Cornell University
Cornell High Energy Synchrotron Source

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.

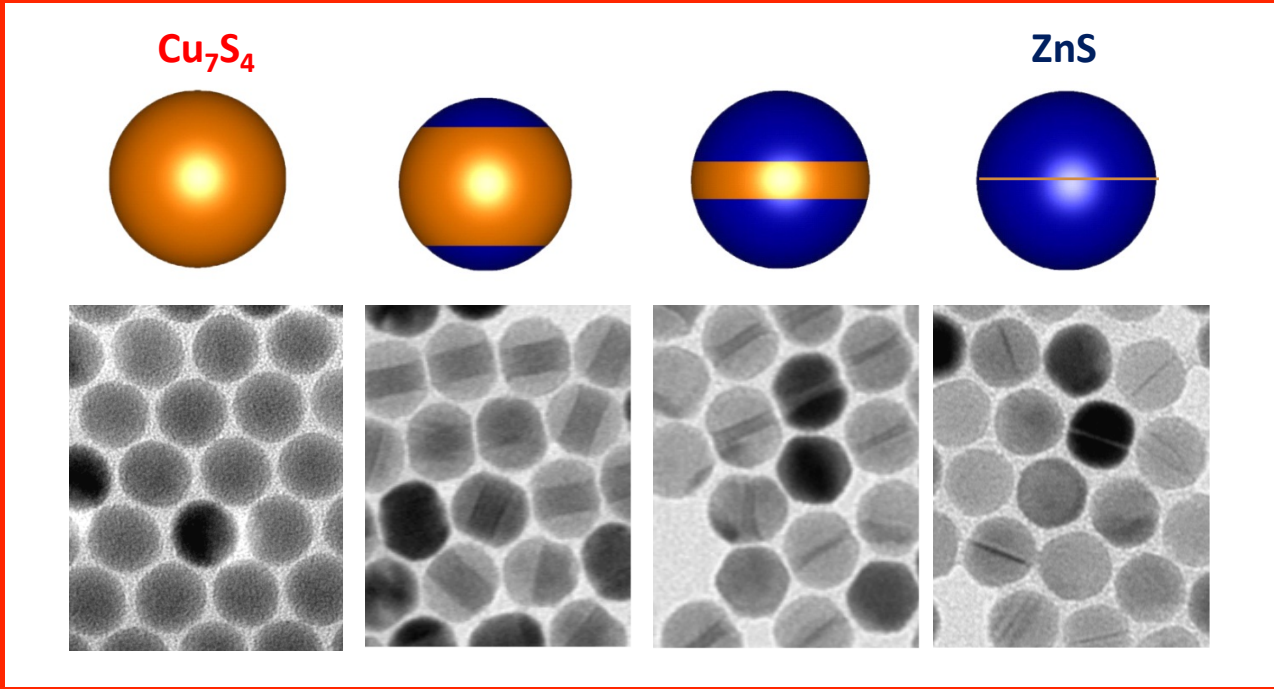
- It can also be synthesized!!

Sphalerite from St. Lawrence County, New York

Image from: www.irocks.com

System of Interest

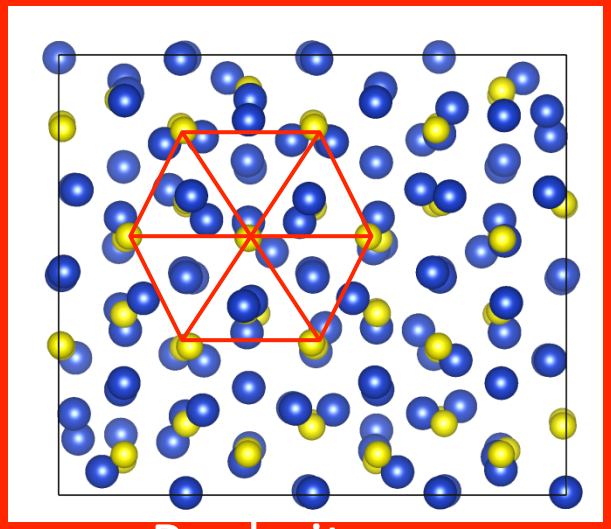
- Copper sulfide nanoparticles transform to zinc sulfide through a process of cation exchange.
- Quenching the reaction at different times allows us to observe different time slices of the reaction



