Correcting XAS Intensity

Corbyn Mellinger

Xu Group Meeting

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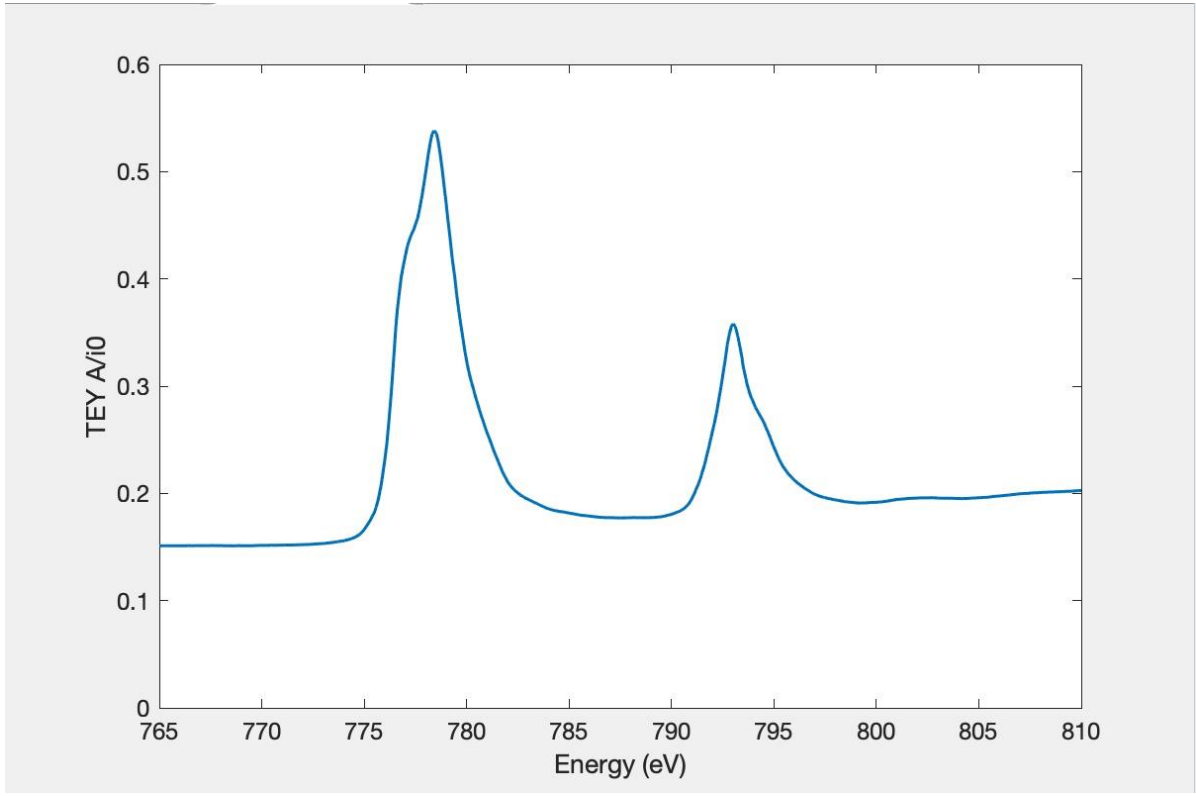
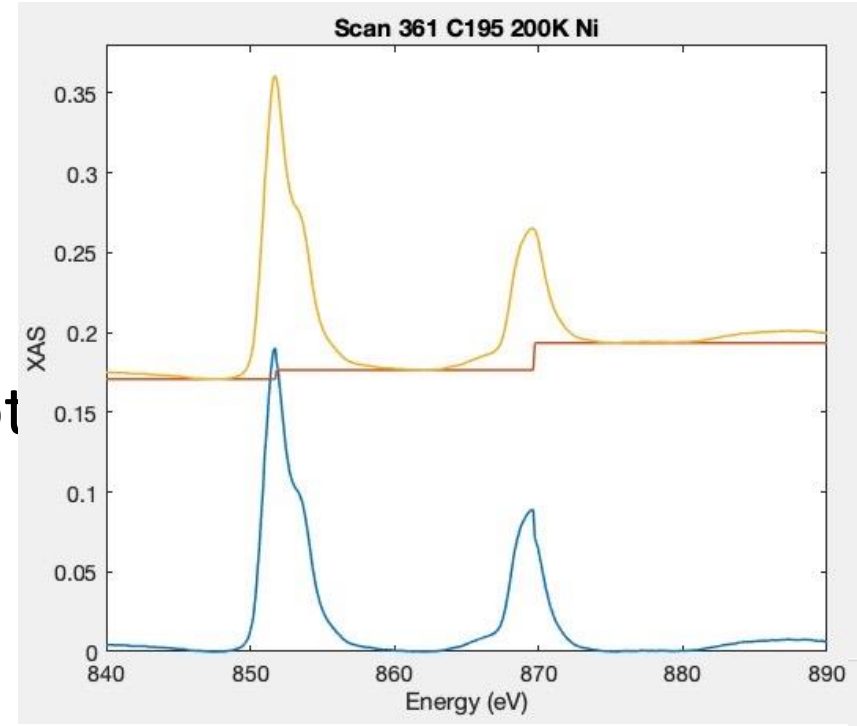
Raw XAS Data

