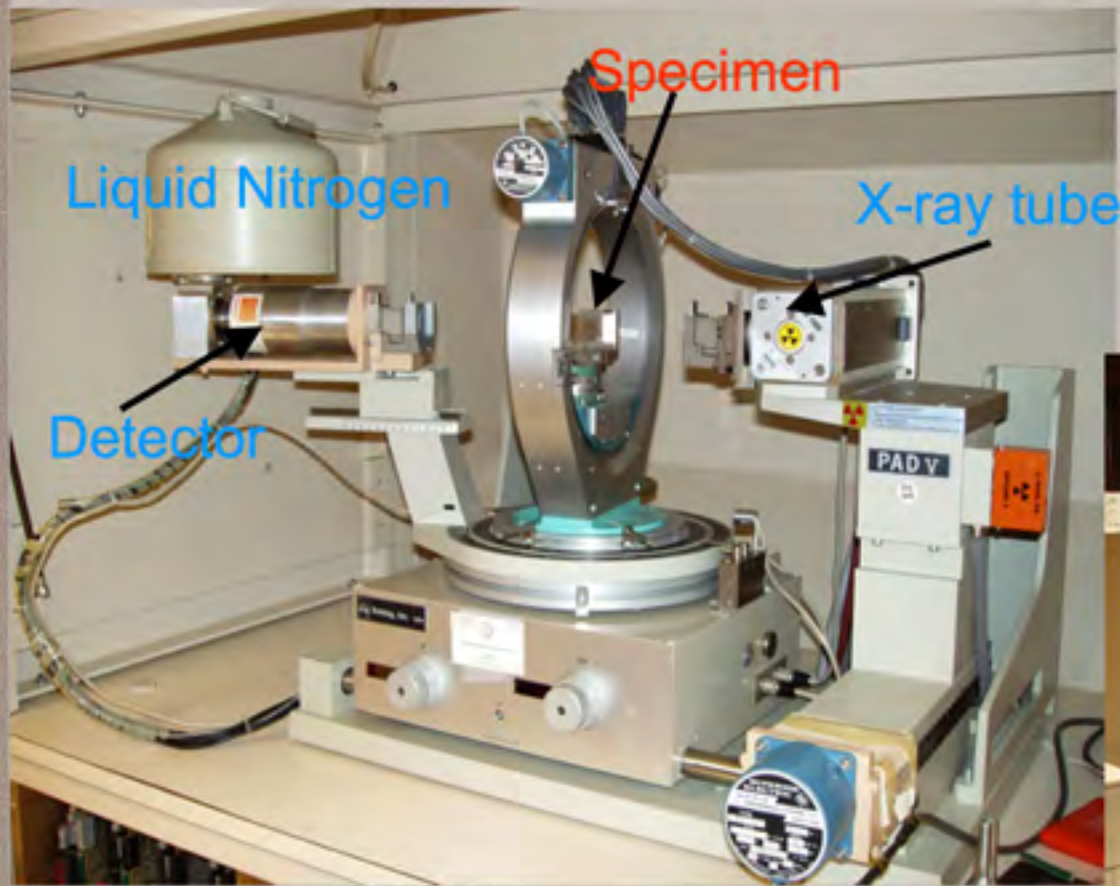




S. W. Bailey
X-ray Diffraction Laboratory

Department of Geology and Geophysics
University of Wisconsin – Madison
Phone: 608-262-0915; 608-890-0925

