System-independent X-ray Characterization of Materials

Stephen Azevedo, Harry E. Martz, Jr., Bill Brown, Kyle Champley, Jeff Kallman, Dan Schneberk, Isaac Seetho, Jerel Smith, Maurice Aufderheide
azevedo3@llnl.gov

Lawrence Livermore National Laboratory
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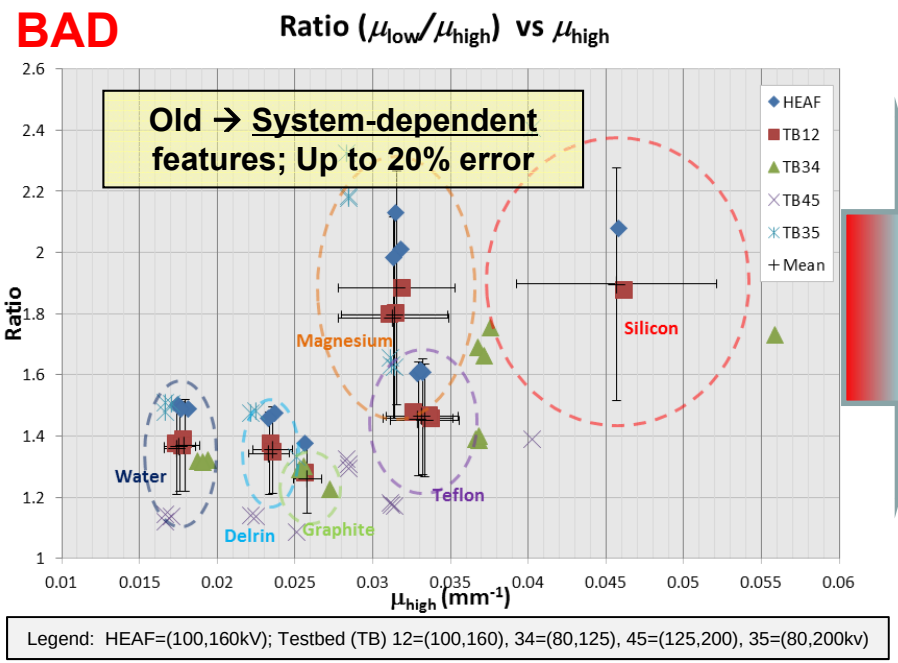
PCD provides more precise X-ray features for detection

- **DHS needs ways to characterize HMEs wrt all X-ray-CT-based EDSs**
  - **As new threats appear, vendors need to know their physics-based X-ray features**
  - **Gov't could measure X-ray features on a non-EDS CT system that maps to EDS**
- **Problem:**
  - **Current X-ray features based on (μ_{high}, μ_{low}) can vary greatly with different scanners looking at the same specimen. Need better discrimintators.**
- **Objective:**
  - **Find a "system-independent" X-ray feature space (with <3% uncertainty)**
- **Results:**
  - **New PCD* method using (ρ_e,Z_e) feature space shows good results on two different scanners and over wide spectral ranges (80 to 200 keV)**
  - **Seven different materials were characterized with PCD in the (ρ_e,Z_e) feature space and demonstrated averages of <2% accuracy and <1% precision**
  - **PCD requires**
    - **Reference materials that span the Z range**
    - **Good knowledge of X-ray spectral response**
    - **No beam-hardening compensation (BHC) needed**
- **PCD may improve Pd/Pfa because of more precise features**

