Prospects for Neutron Tomography and High-Speed Radiography

Les Butler (LSU)
Camden Hubbard (ORNL)
Dayakar Penumadu (U. of Tennessee)

Brief history of chemical analysis

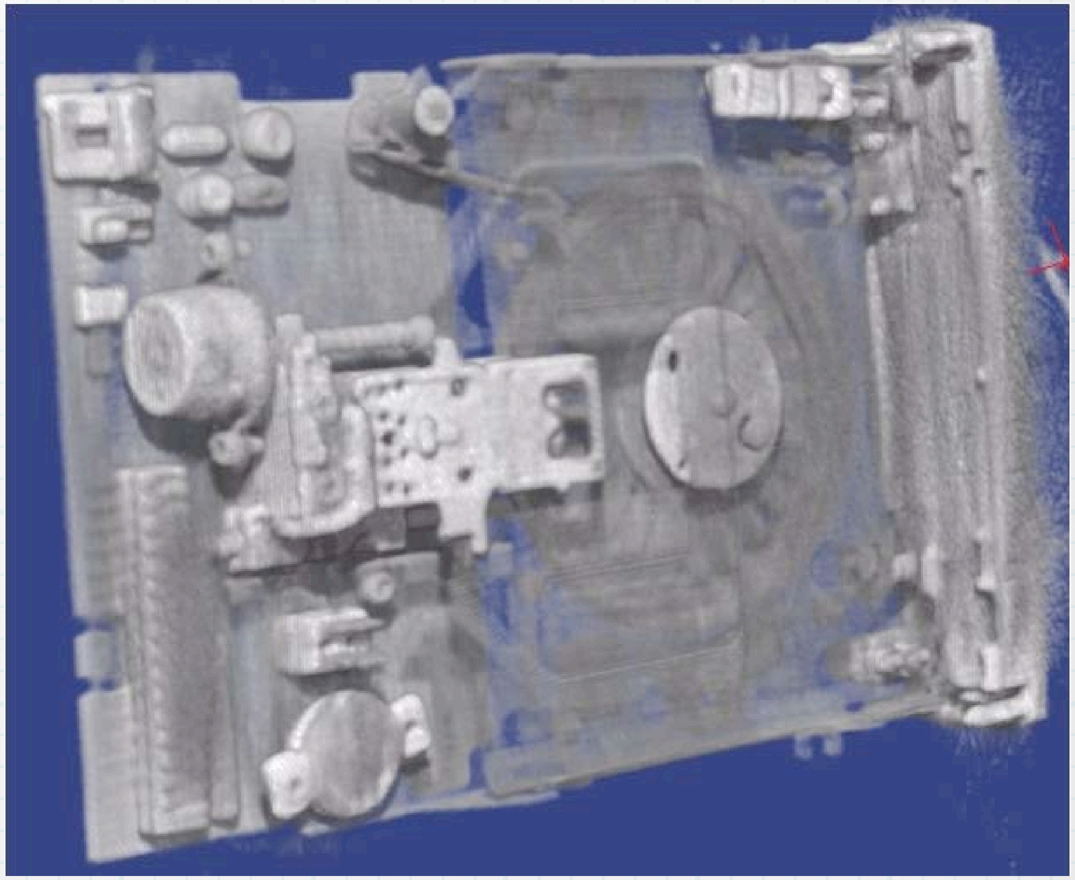
- 19-th century: dissolve sample in nitric acid, ...
- 20-th century: spectroscopy, quantum mechanics, and a line spectra that only a few experts can understand.
- 21-st century: 3D images, convert absorptions into chemical concentrations, make movies and fly-through the sample.

beakers and acid

Sherlock Holmes (asleep)

Neutron Imaging and ORNL:
What unique studies could be done at US high-flux neutron sources?

* Imaging at SNS
  * + high flux
  * + energy analysis via time-of-flight
  * + high L/D
* Imaging at HFIR
  * + high flux
  * - not monochromatic
  * - moderate L/D
  * + wide field of view



Lehmann, 2000

(PSI, Switzerland)

Survey of Chemical Imaging Techniques

* NMR imaging (MRI)
* Electron microscopy tomography
* X-ray tomography
* **Neutron tomography**
* Positron emission tomography

* As chemists, we know chemical signatures, distance scales, and time dependencies vary widely. There is no "best" imaging technique.

Some 3D Methods for Chemical Imaging

Technique	Resolution, Field of View, Expt. Time	Comments
Synch. X–ray	2 μm, 1024^3, 1-8 hrs	> 10 beamlines in US, mature, reliable, great elemental sensitivity for Z ≥ 35 (Br)
^{13}C & ^{31}P MRI	400 μm, 128^3, 6 hrs	lowest S/N, poorest resolution, best chemical speciation
neutron tomo.	50 μm, 1024^3, 2 hrs	~6 beamlines worldwide, some in renovation, elemental sensitivity. US: NIST, UC Davis
electron micro. tomo	2 nm, 512^3, ? hrs	in development; best sample geometry is a thin rod
microtome & 2D EM	2 x 2 x 50 nm, $>1024^3$, >12 hrs	labor intensive; problems with slice-to-slice alignment

Pros & Cons of Neutron Imaging

* - few sources in US; fewer monochromatic sources or time-of-flight sources
* + unique contrast
  * could image soft tissue in presence of metals
  * can image magnetic field structure
* - need better detectors: time and spatial resolution
* - need better information about absorption and scattering cross sections, especially for thermal and cold neutrons
* - small existing US user base at existing sources; SNS tomography user base hard to predict

Preliminary Workshop: April 11, 2005

* Speakers from Paul Scherrer, UC Davis, FRM-II, JINS, HFIR, SNS, MIT, NIST, LSU
* Amount 50 participants from the above and U. Wisconsin, Tufts U., Mayo Clinic
* Tomography results showed seed germination, BMW engine, geology, fuel cell.
* Optics discussed: Kirkpatrick-Baez mirrors
* Imaging techniques: energy selective imaging, phase contrast imaging

Scientific Objectives
"Complex Structure Imaging"

* Chemistry
  * Real-time imaging of blending and chemical reactions through reactor walls. Combine with after-the-fact high resolution imaging and standard spectroscopy.
  * Example: NIST fuel cell images
* Engineering
  * Real-time imaging of operational structures: motors
  * Flow and diffusion processes: lost foam casting
* Biomedial: biopsies
  * Lung: high ^1H contrast helps image alveoli. PM2.5
  * Metal-bone interface: problems with artificial joints

Scientific Objectives
"Complex Structure Imaging"

* Physics
  * Image magnetic field structures with spin polarized neutrons
  * High T_c structures, especially joints
* Nuclear waste remediation
  * Image vitrified waste inside storage casks
* Geology
  * Bio-geology: high ^1H contrast helps search for bacterial growth in rocks.
  * Petroleum: structure and flow of biphasic fluids for advanced oil recovery methods such as CO_2 flooding.

Spallation Neutron Source

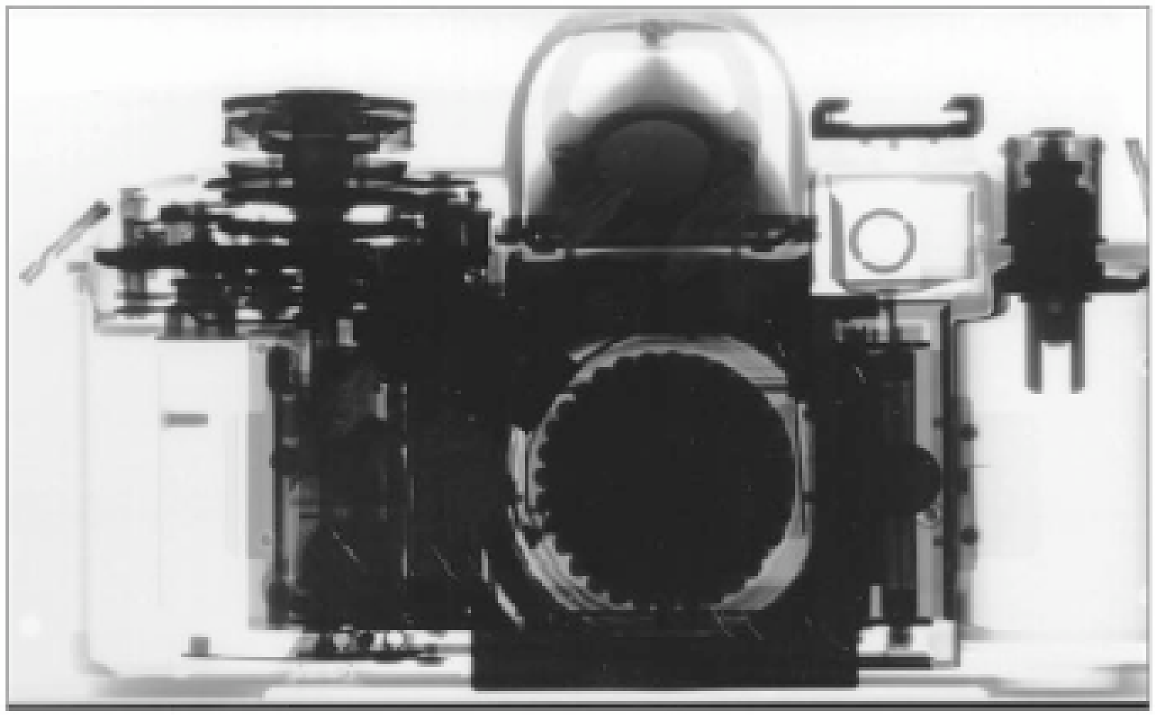
* Neutrons are produced at near-point source by the collision of high-energy protons with a Hg target: 695 ns pulse with 60 Hz rep. rate.
* The experimental hall is about 3/4-populated. Is there room for tomography?

Linear accelerator

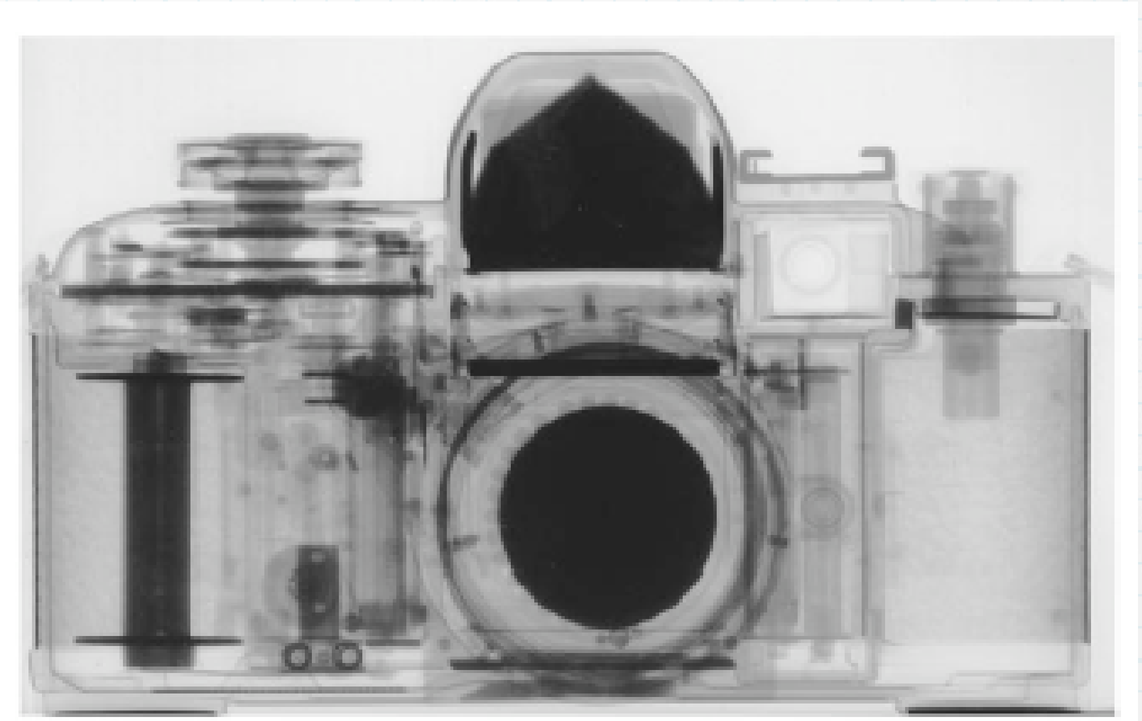
Experimental hall

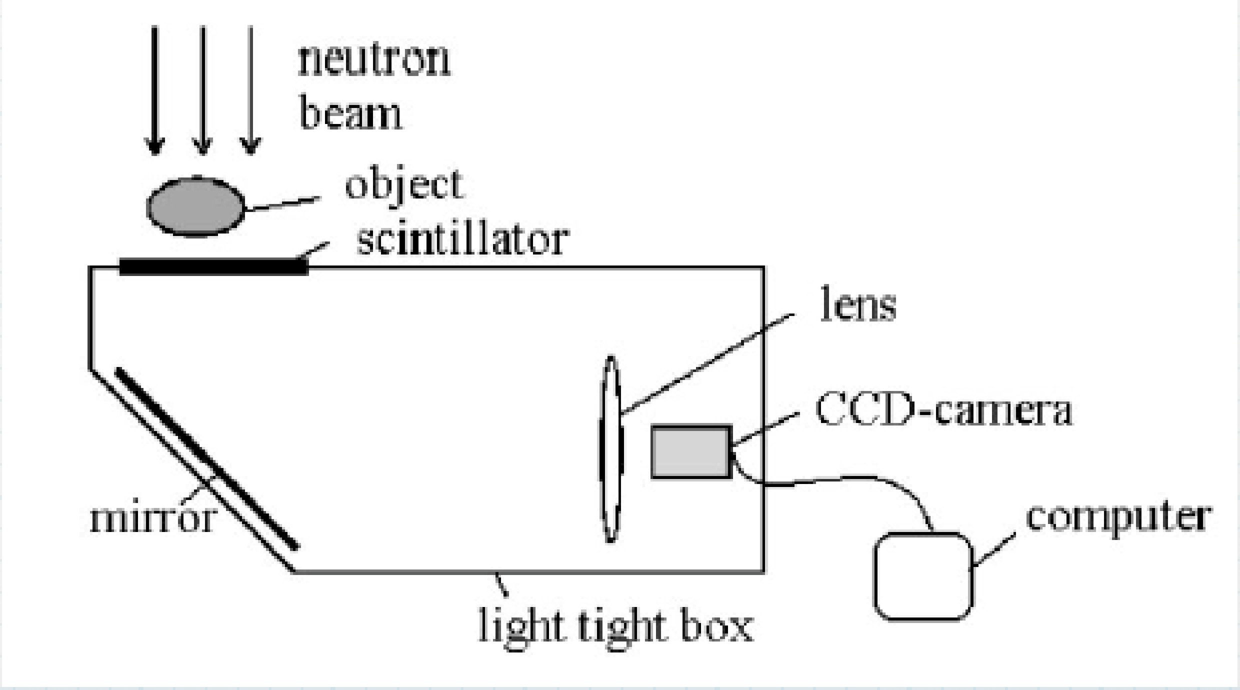
Radiography: X-ray vs neutrons

X-ray: Z-contrast



Neutron: Bragg, nuclear



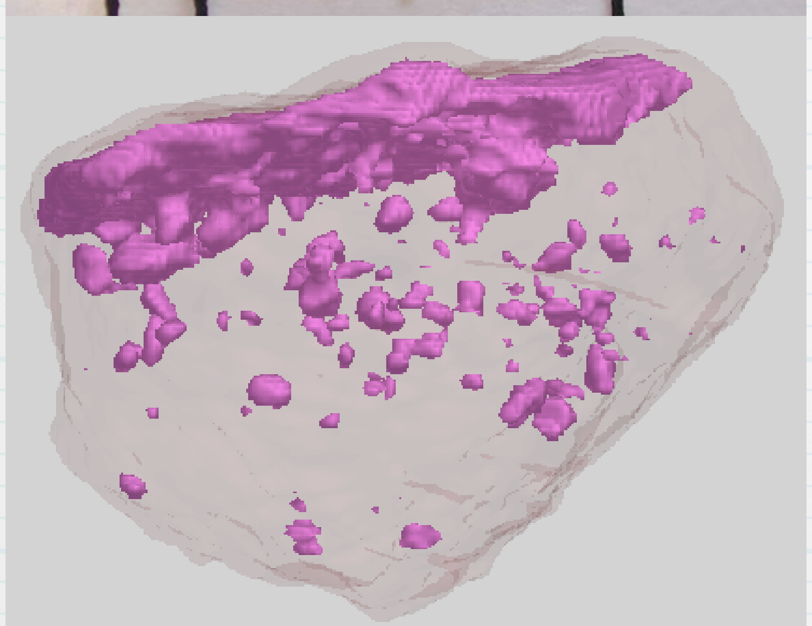


Lehmann, et al. 2000

Neutron Tomography: Geology

* Prof. Dawn Sumner (UC Davis) and MNRC

Endolithic cyanobacteria in sandstone (mm scale)

