X-Ray Diffraction and Cargo Inspection

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Summary

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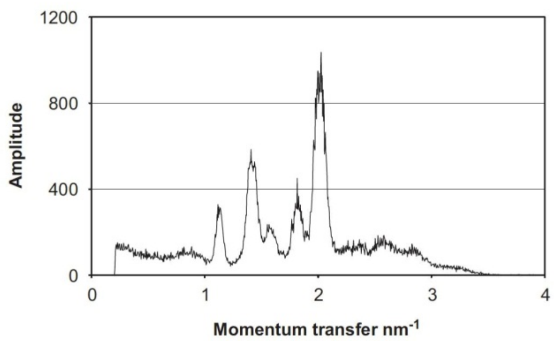
- Iterative reconstruction algorithms show promise for reconstruction of XDI images for checked luggage
  - Good localization and characterization of materials with well-defined Bragg peaks
  - Harder to get accurate reconstruction of liquids and other amorphous materials in the presence of stronger scatterers nearby
  - Need to test on broader classes of liquids, HMEs
- Architectures with photon-counting detectors offer improved reconstruction
  - Must tradeoff cost of detectors, array population vs signal strength
- XDI is less promising for cargo inspection
  - Lower energy requirement, larger dimensions lead to weak signals
  - Irregular shapes make sensing architecture design complex

Motivation

Background:

- Material identification based on conventional X-ray computed tomography (CT) images can be ambiguous
- X-ray diffraction imaging (XDI) systems identify materials based or coherent-scatter form factor – New signature that depends on molecular structure



Coherent-scatter form factor of TNT (Harding '09, Morpho)

XDI currently proposed for luggage inspection

- Existing XDI commercial product
- Much recent research: Brady's group (Duke), BU, others

Morpho XRD 3500 ™

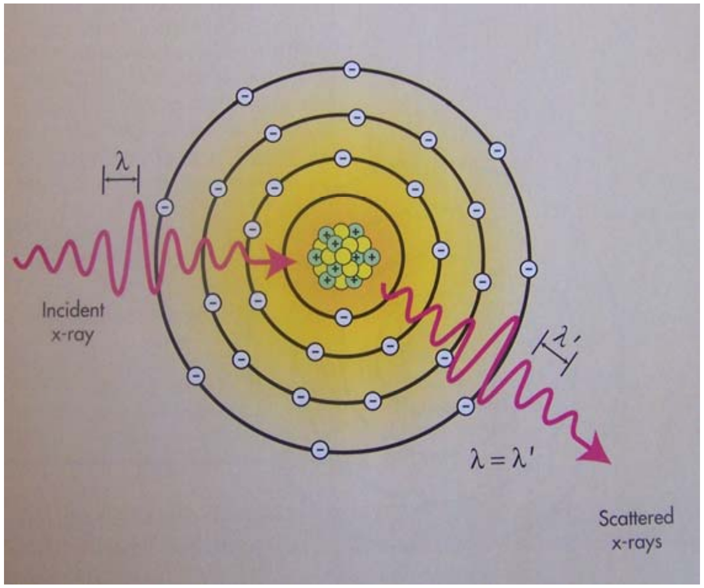
Crawford asks: Can these ideas be used in cargo?

- ?????

Focus of Talk: Discuss XDI, recent progress, and extrapolate on applicability to cargo inspection

Coherent Scattering

- Change in direction of incident photons interacting with the electron layers, but no change in energy (momentum transfer)
- Lower energy photons (15-60 KeV)
  - 12% of photons <30 keV
  - 5% of photons >70 keV
  - Forward scatter, small angles
- Also known as Thompson, or elastic, or Rayleigh Scattering
- Ignored as noise in usual X-ray imaging (transmission)

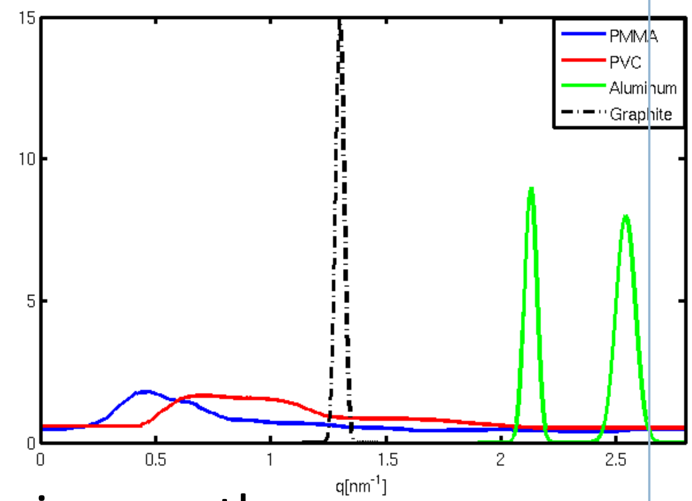


X-ray Diffraction Imaging

- Construct the *coherent-scatter form factor* $|F(q,\boldsymbol{x})|^2$ at all positions x in volume of interest: 4-dimensional function!
  - Expressed as distribution of transferred momentum q that causes the deviation of photon of wavelength λ by angle θ