* **PCD = Photoelectric-Compton Decomposition**

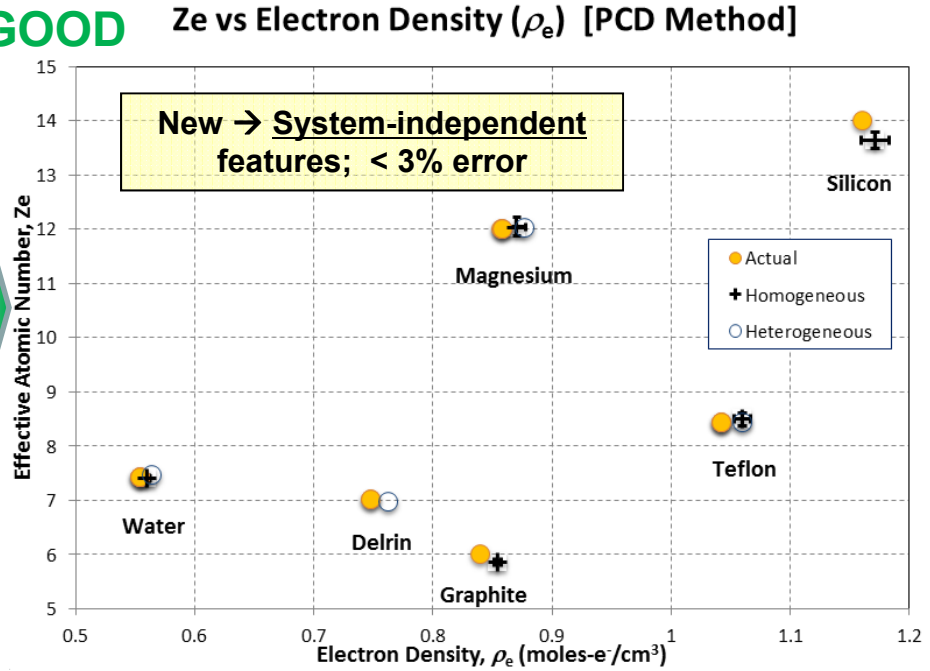
Results Summary leads to Recommendations

BAD



Legend: HEAF=(100,160kV); Testbed (TB) 12=(100,160), 34=(80,125), 45=(125,200), 35=(80,200kv)

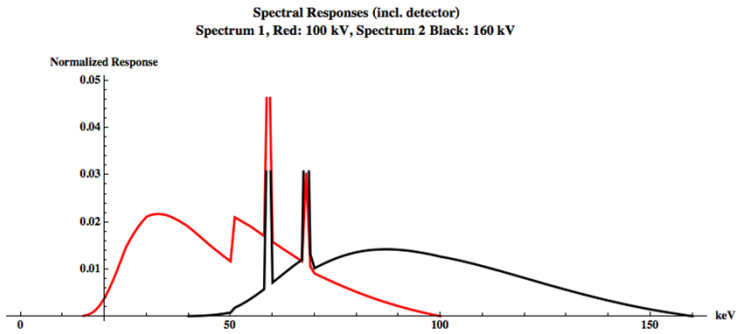
GOOD



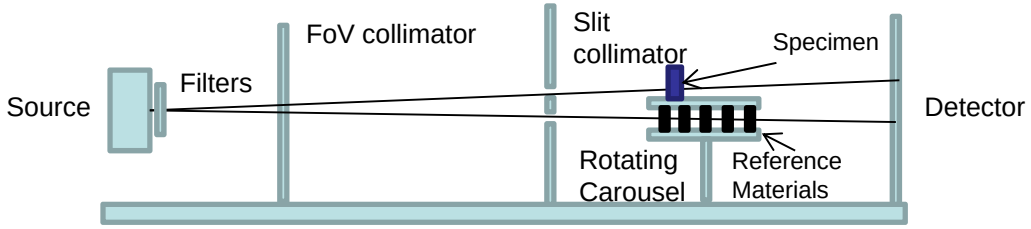
- **New X-ray features (ρ_e,Z_e) gave system-independent results without BHC**
  - **Tested with 7 specimens on 2 different MCT scanners, 2 different detectors and 5 spectra**
- **Recommendations**
  - **Employ Photoelectric-Compton Decomposition (PCD) and (ρ_e,Z_e) features across all MicroCTs at TSL, TAFRL, and LLNL**
  - **Show it translates to EDS and is backward compatible**
  - **Replace (μ_{high}, μ_{low}/μ_{high}) regions of responsibility (RORs) with (ρ_e,Z_e)**

Experiments involved two different MicroCT systems

- **MicroCTs are LLNL-built devices specifically for HME characterization**
  - **Brehmsstrahlung source with end-point energy of up to 450kV**
  - **~150 um isotropic voxels reconstructed**
  - **Two-slit collimator with 2-mm slits to produce fan beam to reduce scatter**
- **Rotating carousel rotates through 400 angles at half-degree intervals**
  - **HME specimen is positioned on the upper level for X-ray features (60-250 mL bottle)**
  - **6 reference samples of known composition on the lower level**
- **The two MicroCTs used (HEAF and TestBed) differed in detector**
  - **HEAF MicroCT used Thales amorphous silicon (AS) panel; Scanned at 100 and 160 kV**
  - **TestBed MicroCT used Perkin-Elmer AS panel; Scanned at 80, 100, 125, 160, 200 kV**
- **Scans were processed pairwise to simulate scanners with very different spectra**