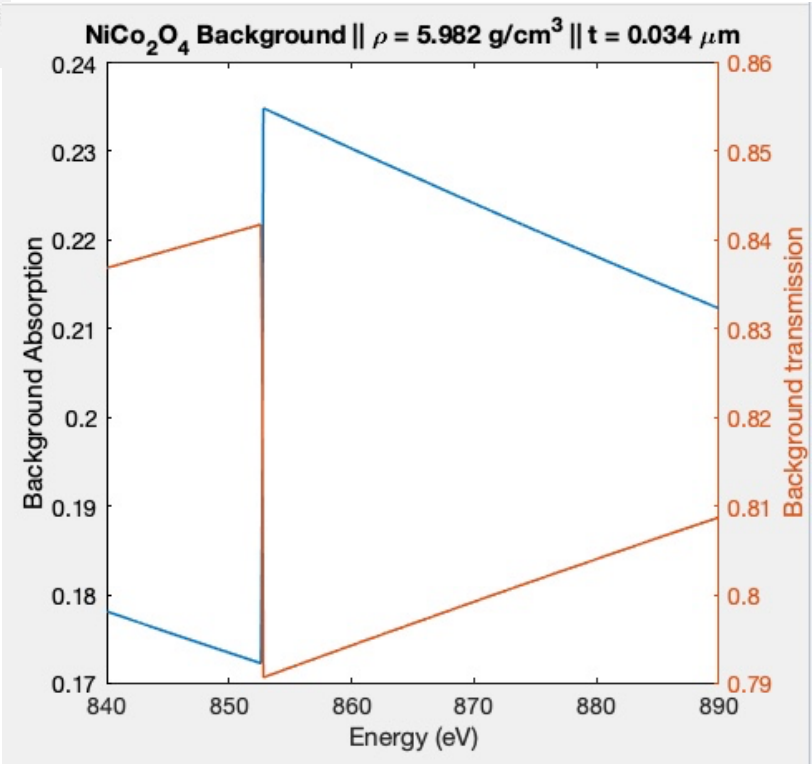
- XAS gives counts normalized to beam intensity
- Depends on many external circumstances (e.g. magnetic field, self-absorption, etc)
  - How to relate this to a *real* physical property of the material?



Background Subtraction

- Can fit to data, but not tied to the real absorption of the element
- Background simulation:
  - https://henke.lbl.gov/optical_constants/filter2.html