$$q = \frac{1}{\lambda}\sin\left(\frac{\theta}{2}\right)$$

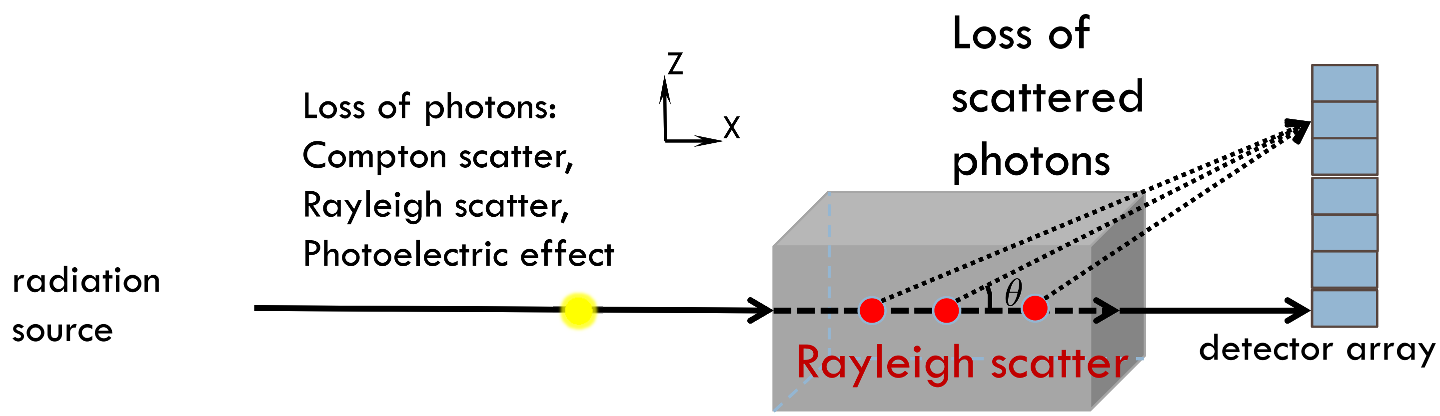
Form factors



  - For crystalline materials, Bragg peaks reveal molecular composition for material discrimination in terms of preferred scattering angles
  - For amorphous materials, or liquids, form factor is smoother

- **Measuring coherent form factor:**
  - Given photon energy wavelength ¸, measure angular deflection µ
  - Given angular deflection µ, measure wavelength ¸

X-ray Diffraction Principles



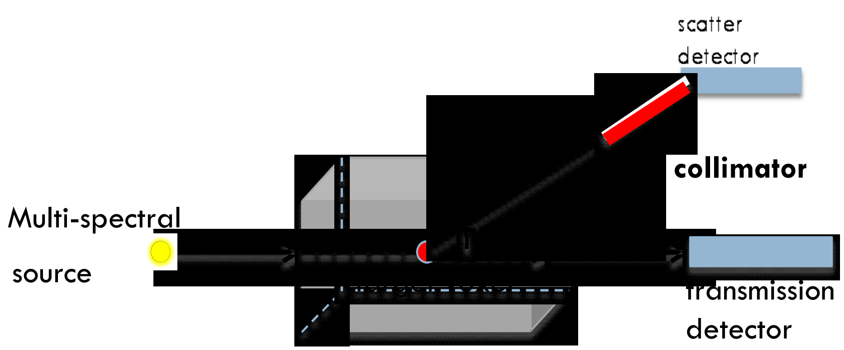
Observations:

- ❑ Fraction of photons that are scattered coherently is small – fraction decreases with increasing photon energy
- ❑ Fraction of photons that are lost to photoelectric effect also decreases with increasing photon energy
- ➔ Low energy Rayleigh scatter will be highly attenuated
- ➔ High energy Rayleigh scatter is less likely

➔ **Weak signals! Limit on effective energy band**

Typical X-ray Diffraction Architecture

- Localize excitation, localize detection
  - Similar to two-photon imaging and other similar localized imaging problems
  - Block secondary scatter whenever possible
  - Many scattered photons fail to reach detector
  - Requires photon-counting detectors



Schematic drawing of XDI system

X-Ray Diffraction: Tomographic Architectures for Stronger Signals

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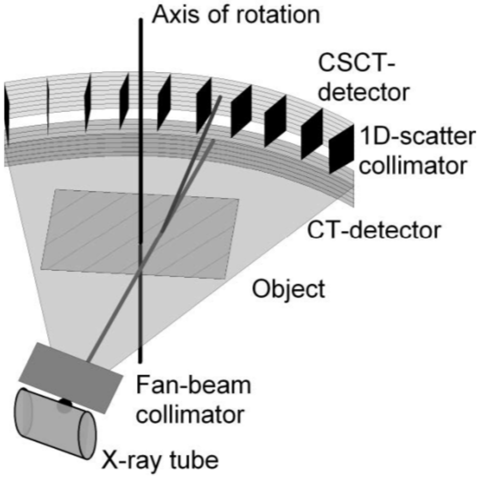
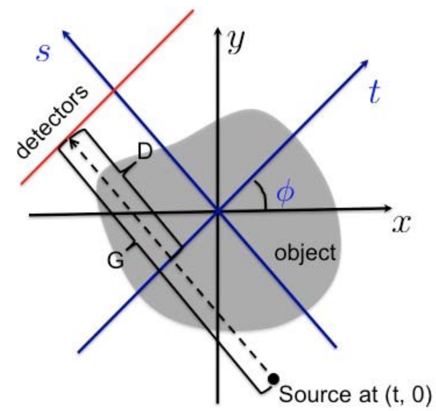
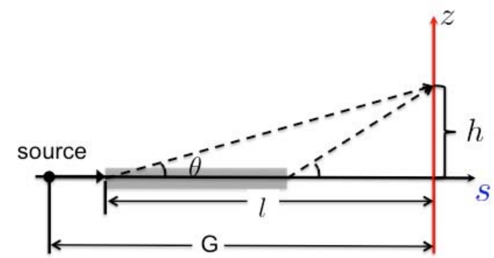
Limited-angle tomography: sheet collimators, vertical scatter mostly