Example Spectra (100kV – red, 160kV – black)



General layout of a MicroCT system

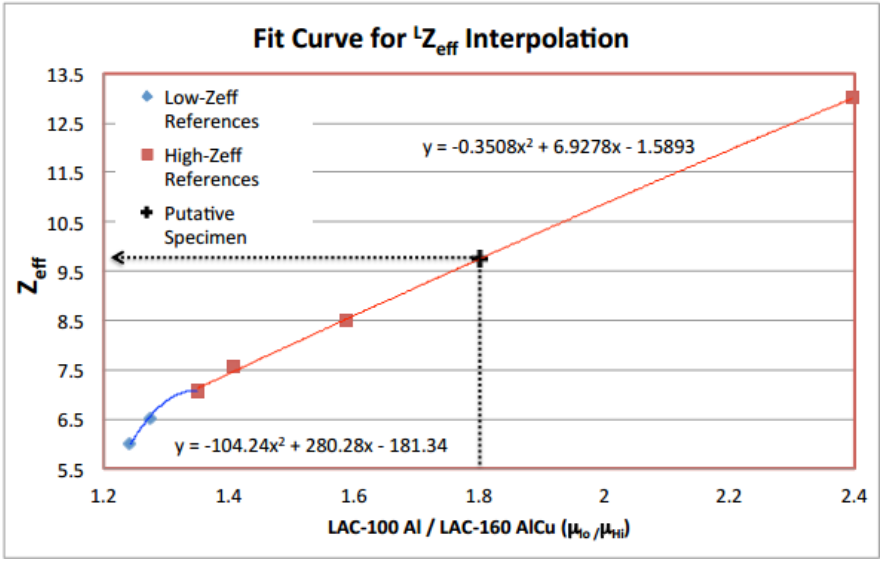
Current Methods: Simple Transfer Function

- Current LLNL processing techniques make use of Z_{eff}, defined as:

$$Z_{eff} = \sqrt[p]{\sum_i a_i (Z_i)^p}$$

  - The a's represent electron fractions contributed by constituent elements, and p is a constant tuned to approximate observed behavior. At the direction of TSL/DHS, we use p = 3.8
- Low- and high-energy measured attenuation values for known reference materials are combined with nominal Z_{eff} values to yield quadratic fit lines between Z_{eff} and attenuation ratio.

- Reference materials are separated into lower and higher Z groups.
- The lower group is used for a quadratic fit, while the upper group uses a constrained quadratic fit to generate a continuous curve.
- The specimen attenuation ratio is entered into the curve equation to yield a $^{L}Z_{eff}$ value, which is plotted against the high-energy attenuation value, in LMHU (where values are normalized such that water at high energy has mean value 1000 and air is zero).



What are Z_e and ρ_e?

- **Z_e is an alternative definition of effective atomic number***
  - **Based on X-ray cross sections for the spectrum used**
  - **Relates the degree of attenuation and scattering using published tables**
  - **ZeCalc is a Java app to calculate Z_e given composition and spectrum**
  - **Calculates ρ_e also if given physical density**

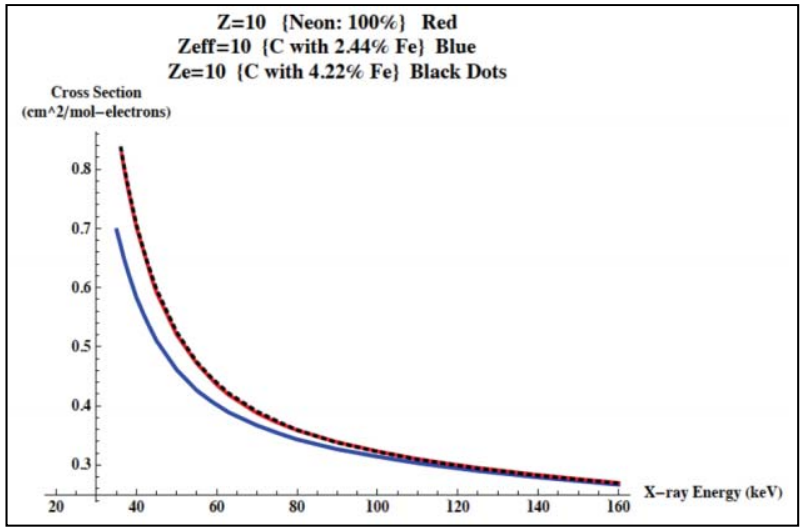
- **ρ_e is the electron density, defined for a single element material as:**

