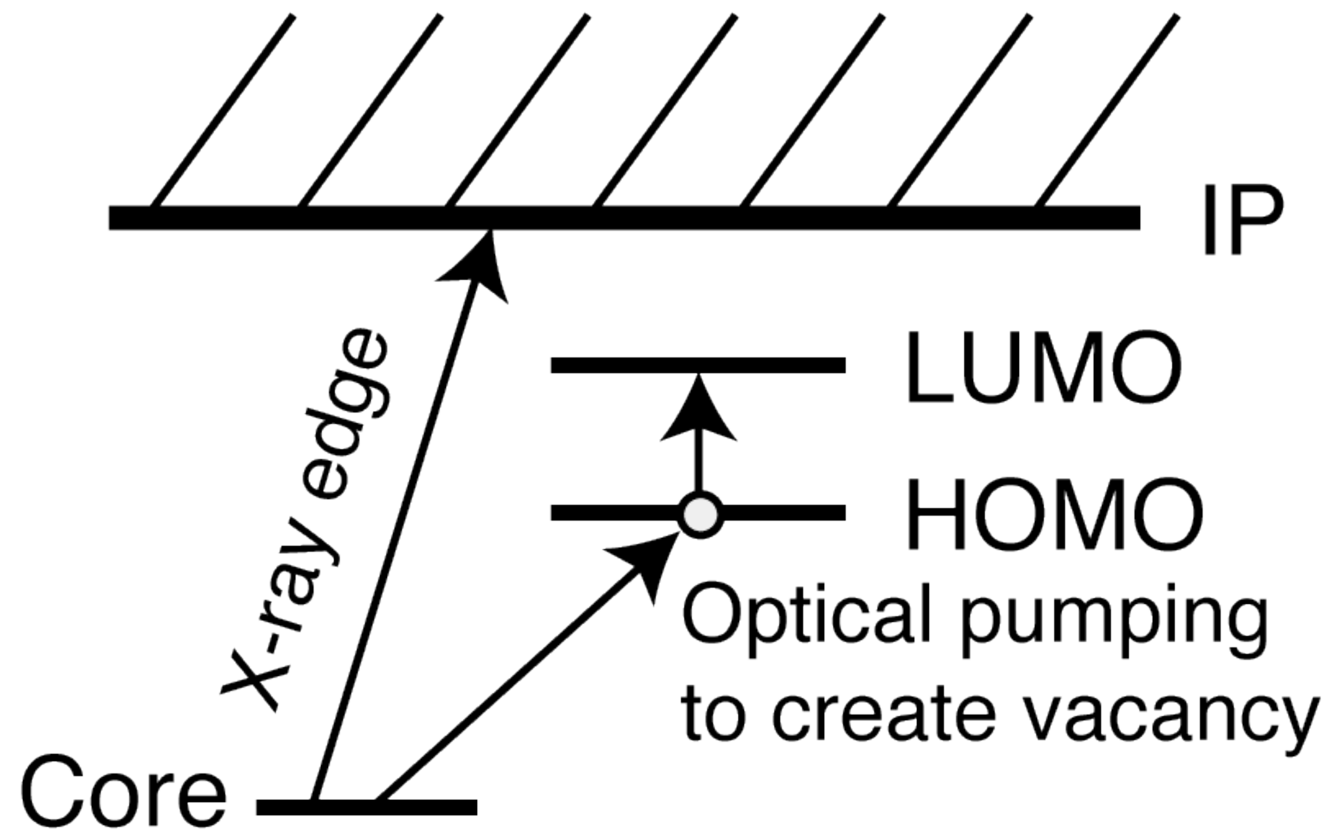
Yogi Berra





Pump-probe: optical transitions with x-ray spatial resolution

- Klems, Phys. Rev. A **43**, 2041 (1991): X-ray Inverse Fluorescence Allowed by Molecular Excitation (XIFAME).
- Watanabe et al., J. Korean Phys. Soc. **32**, 1 (1998): experiments at Photon Factory.
- Jacobsen, SPIE **3925**, 16 (2000).
- Stiel *et al.*, *J. Biochem. Biophys. Meth.* **48**, 239 (2001); Gruszecki *et al.*, *Biochim. Biophys. Acta* **1708**, 102 (2005)



