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Electrochemical cells for neutron diffraction study of Li/Na-ion electrode materials

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In-situ and operando neutron powder diffraction is well established method for studying structural changes in Li-ion electrode materials in real time during battery operation. Quality of diffraction data obtained in operando experiments depends on characteristics of diffractometer (brightness, space resolution) and design and assembly of electrochemical cell. Operando neutron diffraction experiments can be successfully performed with real batteries; however using special designed electrochemical cell allows us to exclude some undesirable reflexes of battery components from diffraction pattern, use Li-metal as counter electrode, decrease background from incoherent scattering elements, be almost independent from commercial machines for battery preparation and considerably reduce a mass of investigated materials.

In this report we present special designed electrochemical cells developed for operando study of Li-ion electrode materials at time-of-flight neutron diffractometers at the IBR-2 neutron source (Dubna, Frank Laboratory of Neutron Physics). The cells are easily assembled in a glove box and demonstrate the excellent parameters of cyclabilities (with graphite electrodes, more than 700 cycles) and absence of leakage current. In dependence of scattering properties of studied materials the measured diffraction patterns can be analyzed by Rietveld method or Peak's profile data analysis. Several successful operando experiments on Li-ion electrode materials using these cells have been performed. In particular, investigation of LiNi0.8Co0.15Al0.05O2 (NCA) cathode material in the electrochemical cell allowed us to reveal the microstructural reasons of phase separation that occurs in cycled NCA during the first charge.

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