- Rotating detectors and tomography algorithms- use either intensity or photon-counting detectors

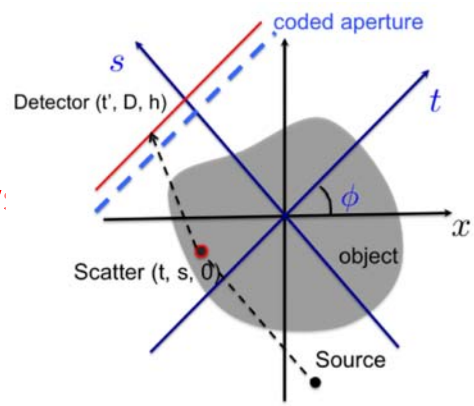


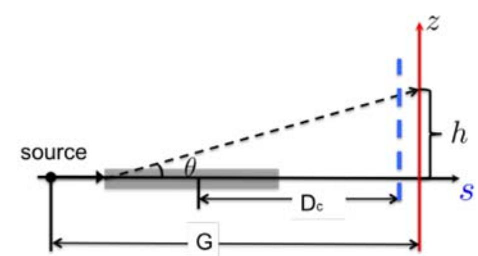




Coded aperture imaging: vertical and horizontal scatter

- Captures more photons, complex inver
problem
- non-rotating source/detectors, limited source locations
- either intensity or photon-counting detectors

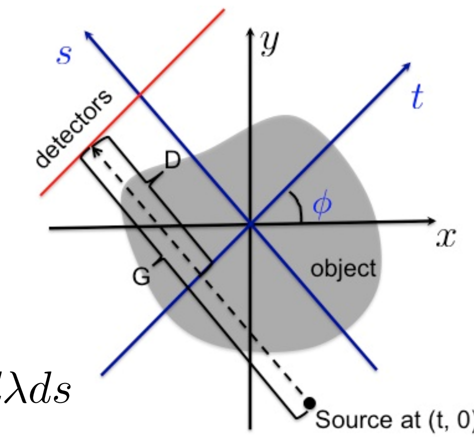




XDI Tomography Models

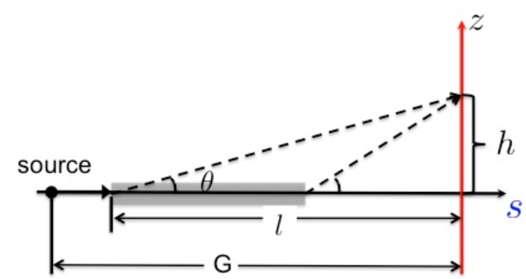
Model depends on architecture :

- Example below for intensity detectors, sheet collimators separating vertical lines of detectors



$$I_\phi(t,h) = \int_0^G \int_{\lambda_min}^{\lambda_max} I_\lambda(t,0)\mathcal{A}_\lambda(t,0,s,0)\mathcal{B}_\lambda(t,s,G,h)\frac{|F(t,s,q)|^2}{[(G-s)^2+h^2]^{3/2}}d\lambda ds$$

$$q = \frac{\sin(0.5\tan^{-1}(\frac{h}{G-s}))}{\lambda} \approx \frac{h}{2\lambda(G-s)}$$



$I_\lambda(t,0)$: incident x-ray intensity at λ;

$\mathcal{A}_\lambda(t,0,s,0)$:attenuation for λ along incoming ray from 0 to s;

$\mathcal{B}_\lambda(s,0,G,h)$:attenuation along the scattered ray from $(s,0)$ to (G,h).

$|F(t,s,q)|^2$:coherent-scatter form factor at location (t,s)

- For photon counting detectors, model changes:

$$I_\phi(t,h,\lambda_0) = \int_0^G \int_{\lambda_0}^{\lambda_0+\Delta} I_\lambda(t,0)\mathcal{A}_\lambda(t,0,s,0)\mathcal{B}_\lambda(t,s,G,h)\frac{|F(t,s,q)|^2}{[(G-s)^2+h^2]^{3/2}}d\lambda ds$$

Reconstruction Algorithms for Tomographic Architectures

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- Iterative reconstruction important
  - Limited view angles in coded aperture imaging
  - Minimize streaking artifacts (worse in form factors than intensity only!)

- Algorithm (IREP):
  - Iterative reconstruction, slice by slice (each slice is 3-D)
  - Look for spatial coherence in form factor reconstructions among
  - Simultaneous segmentation/image formation avoiding smoothing across edges (Ambrosio-Tortorelli)

$$\min_{(\mathbf{x},\mathbf{s})} ||\mathbf{y} - C\mathbf{x}||^2_{W(\mathbf{y})} + \alpha_1^2 \sum_{m=1}^{M} ||\mathbf{D}\mathbf{x}_\mathbf{m}||^\mathbf{2}_{\mathbf{W}_\mathbf{s}} + \varphi_S(\mathbf{s},\gamma)$$

$$W_s = \mathrm{Diag}\left[(1 - [\mathbf{s}]_i)^2\right], \quad \varphi_S(\mathbf{s},\gamma) = \gamma^2 ||\mathcal{D}\mathbf{s}||^2 + \frac{1}{\gamma^2}||\mathbf{s}||^2$$

  - Solve using biquadratic iterative optimization
  - Other algorithms investigated (overcomplete basis representations, …) with similar results.