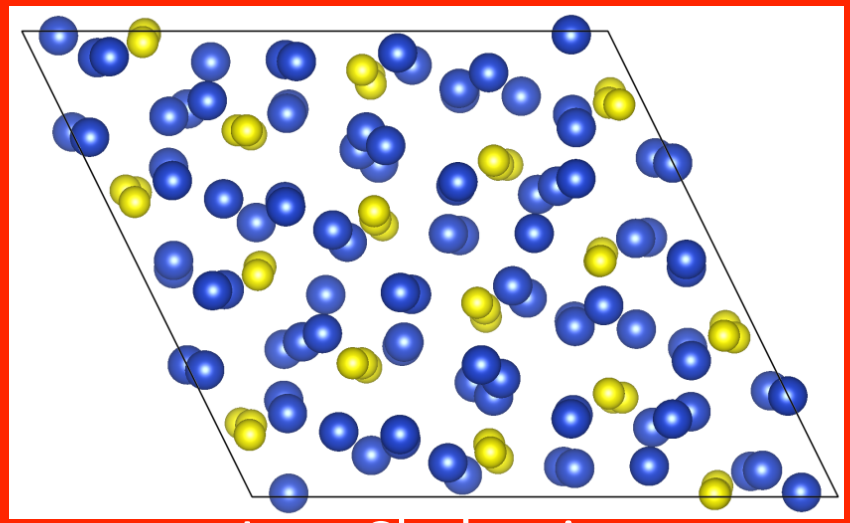
Above image, courtesy of Don-Hyung Ha

System of Interest

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



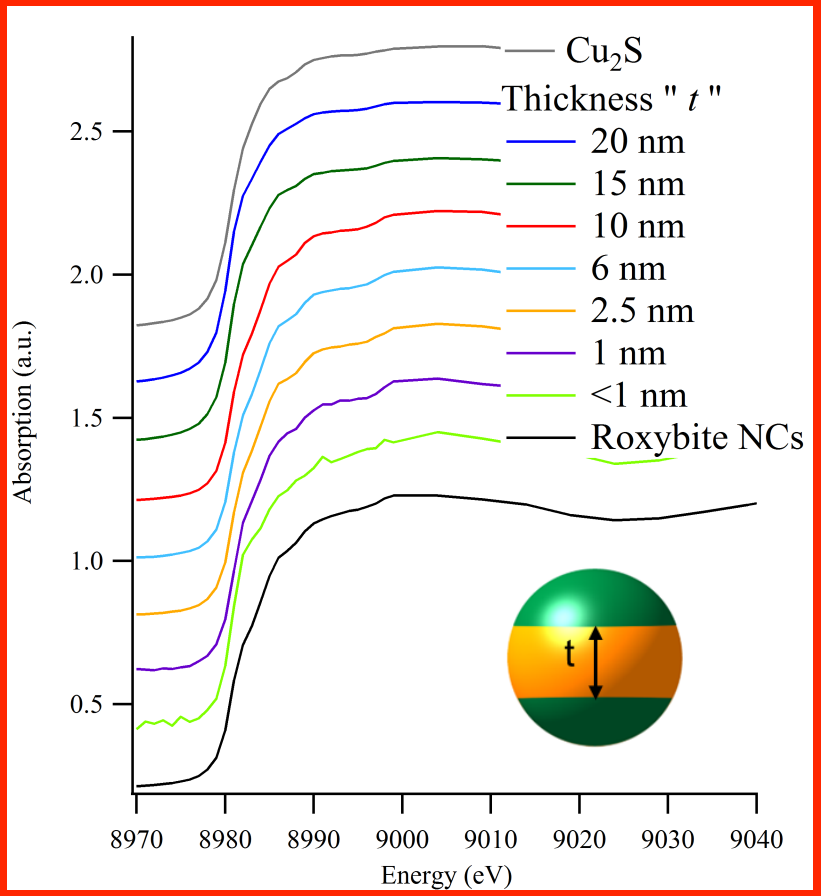
Roxbyite



Low Chalcocite