Scintag PAD V X-ray Diffractionmeter



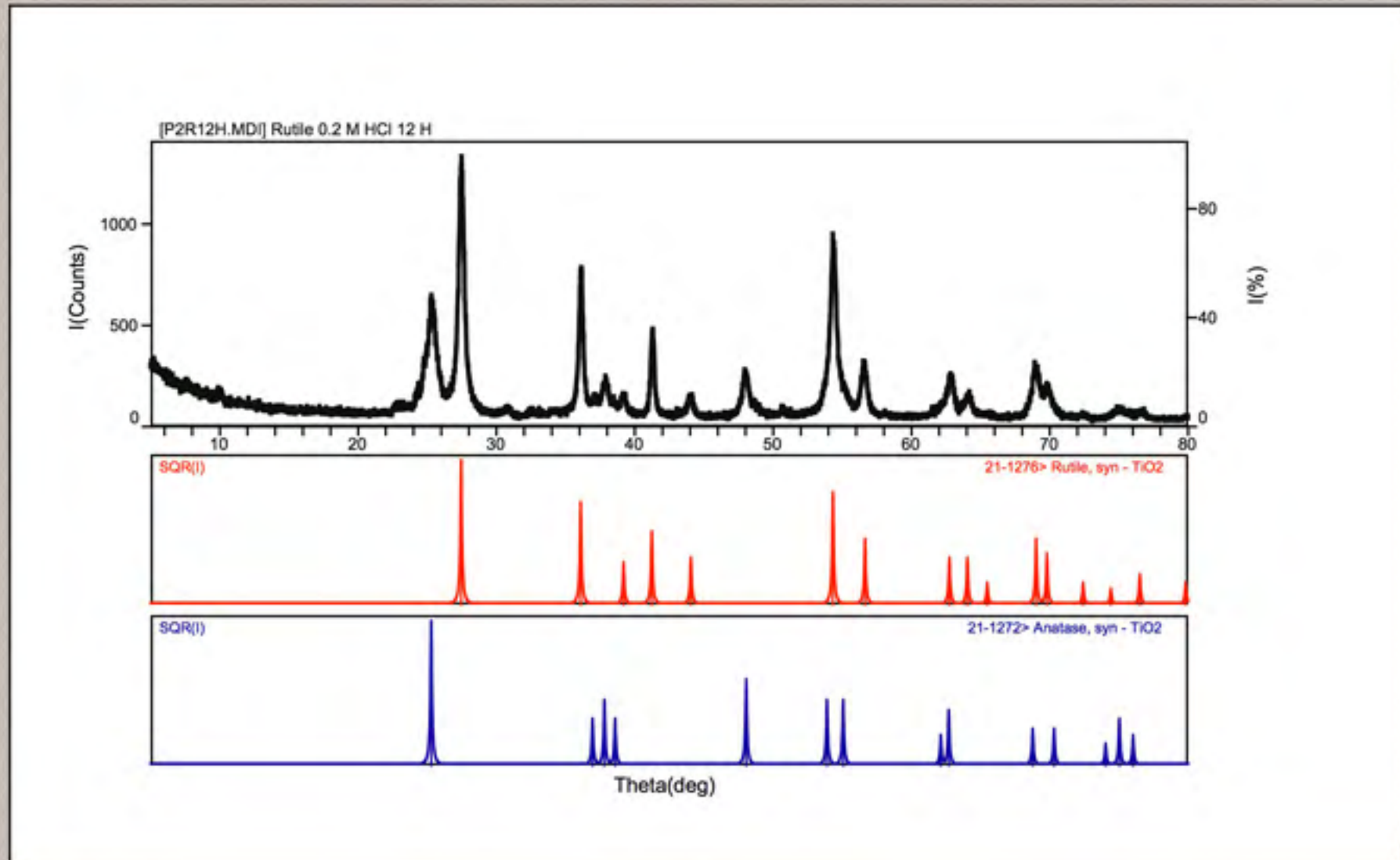
Use Powder Diffraction for...

- Phase identification
- Quantitative analysis
- Unit cell refinement
- Crystal structure refinement
- Crystallite size & strain determination
- Crystallite orientation distribution

Phase Identification

- Matches fingerprint of the unknown with that of a known phase
- The JCPDS powder diffraction file (PDF-2) is a collection of “known” fingerprints
- Software and manual search-match methods

Results of Phase Identification



Quantitative Analysis

- Estimate abundance of each phase present in a polyphase sample
- Qualitative to quantitative depending on method employed
- Standard and standard-less techniques

Unit Cell Refinement

- Least squares refinement of unit cell dimensions from peak positions and indices
- Unit cell dimensions can be correlated to composition, crystal defect concentration, or hydration state