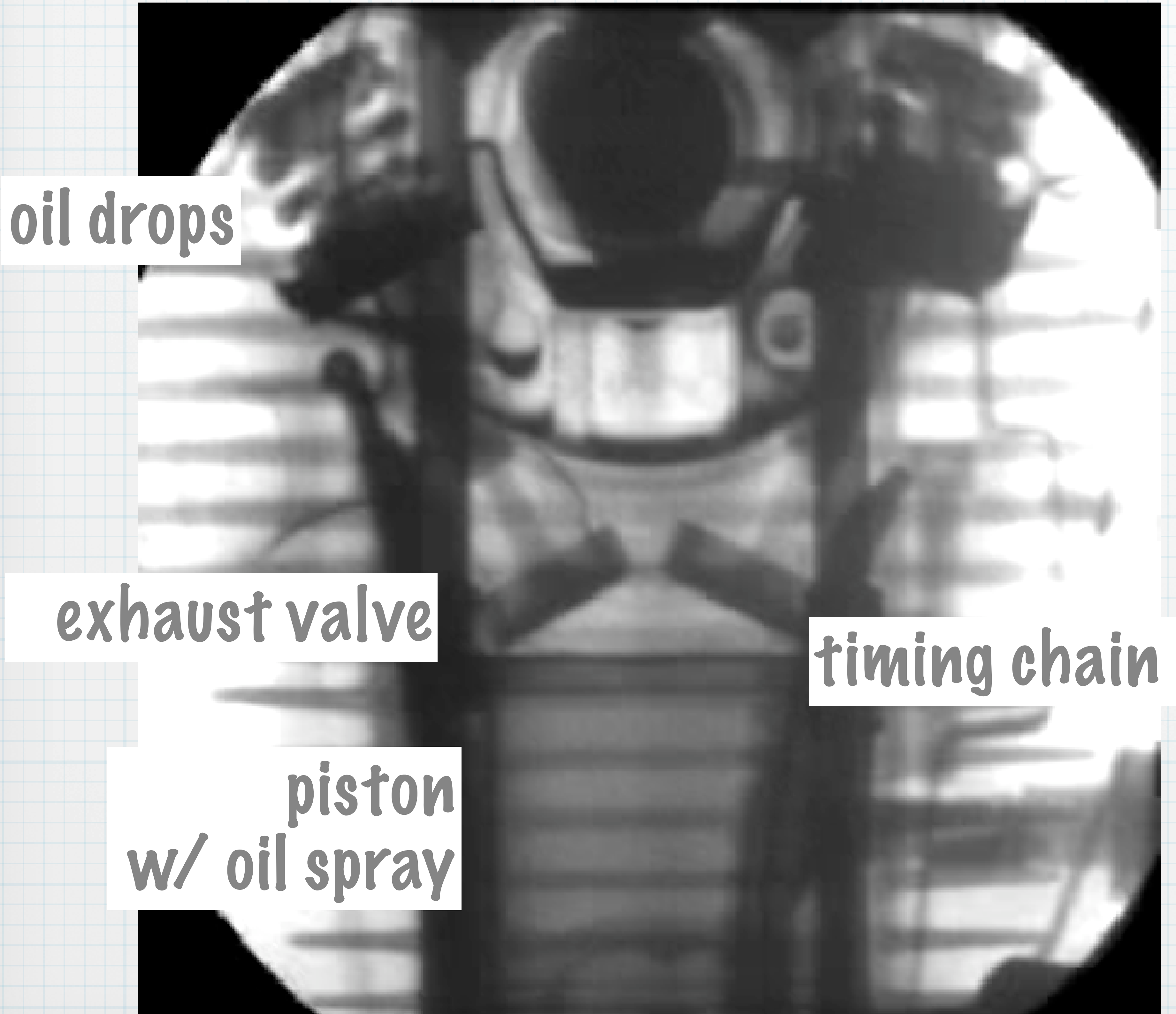


Neutron tomography with volume rendering. High attenuation shown in pink, probably correlating to water in microbial community.

http://www.geology.ucdavis.edu/~sumner/

Examples of Radiography in Engineering

* FRM-II (Munich): air-cooled gas engine



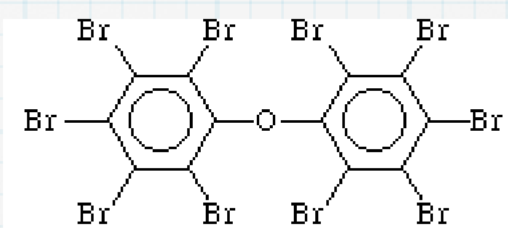
This work uses back projection.

Plans to use discrete tomography for 3D movies.

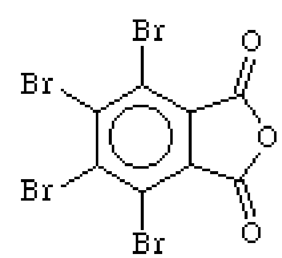
Movie recorded at ILL by G. Frei (PSI), B. Schillinger (FRM-II), and A. Hillenbach (ILL), et al.

Tomography and chemistry: Dispersion of flame retardants in polystyrene

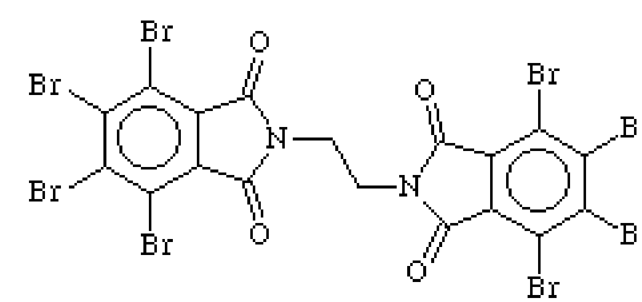
* BT-93, a phthalimide dimer, and antimony(iii) oxide as synergist.
* CRT case can be up to 20 wt% Br.
* How well mixed at the micrometer scale?
* Are the chemical distributions correlated?
* As a function of time, does the system exhibit Ostwald ripening and "blooming"?



1-(2,3,4,5,6-pentabromophenoxy)-2,3,4,5,6-pentabromobenzene (Saytex 102)



3,4,5,6-tetrabromophthalic anhydride (Saytex RB-49)

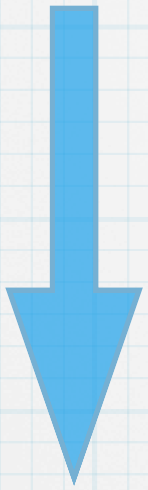


3,3',4,4',5,5',6,6'-octabromo-*N*,*N*'-ethylenediphthalimide (Saytex BT-93)

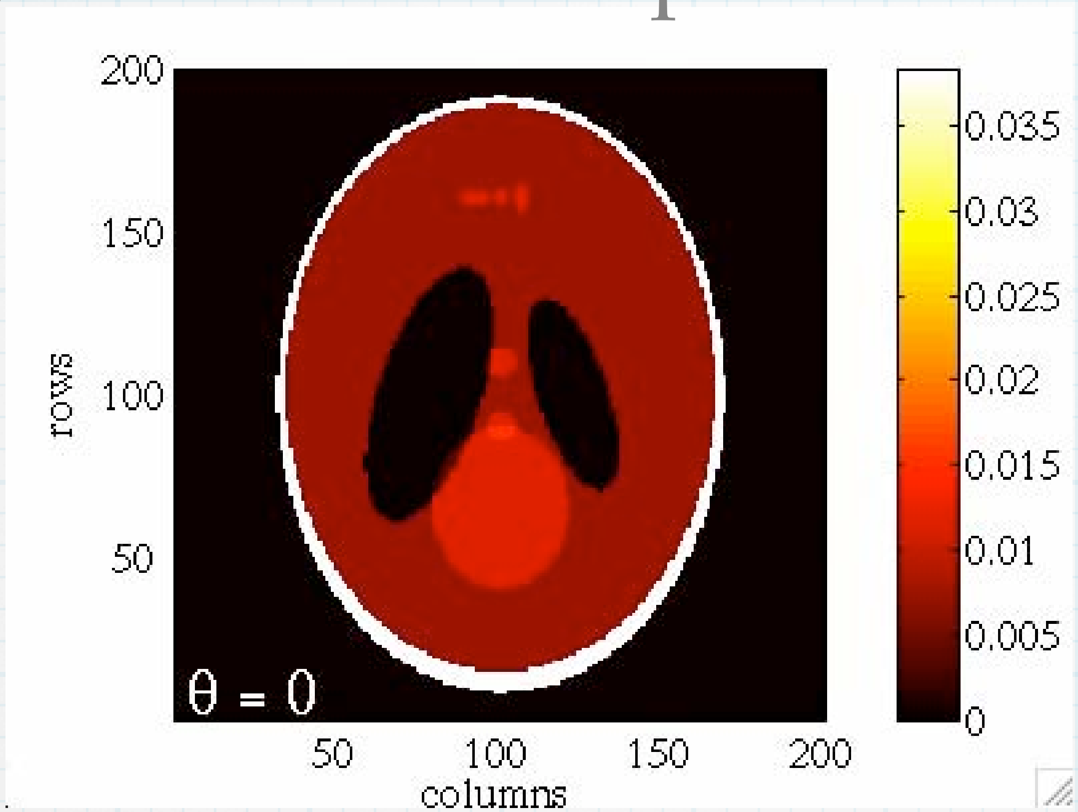
Butler, et al. 2004

What is “tomography”?

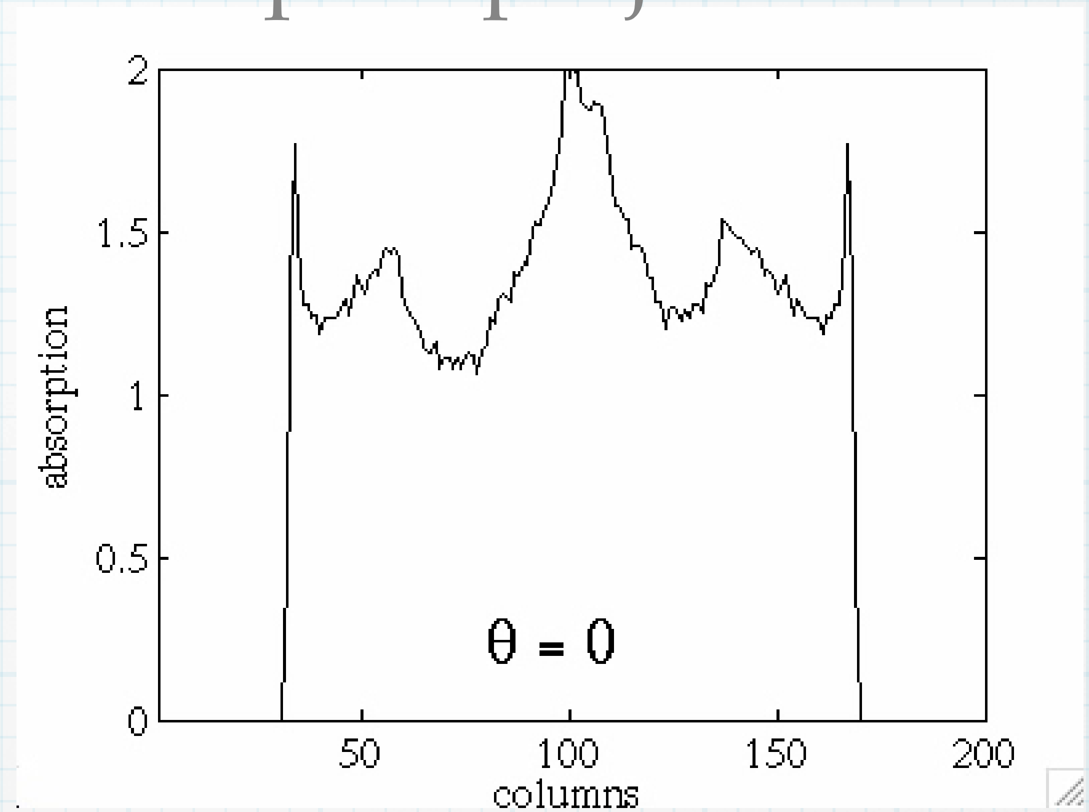
X-rays



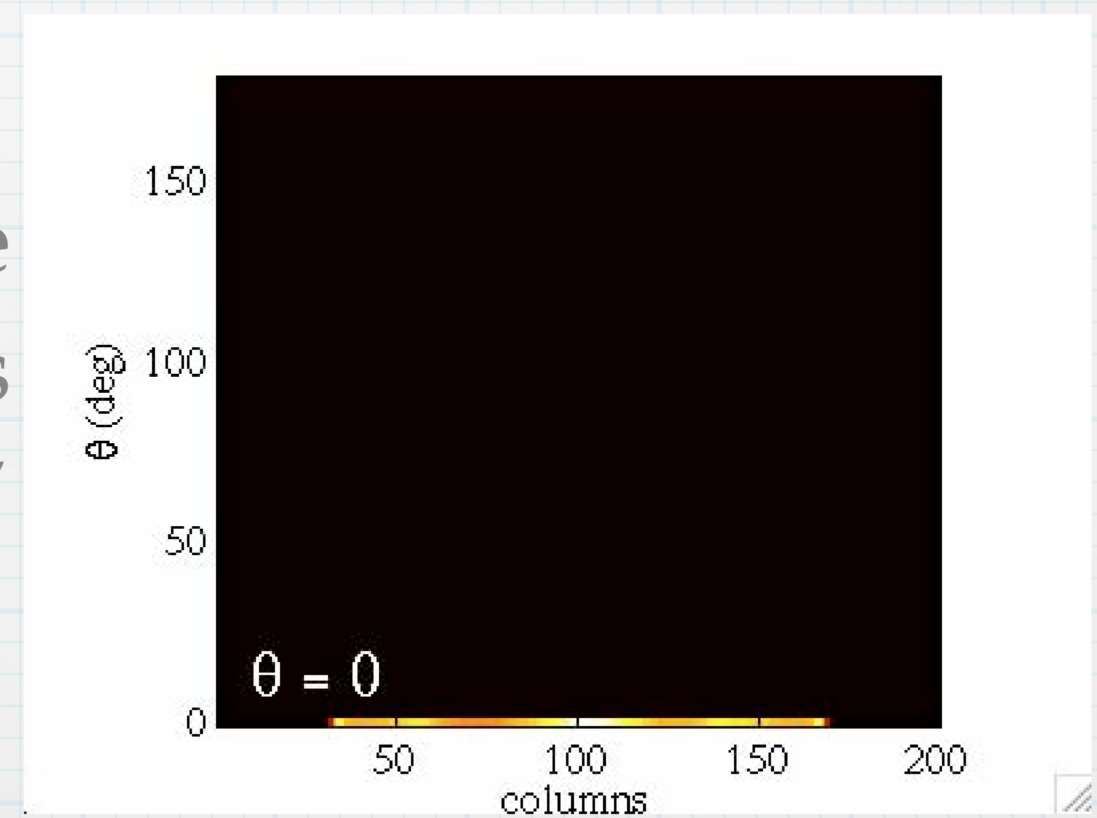
rotate sample



acquire projections

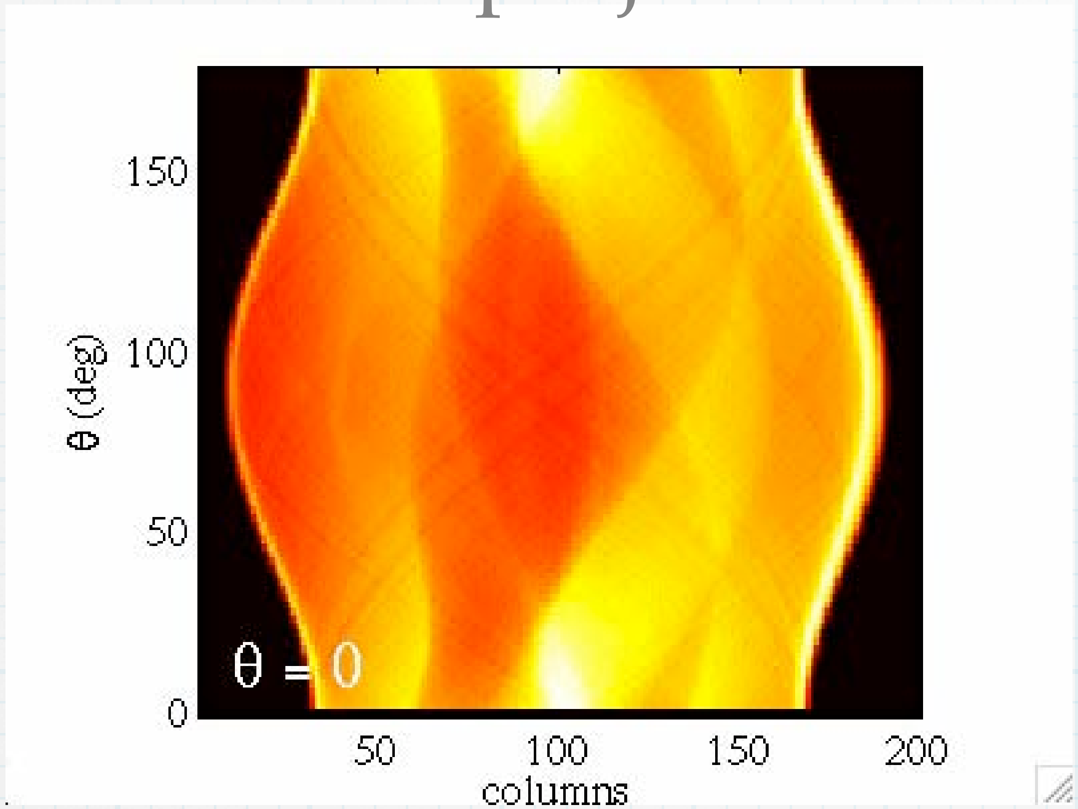


store projections in “sinogram”

