Ideas for early science on DREAM

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I think that first experiments should be as facilitated as possible : no or very short proposal, limited technical complexity (but a cryostat is mandatory) so that future users can get used to the instrument, its capabilities and the associated data treatment (Rietveld refinements).

Magnetic structure determination : These experiments are straightforward (powder in a cryostat) and they are likely to easily transform experiments into science and published papers. This can apply to any inorganic compound that would magnetically order below a given temperature. Areas : magnetism, magneto-electrics, multiferroïcs… Given the high resolution DREAM will provide, compounds for which magnetic ordering are accompanied with changes in the crystal structure could be target compounds.

Materials for Energy : A lot can be done on DREAM regarding materials for energy

- electrode battery materials : Easy early experiments consist in measuring electrode materials either in their pristine state (as synthetized) : this topic includes all new compounds, structural determination from powder diffraction (coupled to X-rays). Example : $Li_2Ni_2W_2O_9$ is a new compound which was recently synthetized and its structure solved (*J. Am. Chem. Soc.* 2023, 145, 23, 12823–12836) : if the analogous compounds $Li_2M_2W_2O_9$ with M=Zn, Co, Fe, Mn… can be synthetized, early experiments on DREAM could be the investigation of their crystal structure.

-electrode materials at different states of charge and discharge : powder recovered from elecrochemical cells that have been cycled. The recovered powder is usually air sensitive so either loading at ESS if an argon glove box is available, or sample holders sent to the users that load and seel them in a glove box. High resolution and high flux (so small quantity of powder) could enable the accurate crystallographic determination of structural changes on cycling, such as cationic migrations, subtle transitions, and defects (antisite defects, stacking faults..). Example : Layered Li- based and Na-based Ni-Mn-Co oxyde compounds, intergrowth structures (Journal of The Electrochemical Society 170(8) 2023)

NMC type compounds (contrast between Ni, Mn, and Co) ; structural modifications (cation migration, phase segregation…) on aging (ex-situ samples), Li localization.

- solid electrolytes : DREAM might be interesting to evaluate Li diffusion paths from measurements either at RT only, or as a function of temperature to be able to refine anisotropic B's and generate bond valence energy landscapes maps from the refined structures to correlate structure with ionic conductivity. Example : argyrodite-type compounds (Nano Energy, Volume 83, May 2021, 105858)

- hybrid perovskites for photovoltaics: many structural phase transitions are reported in the hybrid pervoskites that would benefit from DREAM data

- HER, OER and CO_2 reduction catalysts : in this field, copper-based compounds, alloys, borides/carbides can worth studying at DREAM, on a crystallographic point of view and also regarding the influence of microstructure (nano-objets, influence of the crystallite shapes on the properties..). For example FeB (Acta Crystallographica Section A: Foundations of Crystallography 78, a147-a148) and $Zn_4Si_2O_7Cl_2$ (Angewandte Chemie 135 (26), e202303487) have been reported recently with a structural study from X-rays only.