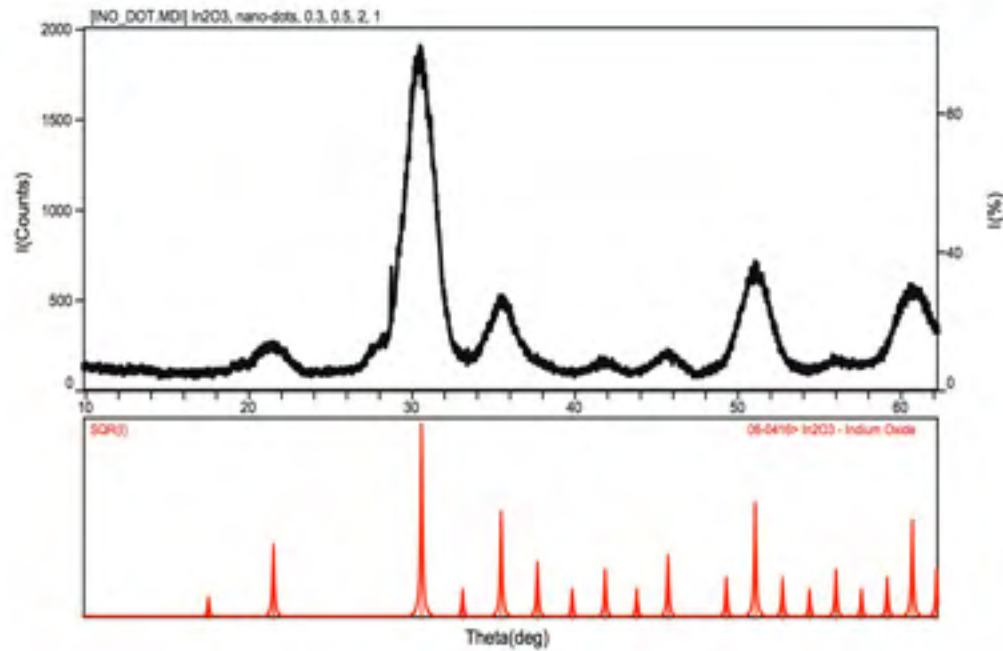
Crystal Structure Refinement

- Rietveld refinement
- Determination of order-disorder effects
- Determination of bond distances and angles
- Multiphase refinement can be used for quantitative analysis

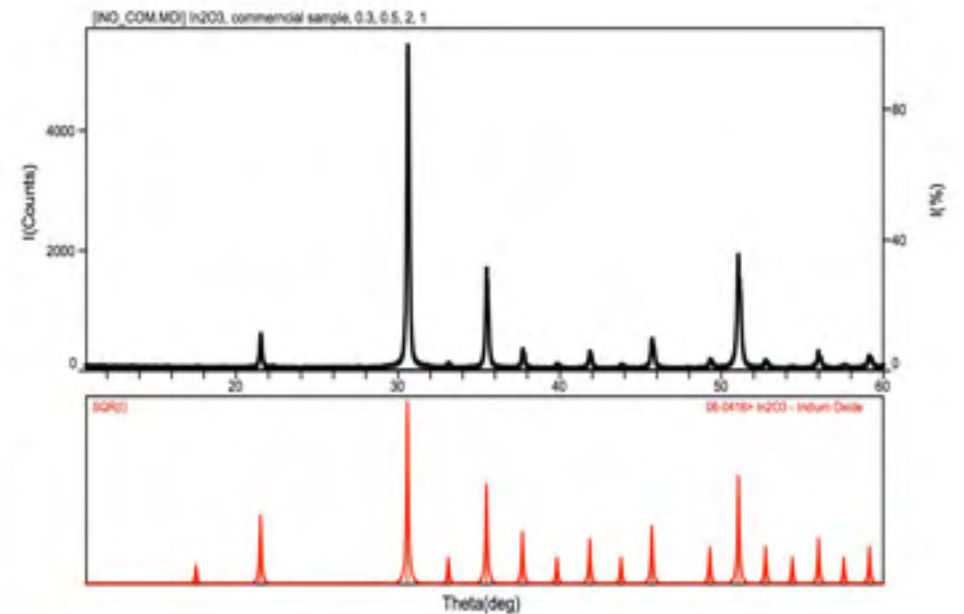
Peak Shape Analysis

- Determination of mean crystallite size and size distributions
- Determination of inhomogeneous residual strain from defects in the crystal
- Qualitative or quantitative depending on method employed

