Ze: an Effective Atomic Number for Polychromatic X-ray Spectra

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Agenda

- What is an “effective atomic number?”
- Cross-sections describe materials.
- Existing approaches to Z_{eff} are inadequate
- A new technique, {Ze, RhoE}, provides an improved approach to characterizing materials with an effective atomic number.
- An Example demonstrates the practical use of {Ze, RhoE}.
- An Application is available to Calculate {Ze, RhoE}.

What is an Effective Atomic Number?

- **An effective atomic number:**
  - Alias: Effective-Z or Z_{eff}
  - "Describes" a complex (non-elemental) material (compound, mixture) as a single number
  - Monoenergetic or Polychromatic spectra
  - Examples Include:
    - Radiography, Computed Tomography (CT)
    - Multi-spectral Radiography
    - Mult-spectral or Dual-energy CT (DECT)
    - Dose to tissue or other materials

X-ray Cross Sections Describe Materials

Beers-Lambert Law for Polychromatic Spectra

$$I[x] = \int dEx\, S[Ex]\, Exp[-(\mu/\rho)[Z, Ex]\, \rho_m\, x]$$

(μ/ρ) is the mass-absorption coefficient (cm^2/g)

Z is the atomic number

Ex is the x-ray energy

ρ_m is the mass density

x is the length of the transmission path

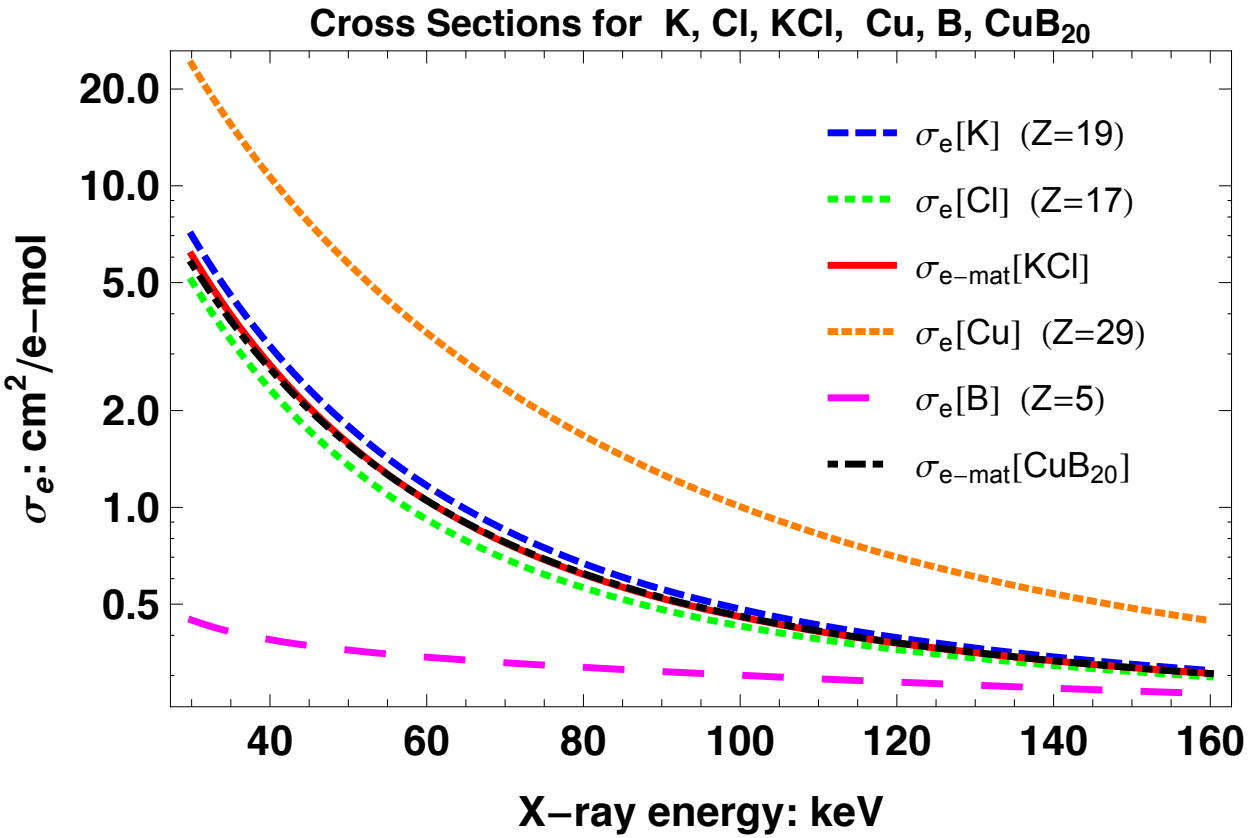
$$I[x] = \int dEx\, S[Ex]\, Exp[-\sigma_e[Z, Ex]\, \rho_e\, x] \qquad \textit{Equation 1}$$