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 roxbyite, and low chalcocite / djurleite are observed at different stages in the reaction.

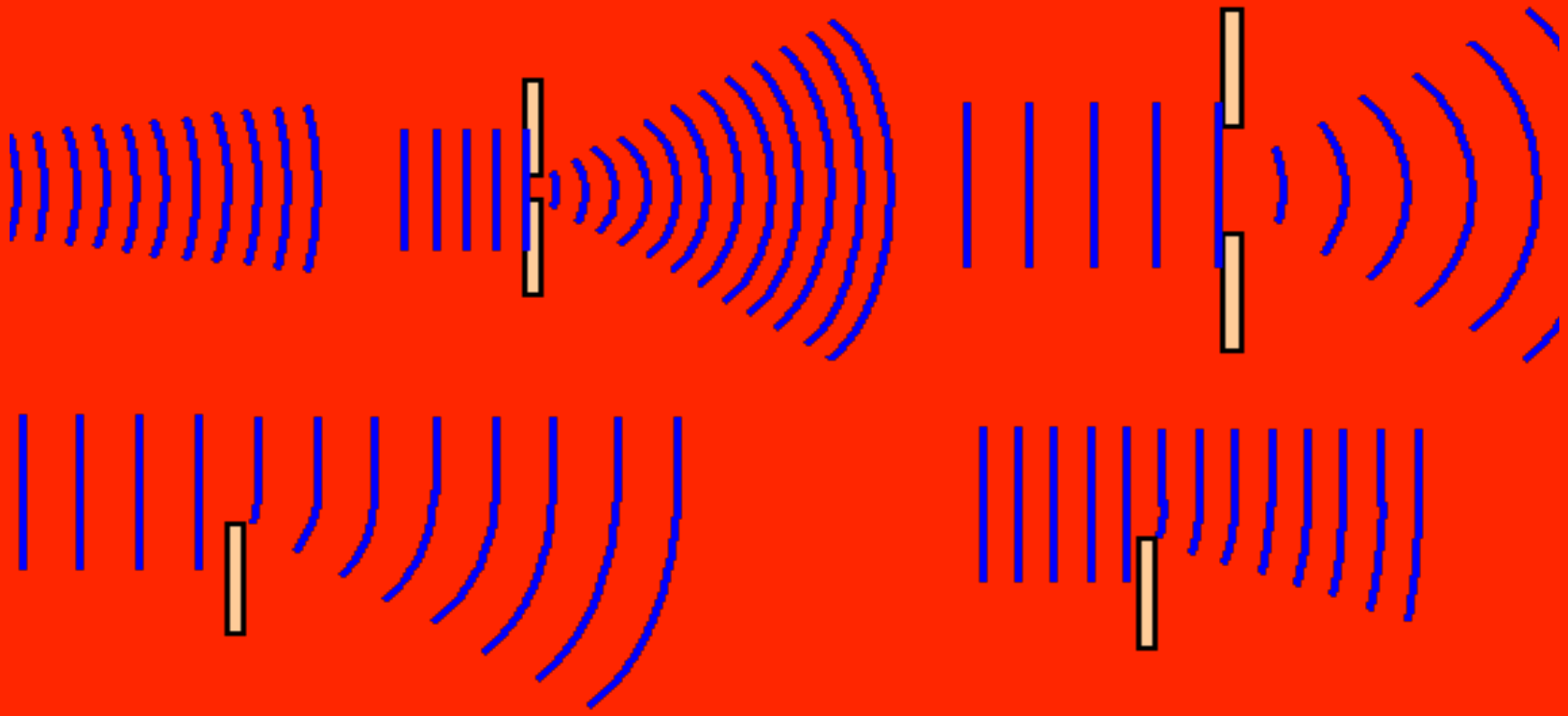


Image taken from:
http://www.schoolphysics.co.uk/age14-16/glance/Waves/Diffraction_/index.html

