

SIMULATION OF TIME-OF-FLIGHT NEUTRON DIFFRACTION USING A NEW SAMPLE KERNEL

S. Y. Lee and E. Ustundag

Department of Materials Science and Engineering, Iowa State University, Ames, IA
50011

L. Li and I. C. Noyan

Department of Applied Physics and Applied Mathematics, Materials Science Program,
Columbia University, New York, NY 10027

B. Clausen

Lujan Center, Los Alamos National Laboratory, Los Alamos, NM 87545

Interpretation of neutron diffraction data is essentially an *inverse problem analysis* that attempts to gain insight into materials from their diffraction patterns. These patterns, however, result from a complex convolution of instrument and specimen contributions. A proper interpretation of diffraction data, therefore, necessitates a systematic comparison of experimental results with sophisticated simulations of the entire diffractometer that includes a sample kernel. In other words, the success of the inverse analysis is largely dictated by the sophistication of the *forward* simulation of the experiment.

As a first step towards an accurate simulation of an engineering neutron diffraction experiment, the widely used Monte Carlo code *McStas* was employed in the simulation of the SMARTS diffractometer at Lujan Center. A new sample kernel was developed that simulates polycrystal deformation via a self-consistent solid mechanics model (the *EPSC* code from Los Alamos). This way, the effects of lattice strain and grain orientation distributions on peak position and profile could be incorporated into the instrument simulation. The simulation also employed the Python-based framework developed in the DANSE project (<http://danse.us>).