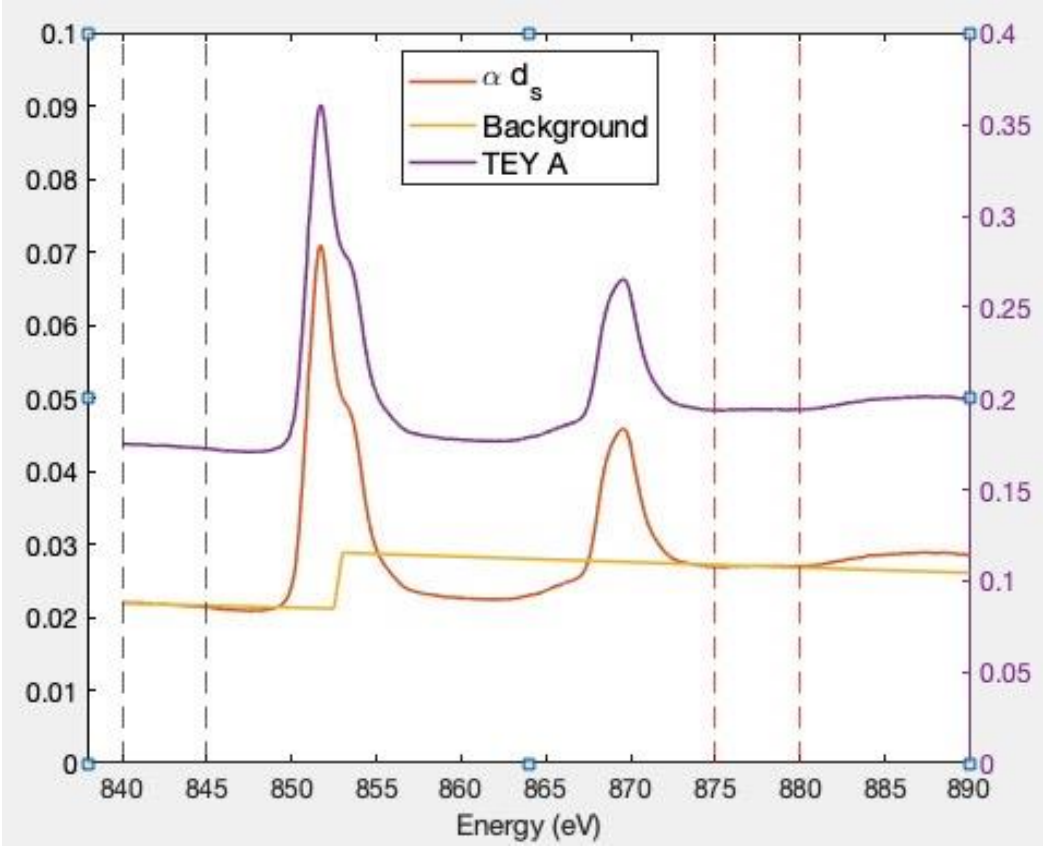




Background Subtraction

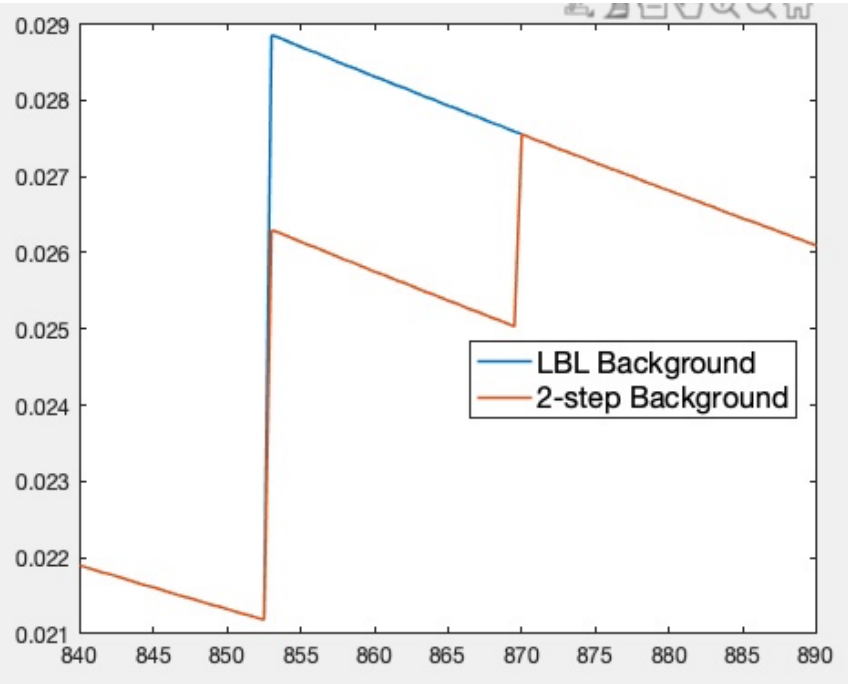
- Transmission factor: T(E) = exp(-αt), t = thickness
- Want absorption(which is what XAS measures)
  - αt = -ln(T(E)) => α = -ln(T(E)) / t