After Stiel (2001): x-ray optical double resonance (XODR)

Sudies of organic photovoltaics

- Organic photovoltaics: cheap, but low efficiency.
- How can efficiency be improved? Trapped excitons?
- Ade *et al.*, XRM 2008

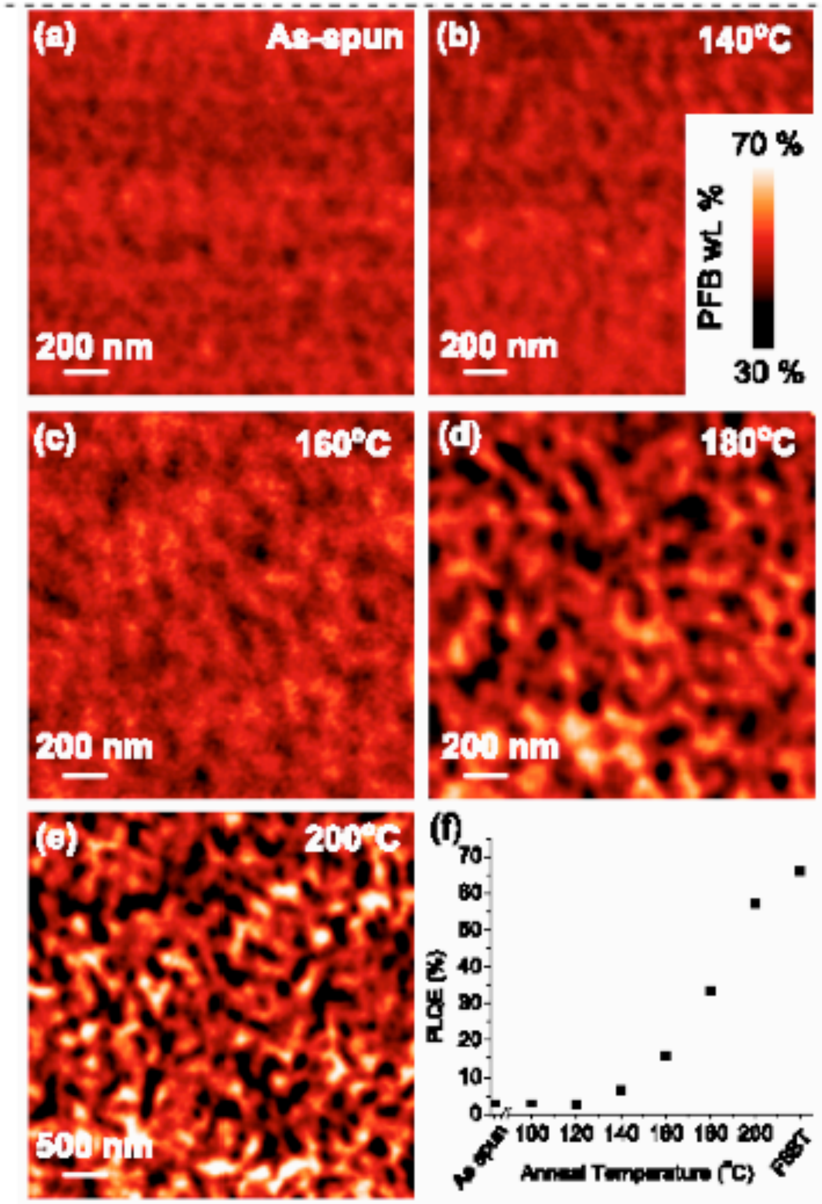
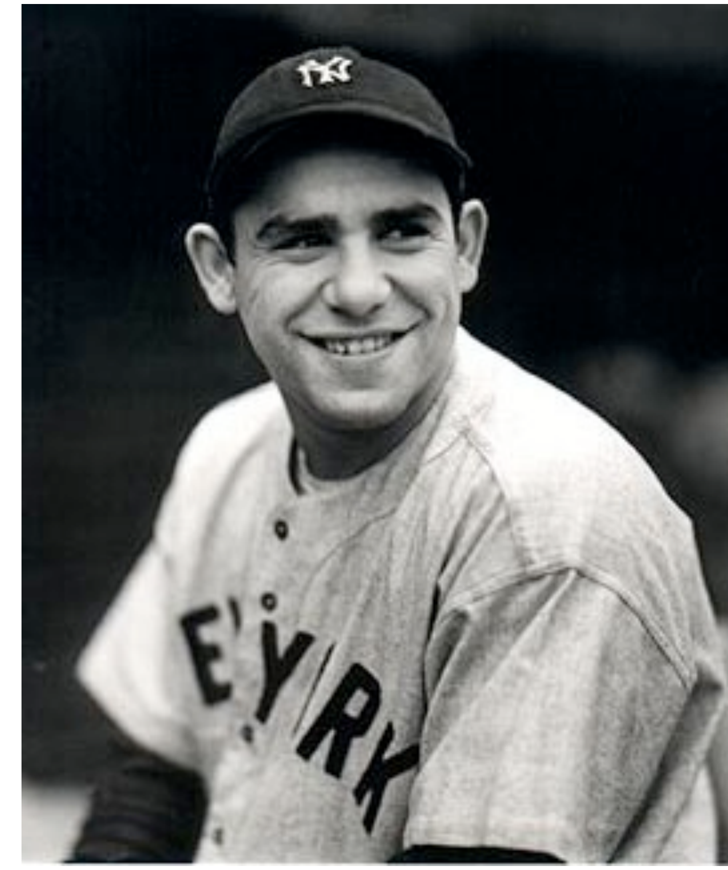