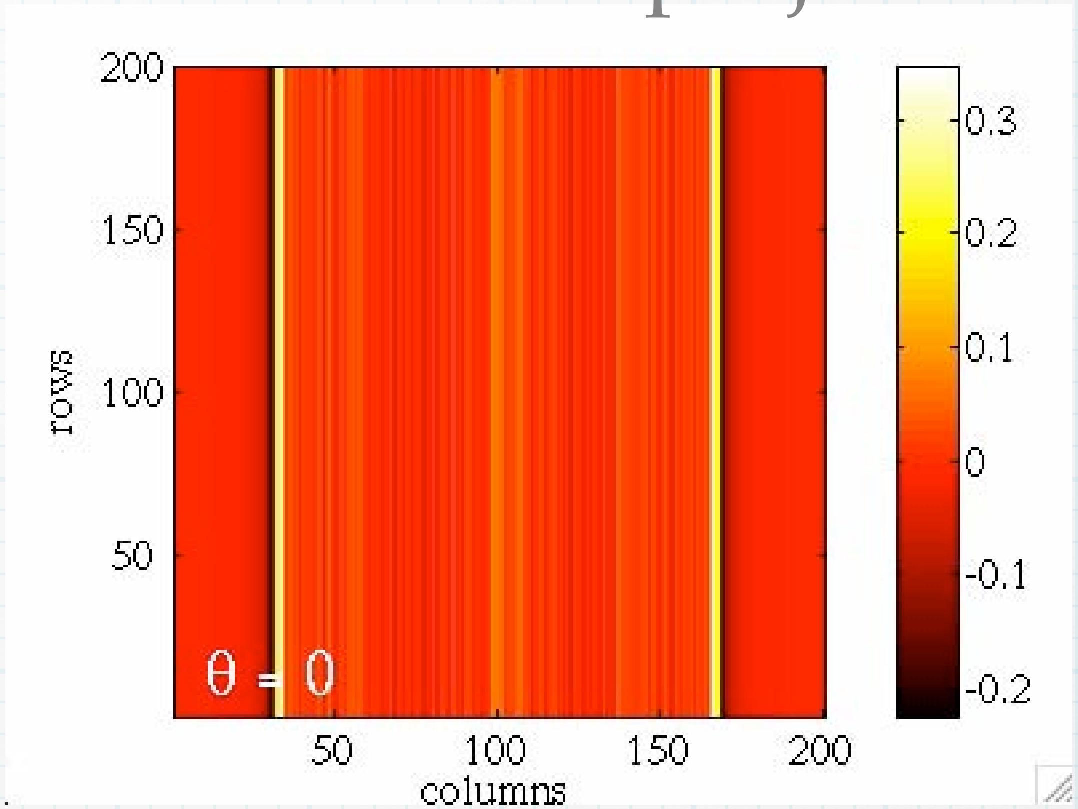


What is "tomography"?

use each projection

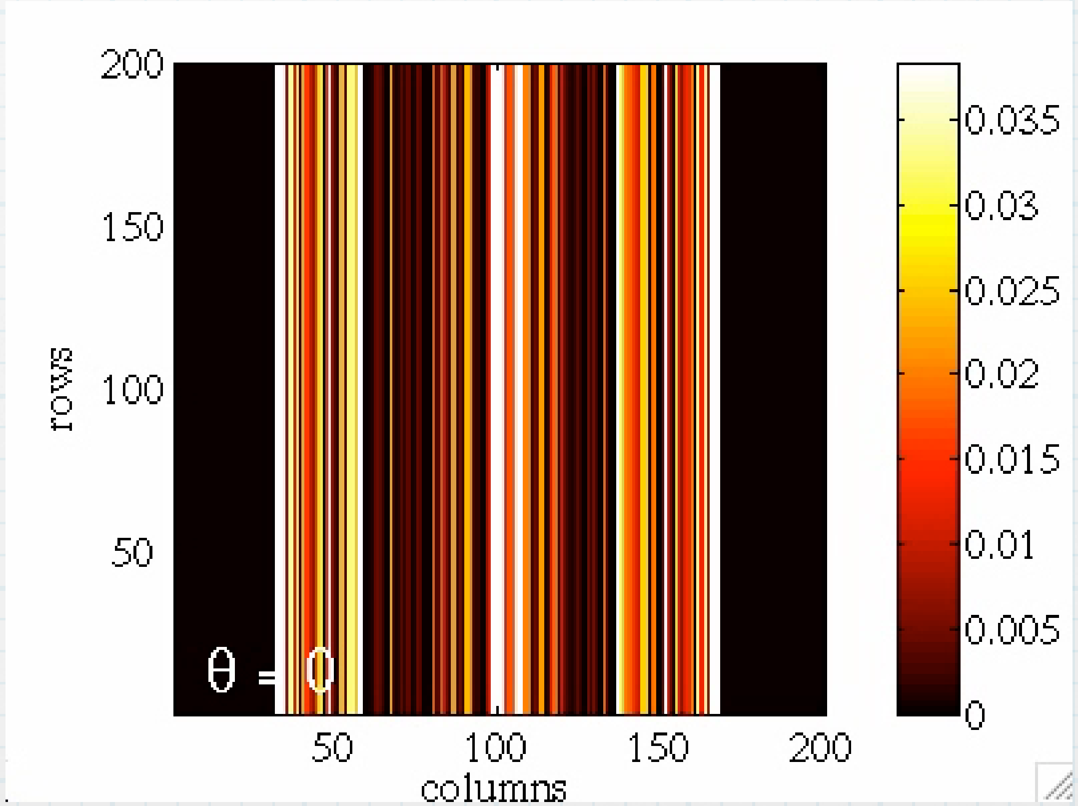


filter and rotate projections



Back-projection reconstruction

sum all projections to reconstruct image

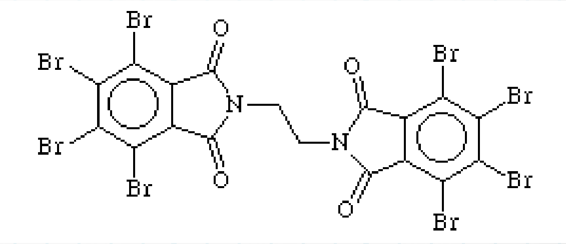


Reconstruction Algorithms

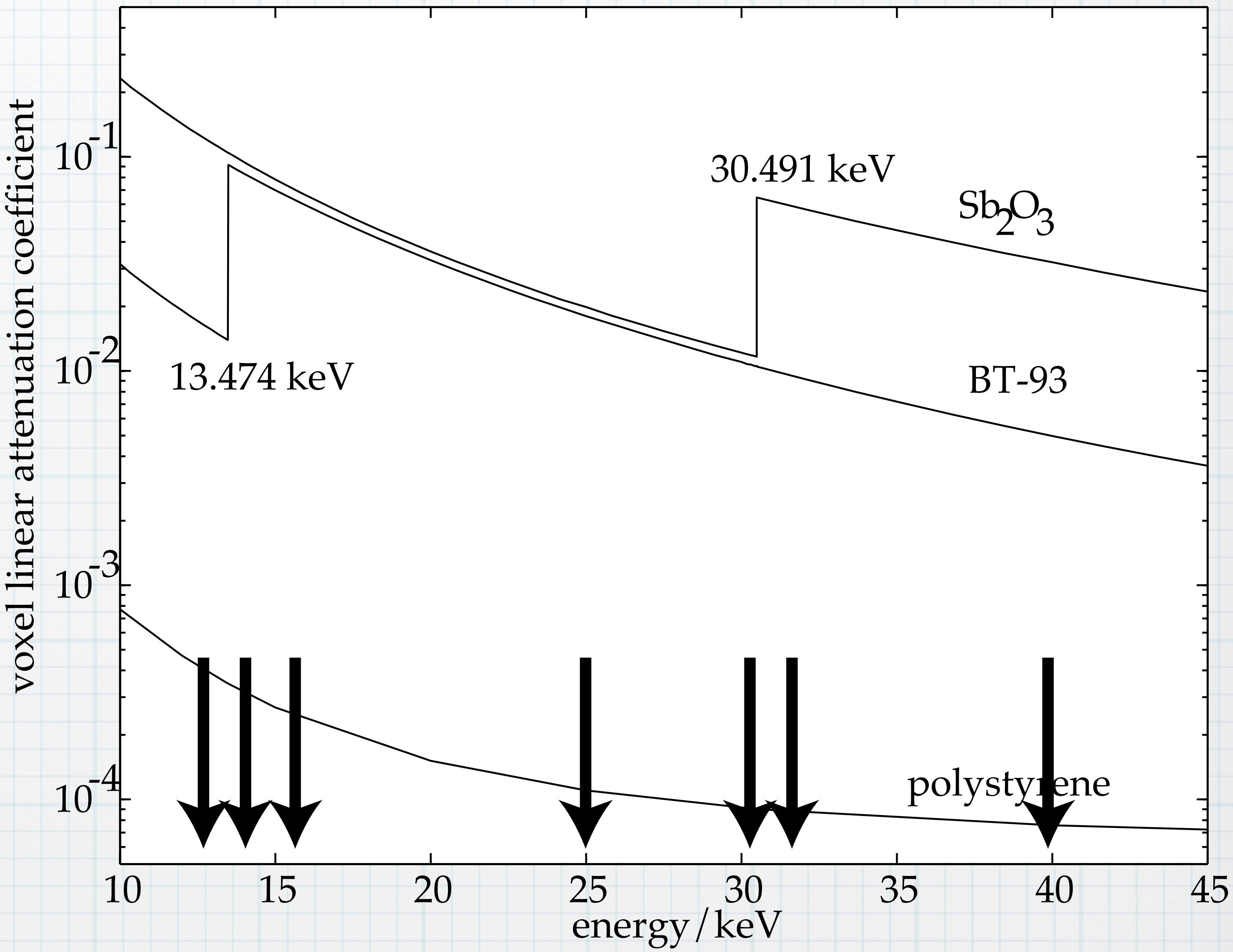
* Back-projection:
  * preserves absorption density information
* Lambda tomography:
  * edge sensitive
  * region of interest imaging
* Discrete tomography:
  * works with minimal number of projections
  * yields binary images, i.e., air and metal
* Algebraic reconstruction:
  * When all else fails:
    * EM tomography: limited field of view

Neutron Tomography Applications

Multispectral Imaging and Composition

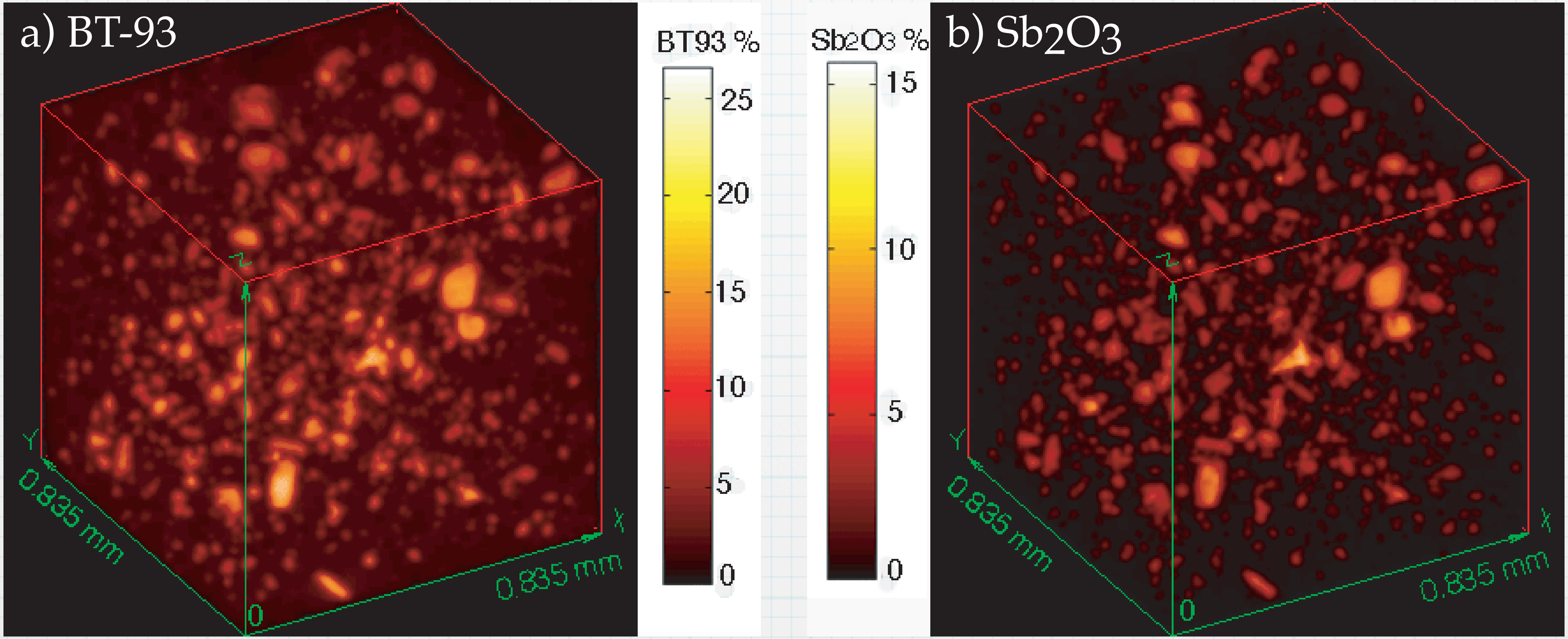


* X-ray absorption edges identify Br and Sb.
* Tomography at X-ray energies spanning Br and Sb absorption images can be converted to Br and Sb 3D composition.
* Independent voxel model with constrained least squares fitting.
* Br and Sb imaged at 7 X-ray energies in 8 hrs beam time.



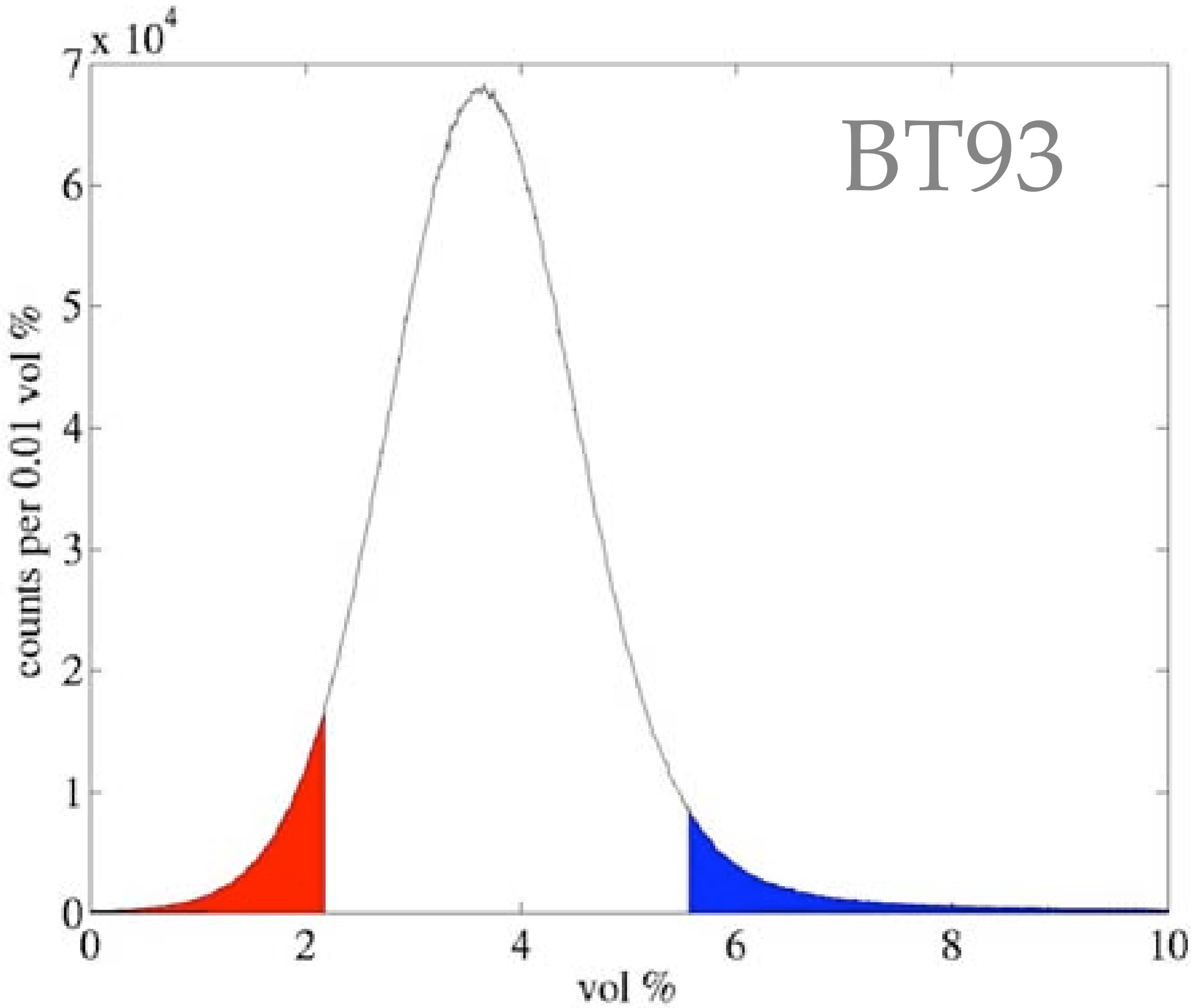
$$Abs_E = Abs_E^{BT93}\,[BT93] + Abs_E^{Sb2O3}\,[Sb2O3] + Abs_E^{poly}\,[polystyrene]$$