$$\rho_e = \frac{\rho Z}{A}$$

, where ρ is mass density and A is atomic mass

- Experimental results show that (Ze, ρ_e) features have better resolution of different materials than methods using the high- and low-energy reconstructions.

- In addition, materials with identical Z_e are shown to have closer x-ray cross section than materials with identical Z_{eff}.

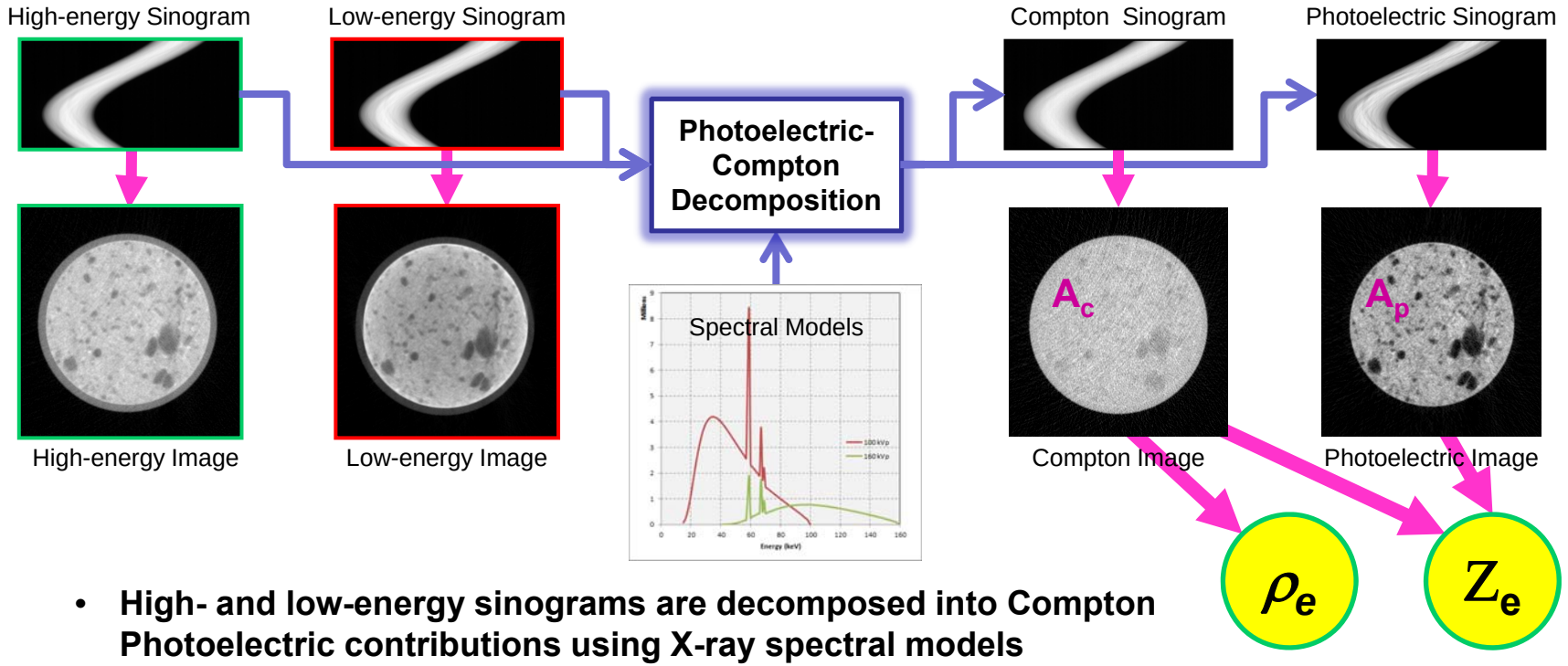


* J. A. Smith, H. E. Martz, J. S. Kallman, *Case for an Improved Effective-Atomic-Number for the Electronic Baggage Scanning Program*, Lawrence Livermore National Laboratory, LLNL-TR-520312, December 14, 2011.