Beam hardening and attenuation correction

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- **Multi-energy attenuation reconstruction needed**?

$$I_\phi(t,h,\lambda_0) = \int_0^G \int_{\lambda_0}^{\lambda_0+\Delta} I_\lambda(t,0)\mathcal{A}_\lambda(t,0,s,0)\mathcal{B}_\lambda(t,s,G,h)\frac{|F(t,s,q)|^2}{[(G-s)^2+h^2]^{3/2}}d\lambda ds$$

  - Frequency-dependent absorption on incoming path and scattered path
- If measure scatter at small angles and: assume attenuation along transmission path is same as attenuation along scatter path and: photon-counting detectors …
  - Normalize scatter signal by transmitted signal

$$J_\phi(t,h,\lambda_0) = \frac{I_\phi(t,h,\lambda_0)}{I_\phi(t,0,\lambda_0)} \approx \int_0^G \int_{\lambda_0}^{\lambda_0+\Delta} \frac{|F(t,s,q)|^2}{[(G-s)^2+h^2]^{3/2}}d\lambda ds$$

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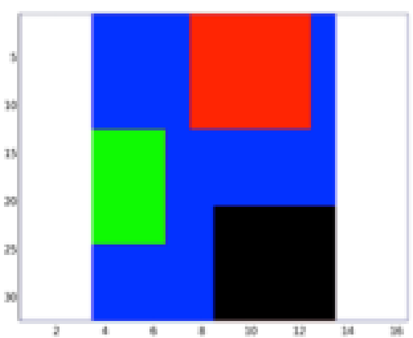
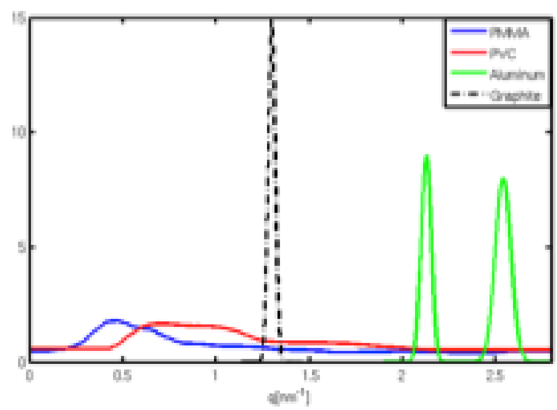
Does this work?

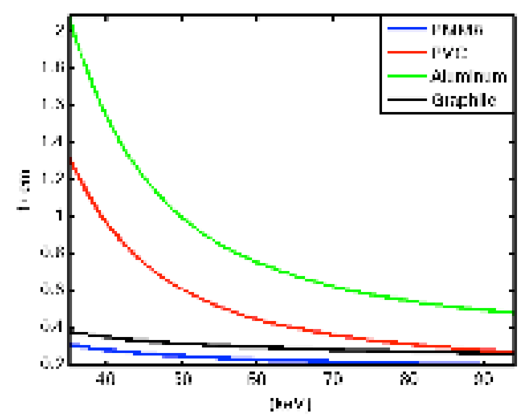
- Compare reconstructions using ratio approximation vs reconstructions using accurate attenuation models
  - Object of size 8*4cm, composed of 4 elements (PMMA, PVC, Aluminum, Graphite)
  - Phantom: tall rectangular solid, 40 cm tall
  - Focus on clutter, interference, attenuation
    - Different attenuation of scatter