σ_e is the mass-absorption coefficient (cm^2/e-mol)

ρ_e is the electron density (e-mol/cm^3)

I[X] is the energy-integrated transmission if: $\int dEx\, S[Ex] = 1.0$

Cross Sections for a Few Elements and Compounds



Cross Sections for Compounds and Mixtures

For a compound with N elements:

$$\sigma_{e-mat}[Ex] = \sum_{i=1}^{N} \alpha_i \sigma_e[Z_i, Ex] \,,$$

$$\alpha_i = n_i Z_i / \sum_{j=1}^{N} n_j Z_j \,.$$

Equation 2

$\sigma_{e\text{-}mat}$ is the electronic cross section of the material

Z_i, n_i are the Z and number of that element in the compound

α_i is the fraction of each mole of electrons provided by element Z_i

We need an effective-Z description of the molecule

$$\sigma_e[Z_{eff}, Ex] \cong \sigma_{e-mat}[Ex]$$

Equation 3

(This equation can only be exact for single-element materials)

Previous Versions of Z_{eff}

– **Mayneord (1937)** (interpolation formula) [1]

$$Z_{eff} = \sqrt[p]{\sum_i^N \alpha_i Z_i^{\,p}}$$

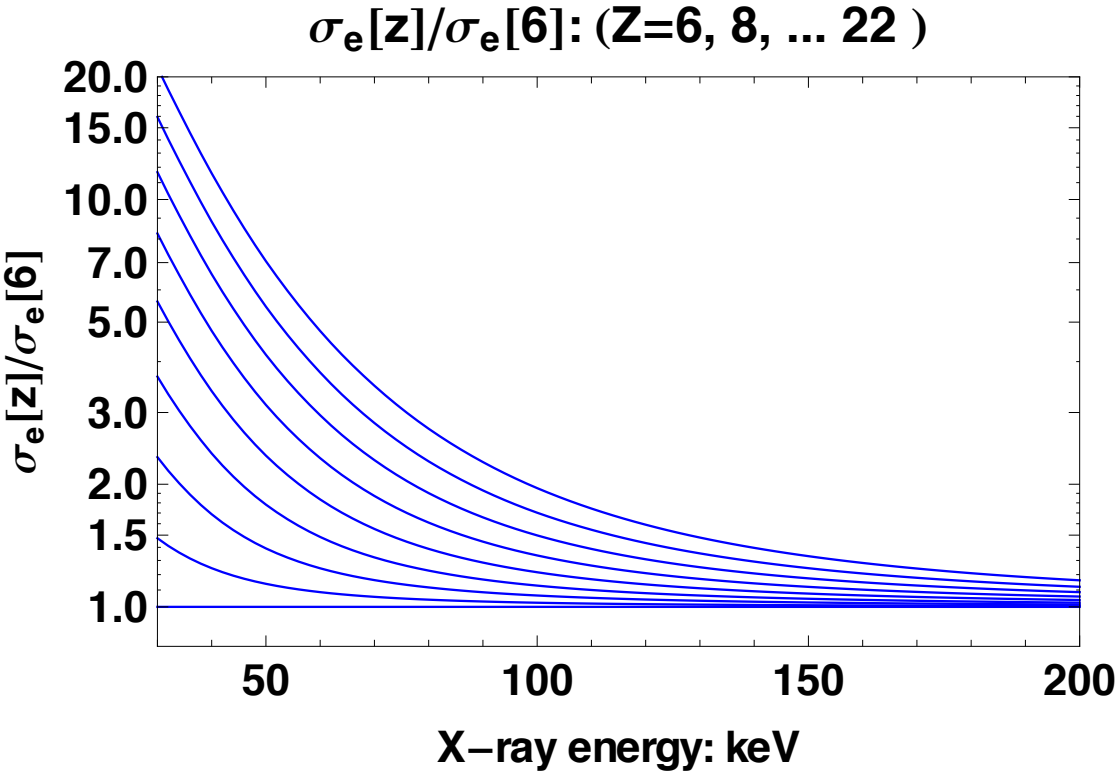
Equation 4

- Typically $3 \leq p \leq 4$ (depends on Ex and Z_i)
- Very common (ubiquitious)
- Cannot write $\sigma_e[Z_{eff}, Ex]$

– **Several other versions** [2–5]

- Provide: $Z_{eff}[Ex]$
- Cannot write $\sigma_e[Z_{eff}, Ex]$

{Ze, RhoE} Strategy



- At high keV, cross-section per e-mol becomes independent of Z
- Low-energy end of spectrum carries most of the Z-dependence
- Ze is simply interpolated into the surface of $\sigma_e[Z, Ex]$

Ze Definition

$$\sigma_{Ze}[Ex] \stackrel{\text{def}}{=} \sigma_e[Ze, Ex] = (1 - \text{frac})\sigma_e[Z_1, Ex] + \text{frac}\ \sigma_e[Z_1 + 1, Ex]$$

$$Z_1 = \text{floor}[Z_e] \text{ and } frac = fractional\_part[Z_e] \qquad \textit{Equation 5}$$

- σ_{Ze}[Ex] is interpolated into σ_e[Z, Ex], using the fractional contribution of electrons from Z1 and Z2 as the interpolation variable.
- σ_e[Z, Ex] (cm2/e-mol) is converted from tabulated cross sections [6–8] σ[Z, Ex] (b/atom), or (μ/ρ) (cm^2/g) and the atomic weight, A:
- $$\sigma_e[\text{Z, Ex}] = \frac{K_0}{Z}\sigma_e[\text{Z, Ex}] = \frac{A}{Z}(\mu/\rho)[\text{Z, Ex}] \qquad \textit{Equation 6}$$

$$K_0 = 0.6022\ cm^2/b - mol\ .$$

- ρ_e and m_e can be calculated from the volumetric mass density, ρ_m, or the areal mass density, $m_m = \rho_m x$

$$\rho_e = \rho_m \sum_{i=1}^{N} w_i Z_i / A_i$$

- $$m_e = m_m \sum_{i=1}^{N} w_i Z_i / A_i\ , \qquad \textit{Equation 7}$$

$$w_i = n_i / \sum_{j=1}^{N} n_j\ .$$

Finding the Best Ze for a Material

- Assigning a Ze to a particular material is done with a least squares fit.
- Minimizing the overall error in the cross section overly emphasizes the low energies where the cross-section differences are greatest, but there is little x-ray transmission.
- It is better to find the Ze that generates the least mean-squared error in transmission:

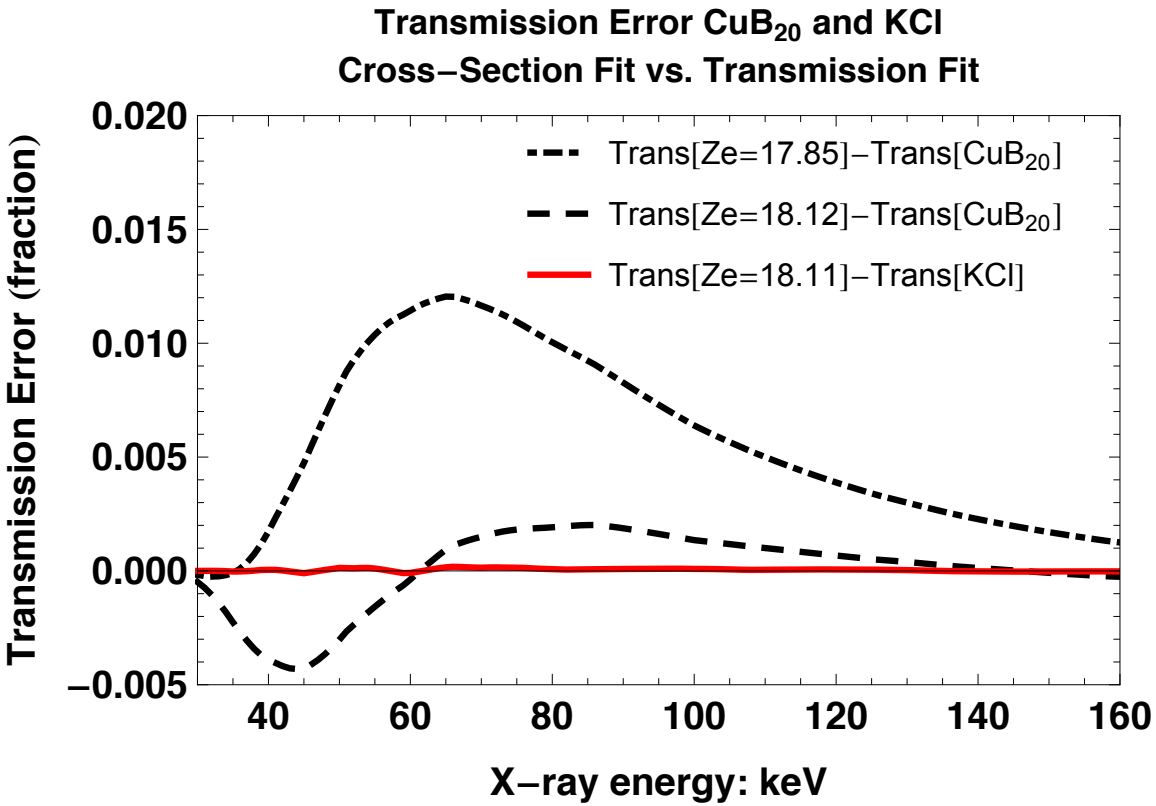
$$\sum_{eMin}^{eMax}(Trans_{e-mat}[Ex] - Trans_{Ze}[Ex])^2 \rightarrow minimum$$