Determine Crystal Sizes

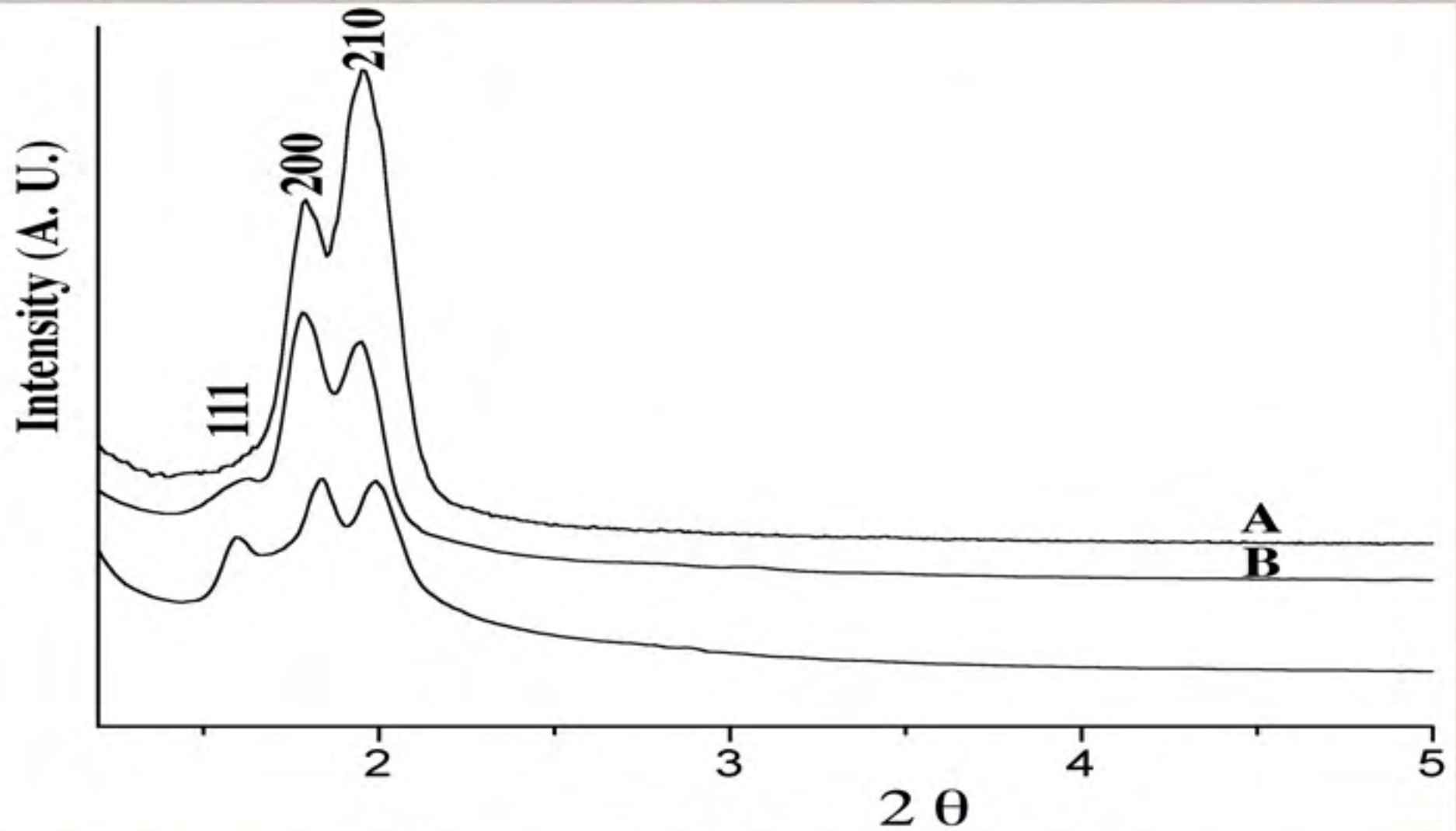


3 nm



40 nm

Low-angle Diffraction for Clays and Meso-phases with Large Unit Cells



Crystallite Orientations

- Determination of deformation textures
- Determination of epitaxial relationships
- Quantification of preferred orientations
- Identification of “statistical cleavage”