Plan view of object in Illumination plane



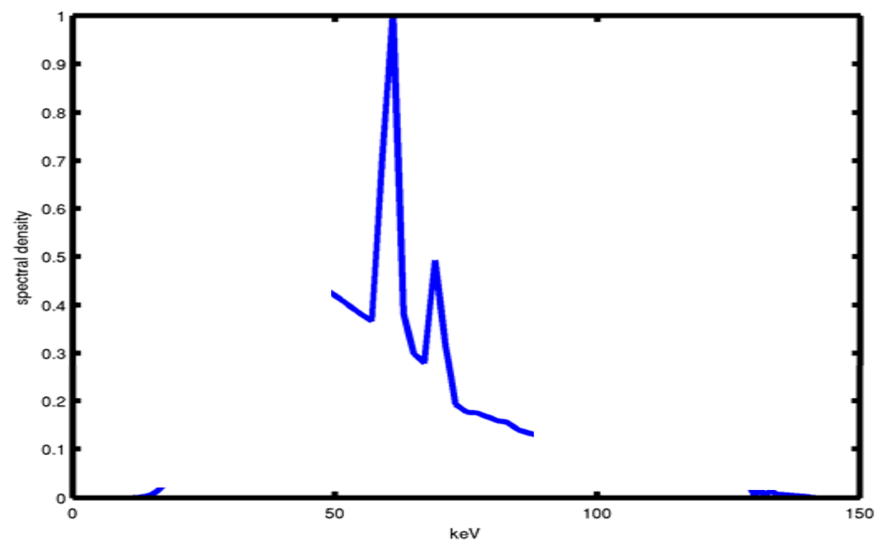
Form factors for elements



Linear attenuation coefficients for elements

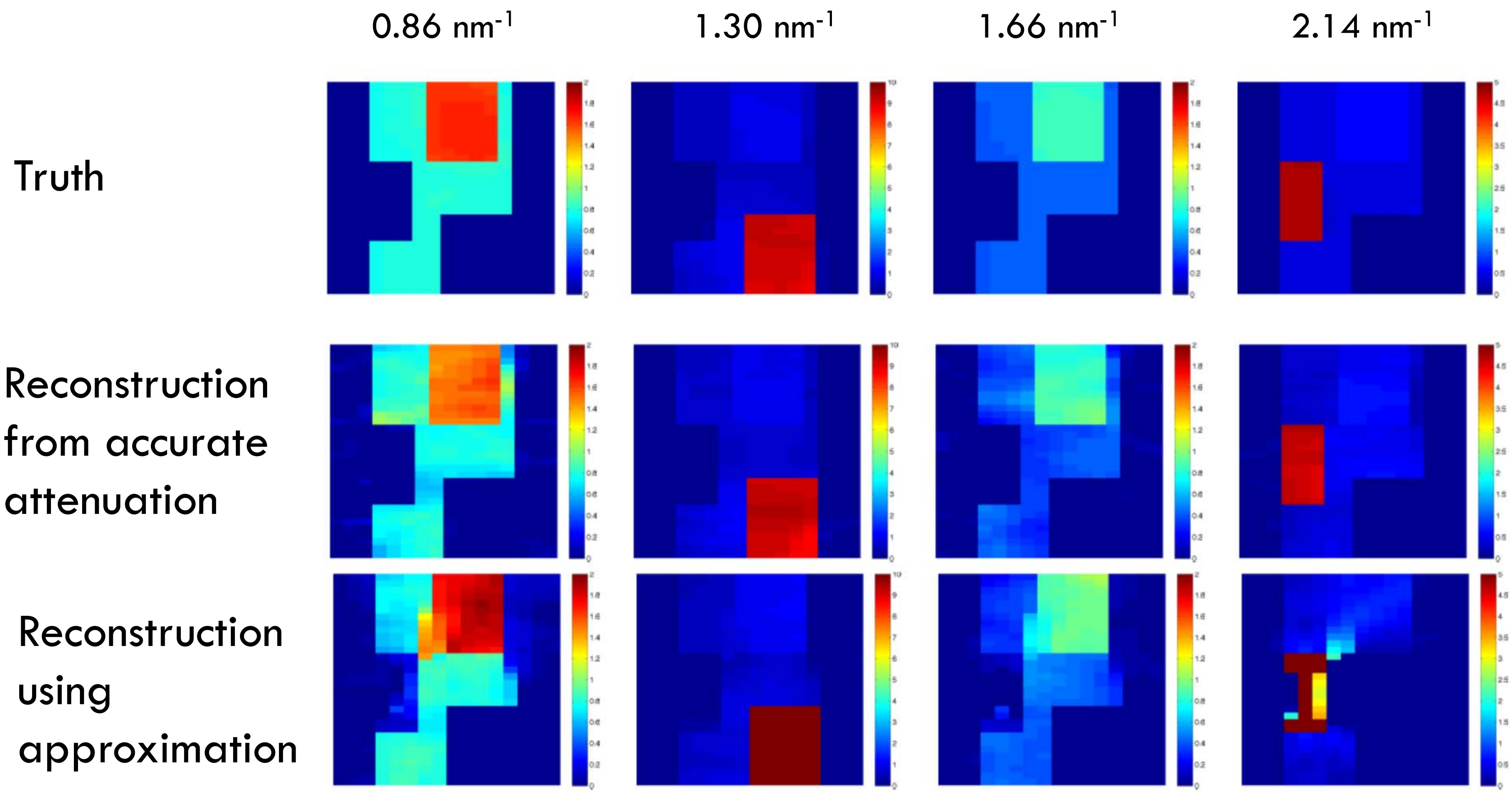
Illumination Variations

- Polychromatic source from 50 keV to 80 keV with basic spectra
- Simulated Monte Carlo photon sources:
  - GEANT 4 with modified Rayleigh scatter, Compton & Photoelectric
  - Analytical model with Poisson noise
  - Sampled spectrum, 30 energy bins



