

SES13-2013-000188

Abstract for an Invited Paper
for the SES13 Meeting of
the American Physical Society

Advances and opportunities for single crystal neutron diffraction¹

CHRISTINA HOFFMANN, Oak Ridge National Laboratory

Two powerful neutron sources at the Oak Ridge National Laboratory, a continuous source (HFIR) and a pulsed source (SNS), offer an exciting suite of next generation instrumentation available for single crystal neutron diffraction (SCND) experiments. The spectrum ranges from traditional monochromatic to (time resolved) polychromatic instruments. A new time resolved neutron single crystal diffractometer is now available for open user access. Time resolved SCND is a powerful tool to sample reciprocal space in a highly effective manner by collecting discrete scattering data within a wide wavelength band. It is exquisitely suited to survey volumes of reciprocal space highly efficiently and provides instantaneous data of the crystal symmetry and crystal quality. Moreover, neutron and X-ray diffraction are complementary techniques. X-ray scattering emphasizes scattering contributions from heavy elements, whereas neutron scattering is equally sensitive to the light element contribution. This can be exploited to resolve hydrogen coordination to metals in metal-hydride compounds or large hydrogen-bonded-frameworks. Furthermore, isotopic substitution studies and magnetic structures can be investigated at the same time due the neutron's magnetic moment. In this contribution we will show recent examples of structure analysis and comparison of neutron data.

¹This research is supported by UT Battelle, LLC under Contract DE-AC05-00OR22725 for the U.S. Dept. Energy, Office of Science.