Abstract

This presentation shows how Rietveld modeling helped to standardize the interpretation of x-ray diffraction data by solving increasingly more complex problems. Rietveld modeling of x-ray diffraction data began in the 1970s. The technique uses structures for each component in a mixture to calculate a theoretical x-ray diffraction pattern. The theoretical pattern is adjusted to match the performance of the x-ray diffractometer being used to acquire the data. The theoretical pattern is compared to the measured pattern and adjusted until the differences are minimized. This process requires a fast computer with the capacity to process multiple structure assignments at once. As computers became more advanced in the 1990s, Rietveld modeling gained momentum and fundamentally changed the way x-ray diffraction data is evaluated. Even the modeling of amorphous phases like oil, water and glass has become a standard practice. Topics of this presentation will include creating a phase filter and how to model amorphous phases as well as estimate their order using the long range order index. A number of the examples included are industrial materials with an emphasis on corrosion samples.

Biography

R. W. Morton, Ph.D.
Dr. Morton has worked as an industrial chemist since 1977. He received his B.S. degree in Chemistry from Missouri Western State University (1979) and graduated with a Ph.D. in Analytical Chemistry– X-ray Spectrometry from the University of Missouri–Kansas City (1987). Dr. Morton began his career in the petroleum industry as an x-ray scientist for Phillips Petroleum Company which is today Phillips 66. He is a leading expert concerning sulfur in fuels and has numerous patents on the chemical removal of sulfur from fuel and gas streams. His instrument designs include the dual wavelength absorption edge spectrometer, the divergent beam diffractometer, and the dual wavelength ultra-low sulfur x-ray spectrometer.

Outside of the petroleum industry, Dr. Morton helped pioneer elemental x-ray imaging (EXI) of irregular 3-dimensional objects. His research led to the discovery of the "chemical fossil" that provided evidence that the chemistry of ancient life is directly related to that of modern animals. EXI was used to retrieve one of the lost works of Archimedes that was erased from recycled parchment many centuries ago. The X-ray images showed that Archimedes understood the concept of infinity and was performing calculus before 200 B.C. Recent EXI sessions at the Stanford Linear Accelerator Center revealed exciting details about the famous "dinobird" Archaeopteryx. Dr. Morton's research has been featured on the Discovery Channel and the National Geographic Channel.