Beam Hardening Correction with Circular Architecture, Column Detectors

- 4 KeV resolution photon counting detectors, 12 views



Works ok…

Beam Hardening Compensation is is Harder with Intensity Detectors

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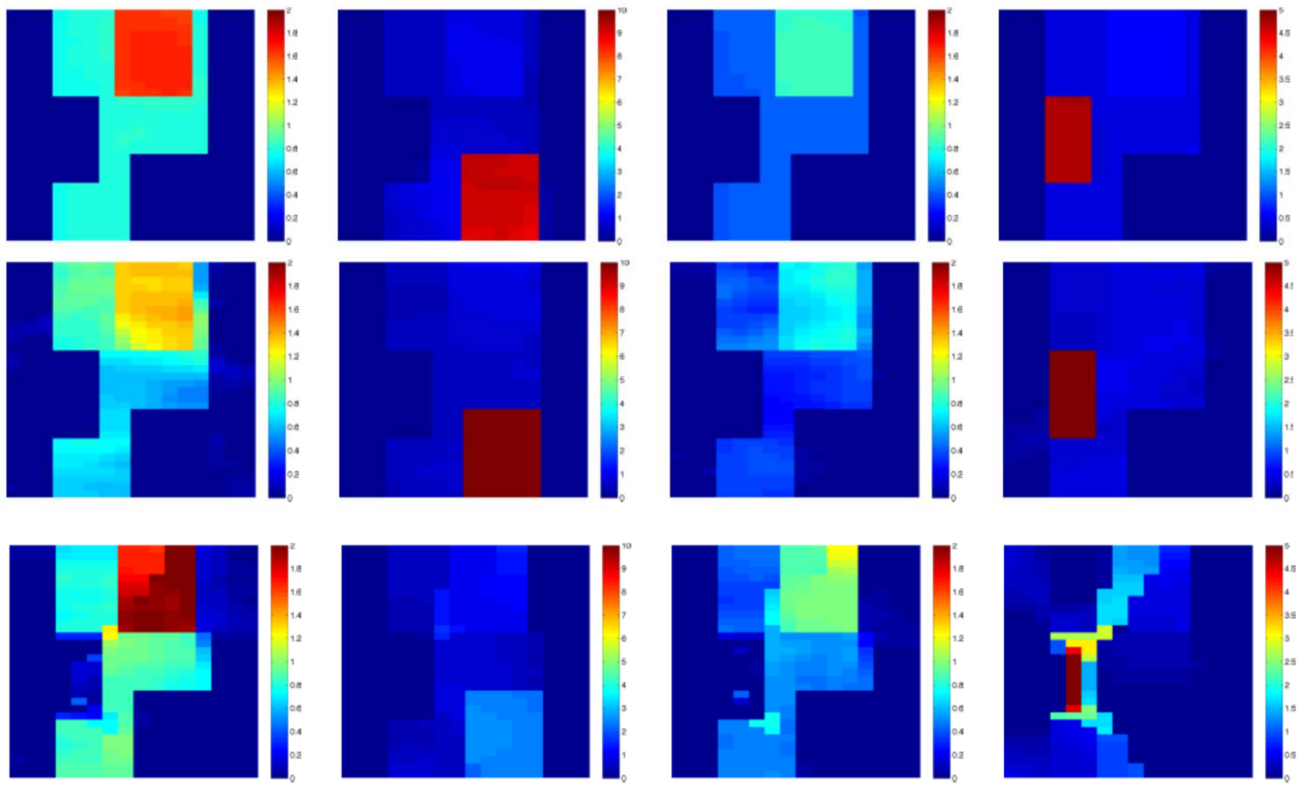
- Intensity detectors, 12 views

