Poster Presentation

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Towards routine study of hydrogenous materials using powder neutron diffraction

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Hydrogen (1H) is an element that is ubiquitous in chemistry and materials science. Neutron diffraction is the preferred technique for studying 1H-containing compounds, but is complicated by the high incoherent scattering cross section, which also varies with wavelength. This variation of scattering cross section as a function of wavelength/energy and chemical environment is not well understood.[1-2] This is surprising as it is the largest contributing factor to the scattering properties used in single crystal and powder neutron diffraction experiments to calculate the optimal sample size for hydrogen containing compounds and the tabulated data are given for fixed neutron velocity of 2200 m s-1 (approximately 1.8 Å). The use and current limitations of certain current generation neutron diffraction instruments to probe 1H materials has recently been described.[3] Here, I present work to validate an empirical correction for the incoherent scattering cross section of 1H as a function of incident neutron wavelength in the range 0.5 - 10 Å using continuous source, monochromatic wavelength measurements. The practical use of this is that a, potentially quantitative, correction for all neutron diffraction data, including time-of-flight (TOF) from pulsed sources, as a function of scattering angle and neutron path length will become possible. Implementation of methodology that allows routine H position definition from easily synthesised material (i.e. non-isotopically enriched, and in polycrystalline or small single crystal (≤ 50 μm) form) for both TOF and monochromatic neutron instruments would be both of widespread application. Additionally, i will present work on an instrument concept for a pulsed monochromatic powder diffractometer for the ESS, which will be built in Lund by the end of the current decade. This diffractometer will aim to specialise in the data collection and analysis of hydrogenous materials using a combination of diffraction and inelastic techniques.

[1] *J. Howard, O. Johnson, A. Schultz et al. J. Appl. Cryst., 1987, 20, 120-122,* ***[2]*** *T. Koetzle, R.McMullan. Research memo C-4, Brookhaven National Laboratory, 1980,* ***[3]*** *C. Wilson, P. Henry, M. Schmidtmann et al. Crystallography Reviews (accepted), 2014, DOI:10.1080/0889311X.2014.886202*

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