Overview of Synchrotron X-Ray Powder Diffraction: Instruments and Case Studies

Peter W. Stephens Department of Physics and Astronomy Stony Brook University Stony Brook, NY 11794-3800 pstephens@stonybrook.edu

Synchrotron radiation has revolutionized the technology of X-ray powder diffraction (XRPD). This is particularly apparent in applications of XRPD to pharmaceutical materials. Starting from the hardware, I will describe several configurations of existing synchrotron beamlines in comparison to the common laboratory Bragg-Brentano instrument. It is important to understand the factors that affect resolution and intensity for any powder diffractometer, and I will illustrate with comparisons of data from several instruments on a couple of challenging samples.

In the second part of the talk, I will describe a few of my projects that were enabled by synchrotron powder diffraction.

- Determining that a particular API was a pure single phase, when NMR suggested otherwise.
- Resolving whether a particular API contained multiple phases, or if preferred orientation was creating confusion.
- Laying the groundwork to challenge the validity of claims in a particular patent, by showing that they could apply to a pharmaceutically acceptable solvate of the same API.