

USING DIFFRACTION PEAKS IN X-RAY FLUORESCENCE SPECTRA FROM THE MARS 2020 PIXL INSTRUMENT FOR MINERAL PHASE IDENTIFICATION. R. E. Schofield¹, J. A. Hurowitz¹, J. B. Parise¹, H. Zhong¹, A. Allwood², D. Flannery², R. Hodyss², ¹Department of Geosciences, Stony Brook University, Stony Brook, NY 11794-2100, renee.schofield@stonybrook.edu. ²NASA-Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, CA 91109.

Introduction: The Planetary Instrument for X-ray Lithochemistry (PIXL), selected for the Mars 2020 rover mission, is a micro-focus X-ray fluorescence instrument with a geometry that is optimized for chemical analysis of sub-millimeter features in rocks and regolith. PIXL's geometry also permits the detection of back-reflected X-rays that arise from diffraction off of crystal lattice planes in minerals exposed to the PIXL X-ray beam. The PIXL instrument geometry

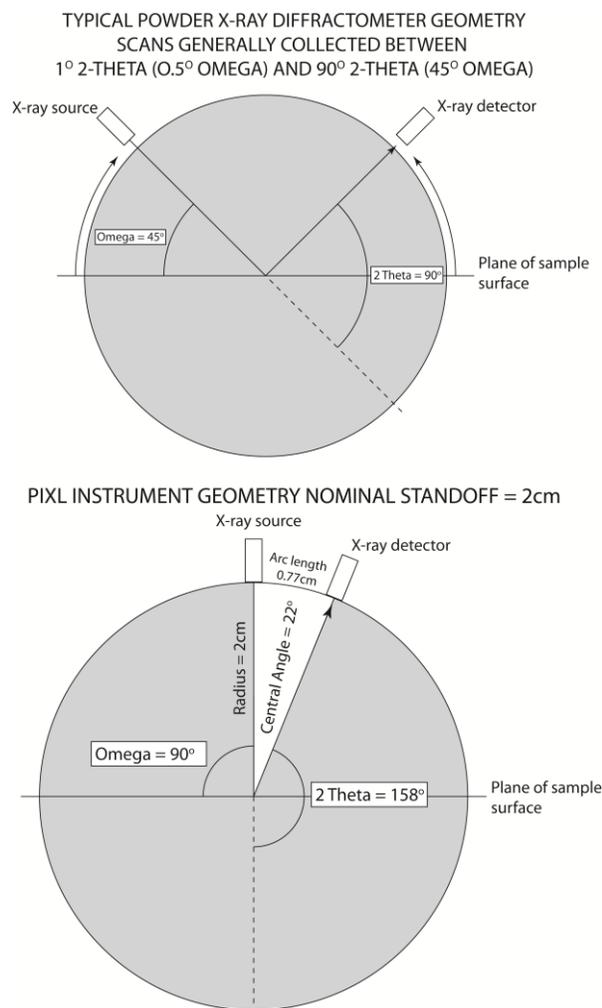


Fig. 1: Line drawing of the unique geometry of PIXL at 2.0 cm standoff compared to the geometry of a typical powder x-ray diffractometer. The JPL PIXL instrument has a stationary sample stage, the x-ray source and detector are fixed relative to each other (at an angle of 22°), and are scanned together in 3-axes across target surfaces.

is distinct from that of a typical powder diffractometer, as shown in **Fig. 1**, but it should be possible to obtain crystallographic information from PIXL energy dispersive X-ray spectra, once its unique back reflection geometry is accounted for (e.g., [1, 2]). The ability to uniquely discriminate between mineral phases, which have more or less identical chemical compositions, using the crystallographic information embedded in PIXL X-ray spectra could provide stronger constraints on mineral and rock origin than chemistry alone. For example, discrimination between anhydrite and gypsum would enable meaningful constraints to be placed on the temperature and salinity of the fluids that those phases were precipitated from (e.g., [3]). Here, we present the results of a set of experiments designed to demonstrate our ability to distinguish between mineral phases of like composition using data collected on a laboratory version of the PIXL instrument at the NASA-Jet Propulsion Laboratory (JPL).