History of Photoelectric-Compton Decomposition

- **Alvarez & Macovsky (1976)**
  - **Decomposition uses photoelectric, Ap, and Compton, Ac, contributions to specify features**
  - **Introduced that full attenuation features at every energy can be represented using a set of energy-independent values**
    - **Do not need many narrow energy bands across a range of interest to characterize a material.**
    - **Instead, scan with a few broad energy peaks over the applicable range, and use the results to validate the system**
  - **Plots are in Ac, Ap feature space**
- **Ying, Naidu, Crawford (2006)**
  - **Propose optimization technique using iso-transmission curve intersections**
  - **Propose scatter, streak and spectral corrections for EDS machines**
  - **Plots are in the Zeff vs high-energy channel feature space**
- **New Photoelectric-Compton Decomposition (PCD)**
  - **Propose calibration of the system to known reference materials**
  - **Propose plot of Ze vs ρ_e to more closely follow material x-ray properties as a transfer method**

Photoelectric Compton Decomposition (PCD) Method



- **High- and low-energy sinograms are decomposed into Compton Photoelectric contributions using X-ray spectral models**
- **These sinograms are reconstructed into Compton (A_c) and Photoelectric (A_p) images**
- **Mean values inside the specimen are calculated: $\bar{a}_c$ and $\bar{a}_p$**
- **Then, $\rho_e = K(\bar{a}_c)$ and $Z_e = k(\bar{a}_p/\bar{a}_c)^{1/n}$**
  - **where K, k and n are empirically determined constants obtained through a calibration procedure using well-known reference materials**

Note that beam-hardening compensation (BHC) is *not* needed.

R&D Experimental Plan: Reference Materials

- **New reference materials were acquired and assayed at LLNL.**
  - **Higher confidence in material composition**
  - **More accurate Ze, ρ_e values for higher confidence in output results**
  - **References selected to expand the range in Z relative to current reference materials**

Material	Diam (mm)	Density g/cm^3	RhoE Mol-e/cm^3	Ze	Nominal Purity %
Graphite	12.956	1.804	0.901	6.00	99.997
Delrin	12.694	1.403	0.748	7.01	copolymer
Teflon	12.707	2.175	1.044	8.44	99.99
Magnesium	12.700	1.736	0.857	12.00	99.98
Silicon	12.620	2.331	1.162	14.00	99.99
Water	10.8	0.998	0.554	7.43	Reagent Grade 1

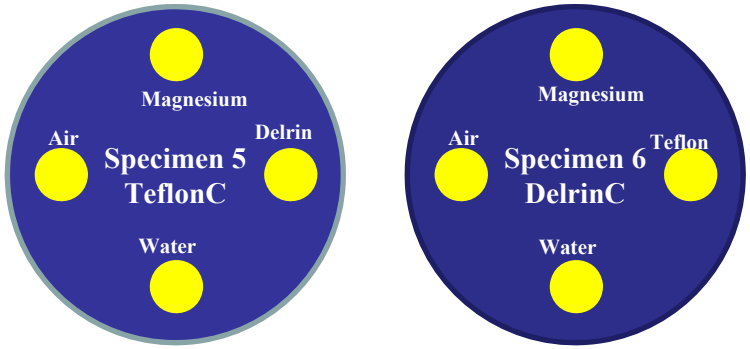
R&D Experimental Plan: Reference Specimens

- Homogeneous Reference Specimens were selected to cover a wide range of Z values (from graphite, Z=6, to silicon, Z=14)
- Specimens matched the composition of corresponding reference materials to establish a baseline on system performance
- Inhomogeneous Reference Specimens were two composite specimens also scanned to examine system behavior for inhomogeneous samples
- All specimens were cylinders measured for size and weight (density)