$$Trans_{e-mat}[Ex] = \mathrm{Exp}[-\sigma_{e-mat}[Ex]\, m_{e-samp}]$$

$$Trans_{Ze}[Ex] = \mathrm{Exp}[-\sigma_{Ze}[Ex]\, m_{e-samp}]\,.$$

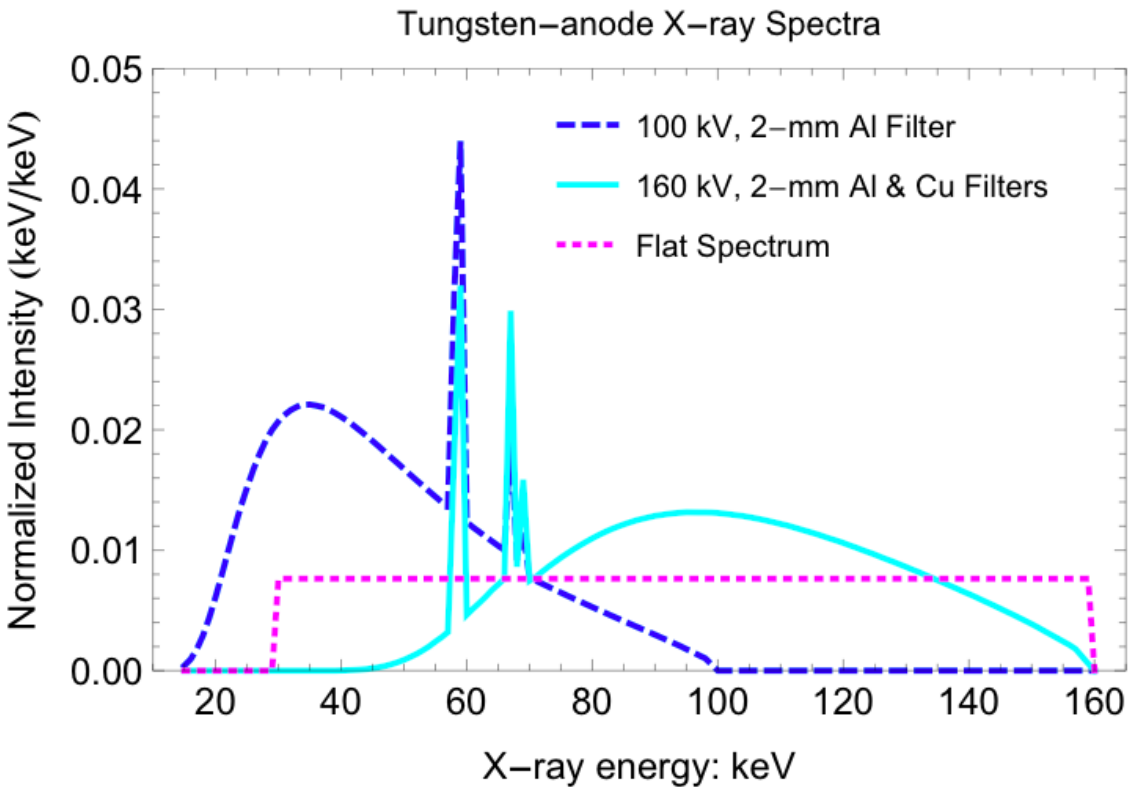