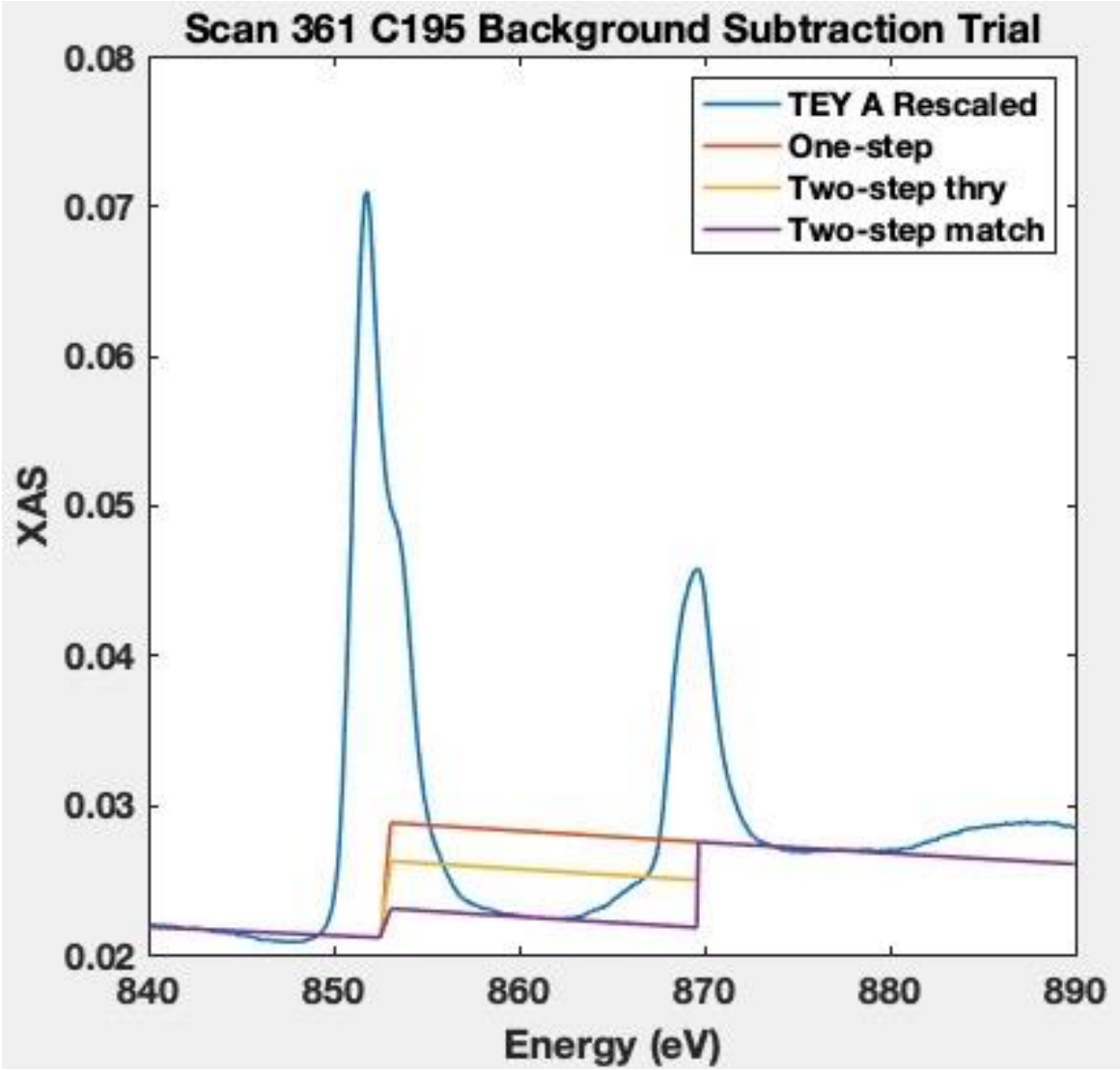
1. Scale the experiment to simulated data at pre-edge, post-edge
2. Subtract background from data to get real



