X-Ray Reflectometry Parameter Uncertainties for Thin SiO\textsubscript{2} Films

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\textbf{ABSTRACT}

The X-ray reflectometry measurement method provides researchers with a powerful tool for determining physical model parameters in thin film stacks. This data analysis is often performed using various optimization-based schemes to generate model refinement. Questions often arise as to the nature of the uncertainty for these optimization solutions. In this work, we apply in-house and collaboration-developed statistical methods for determining uncertainties for structural model solutions on measurements of thin films of SiO\textsubscript{2} on Si. The XRR measurements analyzed were performed at AIST. Our approach is to use Markov Chain Monte Carlo sampling of a Bayesian statistical model of XRR data using a well-established Parratt recursion model with Gaussian roughness and the simplest structural models which can adequately describe the data. Through careful analysis of posterior probability distributions and two-dimensional histograms of structural model parameters, one can establish uncertainties for each structural model parameter. One can also study the absence or presence of solution-space multi-modalities over allowed parameter ranges. The presence of such ranges may indicate the need for more prior information of a given structure, which is required before a single set of parameters can be determined. The figure below shows an example where two sets of solutions are evident in the analysis. The conclusion of this analysis are uncertainty estimates providing the contribution to uncertainty inherent within the XRR modeling method - an uncertainty rarely incorporated in parameter estimations.

\textbf{REFERENCES}