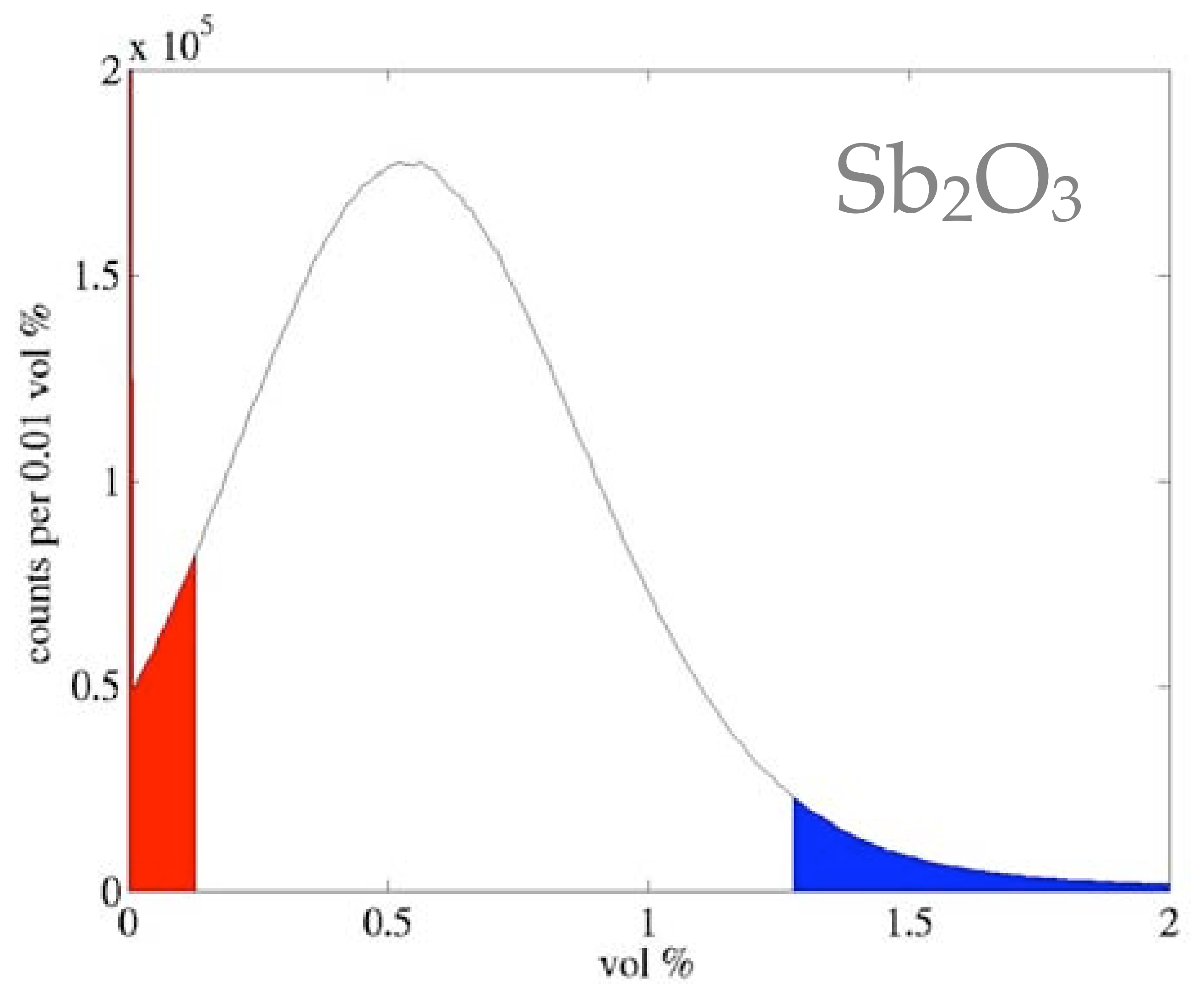
* Least squares fit of X-ray images yields two volumes of data showing BT-93 and Sb_2O_3 concentration distributions. The colorbars show volume percent composition.
* Spatial correlation is obvious. Correlated with mixing order.
* Could have drawn 3-rd volume showing polystyrene.
* Next: metrology on these distributions.



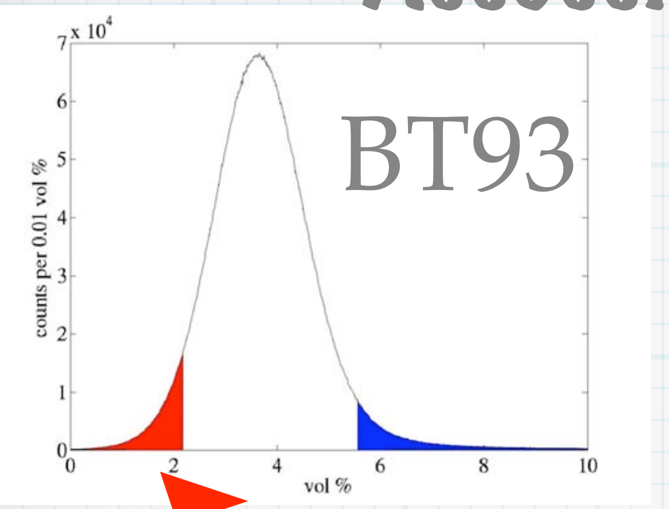
Support: NSF, ACS-PRF, Albemarle Labs: APS, CAMD

* Histograms of vol % throughout the 250x250x250 voxel cube.
* First, "red" shows low concentrations of flame retardants.
  Are the concentrations too low and spatially connected?
  Can a flame exist?
* Second, "blue" shows high concentrations of expensive flame retardants.
  Could money be saved by better mixing?

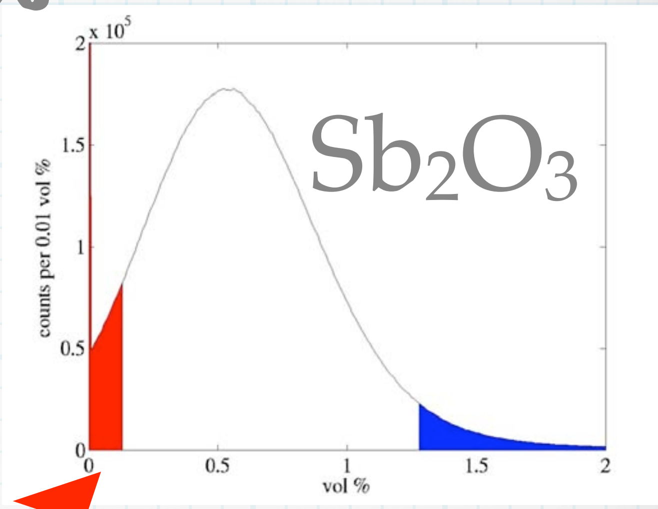




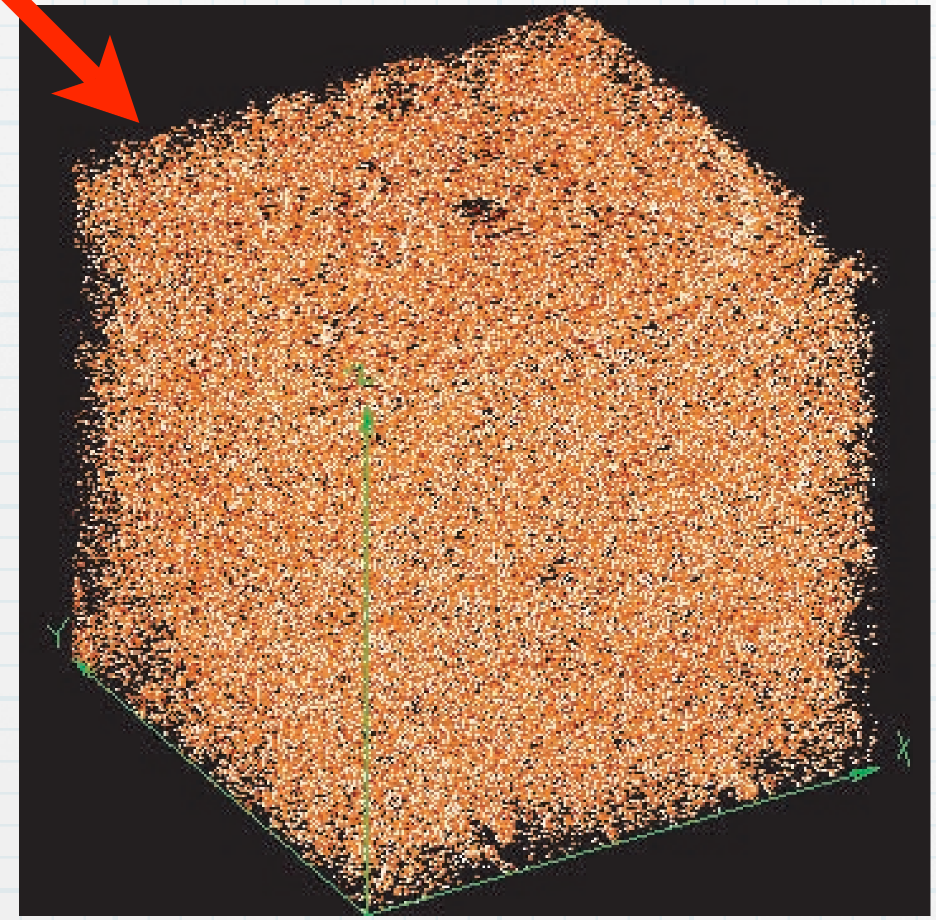
Assessments of dispersions: the extremes



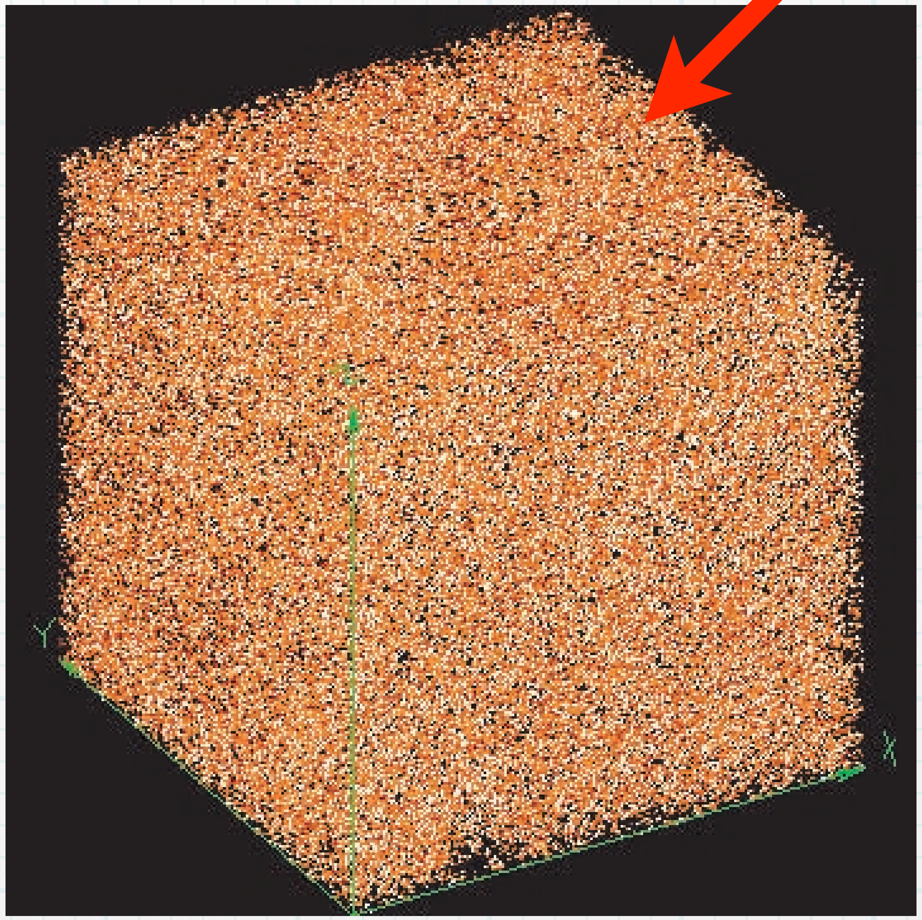
Safety



a) <2.2 vol% BT-93

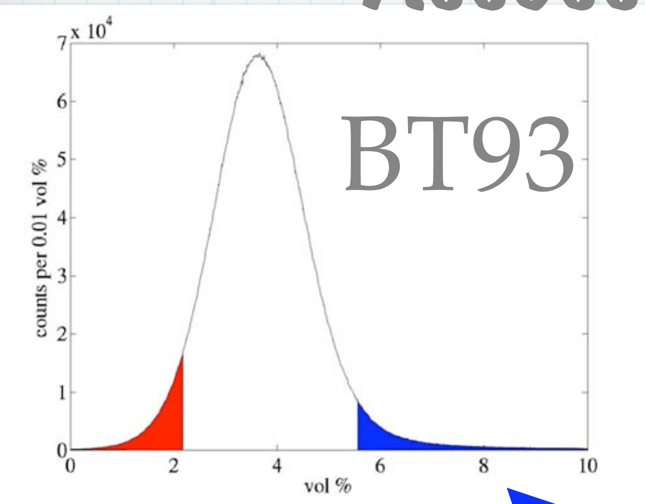


b) <0.1 vol% Sb_2O_3

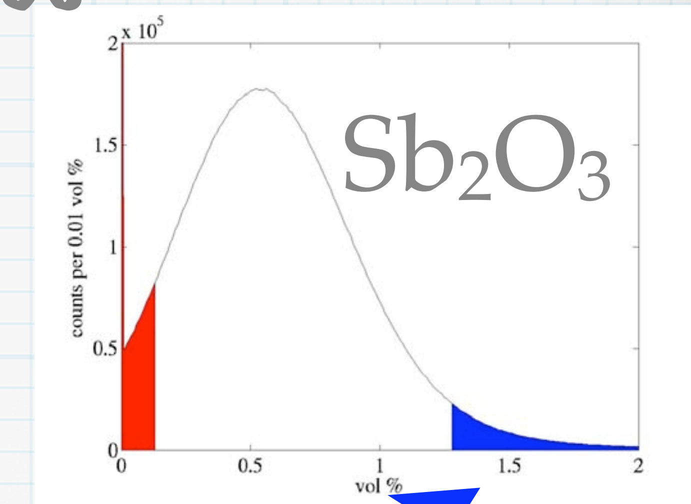


By inspection, there appear to be no large, connected regions in red, that is, no regions large enough to support a flame. Thus, the mixing is judged to be good enough to make a safe material.

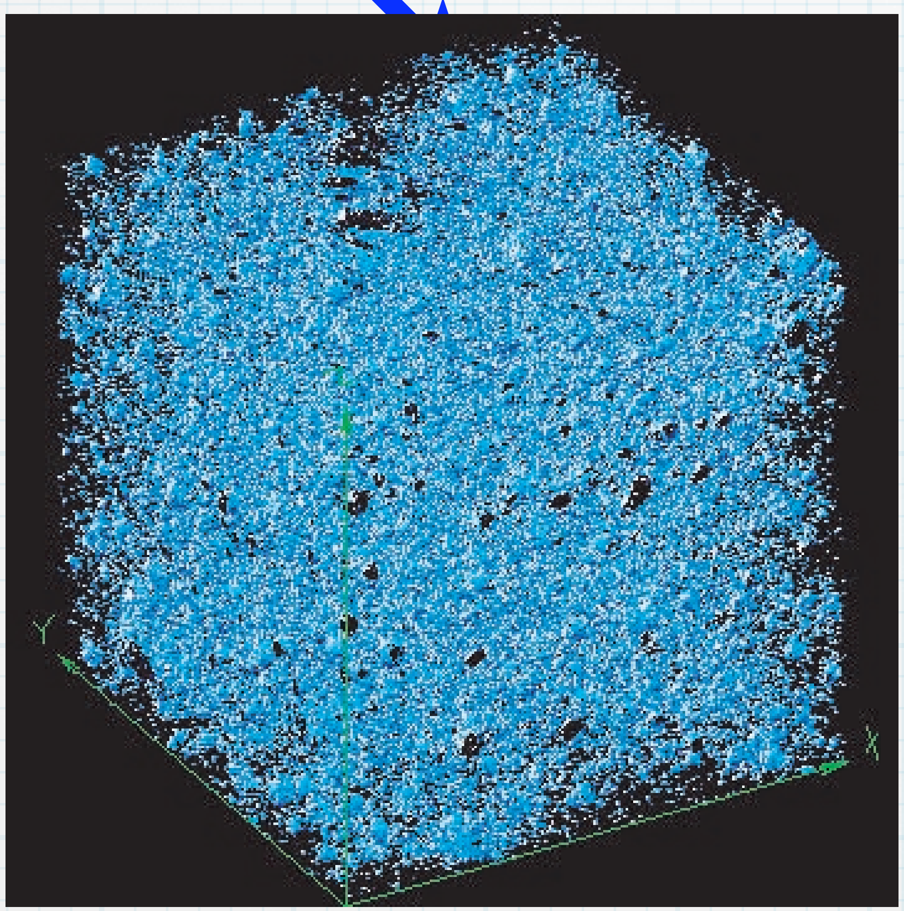
Assessments of dispersions: the extremes