0.86 nm^{-1} | 1.30 nm^{-1} | 1.66 nm^{-1} | 2.14 nm^{-1}

Truth

Reconstruction from accurate attenuation

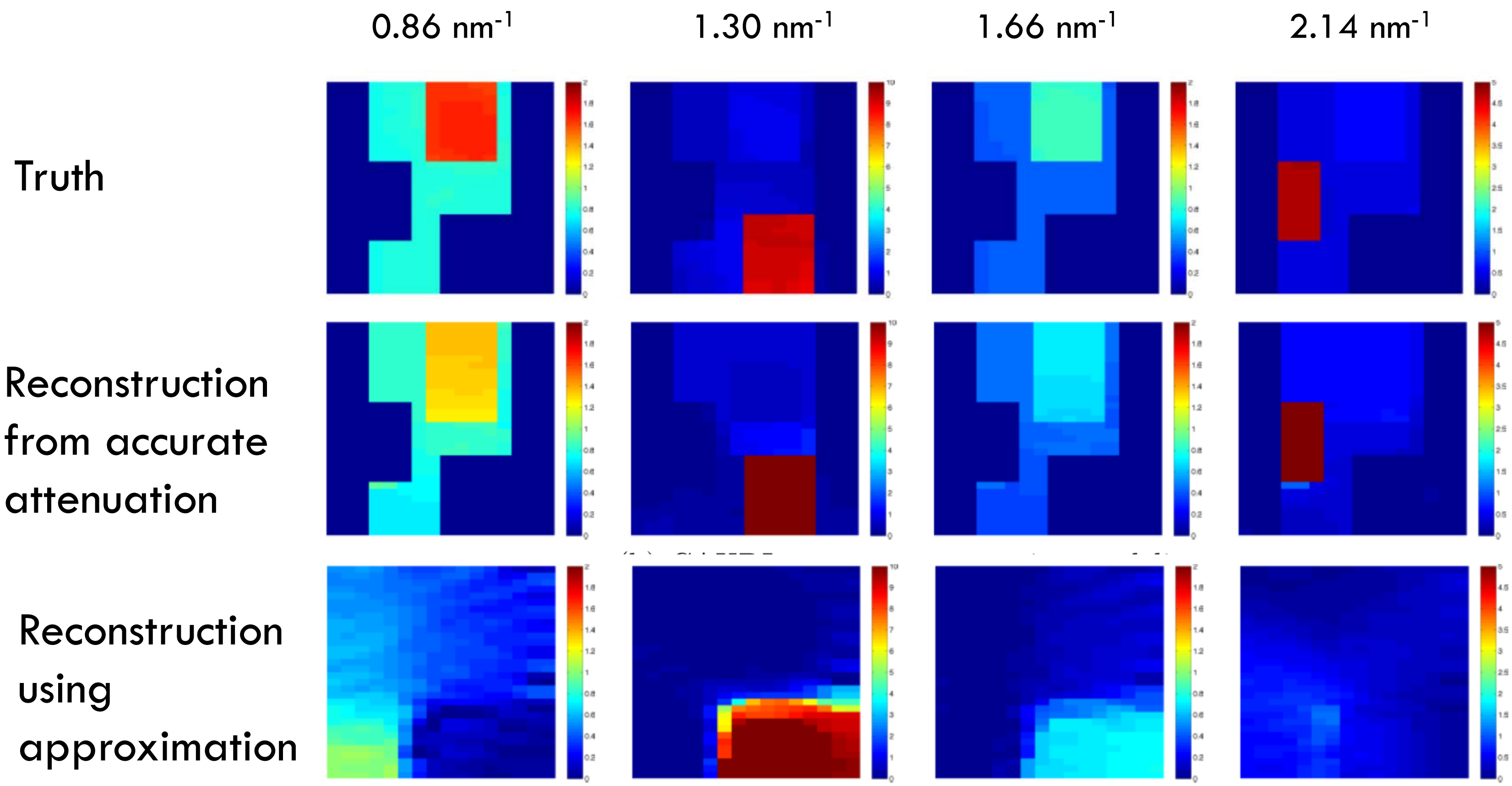
Reconstruction using approximation



Lose structure, size even in aluminum block

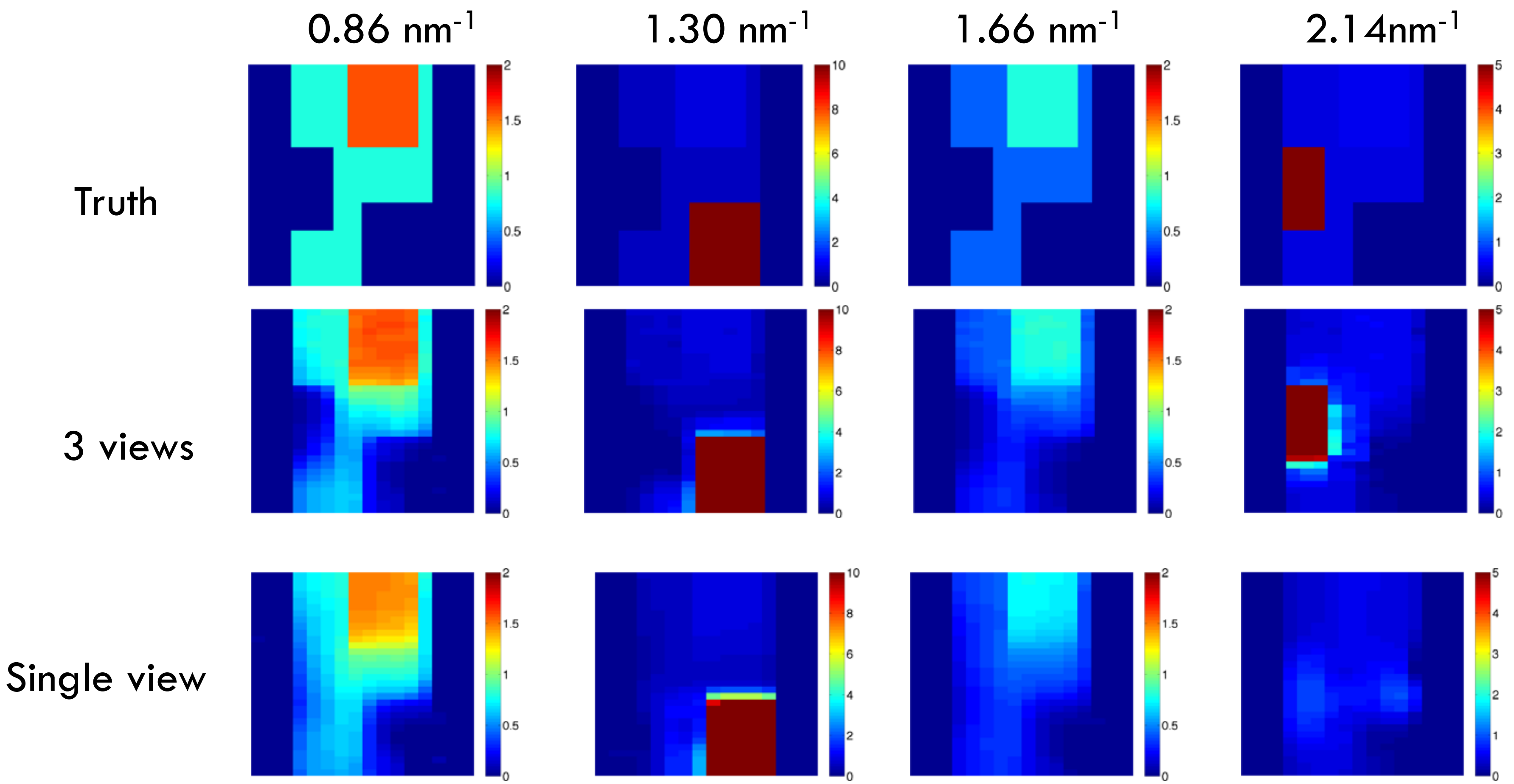
Approximation for coded apertures? No…

- 3 views: (-60, 0, 60 degrees)
- Must have attenuation map for correction



Other Reconstruction Behavior

- Phantom: **Tall rectangular solid**
- Architecture: Coded aperture, 3 views (-60, 0, 60) degrees, vs single view, 0 degrees, with photon-counting detectors, multi-energy illumination



Strong absorption from a single view can reduce scatter signal (no aluminum…)