Adjusting Background

- XMCD theory : twice as many L3 ($p_{3/2}$ -> d) absorptions as L2 ($p_{1/2}$ -> d) absorptions
- Adjust simulation to reflect this





Doesn't always match to the data well; use several types of background in calculation

Background Subtraction

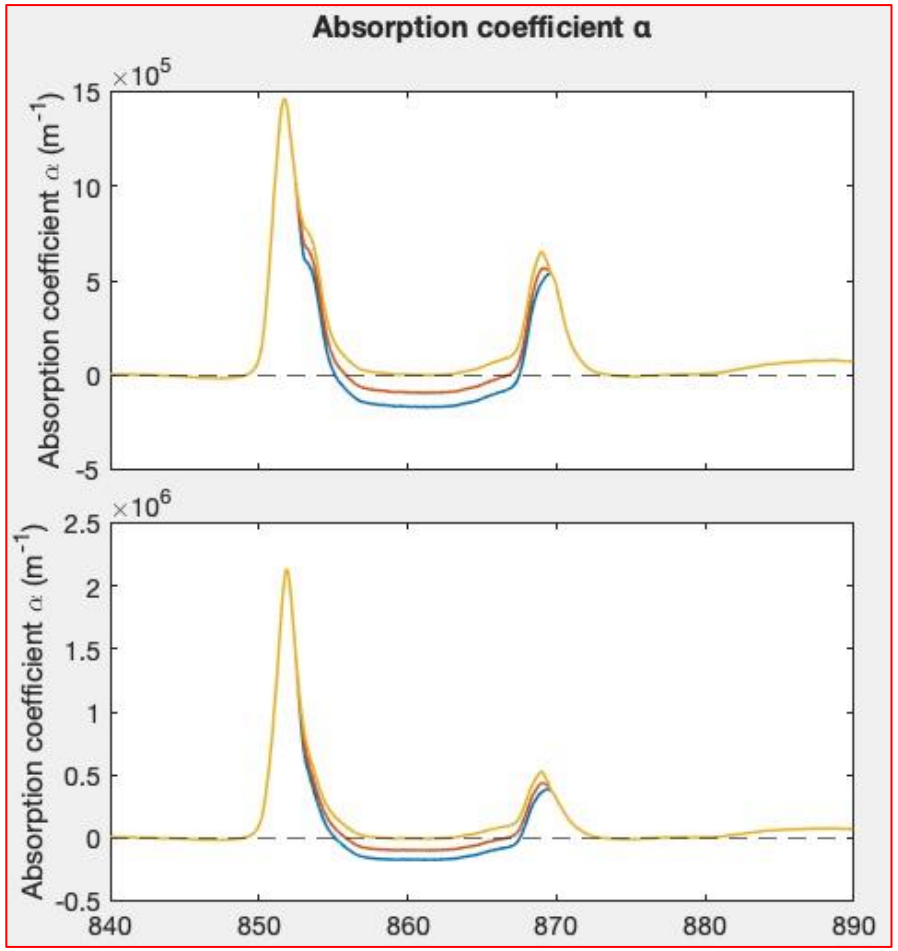
- Once have absorption α, determine **absorption cross section**