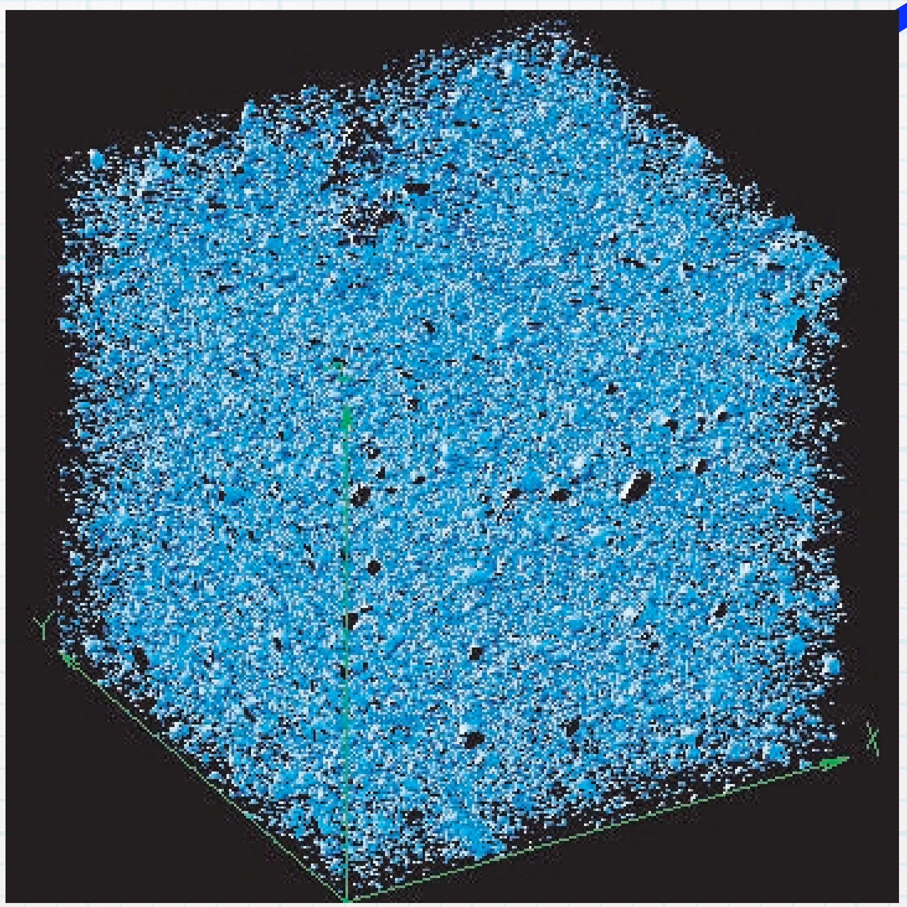
Economy



a) >6.2 vol% BT-93

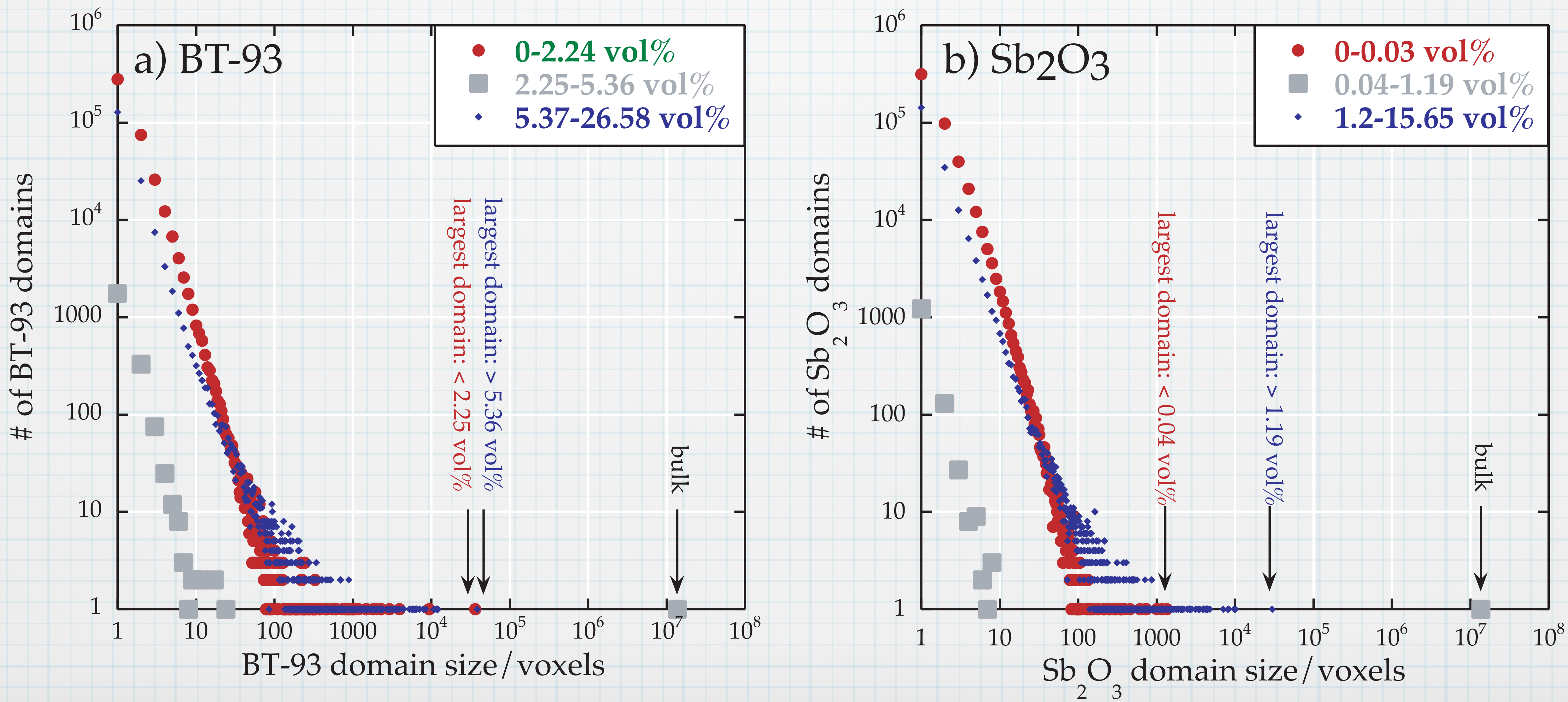


b) >1.5 vol% Sb_2O_3



By inspection, there appear to be domains that could, with better mixing, be reduced in size. Thus, better mixing could reduce the need for the expensive flame retardant materials.

* Domain size distribution for three different concentration ranges: the low and high concentrations (red and blue images) and the intermediate concentration.
* A perfectly homogeneous blend would have one point on these plots at coordinates x=15 million (250^3) and y=1. The pixel labeled "bulk" has nearly these coordinates.
* For safety, the point labeled "largest domain <__ vol%" should be as far to the left as possible.



Need: more 3D image analysis tools and algorithms

http://www.ima.umn.edu

Jan 9-12, 2006 in Minnesota

Workshop goal:
Lock 80 mathematicians,
5 supercomputer folks, and 10 experimentalists
in a room, and
develop new math.

IMA

IMA - Institute for Mathematics and its Applications

Search

more options

SITE MAP

Contact Information

Program Registration

Postdoc/Membership Application

Program Feedback

Material from Talks

Audio/Video

Industrial Programs

Program Solicitation

Calendar

Join our Mailing Lists

Imaging, September 2005-June 2006

IMA Workshop:

3-D Image Acquisition and Analysis Algorithms

January 9-12, 2006

Organizers:

Les Butler
Department of Chemistry
Louisiana State University
lbutler@lsu.edu
http://chemistry.lsu.edu/butler/

Gestur Olafsson
Department of Mathematics
Louisiana State University
olafsson@math.lsu.edu
http://www.math.lsu.edu/~olafsson/

Todd Quinto
Department of Mathematics
Tufts University
todd.quinto@tufts.edu
http://www.tufts.edu/~equinto

Schedule	Participants	Registration	Feedback
Dining Guide			Maps

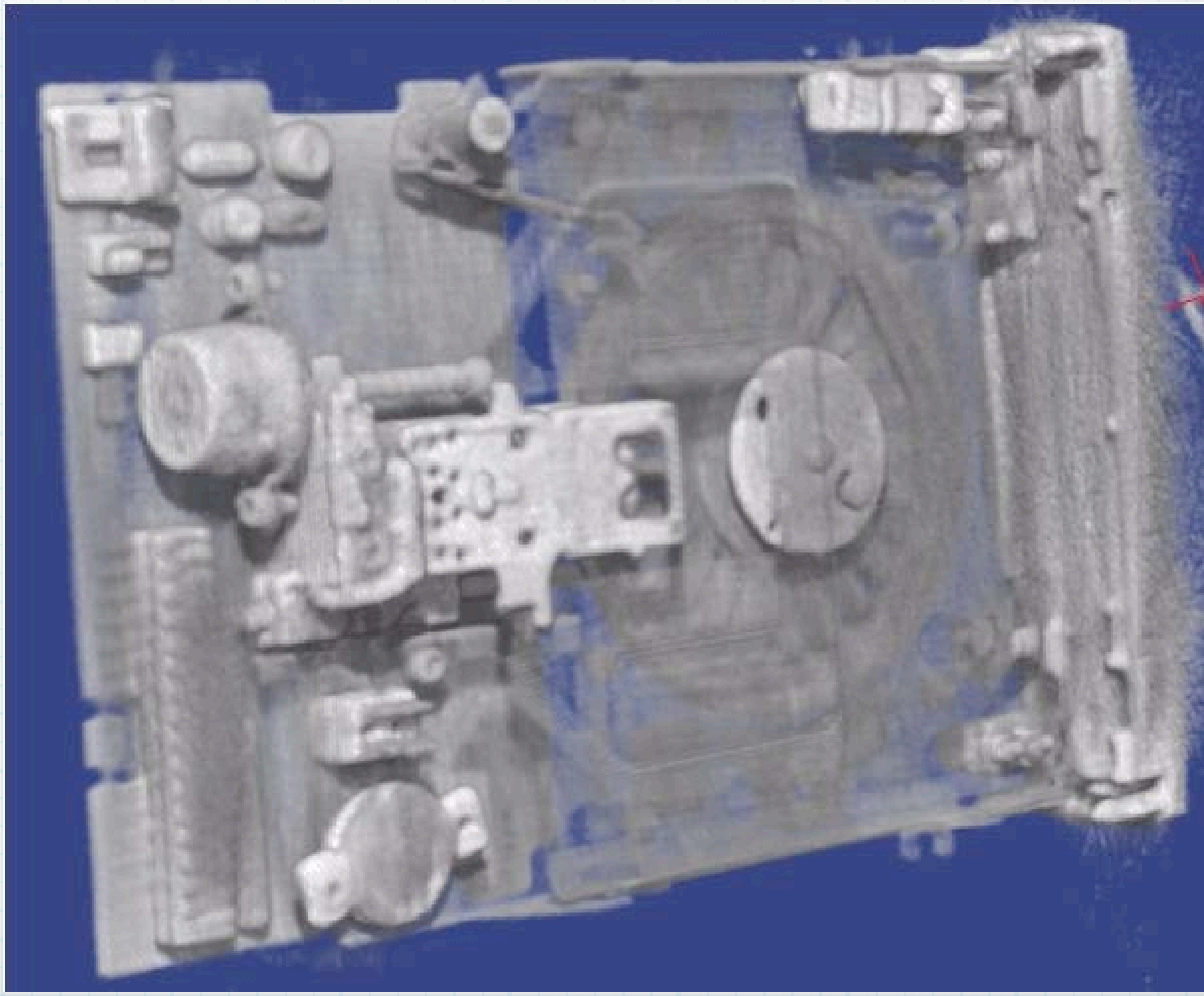
Schedule and list of participants are not yet available.

New mathematics and algorithms are needed for 3-D image acquisition and analysis. The 3-D images come from many disciplines: biomedicine, geology, chemistry, and microfabrication. The mathematics is wide-ranging and includes at least tomography and inverse problems, wavelets, PDE, and conformal mapping. The depth of the problem and the extent of the mathematics argues for multiple, long-duration collaborations that are fostered by a workshop series.

Neutron Tomography in Europe

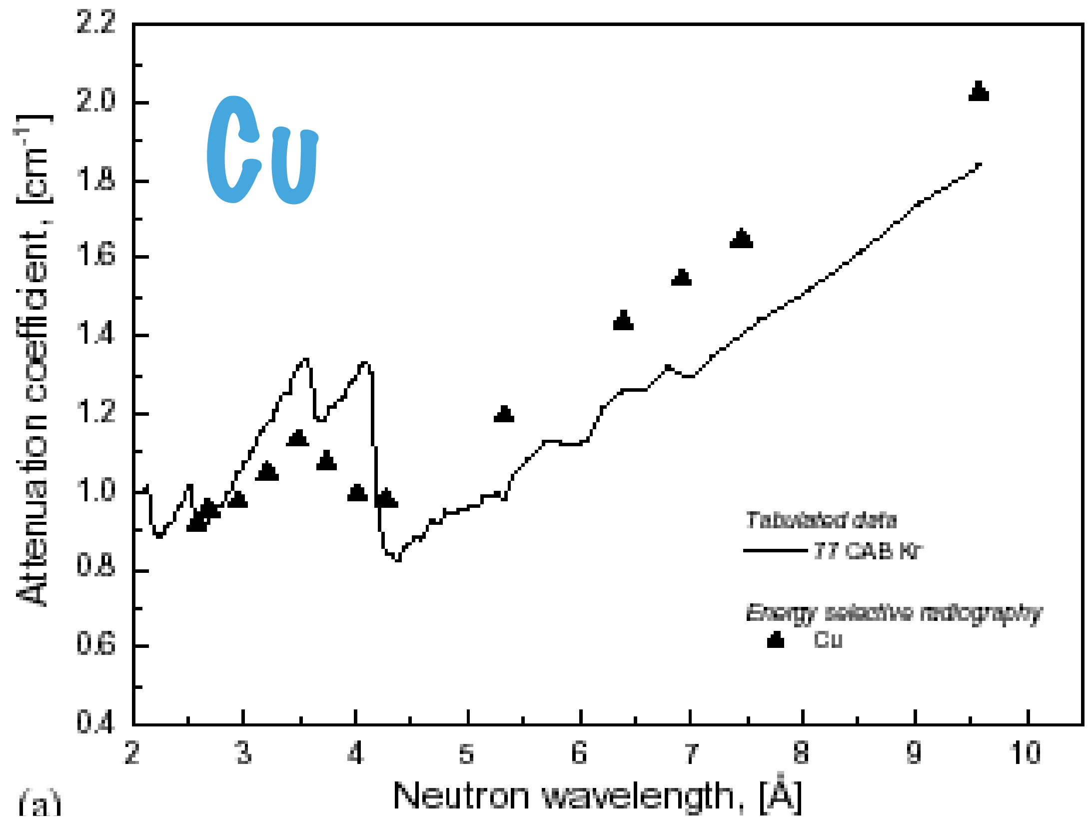
* Floppy disk drive imaged at NEUTRA beam line at Paul Scherrer Institute (ca. 1999)

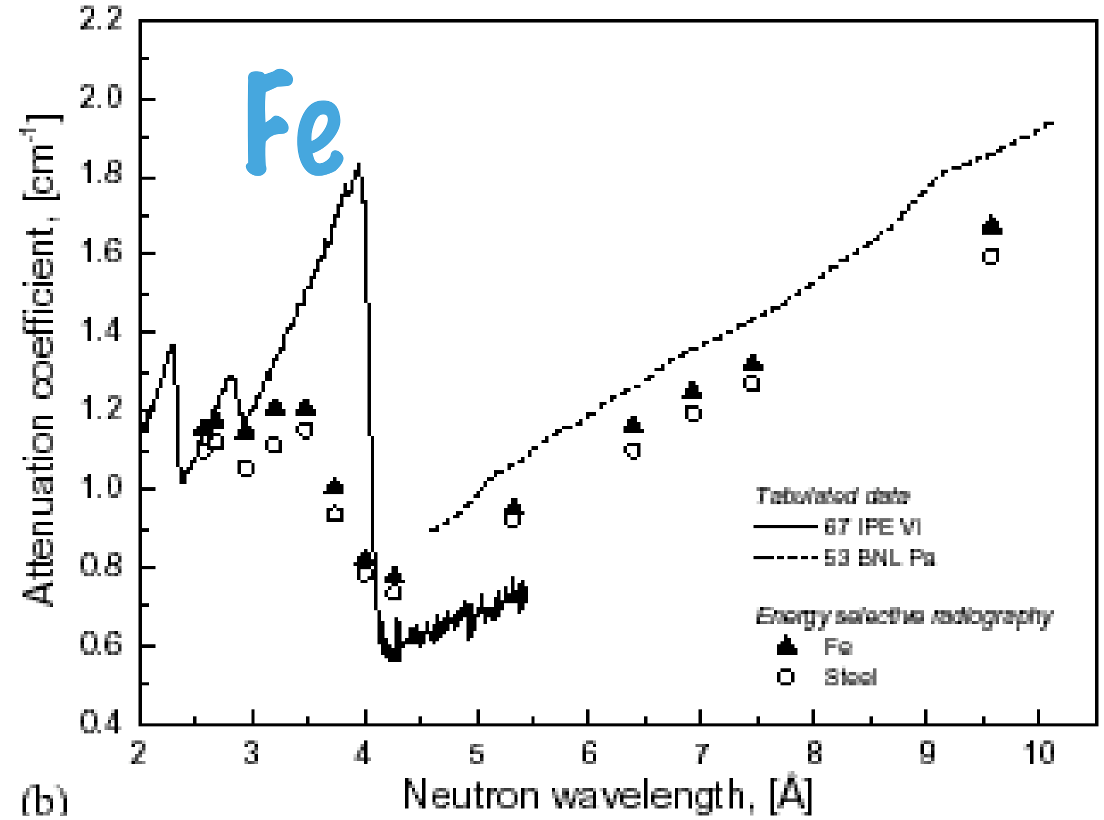
* thermal neutrons from a spallation source.
  Collimation (L/D) = 550.
  Flux = $3x10^6$ n cm^2/s.
  Exposure time 10 - 60 s for 500 µm to 50 µm resolution, 200 projections.
  CCD with 0.4 mm ZnS(Ag) + ^{6}LiF converter/scintillator.