Photon-counting detectors help

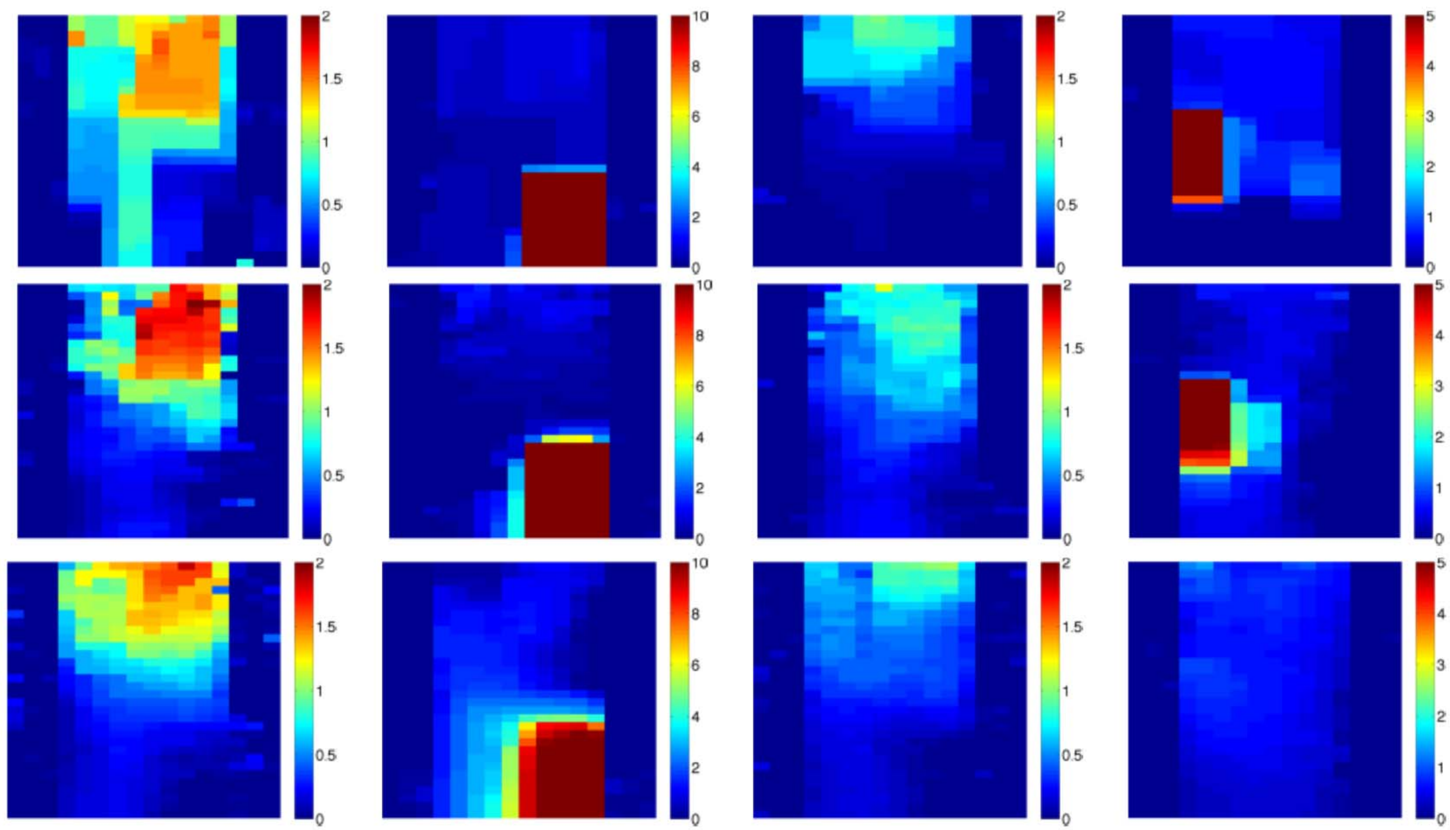
- Phantom: **Tall rectangular solid**
- Architecture: Coded aperture, 3 views (-60, 0, 60) degrees, with intensity detectors and photon-counting detectors , monochromatic vs multi-energy illumination

0.86 nm^{-1} | 1.30 nm^{-1} | 1.66 nm^{-1} | 2.14 nm^{-1}

Single energy

Multi-energy, photon-counting detectors

Multi-energy, intensity detectors



What about XRD Cargo?

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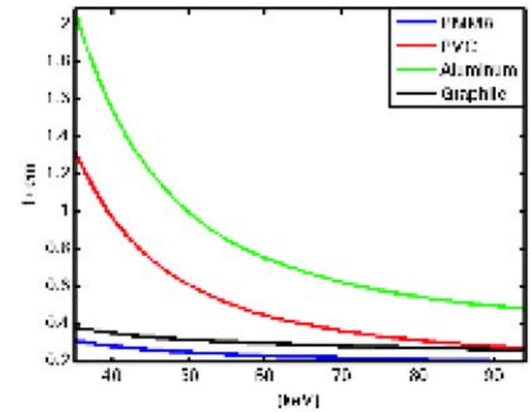

- Energy Levels
  - Need to work at lower energy to get sufficient coherent scatter → LACs of 0.2-0.8
  - Difficult to get coherent scatter for minimum dimension over 15 inches – longer exposure times
- Irregular shapes make tomographic architectures hard
  - Hard to arrange coherent scatter detectors for rotating architecture
  - May have very different length paths for radiation
- Larger minimum dimension ➔ larger arrays needed
  - Photon counting detectors desired
  - Greater expense to populate array
- Increased metal content ➔ increased streaking, attenuation
  - Advanced algorithms required

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