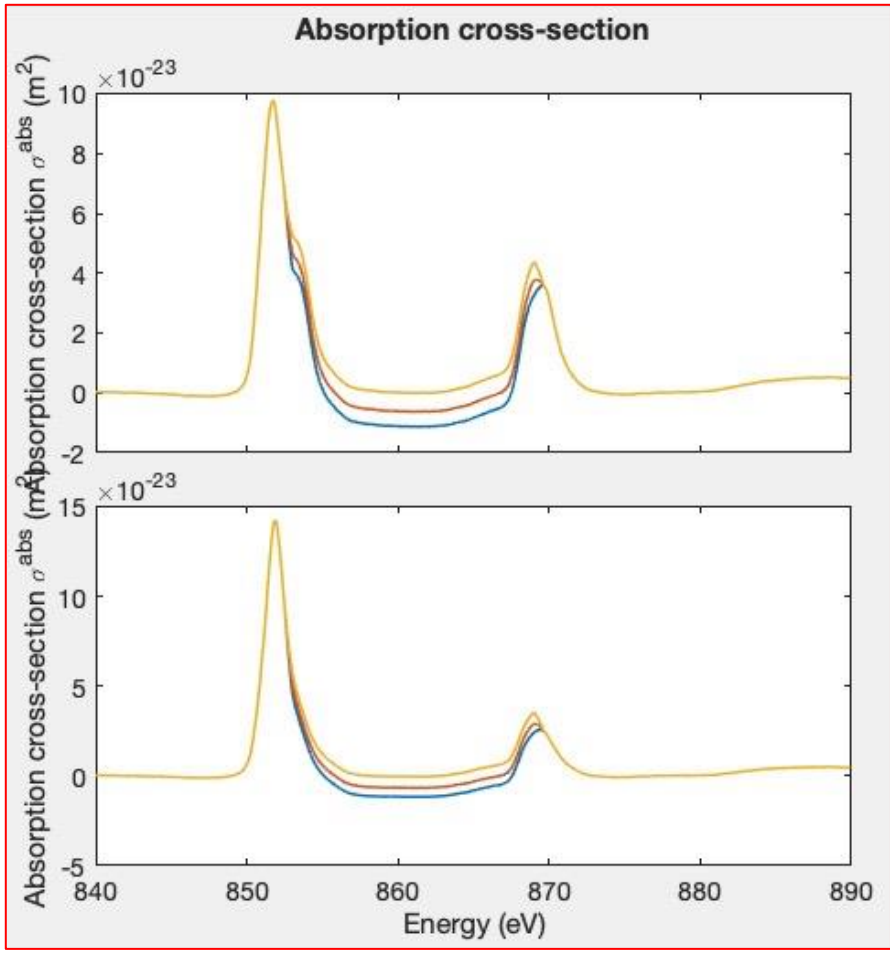
$$\sigma = \alpha / n$$

where:

- α is the absorption coefficient
- n is the atomic number density

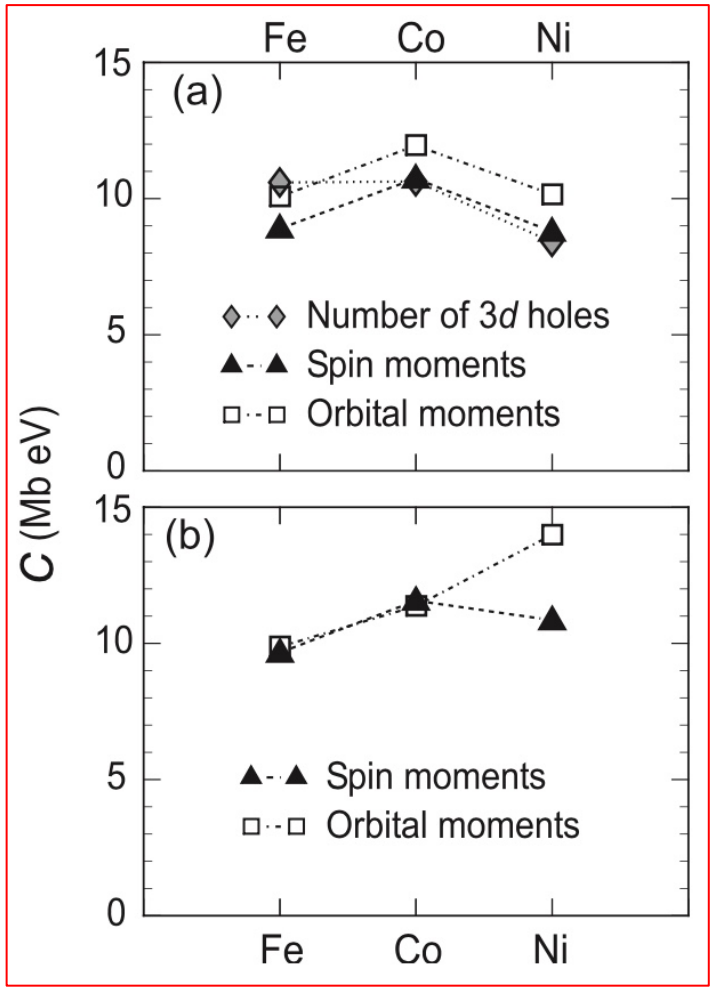
$$\sigma = (\mu/\rho) m_a / N_A$$





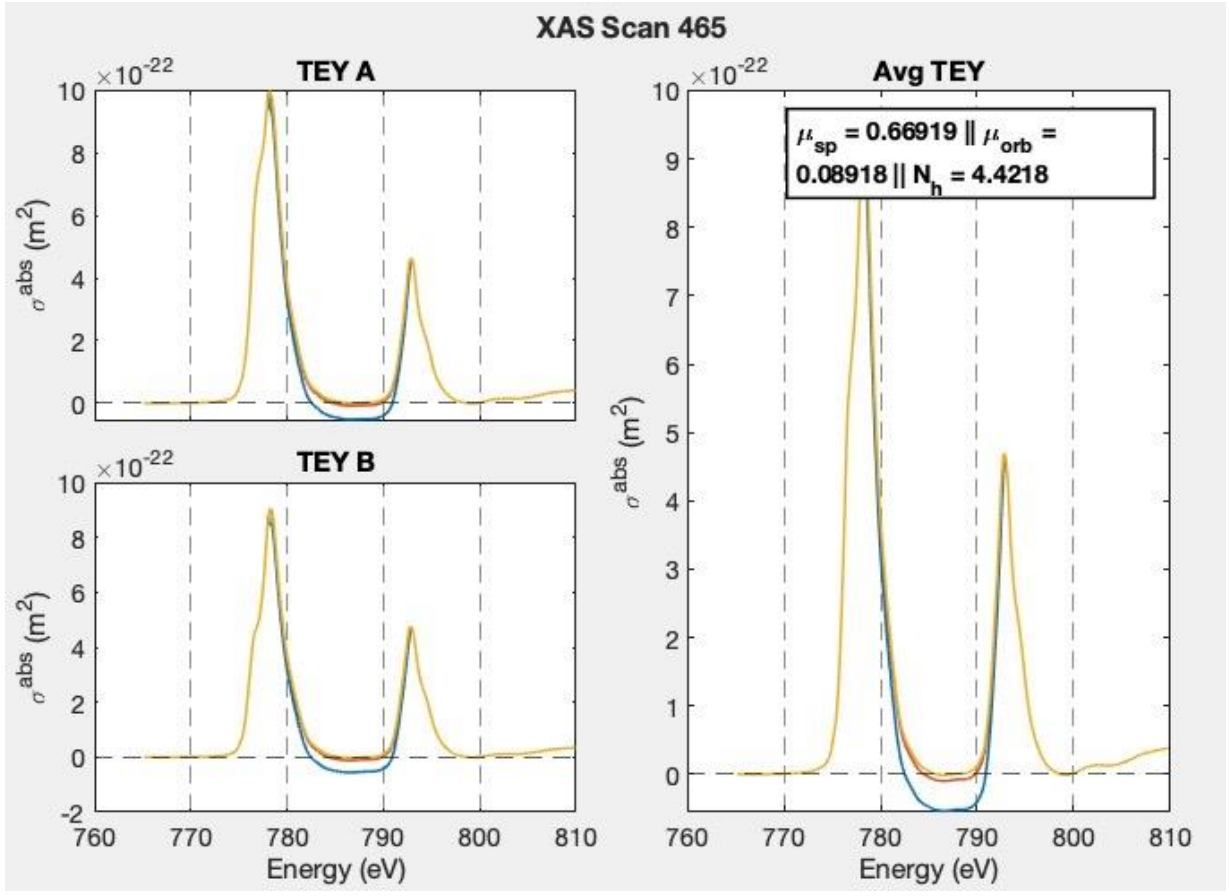
Quantitative Analysis

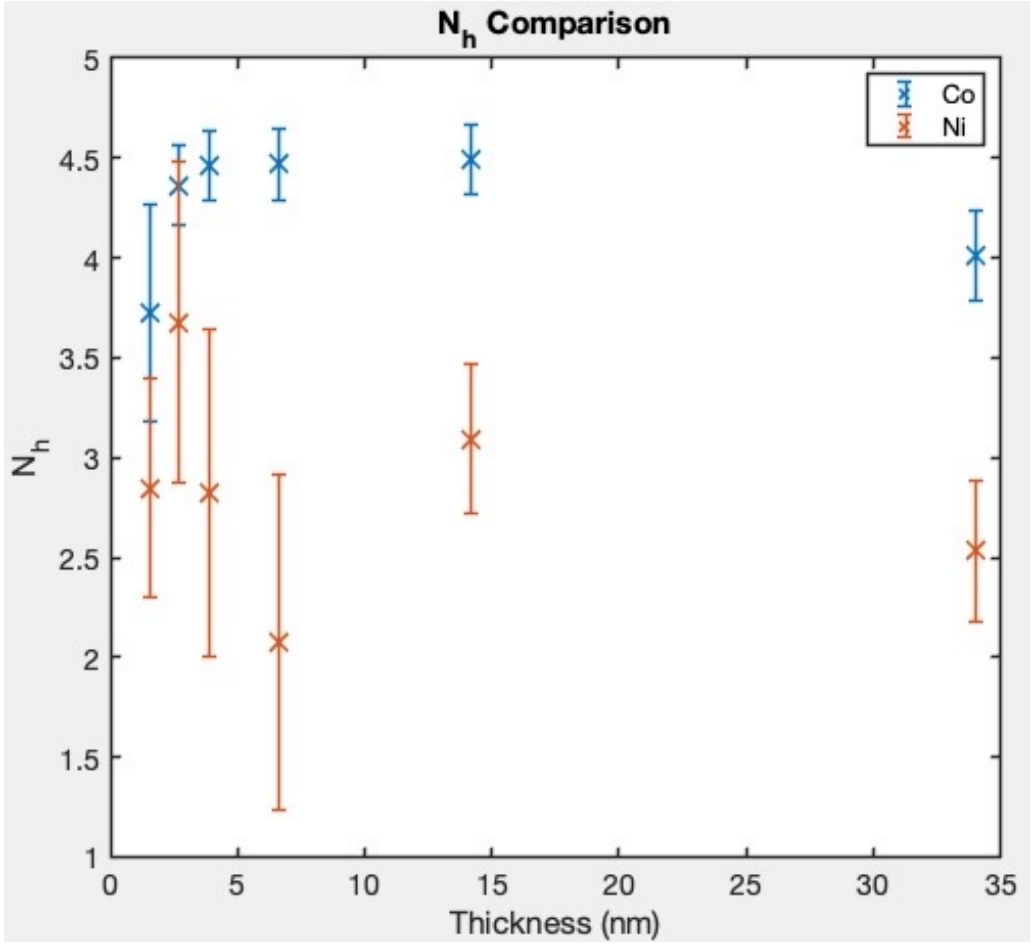
- Can now assign **real values** to the spectrum
- XAS/XMCD Sum Rules
  - $< I > = CN_h$
  - $< A + 2B > = \frac{C}{\mu_B} m_{spin}$
  - $< A + B > = \frac{-3C}{2\mu_B} m_{orb}$
- *C* determined by radial transition element



If the X-ray absorption spectrum is determined in terms of the absolute cross-section (with the dimension [area]) then the measured intensity I, given by the energy integration of the cross-section, has the dimension [area × energy], and therefore C is typically given in conventional units of [Mb eV]. For the $3d$ transition metals it has a value of about 10 Mb eV (see Fig. 9.17) [384].

Example Analyses





Things to Take-Away if You Do This Analysis

1. Convert your data to absorption by matching to a simulated background, thickness, number of atoms
2. Constant *C* determined from the radial transition, can try to determine (see appendix)
3. Remember to account for XAS-active vs XMCD-active atoms
   - e.g. 50% of Co contribute to XMCD, but 100% contribute to XAS

Determining Constant *C*

- $C = \mathcal{A}\mathcal{R}^2 \frac{L}{3(2L+1)}$, and
$$\mathcal{R} = < R_{32} \, |r| \, R_{21} >$$
- Slater's rules :
$$\psi_n = N r^{n^*-1} \exp\left(-(Z-\sigma)\frac{r}{n^* a_0}\right)$$
- Did not work very well for this work (calculated ~20-30 Mb eV; other works give ~10 Mb eV)