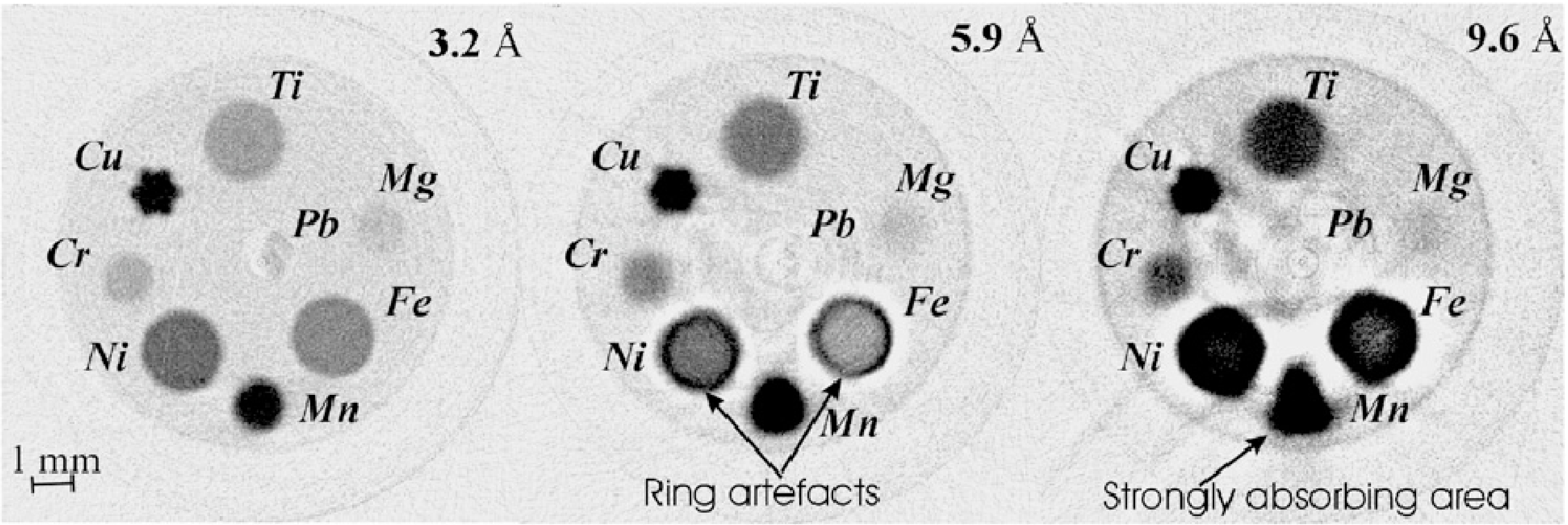


Lehmann, 2000

Cross-sections vs neutron wavelength

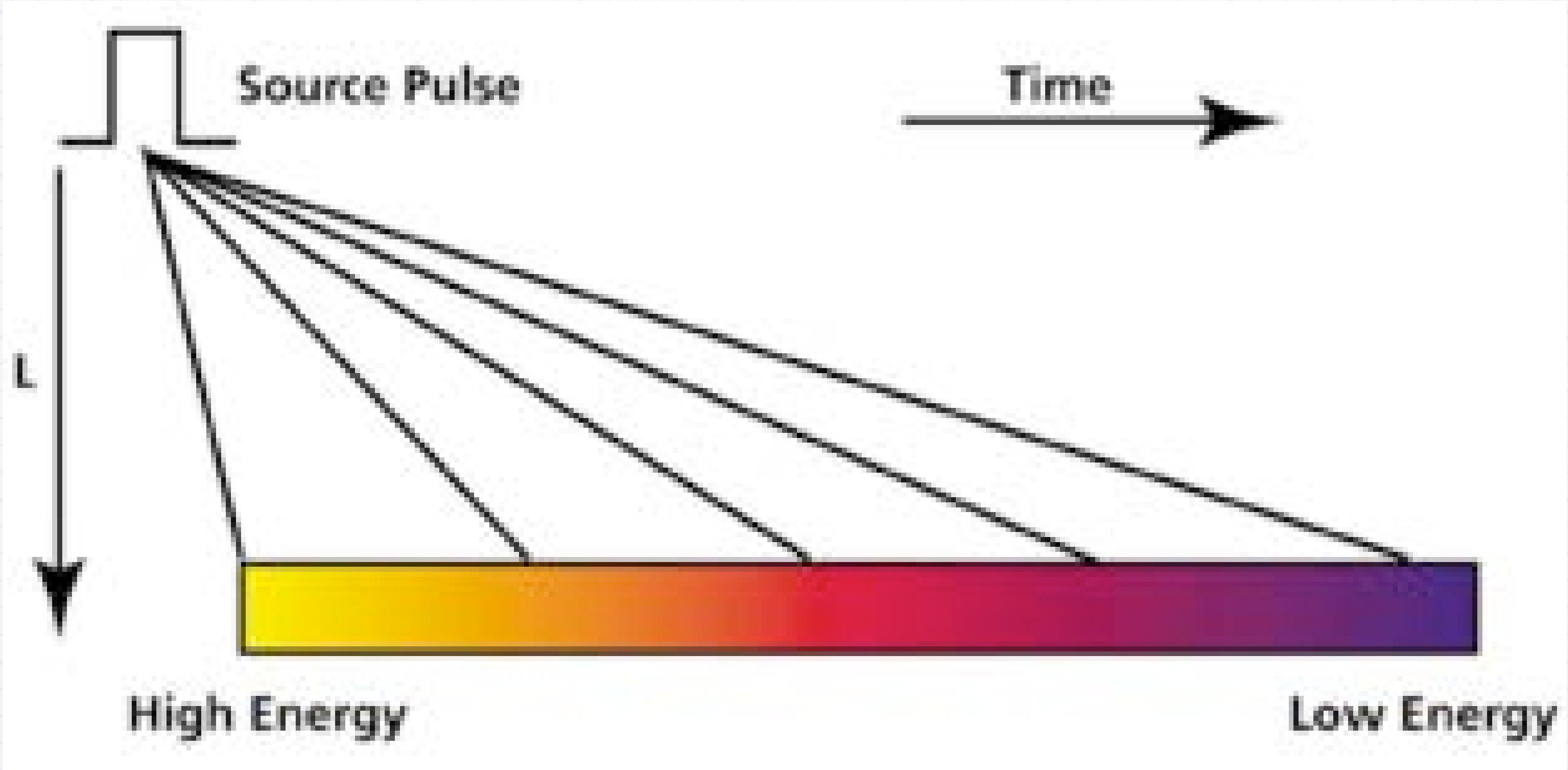




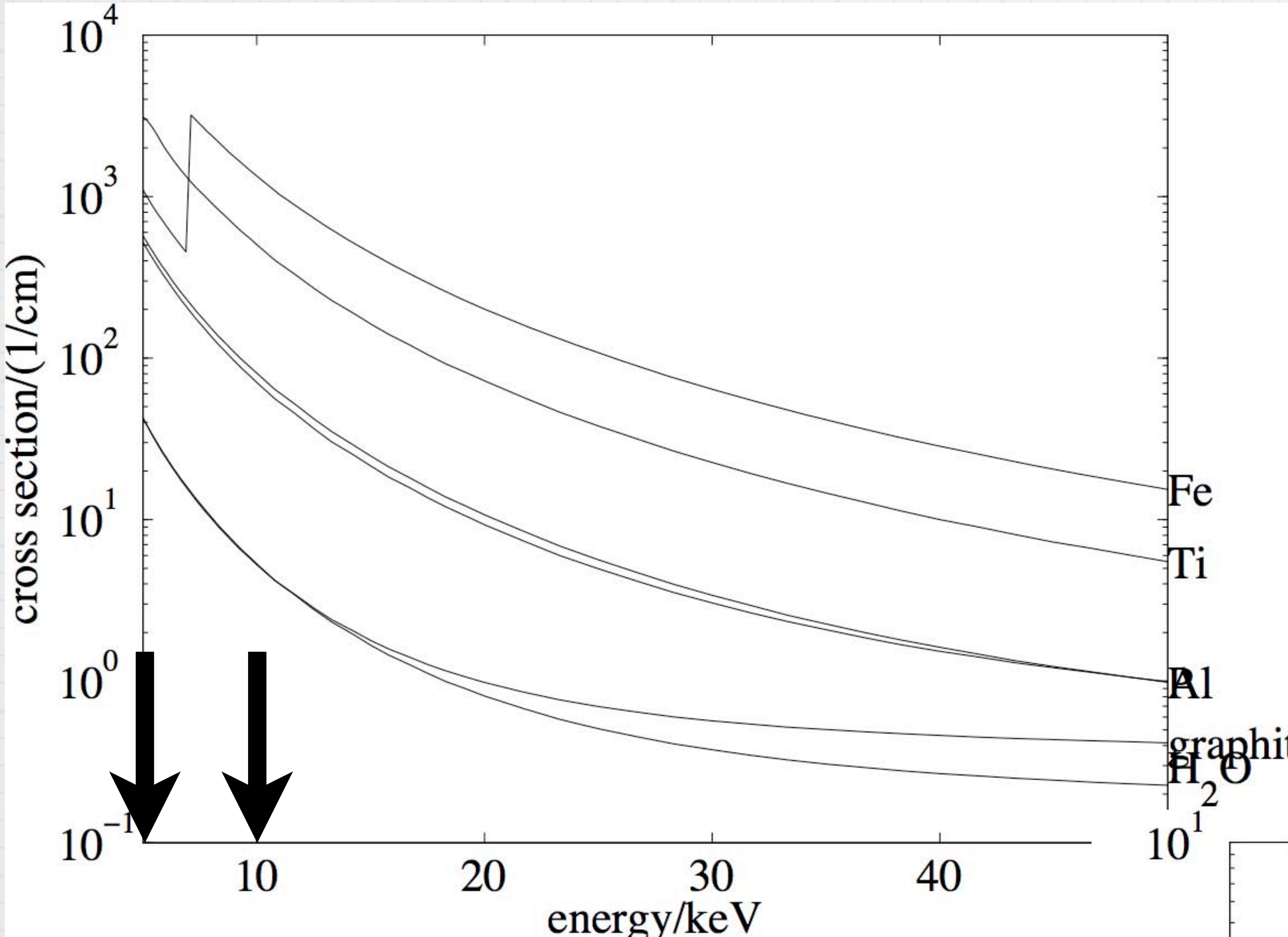


Kardjilov, 2003

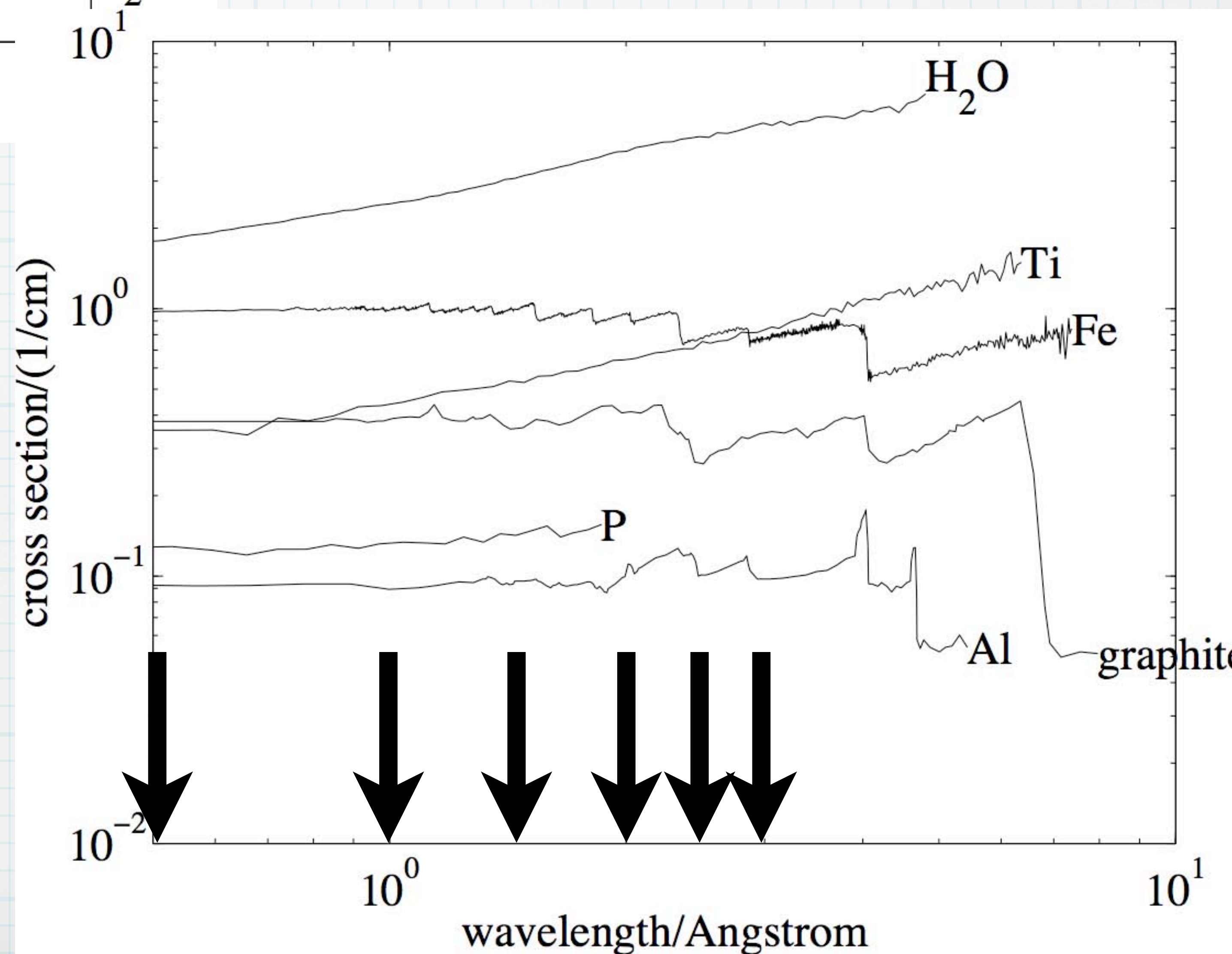
SNS: Energy selection at a pulsed source



* Protons beam: 1.4 MW: 1 GeV, 1.4 mA, 60 Hz rate
* Each pulse: 1.5×10^{14} protons in 695 ns
* Multiple images can be taken in the 16.7 ms after a pulse. Requires fast response scintillators and gated CCDs.