Homogeneous Reference Specimens

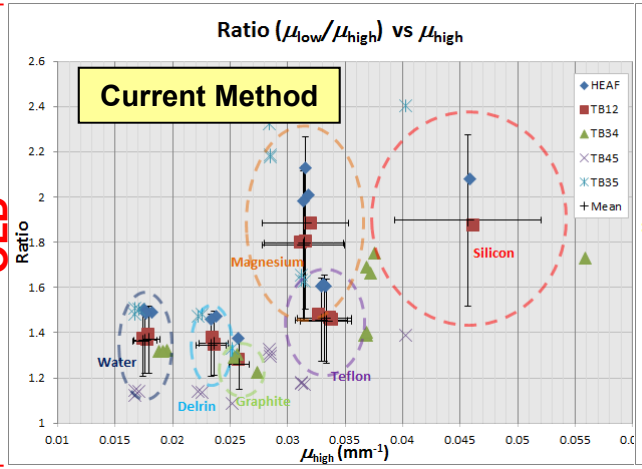
Name	Material	Dia (mm)
Specimen 1	Graphite	50.8
Specimen 2	Teflon	56
Specimen 3	Magnesium	25.4
Specimen 4	Silicon	25.4
Insert A	Teflon	10
Insert B	Delrin	10
Insert C	Magnesium	10
Insert D	Water	10
Substrate 1	Teflon Plug	56
Substrate 2	Delrin Plug	50.8
Specimen 7	Water[2] (60 ml)	36.9/38.9