Equation 8

Finding the Best Ze for a Material (cont.)



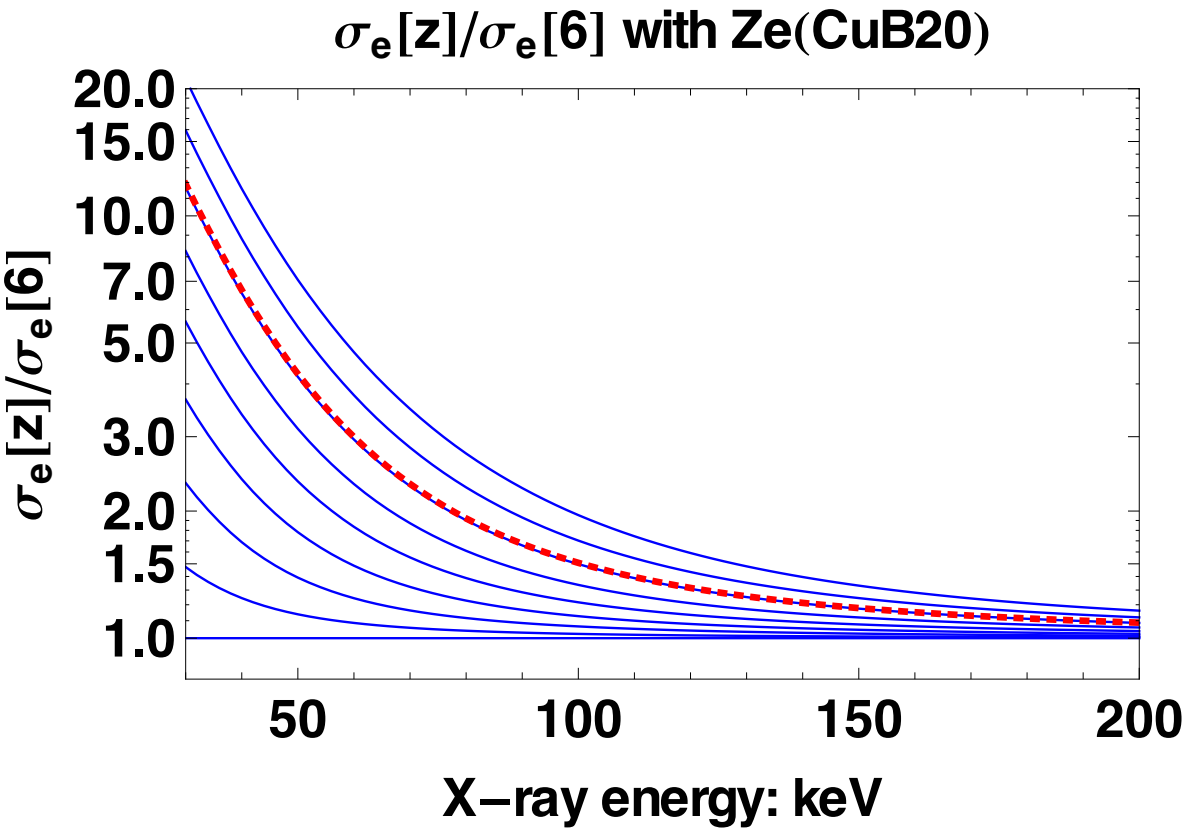
- Transmission is calculated through 2.5 g/cm^2 of material