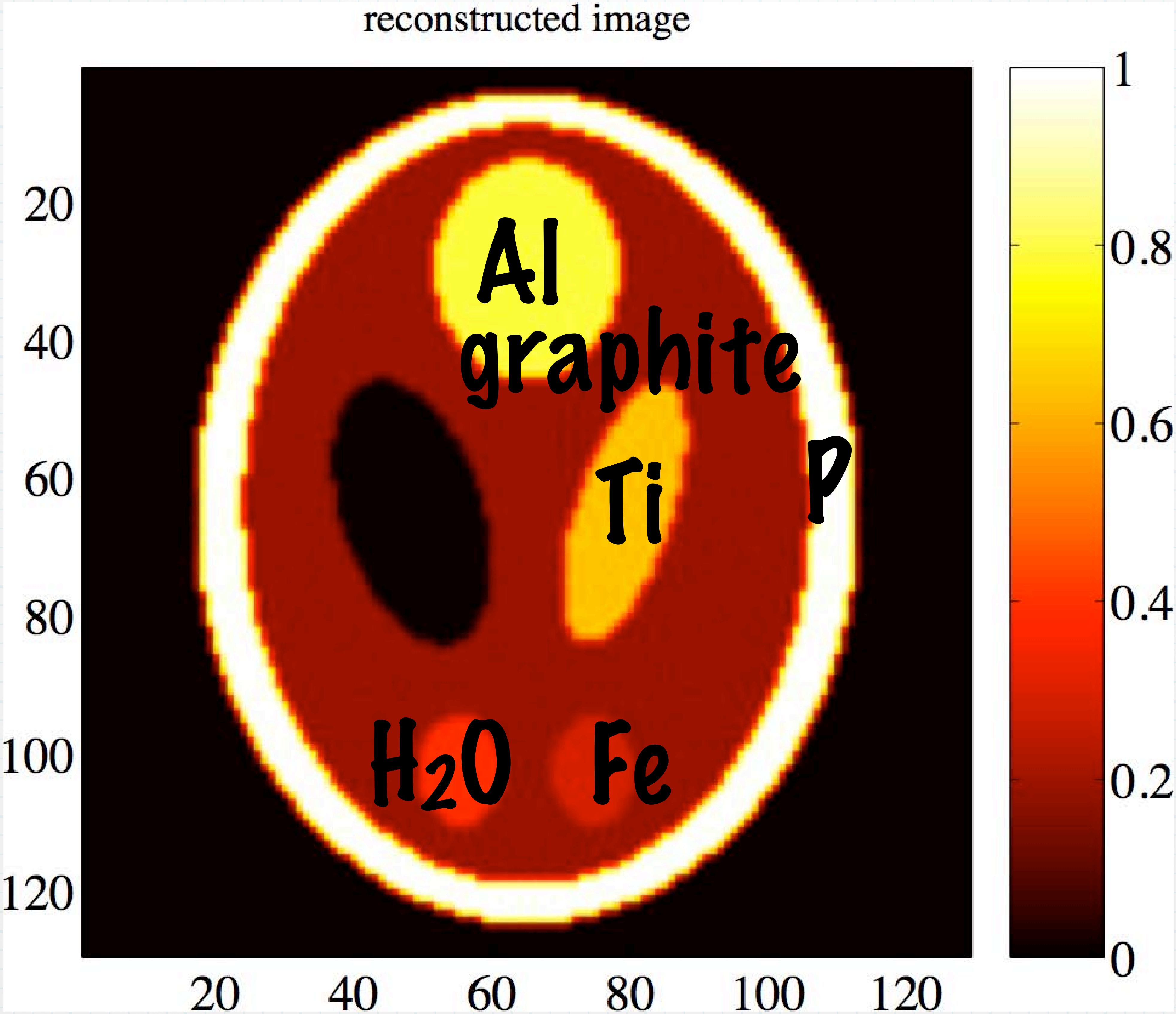


X-ray K-edges: predictable, yet simple structure

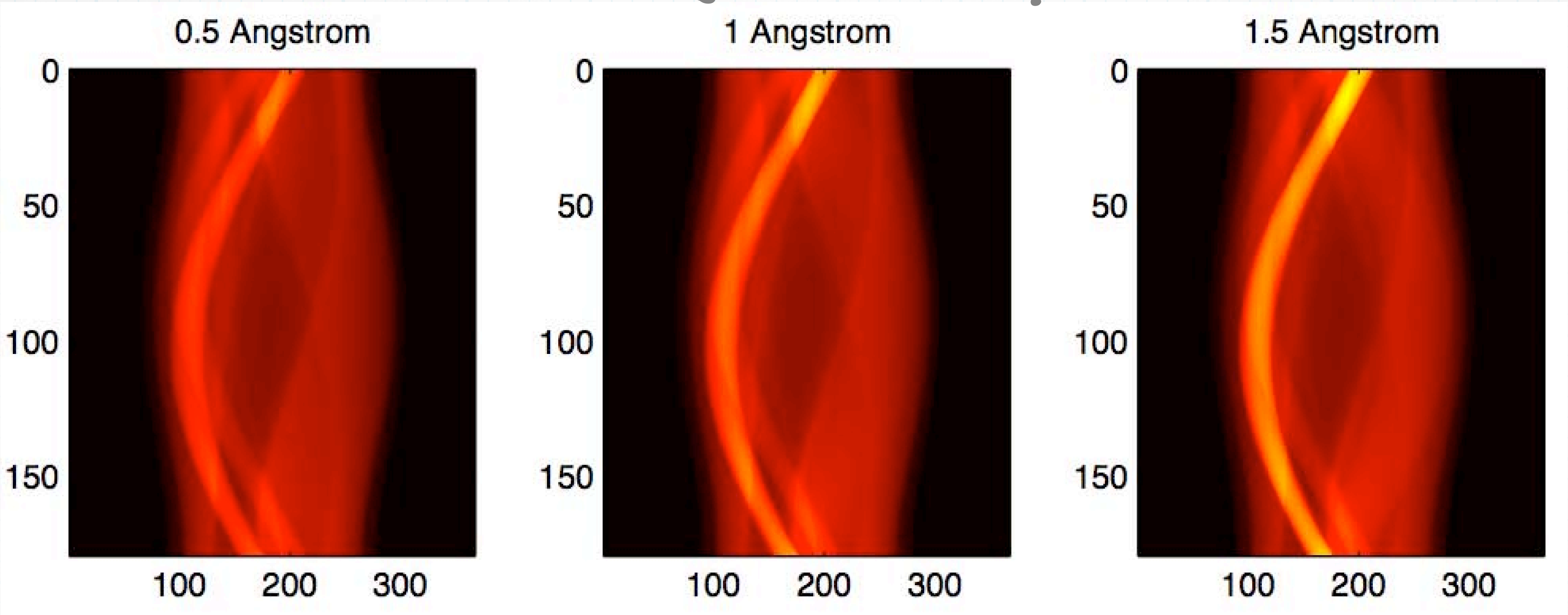


Neutron: richer structure

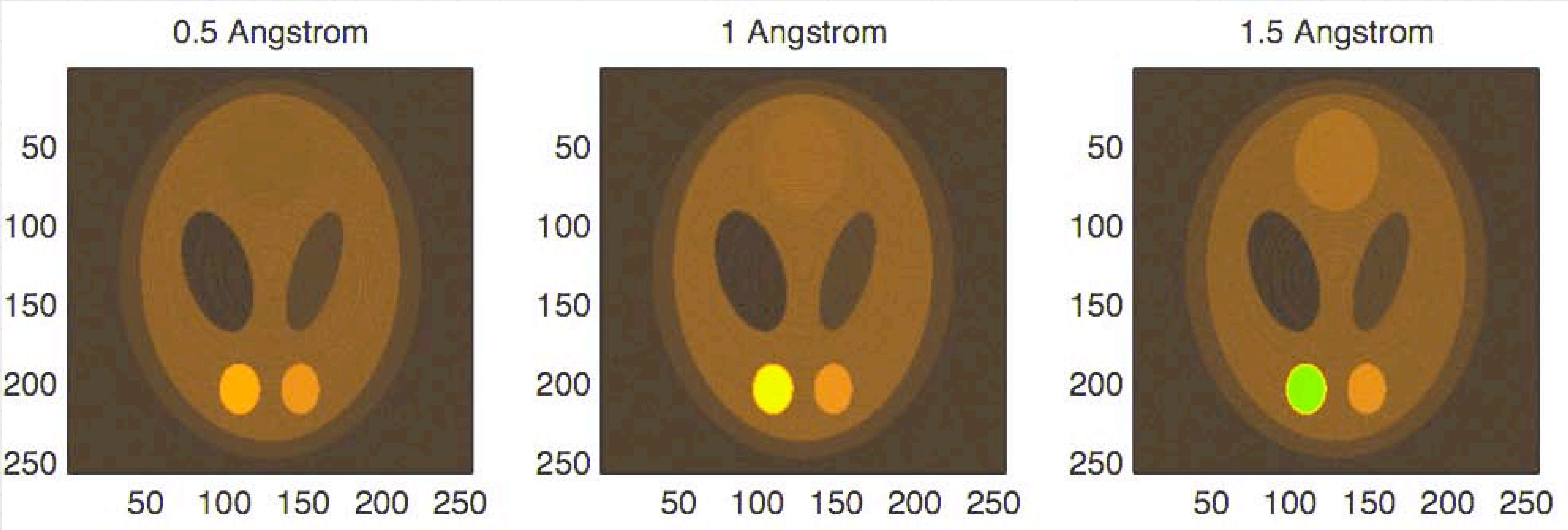
Simulation: Shepp-Logan phantom with materials



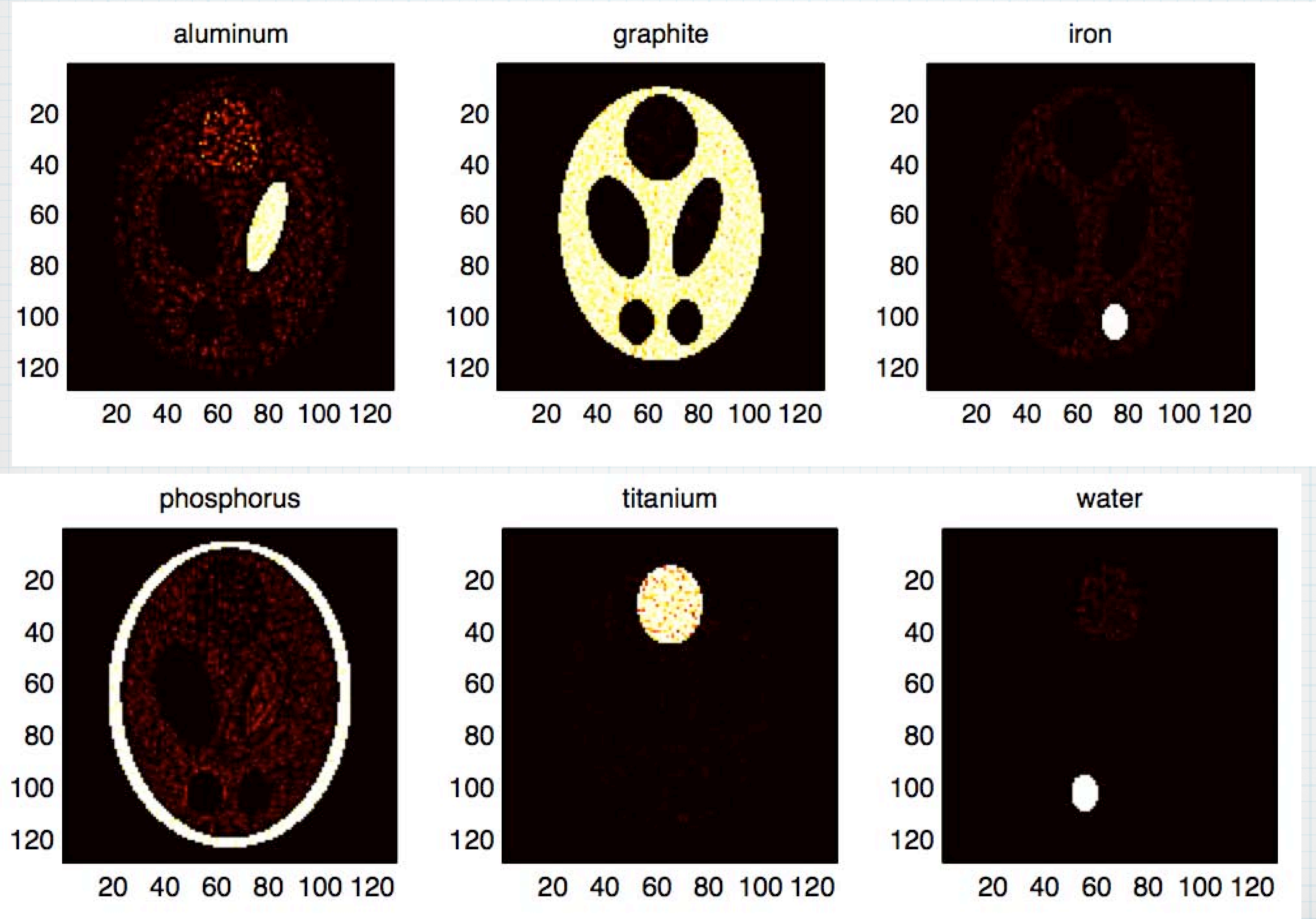
Neutron: sinograms from phantom



Neutron: reconstructed slices



Least-squares fits of composition from images acquired at 0.5 to 3 Å

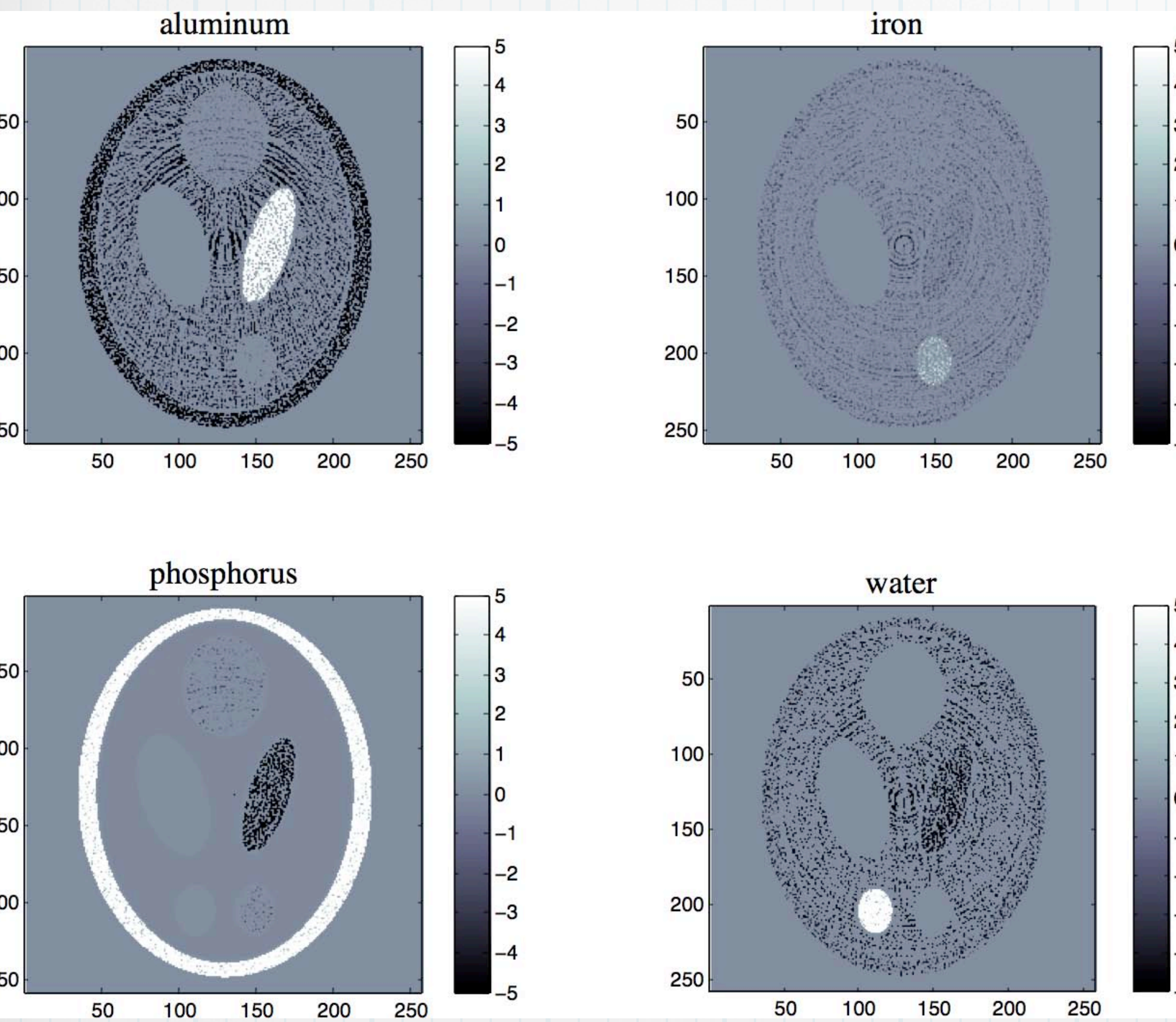


Residuals (%) from least squares fits (simulation)

