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Applications of Neutron diffraction on cathode materials for Na-ion and Li-ion batteries

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High resolution neutron powder diffractometer (HRPD) and High intensity neutron powder diffractometer (HIPD) at China Advanced Research reactor have been opened to users around the world since 2023. Up to now, many experiments in the field of Na-ion and Li-ion batteries have been performed. Here we will introduce the progress of two neutron powder diffractometers and share several meaningful research results. Firstly, we investigated the effect of multiple elements on Na/vacancy ordering, Transition metal (TM) ordering in layered oxide Na_xTMO_2 , thereby explained the performance enhancement mechanism in the view of microstructure. In addition, our users proposed an innovative approach to address structural/chemo-mechanical degradation of LiCoO_2 via the integration of chemical short-range disorder (CSRSD) into LiCoO_2 cathodes. Owing to the opposite sign of neutron-scattering lengths of Li and Co, -1.9 and 2.49 fm, respectively, the Rietveld refinement of NPD data indicated the presence of Li/Co mixing in the crystal structure, which involves the localized distribution of elements within a lattice over spatial dimensions, spanning a few nearest neighbor spacings. Therefore, the rationally designed LiCoO_2 cathode with CSRSD showed increased cycle life and rate capability compared to conventional cathodes.

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