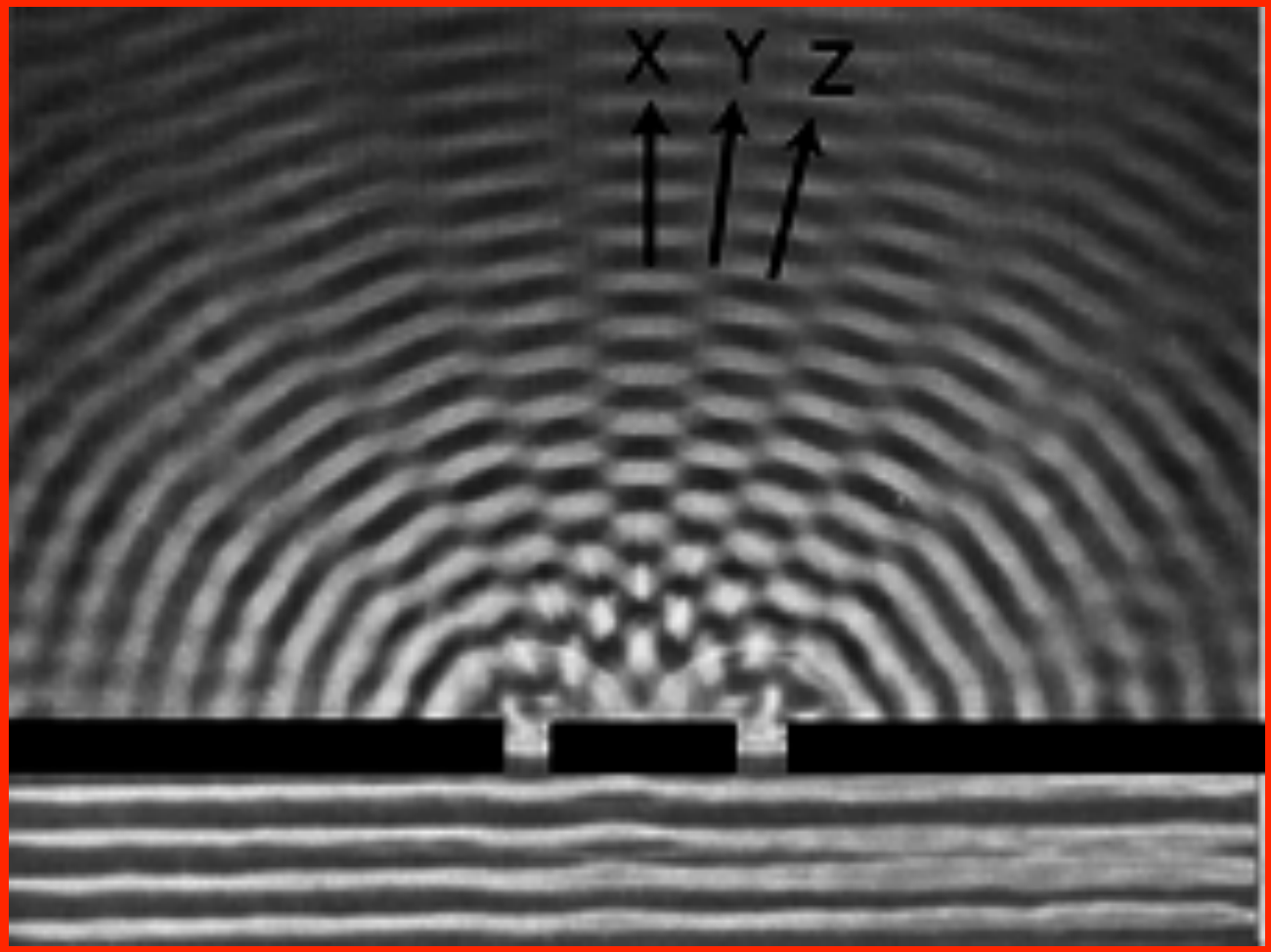
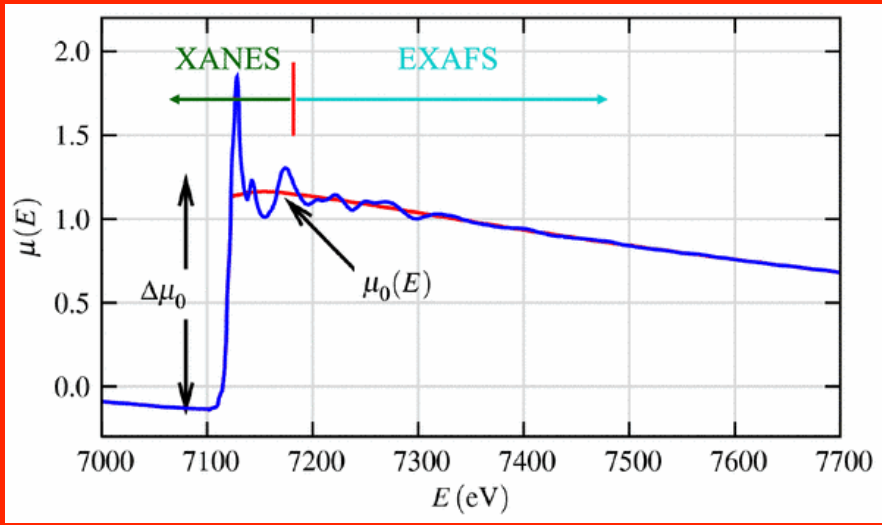