Spectra Used in Evaluating Transmission Errors



- To optimize the Ze fit over a range of energies, a flat spectrum, S[Ex], was used.
- To test the sensitivity of the resulting transmission fit to spectrum, two “typical” spectra (100 kV and 160 kV) were used.

The Transmission-Fit Criterion Selects Ze = 18.12 for CuB_{20}



- The red Ze for CuB_{20} interpolates the cross-section just slightly above the blue Z = 18 curve.

Use of a "Transmission Fit Criterion Minimizes Transmission Errors

			Net Transmission Error (%) by Spectrum		
Material	**Ze**	**Fit Criterion**	**Flat**	**100 kV**	**160 kV**
CuB_{20}	17.85	$\Sigma (\sigma_{e\text{-}mat} - \sigma_{Ze})^2$ => minimum	0.566	0.556	0.690
CuB_{20}	18.12	$\Sigma (Trans_{e\text{-}mat} - Trans_{Ze})^2$ => minimum	0.007	- 0.121	0.096
KCl	18.11	$\Sigma (Trans_{e\text{-}mat} - Trans_{Ze})^2$ => minimum	0.004	0.003	0.006

- **Table 1.** Using a "best fit to cross-section" finds a Ze of 17.85 for CuB_{20}, and greater than ½% errors in calculating the transmission through a layer that is 2.5 g/cm^2 in areal density. Transmission errors are summed over the spectrum, S[Ex].
- In the second row, the transmission error is greatly reduced by using a "best fit to transmission criterion.
- For KCL, both criteria provided the same Ze, and and a minimal transmission error.
- For reference, the calculated transmissions for the Flat, 100 kV, and 160 kV spectra are 42.7%, 17.0 %, and 54.8 % respectively.

Dependence of Ze on Choice of "Representative Layer" (m_m) and Spectrum, S[Ex]

