Understanding the Synthesis of Zinc Sulfide from Copper Sulfide using X-ray Absorption

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Why are we researching?

• Zinc sulfide is **useful** for several applications
  – White pigment
  – Alpha ray detector
  – Semiconductors
  – Manufacturing

• ZnS can be found in nature as minerals: sphalerite and wurtzite.

• It can also be synthesized!!
Sphalerite from St. Lawrence County, New York

Image from: www.irocks.com
System of Interest

- Copper sulfide nanoparticles transform to zinc sulfide through a process of cation exchange.
- Quenching the reaction at different times allows us to observe different time slices of the reaction.

Above image, courtesy of Don-Hyung Ha
System of Interest

- Interestingly, the crystalline structure of the copper sulfide is not consistent throughout the reaction.

Above images, both courtesy of Don-Hyung Ha
How do we know a copper phase change happens?

- The change in copper sulfide phase is evident because of the changing X-ray absorption spectra at each step of the reaction.
- Spectral components from roxbyrite, and low chalcocite / djurleite are observed at different stages in the reaction.
X-Ray absorption

• The part of the X-ray absorption spectra we are most concerned with is called “XANES”, which stands for X-ray Absorption Near Edge Structure.

Left image, courtesy of University of Vienna, http://www.ati.ac.at/index.php?id=247&L=1
Right image, courtesy of S. Woedtke, Ph.D. Thesis
My Task

• Understand how to use WIEN2k and FEFF9, then model the theoretical X-ray absorption spectra for the three different phases of copper sulfide present throughout the synthesis of zinc sulfide nanoparticles.
• FEFF9 uses full multiple scattering (FMS).
• WIEN2k uses density functional theory (DFT).
• Although not perfectly, my theoretical models from FEFF9 and WIEN2k should coincide with each other and the spectra *actually* observed, helping to validate the proposed theory.
Changing the spectrum in FEFF9