Methods: Individual mm-sized crystals of anhydrite, gypsum, microcline, orthoclase, and sanidine were collected from the Stony Brook University Department of Geosciences mineral collection. An aliquot of each was then powdered using an agate mortar and pestle and sieved to less than 100 microns. Mineral identities were verified by powder X-ray diffraction. Sample powders and flat crystal facets were analyzed at JPL at three different vertical distances from the sample; 2.0 cm, 2.5 cm, and 3.0 cm, using a Rh X-ray source powered at 28 kV and 40 microamps, and count times of 600, 1200, and 1800 seconds respectively per vertical distance from the sample. Fluorescent and diffracted X-rays were collected on an energy-dispersive X-ray detector (Amptek FAST X-123 SDD). Using the known instrument geometry and standoff distance, we are able to calculate a 2-theta angle for each X-ray spectrum (Fig. 1), and then use Bragg's Law to convert our energy dispersive X-ray spectra to plots of X-ray intensity versus d-spacing.

Results and Discussion: **Fig. 2** shows energy-dispersive X-ray spectra at variable standoff distance for crystal facets of three potassium feldspar minerals. Fluorescence peaks are denoted by the labeled gray lines, and indicate the presence of Al, Si, K, Ar and Fe. The first three are expected; Ar results from spec-

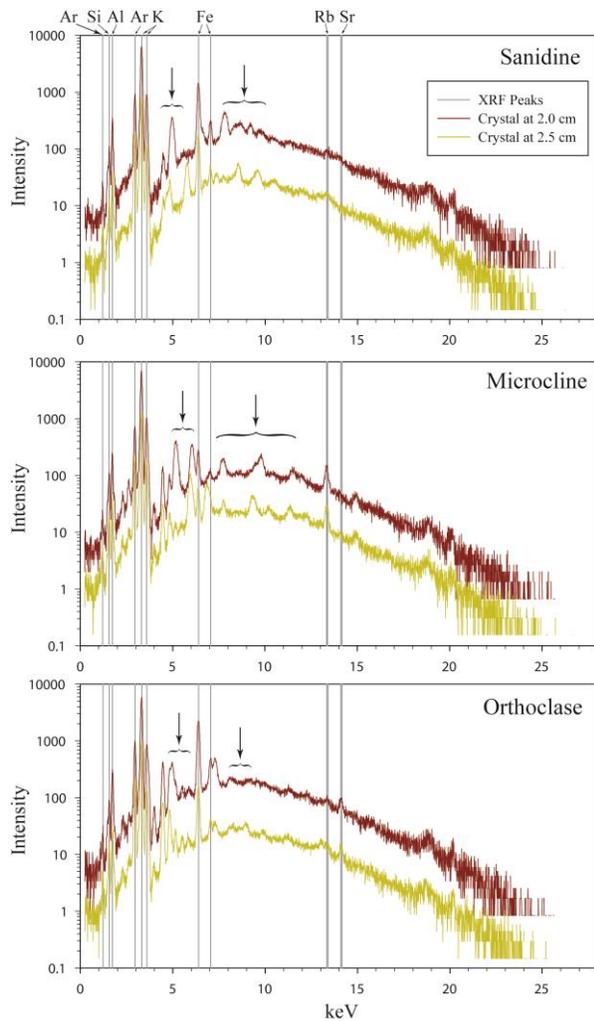


Fig. 3: XRF spectra from PIXL. Crystal samples of three K-feldspars. Spectra in red were taken at a standoff position of 2.0 cm; spectra in yellow were taken at a standoff of 2.5 cm. Fluorescence peaks are labeled with lines through the spectra and diffraction peaks are indicated with arrows.

tral collection in air, and Fe may be present as a contaminant Fe-oxide phase. Also present are a suite of diffraction peaks, denoted by arrows, and readily identified by the fact that they move, appear, and/or disappear as standoff distance is varied during the experiment.

