Diffraction imaging

- Originated by David Sayre
- Developed @ NSLS by Stony Brook group
  (Miao thesis)
- Current work @ ALS, APS, Spring8, BESSYII
- Basic idea: Image non-crystalline object
  by recording diffraction pattern
- Recover lost phase information by "oversampling"
  (pattern continuous, not limited to Bragg peaks)
- Iterative algorithm used in reconstruction

The role of coherent X-ray diffraction

- A technique for 3D imaging of 0.5 – 20 μm isolated objects
- Too thick for EM (0.5 μm is practical upper limit)
- Too thick for tomographic soft X-ray microscopy (depth of focus < 1 μm at 10 nm resolution for soft X-rays even if lenses become available)

Goals

- 10 nm resolution (3D) in 1 - 10μm size biological specimens

  (small frozen hydrated cell, organelle; see macromolecular aggregates)

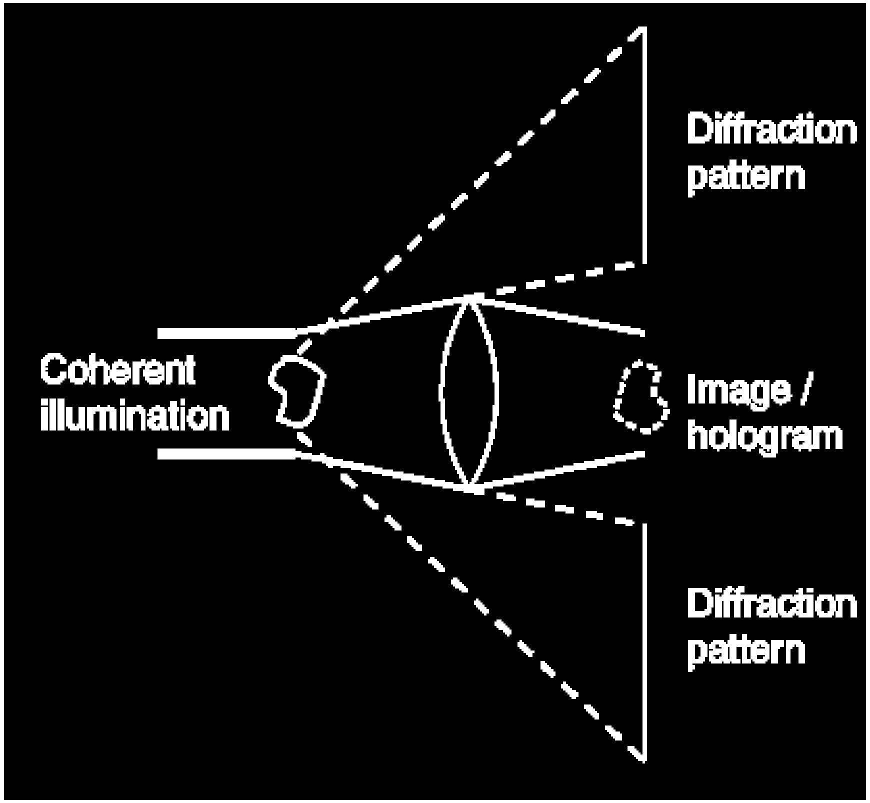
  Limitation: radiation damage!

- <4 nm resolution in less sensitive nanostructures

  (Inclusions, porosity, clusters, composite nanostructures, aerosols…)
  eg: molecular sieves, catalysts, crack propagation

Imaging beyond the lens limit?

- Working from diffraction patterns:
  - No optics-imposed resolution limits!
- Working from images:
  - The lens phases all the Fourier plane information.
  - The lens limits resolution.



- Holography: mix in a reference phase

Where we really want to be

- Collect a high resolution 3D data set in an hour or two
- Reconstruct reliably in a comparable amount of time

Challenges:

1/ getting sufficient coherent photons

- Here is where NSLS II comes in!

2/Choice of energy

- Reconstruction of real objects is easier.
- Electron density becomes more nearly real as energy increases.
- Exposure time scales as E^4 . (Coherent flux for fixed brightness scales as E^{-2}, and cross section scales as E^{-2})
- Best compromise specimen dependent 0.5 – 4 KeV

3/ recording the pattern

- Eliminate higher orders: aperiodic undulator?
- Shielding detector from all but diffracted signal
- Aligning specimen with small beam-spot,
  - Keeping it aligned as specimen is rotated
- Minimizing missing data
  (beam stop, large rotation angles, etc.)
- Dynamic range of detector

