Single crystal diffraction beyond three dimensions: Dynamic structural responses of hydrogen-bonded materials using time filtering of event-based neutron TOF Laue diffraction

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Recent development in detector technology and source power at x-ray and neutron facilities have leveraged the study of the dynamic response of materials under external stimuli using time-resolved diffraction. Such experiments traditionally use hardware solutions to sort data into their respective histogram bins. We have shown a significant advantage of event-based data acquisition over hardware histogramming by enabling postprocessing utilizing a software solution [1]. This approach is made even more powerful for neutron TOF (time-of-flight) Laue diffraction. In addition to volumetric mapping in 3 dimensions, from detector (x,y) positions to wavelength-resolved 3D volume in (x, y, λ) along the neutron TOF direction, we can correlate measured diffraction data with metadata characterizing the applied stimuli (temperature, electric field, etc.) and material response. In this talk, we will present a time-filter approach that leverages the power of event-based diffraction collection on TOPAZ to reduce stroboscopic data representing subsets of the responses to a single cycle of the applied stimulus [1], effectively expanding the measured data beyond three dimensions. We will demonstrate this approach by studying the mechanism that facilitates polarization reorientation in KH2PO4 (KDP) in an alternating applied field using neutron diffraction. Neutron event data collected from a hydrogenated KDP single crystal sample were used to determine how the crystal structure evolves in response to the applied electric fields [2]. Field-dependent diffraction data provide evidence that the reorientation of the macroscopic polarization is associated with a subtle change in displacement in the atomic positions through cooperative hydrogen bonding interactions, indicating that polarization reversal is more complex than a simple inversion of the dipoles.

References

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