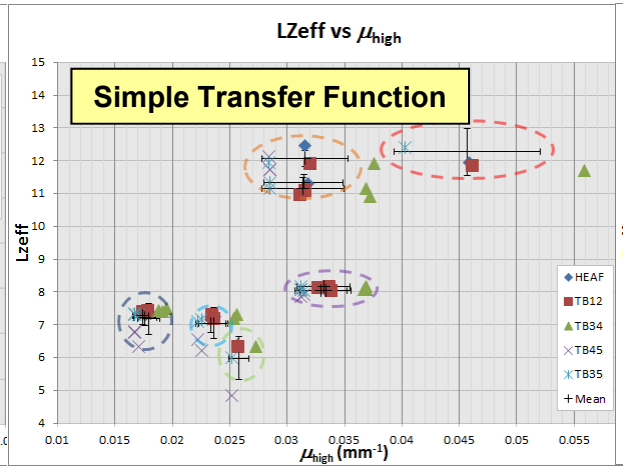
Inhomogeneous Reference Specimens

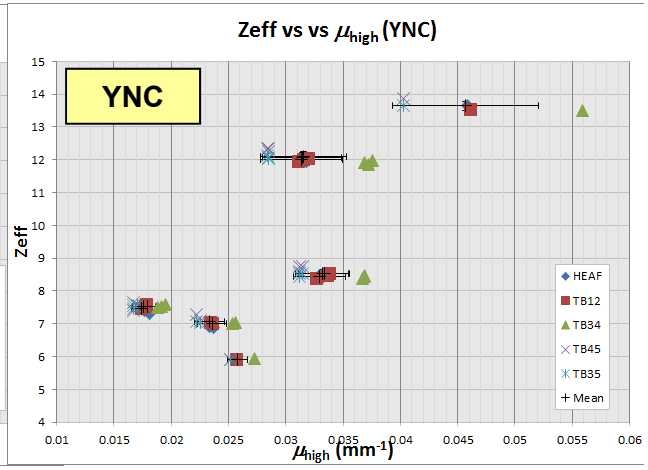


The PCD and DD methods produce similar results

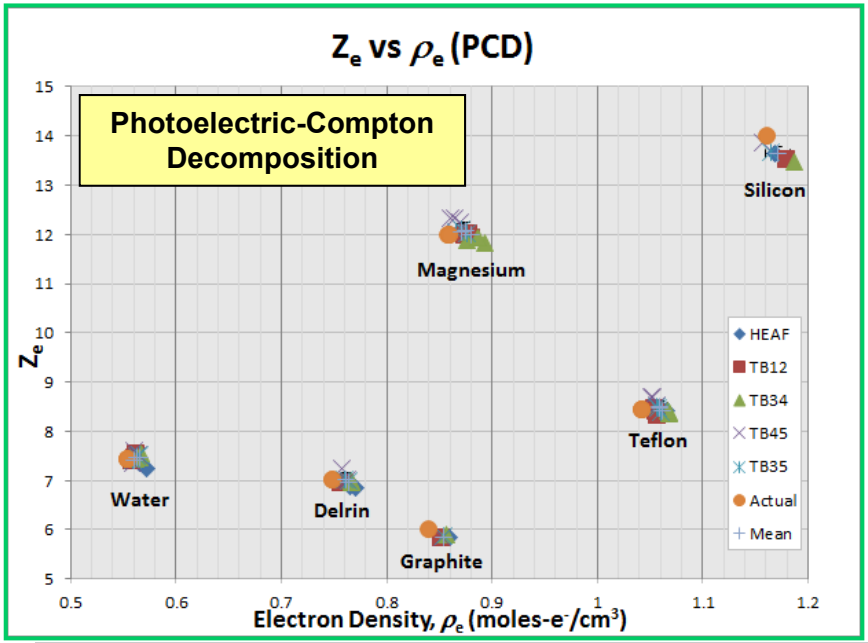
OLD

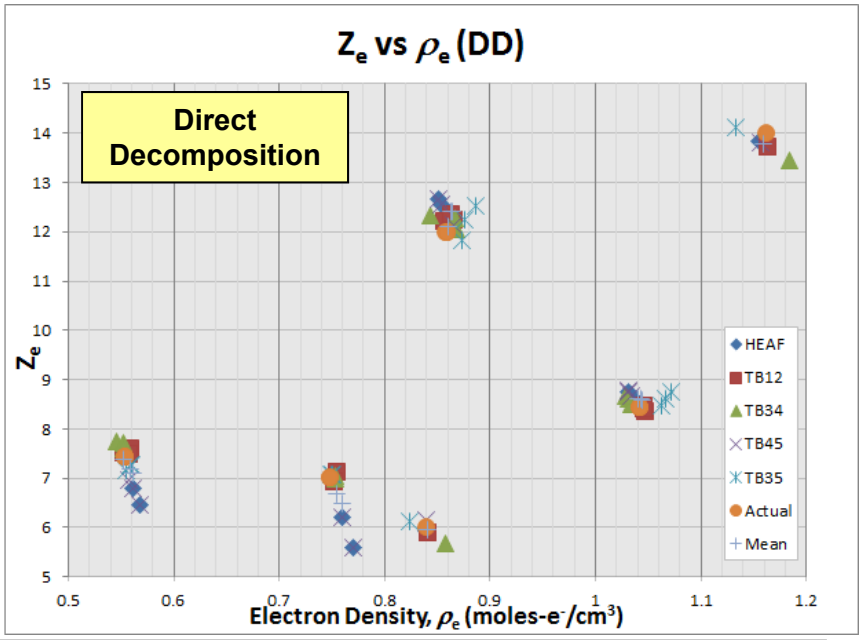






NEW (Proposed)





Legend: HEAF=(100,160kV); Testbed (TB) 12=(100,160), 34=(80,125), 45=(125,200), 35=(80,200kv). . "Actual" is physically measured density and elemental composition.

Precision and accuracy values yield insight into (ρ_e,Z_e)

Average (Mean %)	With RbBr & Refs		Without RbBr & Refs	
	All spectra	100/160 only	All spectra	100/160 only
Ze Precision	1.10	0.72	1.18	0.72
Ze Accuracy	0.87	0.98	0.69	0.84
Rho-e Precision	0.77	0.74	0.64	0.62
Rho-e Accuracy	1.80	1.85	1.66	1.75
mu-lo Precision	14.59	0.21	14.58	0.28
mu-hi Precision	7.72	0.28	7.62	0.38
Worst-case (Max %)	**With RbBr & Refs**		**Without RbBr & Refs**	
	All spectra	100/160 only	All spectra	100/160 only
Ze Precision	3.29	3.63	1.96	2.74
Ze Accuracy	3.73	2.95	2.57	2.93
Rho-e Precision	6.17	5.82	1.03	1.22
Rho-e Accuracy	8.02	7.69	2.43	2.47
mu-lo Precision	23.02	0.73	21.10	0.73
mu-hi Precision	14.47	0.76	14.00	0.76
* Note: actual mu values are not known, so accuracy cannot be computed.				

If systems are nearly the same, μ_{low} and μ_{high} are good. More processing, such as PCD, can slightly increase the error.