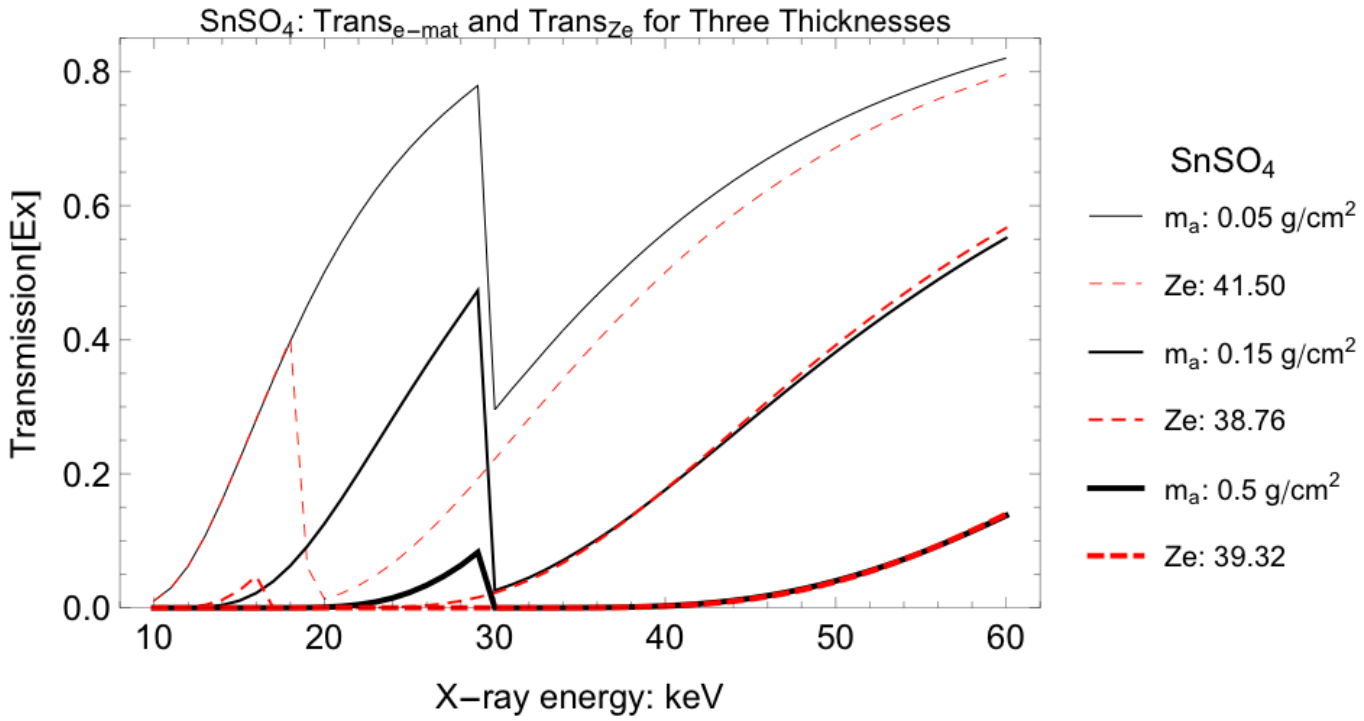
- The fit of Ze to a particular application is adjusted by selecting a spectral range, S[Ex], and a representative-layer areal density (m_m or m_e).
- This adjustment, provides the best approximation for the context of the particular application, but is only effective it the Ze values are relatively insensitive to the exact values of m_m (or $m_{e)}$ and S[Ex].
- Table 2 demonstrates that Ze is indeed insensitive to those values over a broad selection of spectral range and m_m.

Optimized Ze Values are Insensitive to the Selection of Spectrum and m_e

		Areal Density (g/cm2)		
Energy Range (keV)	Material	0.5	2.5	12.5
10 – 60	CH_4	5.14	5.12	5.07
	SiO_2	11.63	11.64	11.64
	$SnSO_4$	N/A[b]	N/A[b]	N/A[b]
30 – 160	CH_4	5.05	5.05	5.03
	SiO_2	11.64	11.64	11.61
	$SnSO_4$	39.80	40.13	40.24
80 - 450	CH_4	4.83	4.83	4.82
	SiO_2	11.58	11.58	11.57
	$SnSO_4$	39.99	40.25	40.46