Figure 1. Composition maps of PFB/F8BT blend films: as-spun (a) and annealed at T=140 °C (b), 160 °C (c), 180 °C (d), and 200 °C (e). (f) Photoluminescence quantum efficiency (PLQE) of annealed blend films and a pure F8BT film.

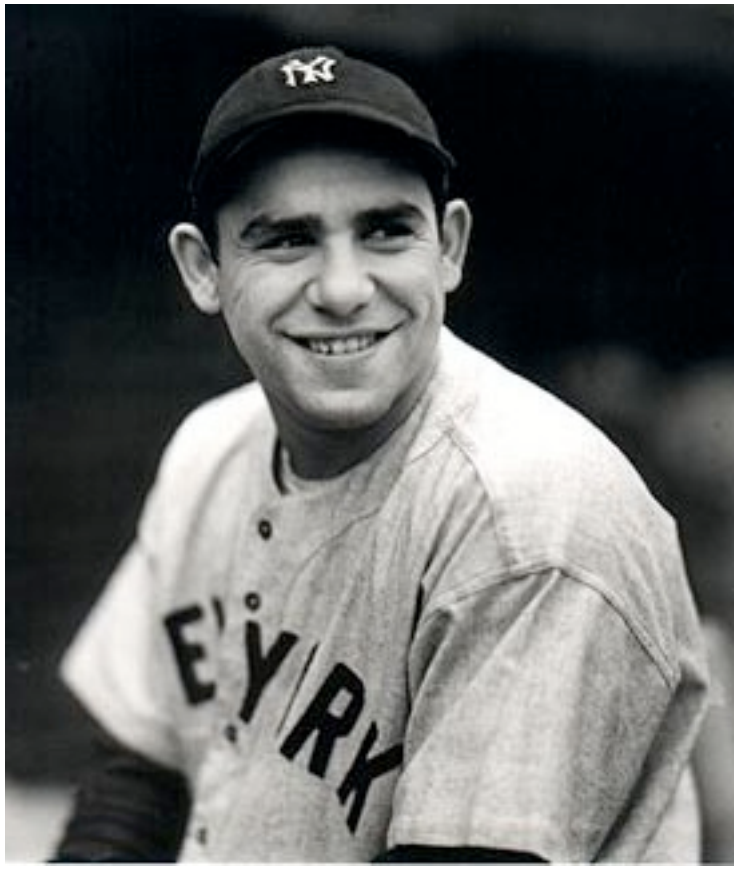
What time is it? You mean now?

- FELS are exciting! It's OK to blow up identical molecules!
- Biological cells, biomass, battery membranes etc. don't come in identical copies!
- We can do a lot with time-averaged brightness, 10 kHz rep rates, and experiment R&D
- Napoleon wanted his soldiers to march in the shade...



Yogi Berra

We're lost, but we're making good time!



Yogi Berra

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