Plotted on a d-spacing axis, **Fig. 3** shows the spectra from a more crystallographic point-of-view. Here the approximate position of the fluorescence peaks are labeled, and the diffraction peaks are also noted. Ultimately, these figures will be used for comparison to tabulated values of d-spacings, which are available in crystallographic databases, such as the ICDD PDF-4 database or the RRUFF database, in order to assign the reflections to specific crystallographic planes in each mineral. To first-order, comparison between spectra collected from the different K-feldspar miner-

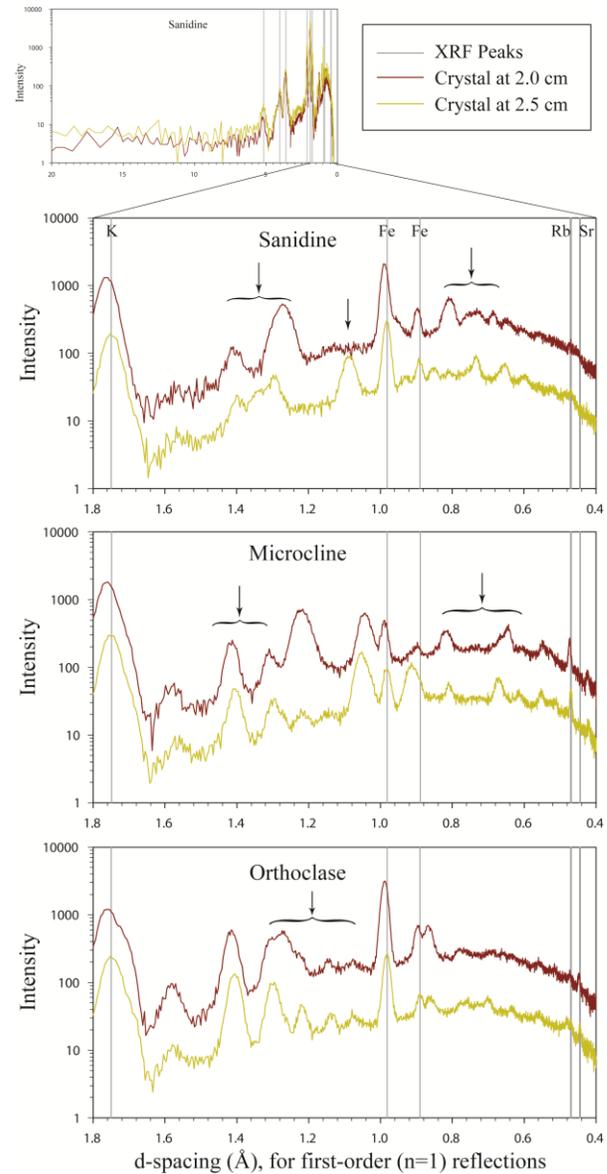


Fig. 2: X-ray intensity plotted against d-spacing calculated for first-order Bragg reflections. A full scale spectrum is shown for sanidine at the top, and a smaller range of d-spacing values for each mineral is shown below to better illustrate diffraction peaks present in the X-ray spectra.

als at the same standoff distance reveals differences in the number, position, and intensity of diffracted X-rays. Accordingly, our work, and that of [1, 2] indicates that it should, in principal, be possible to use diffracted X-rays in PIXL X-ray spectra to distinguish between mineral phases that can not be uniquely identified on the basis of chemical composition alone.

References: [1] Hansford G. M. (2009) *RSI*, 80, 073903. [2] Hansford G. M. (2011) *JAC*, 44, 514-525. [3] Hardie L. A. (1967) *AM*, 52, 171-200.