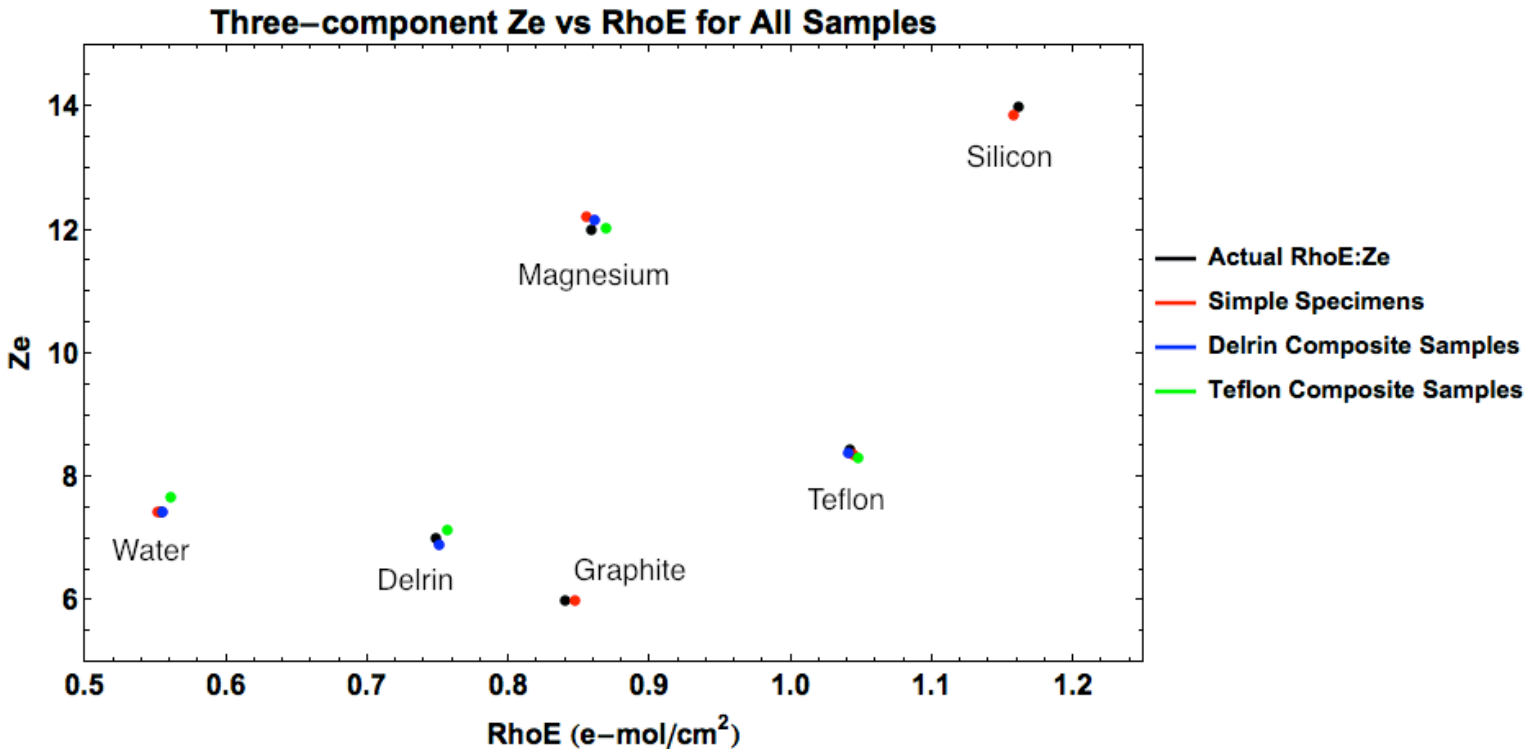
- **Table 2.** Ze was calculated for three materials, three different "representative-layer" thicknesses and three spectral regions. The Ze were relatively insensitive to these parameters.
- [b] SnSO4 was not an appropriate candidate for Ze at these energies (next slide)

X-ray Absorption Edges are not Compatible with effective-Z models



- X-ray absorption edges can cause a discontinuity in the absorption/ transmission of spectra through a material. This behavior cannot in general be approximated except by the specific element causing the discontinuity

Example of Ze Usage



- An example of Ze and ρ_e (RhoE) used to discriminate materials is illustrated by recent data showing a three-spectrum decomposition of a variety of simple and complex specimens.

An application is available for calculation Ze rhoe

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ZeCalc Algorithm Details

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- ZeCalc (a Java app.) calculates Ze based on the transmission-fit criterion for:
  - 10 keV ≤ Ex ≤ 500 keV, including 3 tungsten bremsstrahlung spectra
  - 1 ≤ Ze ≤ 100
  - 0.5 ≤ mm ≤ 12.5 g/cm^2
  - Outputs: Ze, optional ρ_e, Graphs of Z[Ex], Transmission vs. Ex, Transmission Error vs. Ex.
  - For more information, contact the authors.

Summary

- Ze provides a practical tool for obtaining an accurate approximation to the energy-dependent cross section for transmission measurements using polychromatic spectra.
- This tool can be used for quantitative measurements on compounds and mixtures over energies from 10–1000 keV.
- A more detailed technical discussion of this material will be submitted for publication in *Nuclear Instruments and Methods Part B.* in the near future.

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