Challenges

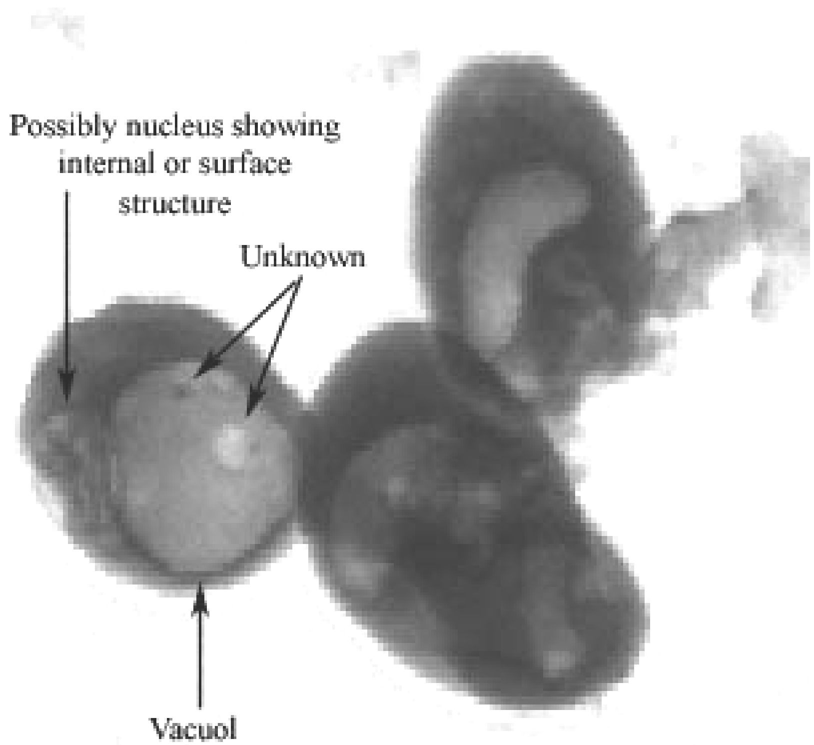
4/reconstruction

5/ damage

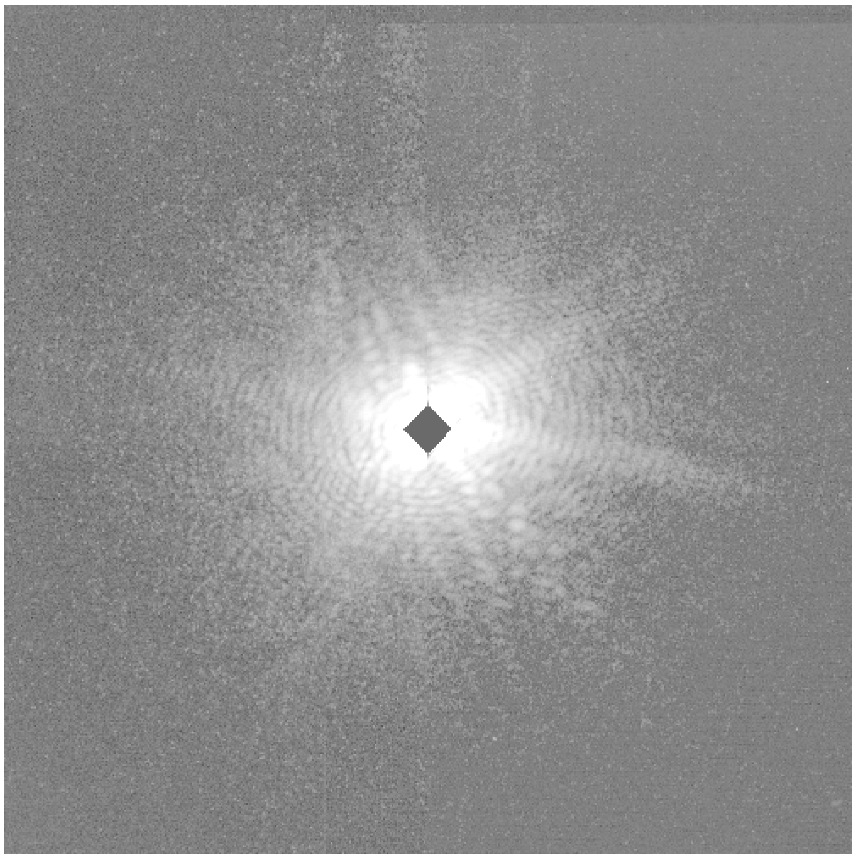
The ultimate limitation for radiation-sensitive materials only

Low temperature helps, but not in chemical mapping

Freeze-dried yeast cells



Diffraction pattern from freeze-dried yeast cell



- ln √ I
- Combination of multiple exposures
- Edge of figure: 45 nm

  pattern extends half way