Bayesian refinement of full profile diffraction patterns for uncertainty quantification

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Advancements in x-ray and neutron characterization instruments provide the ability to examine the structures of newly developed materials. Full profile diffraction patterns collected from these instruments can be analyzed through Rietveld refinements using least-squares fitting routines to obtain sample, structural, lattice, and instrumental parameters. An alternative statistical framework using a Bayesian analysis method can also be applied to full profile fitting in order to quantify the uncertainty in the model parameters [1]. In Bayesian inference, parameters are taken to be random variables having associated posterior distributions. This representation provides descriptive insight to the uncertainties in the parameters and the model fits. In this work, Rietveld refinements are initially performed with GSAS-II [2] on the metastable perovskite material system of $(Ba_{1-x}Sn_x)(Zr_{0.5}Ti_{0.5})O_3$ (BSZT) [3]. The Bayesian refinement method is then employed to enrich the model information, specifically to provide higher fidelity uncertainty quantification on the atomic occupancies and positions. The effects of refining instrumental parameters via the Bayesian method are also investigated. [1] C. M. Fancher, Z. Han, I. Levin, K. Page, B. J. Reich, R. C. Smith, A. G. Wilson, and J. L. Jones, "Use of Bayesian Inference in Crystallographic Structure Refinement via Full Diffraction Profile Analysis," Scientific Reports, Vol. 6, No. 31625 (2016). http://dx.doi.org/10.1038/srep31625 [2] B. H. Toby and R. B. Von Dreele, "GSAS-II: the genesis of a modern open-source all purpose crystallography software package," Journal of Applied Crystallography, Vol. 46, No. 2, pp. 544-549 (2013). doi:10.1107/S0021889813003531 [3] S. O'Donnell, C. C. Chung, A. Carbone, R. Broughton, J. L. Jones, and P. A. Maggard, "Pushing the Limits of Metastability in Semiconducting Perovskite Oxides for Visible Light-Driven Water Oxidation," Chemistry of Materials, Vol. 32, No. 7, pp. 3054-3064 (2020). https://dx.doi.org/10.1021/acs.chemmater.0c00044