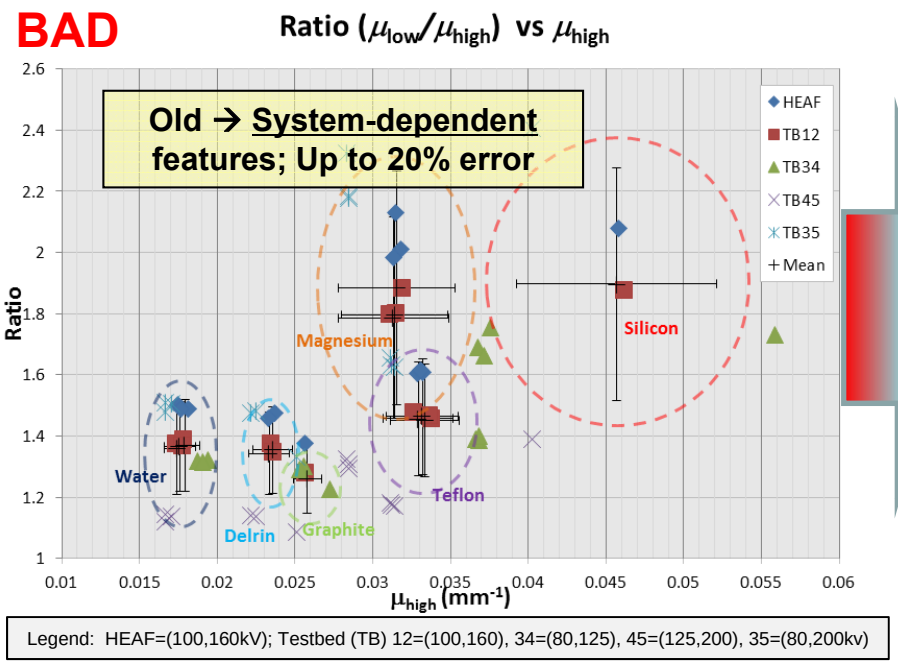
If systems are not the same, (ρ_e,Z_e) is much better.

If materials are beyond the Z of reference materials, some of the worst-case (ρ_e,Z_e) errors are slightly higher; they are still better than μ_{low} and μ_{high}.

(ρ_e,Z_e) is a valid new System-independent X-ray feature space.

Results Summary leads to Recommendations

BAD



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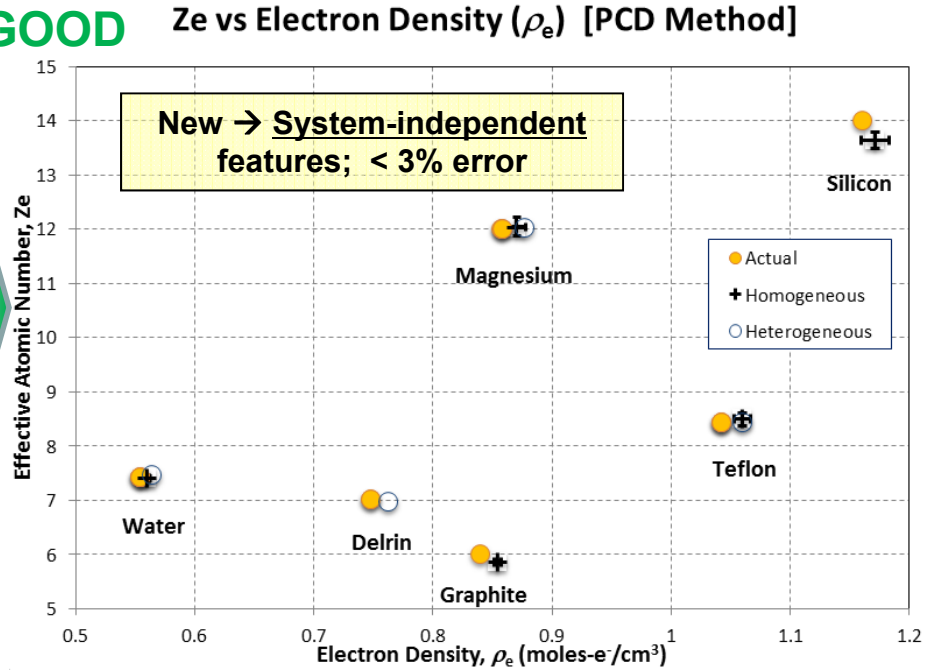

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