Contribution ID: **26** Type: **Invited**

Ionic diffusion in battery cathods, e.g. Na0.7CoO2

Tuesday 19 July 2016 09:50 (20 minutes)

Diffusion is one of the key areas in neutron spectroscopy. The accessible time scale covers fortunately the ionic diffusion in battery cathodes. Evenly important that state-of-the art instrumentation provides sufficient intensity and signal-to-noise ratio for measuring ionic diffusion in a host material, although pushing the experimental possibilities to the limits.
This talk will focus on atomic scale Na diffusion in Na_xCoO_2, which is the Na analogue of the commercially used Li compound. It belongs to the layered transition-metal oxide family with promising properties for commercial applications. Temperature dependent neutron powder diffraction (HRPT, PSI) revealed two phase transitions (at about T_A=290K and T_B=400K), which are connected to successive opening of Na diffusion paths. Between T_A and T_B the lattice deforms in a way that Na sides gets closer to each other allowing for quasi-1D (zig-zag) diffusion. Above T_B Na diffusion occurs in a plane via jumps on the hexagonal lattice.
Inelastic fixed window scans from MARS, PSI (δE=13μeV) and from IN16b, ILL (δE=0.85μeV) indicate sudden change in the dynamics at the phase transition temperatures. At both instruments quasielastic spectrum is present above T_B, whereas at the new IN16b the QENS intensity is continuously increasing from T_A. The later being especially important because of probing the diffusion in the temperature range relevant for application. Puzzling is however the comparison of the results with muon-spin relaxation (μ^+SR) data, which will be discussed in detail. This technique has been successfully applied in the last years to measure ionic diffusion in this type of materials. Although these results are only the first steps, the relevance of neutron scattering in fundamental understanding of ionic diffusion at the atomic scale is unquestionable for the design of novel cathode materials.

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Session Classification: Session III: Batteries 1 (Chair: Michael Hofmann)

Track Classification: Energy storage & transformation