The use of Bayesian inference in the characterization of materials and thin films

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Materials development remains limited by our ability to "see" and characterize newly synthesized materials. Over the past decades, great advancements have been made 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 the least squares method (1969). In this talk, I will introduce 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 [1-3]. 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 ferroelectric ceramics and thin films, we demonstrate that these probability distributions can be readily propagated into new calculated parameters related to domain reorientation [4]. 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.

References

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