Use of Bayesian Inference in Characterization of Ceramic Materials: An Introduction and Applications in Ferroelectrics

Jacob L. Jones, Thanakorn Iamsasri, Jonathon Guerrier, Chris M. Fancher, John E. Daniels, Alexandra Larsen, Alyson G. Wilson, Brian Reich, and Ralph C. Smith
[1]Materials Science and Engineering, North Carolina State University
911 Partners Way, Raleigh, NC 27695
[2]Materials Science and Engineering, University of New South Wales
Sydney NSW 2052, Australia
*Jacob Jones: jacobjones@ncsu.edu

Materials development remains limited by our ability to "see" and characterize newly synthesized materials. Over the past decades, great advancements have been seen in X-ray and neutron characterization instruments. However, the analysis of data from such instruments has progressed slowly, an example being the Rietveld method for refinement of crystallographic structures using least squares (1969). In this talk, I will introduce to the materials researcher the alternative statistical framework of Bayesian statistics and its application to analysis of diffraction data when employed in conjunction with a Markov Chain Monte Carlo (MCMC) algorithm. The talk will include a basic introduction and application to modeling single reflections, doublets from ferroelastic degenerate reflections, and the entire pattern (full profile). The parameters in the new models represent structure using probability distributions, treating solutions probabilistically with improved uncertainty quantification. For ferroelectrics, we demonstrate that these probability distributions can be readily propagated into new calculated parameters related to domain reorientation. The conventional least squares solutions and its confidence intervals will be compared/contrasted to the new approach and its credible intervals. The new approach offers more confident structure-property correlations.

T. Iamsasri, J. Guerrier, G. Esteves, C. M. Fancher, A. Wilson, R. Smith, E. Paisley, R. Johnson-Wilke, J. Ihlefeld, N. Bassiri-Gharb and J. L. Jones, "A Bayesian Approach to Modeling Diffraction Profiles and Application to Ferroelectric Materials," Journal of Applied Crystallography, accepted (2017).

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 http://www.nature.com/articles/srep31625