Instructor Notes

Introduction to X-ray Diffraction Learning Module

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This module provides an introduction to *X-ray Diffraction (XRD).*

XRD is a versatile, non-destructive technique that reveals detailed information about the chemical composition and crystallographic structure of materials. It is utilized in a variety of settings ranging from chemistry and materials to geology and biological sciences.

Objective

This module is aimed at presenting the basic theory and applications of X-ray Diffraction to a novice user. It focuses on the application of Powder XRD to identify unknown crystalline samples.

The module is designed with learning activities for the students. The activities are interactive and inquiry based. Activities also include web-links to interactive applets to aid in student understanding.

The activities can be completed independently or in a classroom/laboratory setting. The Learning activity on Crystallography utilizes a freeware program called Powdercell. Crystal structure files have been created for this specific module and are available to open in this program for student analysis.

Note: In addition to the learning activities there is a section on the module that gives a historical perspective on X-ray diffraction.

Learning Activities

The learning activities web-based but have also been broken up into separate .pdf files that could be printed or utilized online.   They are designed to build off of each other but could be used independently depending on student background.

1) X-rays
2) Diffraction and Bragg's Law
3) Crystallography
4) Instrument Design

X-ray Learning Activity: The activity is designed to get students to think about why one would use X-rays to probe a material.   It lead is into the second activity about diffraction.

Diffraction and Bragg's Law Learning Activity: This is an interactive tutorial that walks through diffraction, constructive/deconstructive interference and Bragg's Law.   The activity includes a useful applet on Bragg's law that allows students to modify wavelength, theta, and inter-atomic distances of a lattice to see how that effect diffraction.

Crystallography Learning Activity: This is an interactive tutorial that provides an overview of how X-rays can provide information on the structure of material. It does not go into a detailed understanding of crystal structures, but does provide an introduction into some common lattices and the concept of the unit cell. The activity uses a freeware program Powdercell to examine powder patterns of materials. The activity is designed so crystal structures are already created to be opened up in the program (concepts of unit cells, and point groups not needed). By working through the module students are able to understand how symmetry and intensity effect diffraction and can predict relationships between cell and powder diffraction pattern.

The Powdercell files needed for this activity can be accessed on the homepage for Crystallography.

Instrument Design Learning Activity: This activity is designed to get students to think about important factors in instrument design for XRD analysis rather than providing a list of detectors and sources. It is focused on the design commonly seen for powder XRDs.

References:

Matter Online Tutorial on Diffraction
Excellent interactive tutorial on all aspects of diffraction phenomena, with a section on XRD. Produced by a non-profit consortium of Materials Science departments in Universities in the UK. Highly recommended. Some aspects may be too technical for a novice user.

Applet using Bragg's Law (they include the Java code for this)
http://www.eserc.stonybrook.edu/ProjectJava/Bragg/

Powdercell is a freeware program that can be downloaded.
Werner, K. Nolze, G. *Powder Cell 2.3* Powdercell is a freeware program that can be downloaded.
http://www.ccp14.ac.uk/ccp/web-mirrors/powdcell/a_v/v_1/powder/e_cell.html