X-ray

low residuals for Fe
high residuals for others

Al Fe



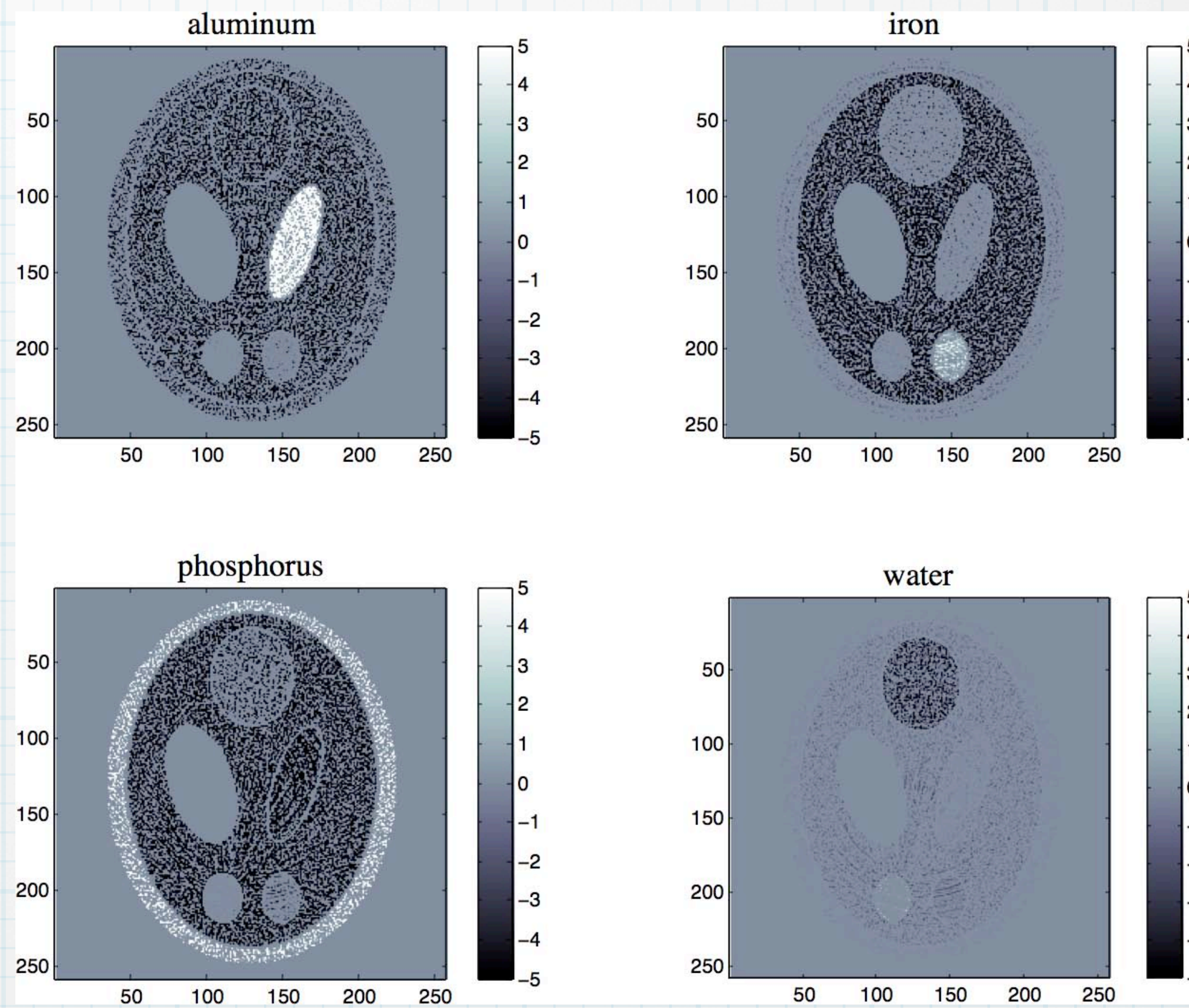
P H_2O

s.d. >20%

Neutron

low residuals for all elements

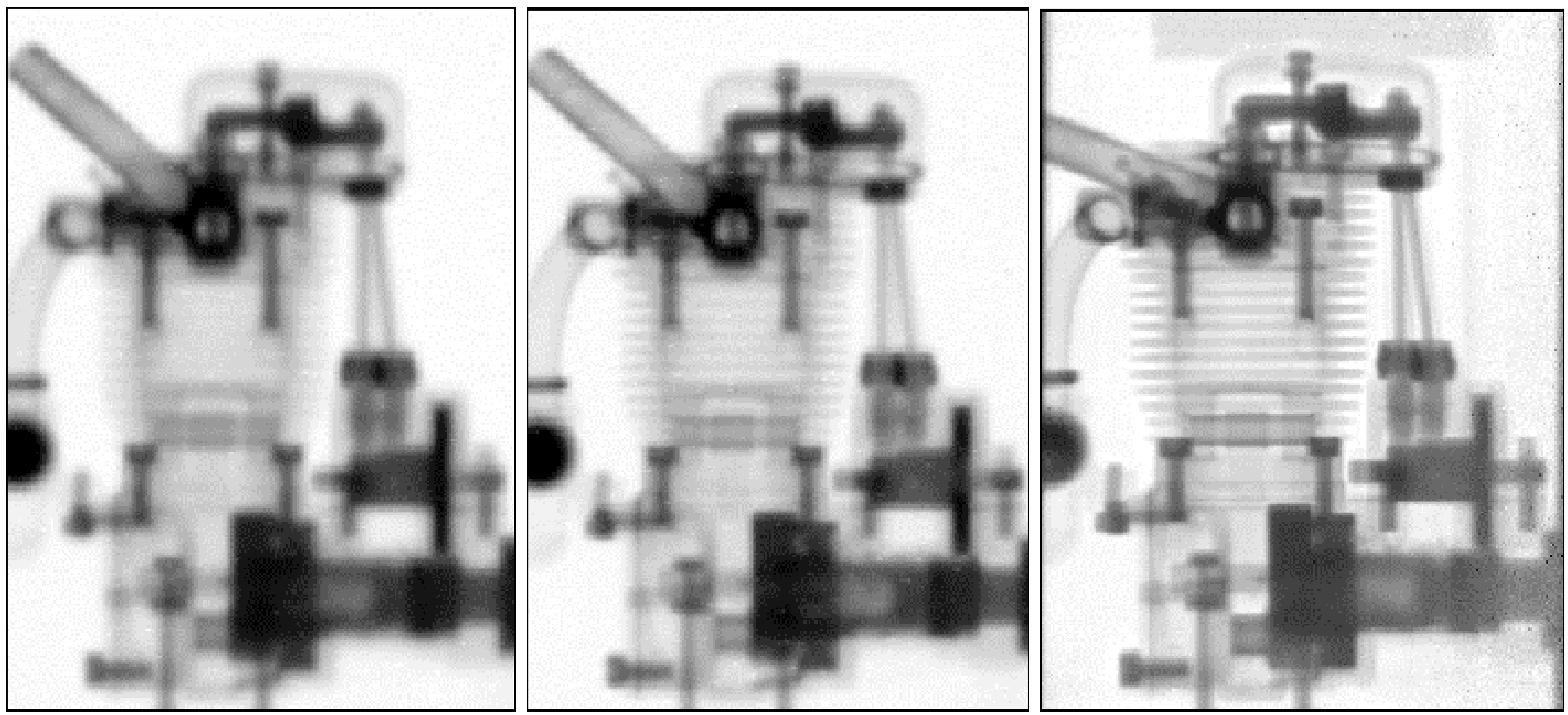
Al* Fe



P H_2O

*Al and Ti fits are moderately correlated.
Better fitting possible with images acquired at $\lambda > 3$ Å

Need high L/D



ŁD = 71 115 320

L = length of collimator

D = diameter of the aperture

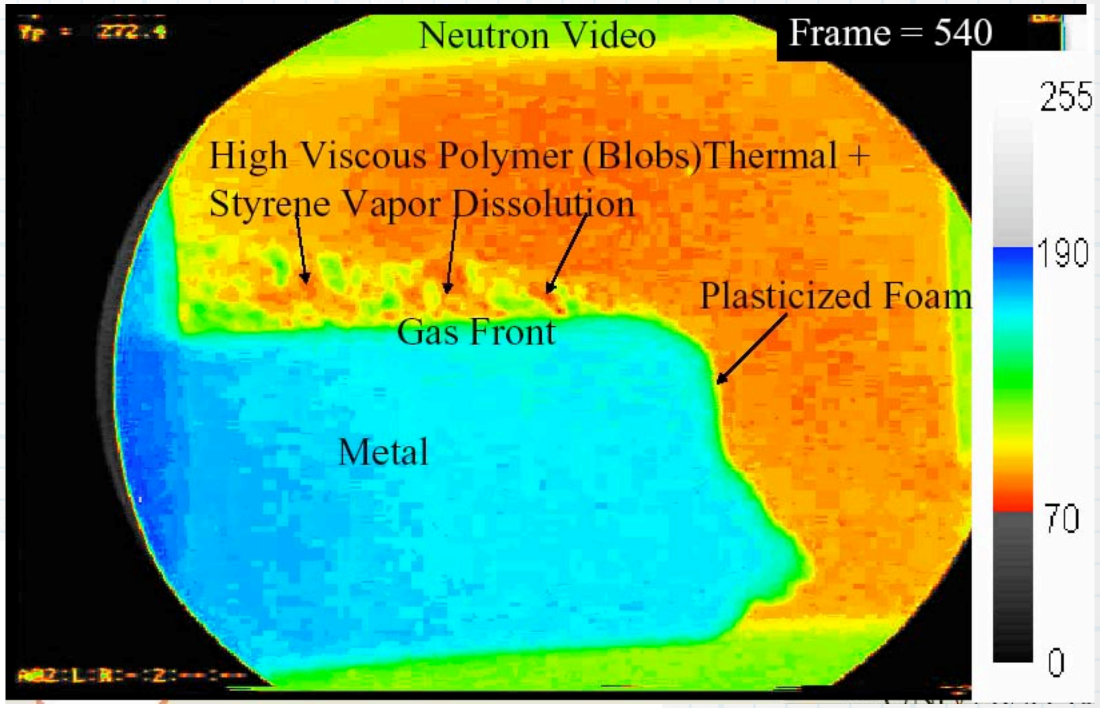
Lehmann, 2000

acquisition times not reported

Radiography: Prof. D. Penumadu, U. Tenn.

Movies of molten Al flow in lost foam casting show polystyrene melt and gas formation.

Imaging at MNRC; support from GM.



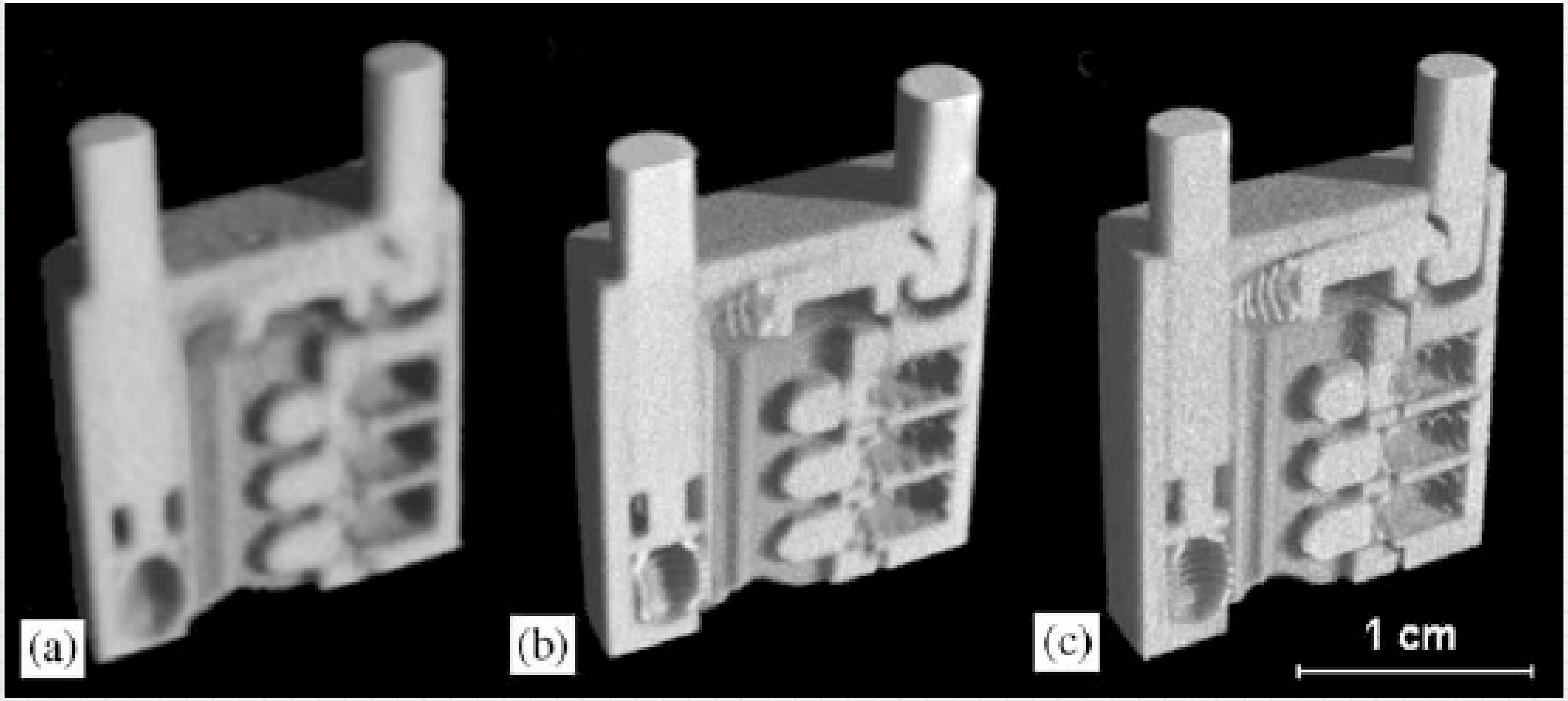
Engines Powered by Lost Foam Casting

GM's 2002 Chevrolet TrailBlazer
http://www.canadiandriver.com/articles/jk/02trailblazer.htm

GM's Vortec 4200 inline 6-cylinder engine
Source: http://www.canadiandriver.com/articles/jk/at_010424.htm

Need Monochromatic

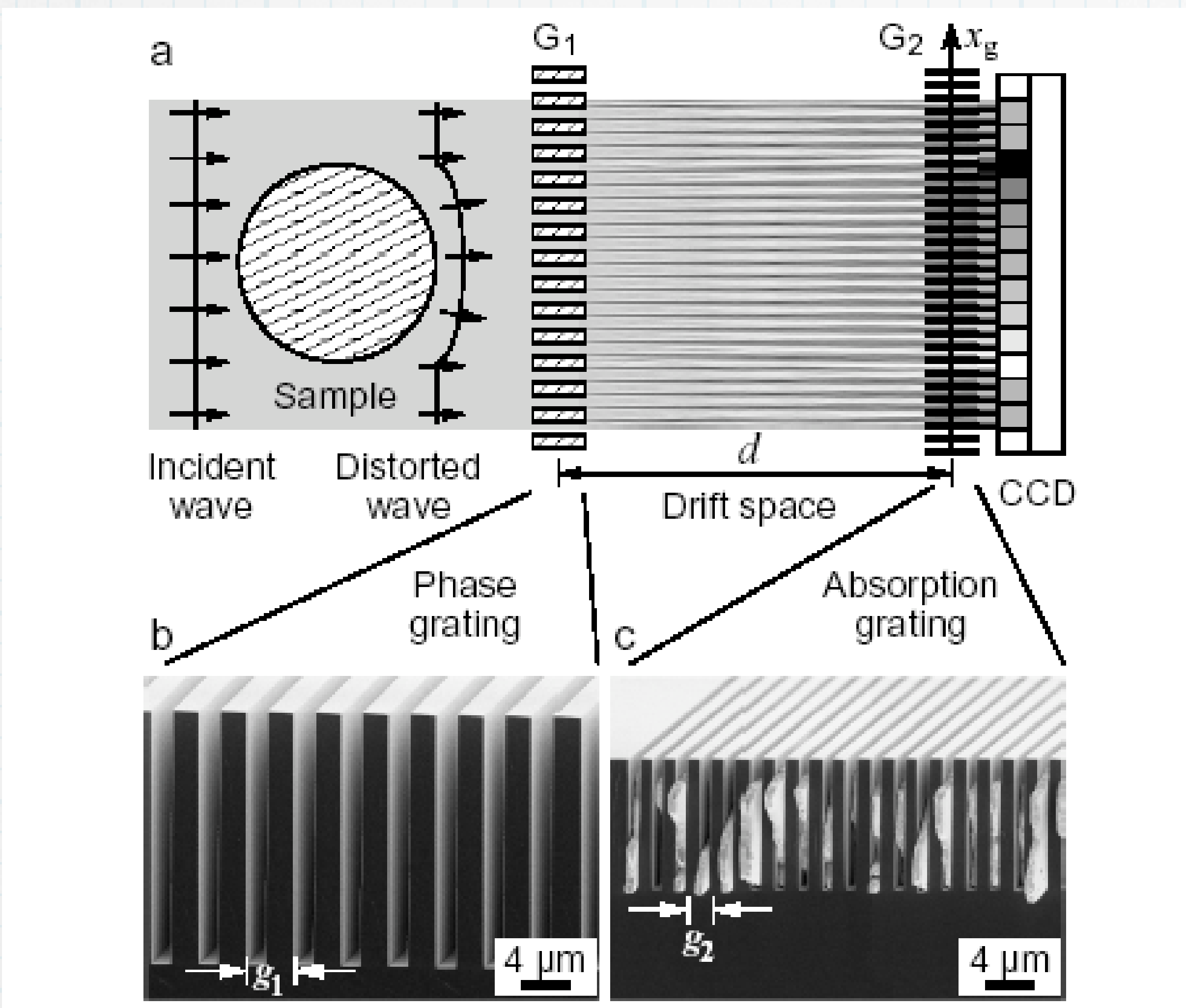
* PSI: white beam (cold neutrons) has higher flux, 2 s per projection, while 2.7 Å requires 80 s per projection
* small padlock; CCD/scintillator $^{6}LiF/ZnS(Ag)$
* (a) white beam with 0.42 mm thick scintillator
  (b) white beam with 0.10 mm thick scintillator
  (c) 2.7 Å with 0.10 mm thick scintillator

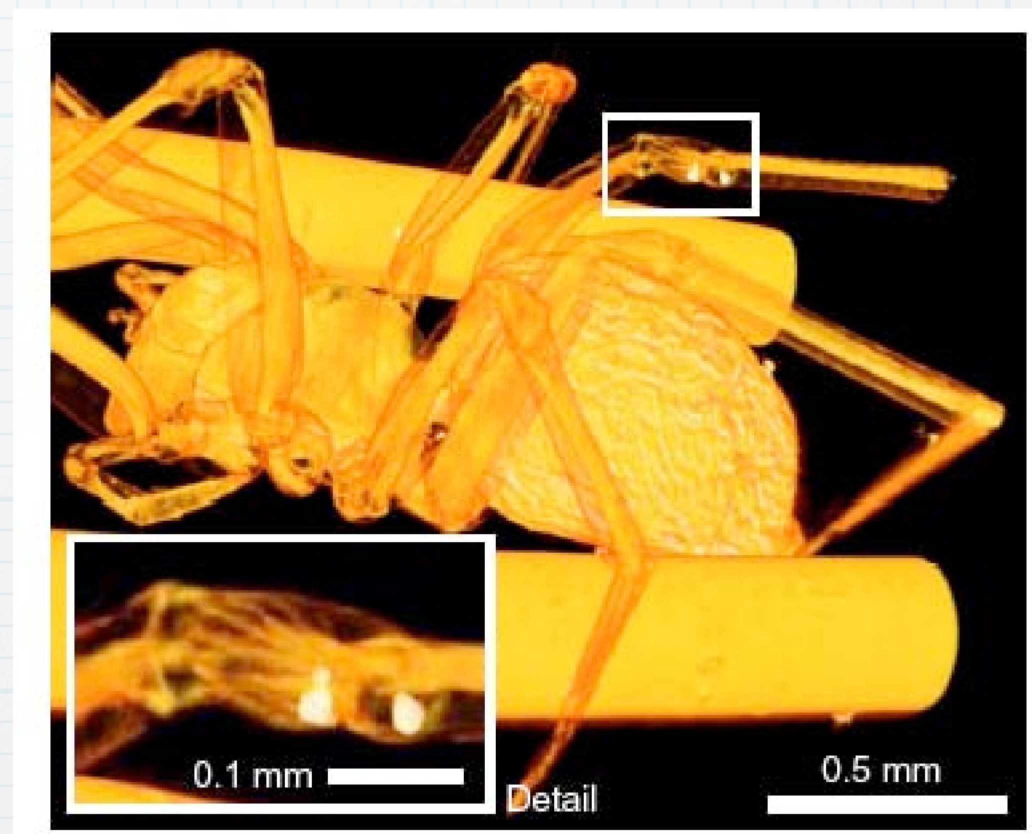


Baechler, et al., 2002

Need Optics ?

* Why optics?   Correct for low L/D
* Example: Grating interferometer used X-ray tomography to improve results of phase contrast imaging w/ poor source.





Weitkamp, 2005

Status

* Instrument capabilities not well defined.
  * Image resolution? Energy range? Time?
  * beamline length? L/D options?
  * Optics? Spin polarizer?
  * Sample sizes: 0.1 g to 100 kg?
* User base?
  * geology, biomedical (bone/metal @ 4 mm diameter), engineering, materials science, chemistry?

Scientific Objectives
"Complex Structure Imaging"

* Chemistry
  * Real-time imaging of blending and chemical reactions through reactor walls. Combine with after-the-fact high resolution imaging and standard spectroscopy.
  * Example: NIST fuel cell images
* Engineering
  * Real-time imaging of operational structures: motors
  * Flow and diffusion processes: lost foam casting
* Biomedial: biopsies
  * Lung: high ^1H contrast helps image alveoli. PM2.5
  * Metal-bone interface: problems with artificial joints

Scientific Objectives
"Complex Structure Imaging"

* Physics
  * Image magnetic field structures with spin polarized neutrons
  * High T_c structures, especially joints
* Nuclear power
  * Image vitrified waste inside storage casks
* Geology
  * Bio-geology: high ^1H contrast helps search for bacterial growth in rocks.
  * Petroleum: structure and flow of biphasic fluids for advanced oil recovery methods such as CO_2 flooding.