DREAM – First Science Ideas – J.P. Attfield

Overview: During commissioning DREAM will have relatively low flux and similar performance to WISH@ISIS or POWGEN@SNS. Early science should demonstrate the instrument capabilities, with some benchmarking against other instruments (e.g. showing that Rietveld-refined crystal structures of standard materials are similar to previous reports), but also aim to produce new science from the start.

Initial experiments:

These should be powder diffraction experiments on large samples at room temperature;

1. Standards e.g. Si; and cubic structures with few variable parameters e.g. Y2O3 to check Rietveld results including Q-dependent effects such as temperature factors and absorption.

2. More complex materials with some structural subtleties or magnetic orders e.g. transition metal monoxides are NaCl types but have small lattice distortions below magnetic transitions e.g. MnO 120 K, NiO 520 K. (NiO peak splitting at 300 K was an early HRPD@ISIS highlight.) Complex oxide/ phosphate/silicate structures as more complex refinements. Perhaps even a zeolite such as sodalite.

More challenging experiments:

Variable T, smaller or hydrogenous samples (also variable time for kinetics or batteries – ideas from Gwen Rousse)

1. Variable T studies of materials showing structural and/or magnetic transitions, e.g. Fe2O3 (Morin transition at 260 K), perovskites CaTiO3, LaCrO3 (TN = 280 K) etc. More challenging; magnetite Fe3O4 over wide T-range from below Verwey transition (120 K) to above Curie (Tc = 860 K) (compare against variable T XPDF study; *G. Perversi et al*. Nature Comm., **10**, 2857 (2019) – any subtle changes around Tc will be important).

2. Small samples e.g. cation-ordered perovskites from high pressure synthesis. Our experience is that 50-100 mg is acceptable for ~6-8 hrs data collection on WISH@ISIS. AA'BB'O6 double double perovskites (DDP) are good test cases and also a source of new materials. Structures are tetragonal ($P4_2/n$, $a,c \approx 7.5$ Å) with some cation inversion disorder. Tc's vary from 10 to 500 K. Most have simple k = (000) ferrimagnetic structures, e.g. CaCuFeReO6 Tc = 500 K (*E. Solana-Madruga et al.* Angew. Chem., **61** 9497 (2022)). Occasionally more complex spin structures; $CaMnCoWO_6$ has an unusual combination of commensurate and incommensurate spin orders (Mn-site k = (0.5 0.5 0.5) and Co-site k = (0.5 0.42 0.5)) below T_C = 18 K (*K. Ji et al*, ZAAC, 2023). Newly synthesised DDP compositions can be provided for DREAM commissioning.

3. H-containing samples; metal hydroxides, hydroxysalts, small organics, perhaps a MOF.