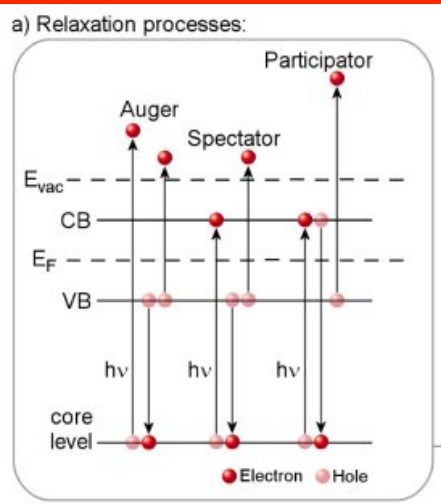
Image taken from:

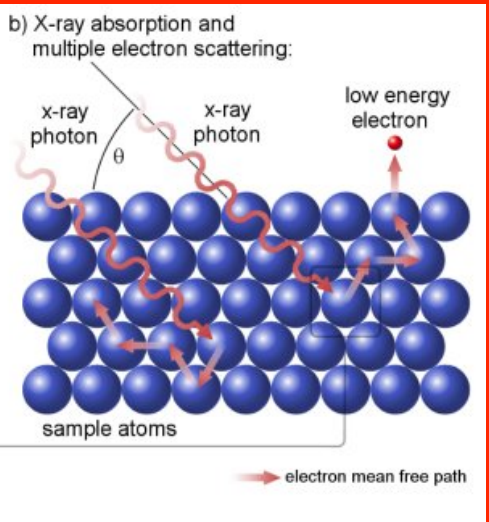
http://www.lightandmatter.com/html_books/lm/ch32/ch32.html

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